

Supporting Information

**Single-Step Synthesis of Atropisomers with Vicinal C–C and C–N
Diaxes by Cobalt-Catalyzed Atroposelective C–H Annulation**

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Content

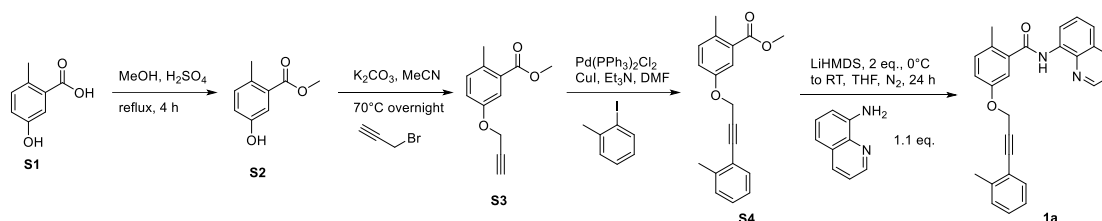
1. General Information.....	2
2. Synthesis and Characterization of Substrates.....	3
3. Synthesis of Chiral Ligands	28
4. Optimization of Reaction Conditions.....	35
5. General Procedure for Atroposelective C–H Annulation and Characterization of Products...39	
5.1. Synthesis and characterization of 5a	39
5.2. General Procedure for Intramolecular Atroposelective C–H Annulation.....	40
5.3. Characterization of Products	41
5.4. Gram-Scale Synthesis of 2a	68
6. Optical Properties.....	70
6.1. Uv-vis and CD spectra	70
6.2. Fluorescence Spectra.....	72
6.3. Circular polarized luminescence (CPL) spectra.....	73
6.4. Photoluminescence Quantum Yield (PLQY)	75
7. Measurements of Rotation Barriers of 5a and 2f	76
7.1. Experimental Procedure	76
7.2. Data processing	76
8. Computational Studies of Atropisomerization of 2a , 2c , 2d , 2e , 2f , 5a and 6	81
8.1. Computational Details.....	81
8.2. Diagrams of Atropisomerization	82
8.3. Structures of Transition States	85
8.4. Computational Research on Concerted Rotation Pathways	89
8.6. Cartesian Coordinates of Computed Species	95
9. Synthesis of Quasi-Intermediate	302
10. X-ray Crystallographic Data of 2a , 2d , 2m and QI	303
11. Reference	311
12. NMR Spectra	312

1. General Information

Unless otherwise specified, all reagents were purchased from commercial suppliers (Bide Pharmatech, Energy Chemical, TCI, Aldrich, Alfa and J&K) and directly used without further purification. NMR spectra were recorded on a Bruker AV-400 or a Zhongke-Niujin 400 NMR spectrometer operating for ^1H NMR at 400 MHz, ^{13}C NMR at 101 MHz, ^{19}F NMR at 376 MHz using TMS as internal standard ($\delta = 0.00$). The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, hept = septet, m = multiplet, brs = broad singlet. Mass spectroscopy data of the products were collected on an HRMS-TOF instrument. The ee and dr values were determined on Shimadzu LC-20A HPLC system using CHIRALPAK column unless notified. Emission spectra were measured with a Shimadzu RF-6000 spectrometer. Circular polarized luminescence (CPL) spectra were measured on a JASCO CPL-300 spectrometer. Absorption spectra and circular dichroism (CD) spectra were measured on a Jasco J-1500-150ST CD spectrometer. Optical rotation data were obtained on a PerkinElmer Model 341 Polarimeter.

2. Synthesis and Characterization of Substrates

2-Methyl-*N*-(quinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (**1a**)



General Procedure A:

25.0 g (164 mmol) of 2-methyl-5-hydroxybenzoic acid **S1** and 250 mL of methanol were added into a 500 mL round-bottom flask, to which was added dropwise 2 mL of conc. sulfuric acid under stirring. The mixture was heated to reflux in an oil bath and refluxed for 4 h. Then it was cooled to near room temperature. 2/3 of the methanol was removed by rotary evaporation. Remaining liquid was poured into 300 mL of iced water and 200 mL of ether. The aqueous phase was extracted twice with ether (50 mL). The organic phase was washed with saturated sodium bicarbonate solution and brine then dried with anhydrous sodium sulfate. Then ether was removed by rotary evaporation and in vacuo giving methyl 2-methyl-5-hydroxybenzoate **S2** as off-white solid (18.5 g, 68%).

General Procedure B:

S2 (8.31 g, 50.0 mmol), potassium carbonate (17.25 g, 125 mmol) and 150 mL of acetonitrile were added into a 250 mL round-bottom flask, to which was added slowly propargyl bromide (4.14 mL, 55 mmol). The mixture was stirred and heated to 70°C in an oil bath overnight. The mixture was cooled to room temperature. Solvent was removed by rotary evaporation. To the residue were added 100 mL of water and 100 mL of ether. The aqueous phase was extracted twice with ether (50 mL). The organic phase was washed with brine then dried with anhydrous sodium sulfate. Then ether was removed by rotary evaporation and in vacuo giving methyl 2-methyl-5-((prop-2-yn-1-yl)oxy)benzoate **S3** as white solid (10.13 g, 99%).

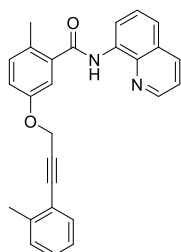
General Procedure C:

S3 (4.08 g, 20.0 mmol), 2-iodotoluene (5.23 g, 24 mmol), Pd(PPh₃)₂Cl₂ (281 mg, 0.4 mmol), CuI (152 mg, 0.8 mmol), 20 mL of DMF and 20 mL of triethylamine were added into a 100 mL round-bottom flask under nitrogen atmosphere. The mixture was stirred at 25°C overnight. To the mixture were added 100 mL of water and 100 mL of ether. The aqueous phase was extracted twice with ether (50 mL). The organic phase was washed with water and brine then dried with anhydrous sodium sulfate. Purification by flash chromatography (5:95 EA:PE) gave methyl 2-methyl-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzoate **S4** as light yellow oil (3.67 g, 62%).

General Procedure D:

Commercially available 8-aminoquinoline was purified by column chromatography (eluent: DCM) prior to use. 8-aminoquinoline (1.81 g, 12.6 mmol) was added into a 250 mL 2-necked round-bottom flask which was then flushed with nitrogen. **S4** (3.36 g, 11.4 mmol) dissolved in 45 mL of dry THF

was added into the flask via a syringe. The mixture was stirred and cooled with ice, to which LiHMDS THF solution (1 M, 23 mL) was added dropwise. The mixture was stirred at room temperature for 24 h. Methanol (5 mL) was added to the mixture in order to quench the reaction and solvent was removed by rotary evaporation. Purification by flash chromatography (3:30:67 EA:DCM:PE) gave 2-methyl-*N*-(quinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide **1a** as light yellow solid (4.14 g, 90%).

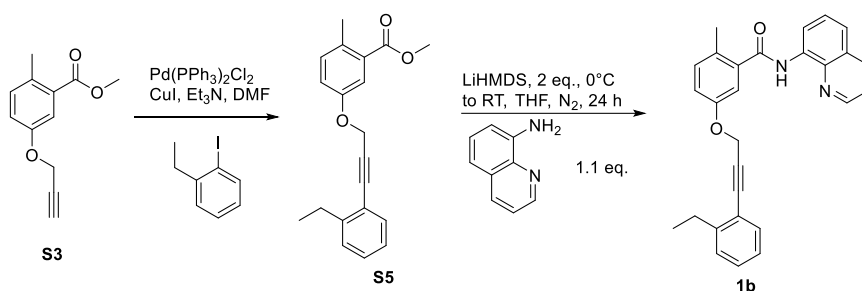


¹H NMR (400 MHz, Chloroform-*d*) δ 10.21 (s, 1H), 8.93 (dd, $J = 7.4, 1.5$ Hz, 1H), 8.66 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.17 (dd, $J = 8.2, 1.7$ Hz, 1H), 7.65 – 7.50 (m, 2H), 7.46 – 7.35 (m, 3H), 7.25 – 7.17 (m, 2H), 7.16 – 7.06 (m, 3H), 5.00 (s, 2H), 2.54 (s, 3H), 2.36 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.81, 155.80, 148.29, 140.60, 138.57, 137.40, 136.32, 134.64, 132.36, 132.21, 129.42, 129.20, 128.69, 127.97, 127.40, 125.47, 121.96, 121.83, 121.67, 117.05, 116.56, 114.09, 87.44, 86.45, 57.00, 20.65, 19.32.

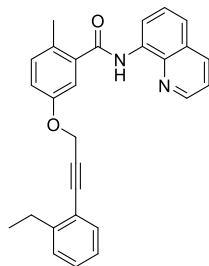
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{27}H_{23}N_2O_2^+$ 407.1754; found: 407.1757.

5-((3-(2-Ethylphenyl)prop-2-yn-1-yl)oxy)-2-methyl-*N*-(quinolin-8-yl)benzamide (**1b**)



S5 was prepared according to **General Procedure C** on a 6.08 mmol scale. Purification by flash chromatography (3:97 EA:PE) gave **S5** as a yellow oil (0.594 g, 32%).

1b was prepared according to **General Procedure D** on a 1.89 mmol scale. Purification by flash chromatography (3:20:77 EA:DCM:PE) gave **1b** as a yellow oil (0.458 g, 58%).

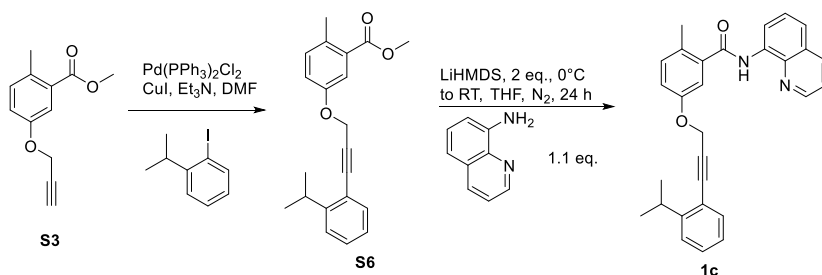


¹H NMR (400 MHz, Chloroform-*d*) δ 10.22 (s, 1H), 8.93 (dd, $J = 7.4, 1.5$ Hz, 1H), 8.65 (dd, $J = 4.3, 1.7$ Hz, 1H), 8.16 (dd, $J = 8.4, 1.7$ Hz, 1H), 7.64 – 7.51 (m, 2H), 7.45 – 7.34 (m, 3H), 7.24 (td, $J = 5.8, 5.0, 3.3$ Hz, 2H), 7.16 (d, $J = 8.2$ Hz, 1H), 7.13 – 7.05 (m, 2H), 5.00 (s, 2H), 2.72 (q, $J = 7.6$ Hz, 2H), 2.54 (s, 3H), 1.13 (t, $J = 7.6$ Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.83, 155.83, 148.33, 146.64, 138.60, 137.43, 136.33, 134.68, 132.55, 132.39, 129.22, 128.95, 127.98, 127.93, 127.42, 125.57, 121.85, 121.70, 121.29, 117.06, 116.55, 114.14, 87.02, 86.26, 57.01, 27.63, 19.36, 14.79.

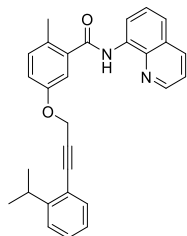
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{28}H_{25}N_2O_2^+$ 421.1911; found: 421.1912.

5-((3-(2-Isopropylphenyl)prop-2-yn-1-yl)oxy)-2-methyl-N-(quinolin-8-yl)benzamide (1c)



Methyl 5-((3-(2-isopropylphenyl)prop-2-yn-1-yl)oxy)-2-methylbenzoate **S6** was prepared according to **General Procedure C** on a 15.0 mmol scale. Purification by flash chromatography (5:95 EA:PE) gave **S6** as yellow liquid (2.23 g, 46%).

5-((3-(2-isopropylphenyl)prop-2-yn-1-yl)oxy)-2-methyl-N-(quinolin-8-yl)benzamide **1c** was prepared according to **General Procedure D** on a 6.00 mmol scale. Purification by flash chromatography (20:80 EA:PE) gave **1c** as yellow solid (2.20 g, 84%).



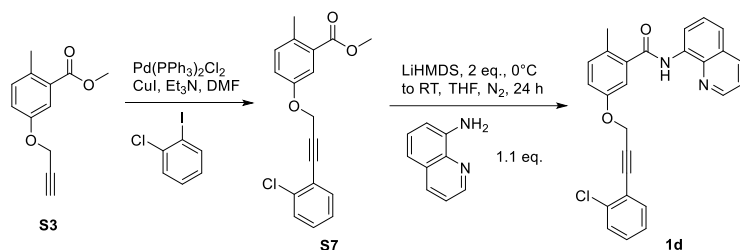
¹H NMR (400 MHz, Chloroform-*d*) δ 10.22 (s, 1H), 8.93 (dd, $J = 7.5, 1.5$ Hz, 1H), 8.64 (dd, $J = 4.3, 1.7$ Hz, 1H), 8.16 (dd, $J = 8.2, 1.7$ Hz, 1H), 7.64 – 7.50 (m, 2H), 7.45 – 7.35 (m, 3H), 7.31 – 7.19 (m, 4H), 7.13 – 7.05 (m, 2H), 5.01 (s, 2H), 3.34 (hept, $J = 6.9$ Hz, 1H), 2.54 (s, 3H), 1.16 (d, J

= 6.9 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.76, 155.80, 150.89, 148.28, 138.56, 137.37, 136.29, 134.65, 132.62, 132.34, 129.23, 129.03, 127.95, 127.38, 125.44, 124.87, 121.80, 121.65, 120.93, 117.09, 116.52, 114.17, 87.18, 86.30, 57.02, 31.47, 23.04, 19.33.

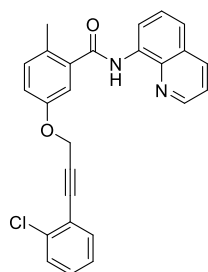
HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{29}\text{H}_{27}\text{N}_2\text{O}_2^+$ 435.2067; found: 435.2067.

5-((3-(2-Chlorophenyl)prop-2-yn-1-yl)oxy)-2-methyl-*N*-(quinolin-8-yl)benzamide (**1d**)



Methyl 5-((3-(2-chlorophenyl)prop-2-yn-1-yl)oxy)-2-methylbenzoate **S7** was prepared according to **General Procedure C** on a 4.00 mmol scale. Purification by flash chromatography (5:95 EA:PE) gave **S7** as a light-yellow liquid (0.708 g, 56%).

5-((3-(2-chlorophenyl)prop-2-yn-1-yl)oxy)-2-methyl-*N*-(quinolin-8-yl)benzamide **1d** was prepared according to **General Procedure D** on a 2.19 mmol scale. Purification by flash chromatography (5:10:85 EA:DCM:PE) gave **1d** as a yellow solid (0.496 g, 53%).

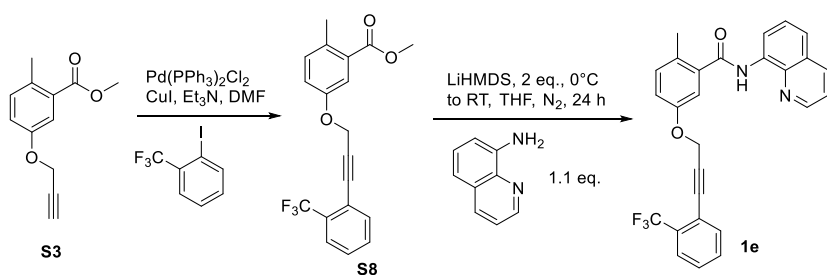


^1H NMR (400 MHz, Chloroform-*d*) δ 10.21 (s, 1H), 8.94 (d, $J = 7.4$ Hz, 1H), 8.68 (d, $J = 4.2$ Hz, 1H), 8.16 (d, $J = 8.2$ Hz, 1H), 7.58 (dt, $J = 16.3, 8.1$ Hz, 2H), 7.49 – 7.37 (m, 3H), 7.34 (d, $J = 8.0$ Hz, 1H), 7.26 – 7.20 (m, 2H), 7.19 – 7.08 (m, 2H), 5.01 (s, 2H), 2.54 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.79, 155.73, 148.26, 138.56, 137.41, 136.30, 136.23, 134.63, 133.66, 132.38, 129.74, 129.30, 129.23, 127.95, 127.38, 126.38, 122.11, 121.82, 121.65, 116.99, 116.54, 114.17, 88.83, 84.20, 56.88, 19.32.

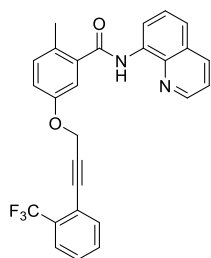
HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{26}\text{H}_{20}\text{ClN}_2\text{O}_2^+$ 427.1208; found: 427.1210.

2-Methyl-*N*-(quinolin-8-yl)-5-((3-(2-(trifluoromethyl)phenyl)prop-2-yn-1-yl)oxy)benzamide (**1e**)



Methyl 5-((3-(2-(trifluoromethyl)phenyl)prop-2-yn-1-yl)oxy)-2-methylbenzoate **S8** was prepared according to **General Procedure C** on a 6.00 mmol scale. Purification by flash chromatography (5:95 EA:PE) gave **S3** as a light-yellow liquid (1.08 g, 52%).

5-((3-(2-(trifluoromethyl)phenyl)prop-2-yn-1-yl)oxy)-2-methyl-*N*-(quinolin-8-yl)benzamide **1e** was prepared according to **General Procedure D** on a 3.01 mmol scale. Purification by flash chromatography (2:20:78 EA:DCM:PE) gave **1e** as a yellow oil (0.542 g, 39%).



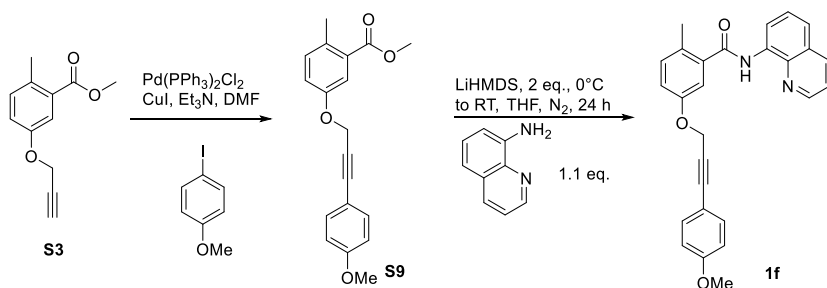
¹H NMR (400 MHz, Chloroform-*d*) δ 10.20 (s, 1H), 8.93 (d, $J = 7.8$ Hz, 1H), 8.69 (dd, $J = 4.3, 1.7$ Hz, 1H), 8.17 (dd, $J = 8.2, 1.7$ Hz, 1H), 7.58 (dtd, $J = 14.8, 8.0, 1.9$ Hz, 4H), 7.48 – 7.33 (m, 4H), 7.24 (s, 1H), 7.10 (dd, $J = 8.4, 2.7$ Hz, 1H), 4.99 (s, 2H), 2.54 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.83, 155.83, 148.34, 138.61, 137.52, 136.37, 134.69, 134.44, 132.48, 131.71(q, $J_{C-F} = 30.4$), 131.48, 129.35, 128.59, 128.02, 127.40, 125.82(q, $J_{C-F} = 5.0$), 123.45(q, $J_{C-F} = 271.9$), 121.94, 121.73, 120.41, 116.79, 116.60, 114.34, 89.44, 83.34, 56.82, 19.41.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -62.24.

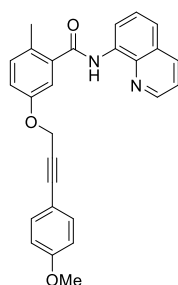
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{27}H_{20}F_3N_2O_2^+$ 461.1471; found: 461.1475.

5-((3-(4-Methoxyphenyl)prop-2-yn-1-yl)oxy)-2-methyl-*N*-(quinolin-8-yl)benzamide (**1f**)



Methyl 5-((3-(4-methoxyphenyl)prop-2-yn-1-yl)oxy)-2-methylbenzoate **S9** was prepared according to **General Procedure C** on a 5.00 mmol scale. Purification by flash chromatography (8:92 EA:PE) gave **S9** as a light yellow liquid (0.653 g, 42%).

5-((3-(4-methoxyphenyl)prop-2-yn-1-yl)oxy)-2-methyl-N-(quinolin-8-yl)benzamide **1f** was prepared according to **General Procedure D** on a 2.19 mmol scale. Purification by flash chromatography (10:90 acetone:PE) and recrystallization in DCM/hexane gave **1f** as an off-white solid (0.609 g, 72%).

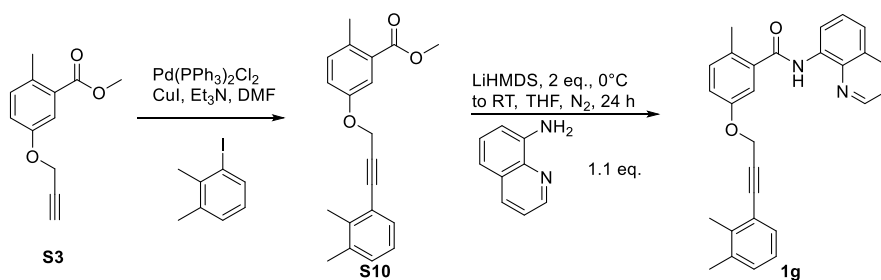


¹H NMR (400 MHz, Chloroform-*d*) δ 10.22 (s, 1H), 8.94 (d, $J = 7.4$ Hz, 1H), 8.70 (dt, $J = 3.8, 1.8$ Hz, 1H), 8.18 (dd, $J = 8.3, 1.9$ Hz, 1H), 7.66 – 7.50 (m, 2H), 7.47 – 7.32 (m, 4H), 7.25 (d, $J = 10.4$ Hz, 2H), 7.08 (dt, $J = 8.5, 2.2$ Hz, 1H), 6.84 – 6.73 (m, 2H), 4.94 (s, 2H), 3.79 (s, 3H), 2.54 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.83, 159.88, 155.88, 148.30, 138.58, 137.40, 136.32, 134.66, 133.42, 132.38, 129.16, 127.97, 127.40, 121.82, 121.66, 116.94, 116.55, 114.23, 113.97, 113.87, 87.46, 82.25, 57.06, 55.27, 19.31.

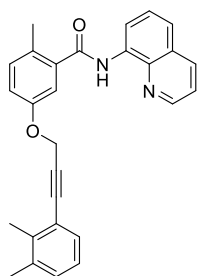
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{27}H_{23}N_2O_3^+$ 423.1703; found: 423.1703.

5-((3-(2,3-Dimethylphenyl)prop-2-yn-1-yl)oxy)-2-methyl-N-(quinolin-8-yl)benzamide (**1g**)



S10 was prepared according to **General Procedure C** on a 5.00 mmol scale. Purification by flash chromatography (4:96 EA:PE) gave **S10** as a yellow oil (0.864 g, 56%).

1g was prepared according to **General Procedure D** on a 2.76 mmol scale. Purification by flash chromatography (3:20:77 EA:DCM:PE) gave **1g** as a yellow oil (1.04 g, 90%).

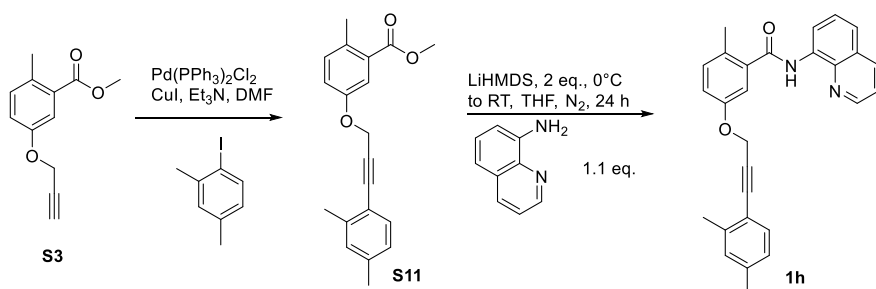


¹H NMR (400 MHz, Chloroform-*d*) δ 10.21 (s, 1H), 8.93 (d, *J* = 7.5 Hz, 1H), 8.64 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.63 – 7.51 (m, 2H), 7.45 – 7.36 (m, 2H), 7.30 – 7.21 (m, 2H), 7.13 – 7.04 (m, 2H), 6.99 (t, *J* = 7.6 Hz, 1H), 5.00 (s, 2H), 2.54 (s, 3H), 2.30 (s, 3H), 2.21 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.84, 155.90, 148.30, 138.98, 138.62, 137.45, 136.75, 136.30, 134.70, 132.38, 130.30, 130.13, 129.20, 127.99, 127.41, 125.27, 122.12, 121.83, 121.67, 117.13, 116.57, 114.14, 87.17, 86.88, 57.12, 20.27, 19.32, 17.42.

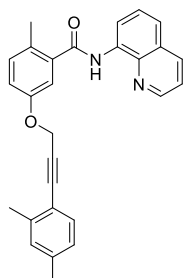
HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₂₈H₂₅N₂O₂⁺ 421.1911; found: 421.1913.

5-((3-(2,4-Dimethylphenyl)prop-2-yn-1-yl)oxy)-2-methyl-N-(quinolin-8-yl)benzamide (**1h**)



S11 was prepared according to **General Procedure C** on a 9.646 mmol scale. Purification by flash chromatography (4:96 EA:PE) gave **S11** as a yellow oil (1.007 g, 34%).

1h was prepared according to **General Procedure D** on a 2.76 mmol scale. Purification by flash chromatography (3:15:82 EA:DCM:PE) gave **1h** as a yellow oil (1.10 g, 80%).



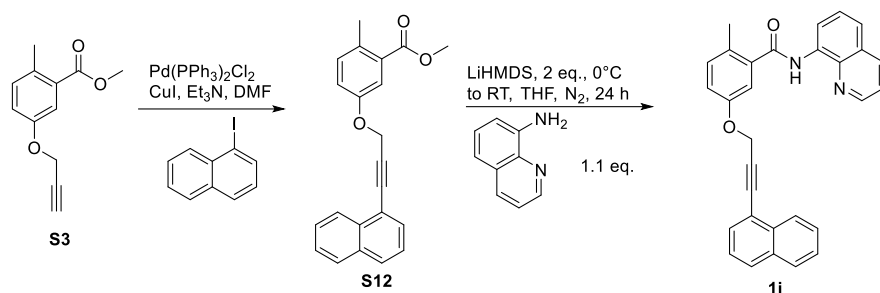
¹H NMR (400 MHz, Chloroform-*d*) δ 10.21 (s, 1H), 8.93 (d, *J* = 7.4 Hz, 1H), 8.67 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.59 (t, *J* = 7.9 Hz, 1H), 7.54 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.42 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.38 (d, *J* = 2.7 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.23 (s, 1H), 7.10 (dd, *J* = 8.5, 2.7 Hz, 1H), 6.96 (s, 1H), 6.89 (d, *J* = 7.8 Hz, 1H), 4.99 (s, 2H), 2.53 (s, 3H), 2.32 (s, 3H),

2.29 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.88, 155.94, 148.37, 140.51, 138.86, 138.66, 137.47, 136.36, 134.74, 132.41, 132.20, 130.33, 129.22, 128.03, 127.46, 126.34, 121.87, 121.71, 119.01, 117.11, 116.61, 114.22, 86.77, 86.72, 57.17, 21.46, 20.61, 19.38.

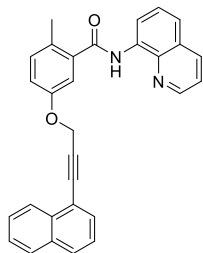
HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{28}\text{H}_{25}\text{N}_2\text{O}_2^+$ 421.1911; found: 421.1913.

2-Methyl-5-((3-(naphthalen-1-yl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (**1i**)



Methyl 2-methyl-5-((3-(naphthalen-1-yl)prop-2-yn-1-yl)oxy)benzoate **S8** was prepared according to **General Procedure C** on a 10.0 mmol scale. Purification by flash chromatography (10:90 EA:PE) gave **S12** as a light-yellow solid (2.71 g, 82%).

2-methyl-5-((3-(naphthalen-1-yl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide **1i** was prepared according to **General Procedure D** on a 4.03 mmol scale. Purification by flash chromatography (20:80 EA:PE) gave **1i** as a yellow solid (0.869 g, 49%).

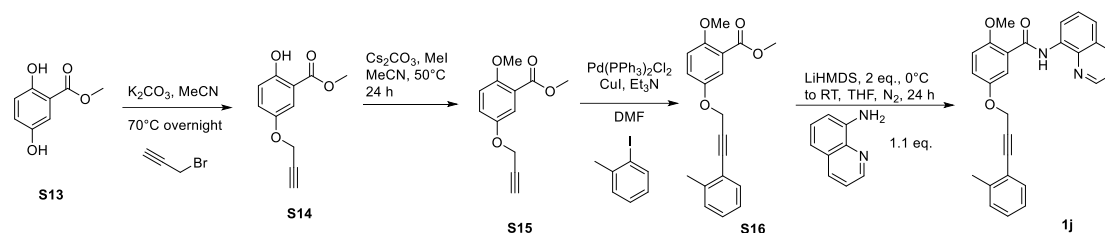


^1H NMR (400 MHz, Chloroform-*d*) δ 10.22 (s, 1H), 8.94 (d, $J = 7.5$ Hz, 1H), 8.58 (dd, $J = 4.1, 1.8$ Hz, 1H), 8.21 (d, $J = 7.9$ Hz, 1H), 8.14 (dd, $J = 8.2, 1.6$ Hz, 1H), 7.84 – 7.76 (m, 2H), 7.67 (d, $J = 7.2$ Hz, 1H), 7.63 – 7.32 (m, 7H), 7.30 – 7.23 (m, 2H), 7.16 (dt, $J = 8.5, 2.1$ Hz, 1H), 5.11 (s, 2H), 2.55 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.80, 155.84, 148.24, 138.54, 137.47, 136.25, 134.63, 133.30, 133.01, 132.44, 130.86, 129.32, 129.18, 128.16, 127.94, 127.37, 126.91, 126.42, 126.01, 125.06, 121.81, 121.62, 119.79, 117.20, 116.54, 114.16, 88.46, 85.69, 57.14, 19.34.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{30}\text{H}_{23}\text{N}_2\text{O}_2^+$ 443.1754; found: 443.1754.

2-Methoxy-*N*-(quinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (**1j**)



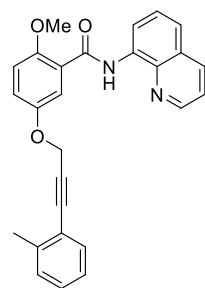
Methyl 2-hydroxy-5-(prop-2-yn-1-yloxy)benzoate **S14** was prepared according to **General Procedure B** on a 25.0 mmol scale. Purification by flash chromatography (20:80 EA:PE) gave **S14** as white crystal (4.00 g, 78%).

General Procedure E:

S14 (2.06 g, 10 mmol), caesium carbonate (8.15 g, 25 mmol), 100 mL of acetonitrile and methyl iodide (0.9 mL, 15 mmol) were added into 250 mL round-bottom flask. The mixture was and heated to 50°C in an oil bath and stirred for 24 h. The mixture was cooled to room temperature and filtered through celite. Solvent was removed by rotary evaporation. Purification by flash chromatography (15:85 EA:PE) gave methyl 2-methoxy-5-(prop-2-yn-1-yloxy)benzoate **S15** as white crystal (2.19 g, 99%).

Methyl 2-methoxy-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzoate **S16** was prepared according to **General Procedure C** on a 7.50 mmol scale. Purification by flash chromatography (30:70 EA:PE) gave **S16** as a light-yellow liquid (1.63 g, 70%).

2-methoxy-*N*-(quinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide **1j** was prepared according to **General Procedure D** on a 5.16 mmol scale. Purification by flash chromatography (10:10:1 DCM:PE:EA) gave **1j** as an off-white solid (1.87 g, 86%).

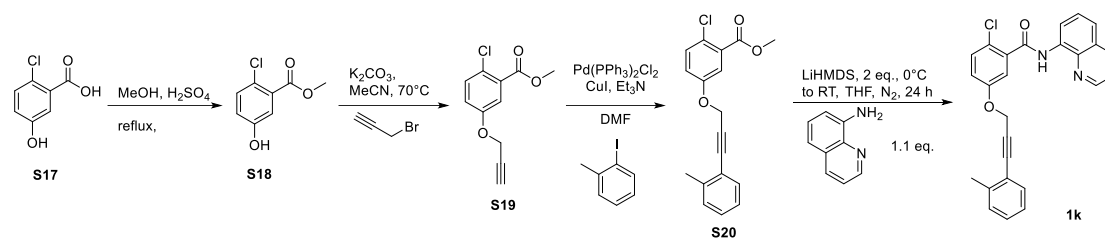


¹H NMR (400 MHz, Chloroform-*d*) δ 12.44 (s, 1H), 9.03 (dd, $J = 7.6, 1.4$ Hz, 1H), 8.87 (dd, $J = 4.3, 1.5$ Hz, 1H), 8.16 (dd, $J = 8.3, 1.6$ Hz, 1H), 8.07 (d, $J = 3.2$ Hz, 1H), 7.58 (t, $J = 7.9$ Hz, 1H), 7.52 (dd, $J = 8.3, 1.3$ Hz, 1H), 7.48 – 7.39 (m, 2H), 7.23 – 7.07 (m, 4H), 7.04 (d, $J = 8.9$ Hz, 1H), 5.02 (s, 2H), 4.17 (s, 3H), 2.38 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.13, 152.63, 152.01, 148.28, 140.65, 139.27, 136.25, 135.70, 132.22, 129.38, 128.61, 128.10, 127.57, 125.44, 122.94, 122.08, 121.55, 121.45, 120.89, 117.55, 117.37, 113.16, 87.65, 86.25, 57.44, 56.74, 20.68.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{27}H_{23}N_2O_3^+$ 423.1703; found: 423.1704.

2-Chloro-*N*-(quinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (**1k**)

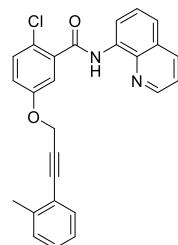


Methyl 2-chloro-5-hydroxybenzoate **S18** was prepared according to **General Procedure A** on a 58 mmol scale. Off-white solid (5.94 g, 55%).

Methyl 2-chloro-5-(prop-2-yn-1-yloxy)benzoate **S19** was prepared according to **General Procedure B** on a 20.0 mmol scale. Purification by flash chromatography (10:90 EA:PE) gave **S19** as white solid (2.81 g, 63%).

Methyl 2-chloro-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzoate **S20** was prepared according to **General Procedure C** on a 6.00 mmol scale. Purification by flash chromatography (10:90 EA:PE) gave **S20** as a light yellow liquid (1.20 g, 64%).

2-chloro-*N*-(quinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide **1k** was prepared according to **General Procedure D** on a 3.46 mmol scale. Purification by flash chromatography (6:10:84 EA:DCM:PE) gave **1k** as an off-white solid (1.34 g, 91%).

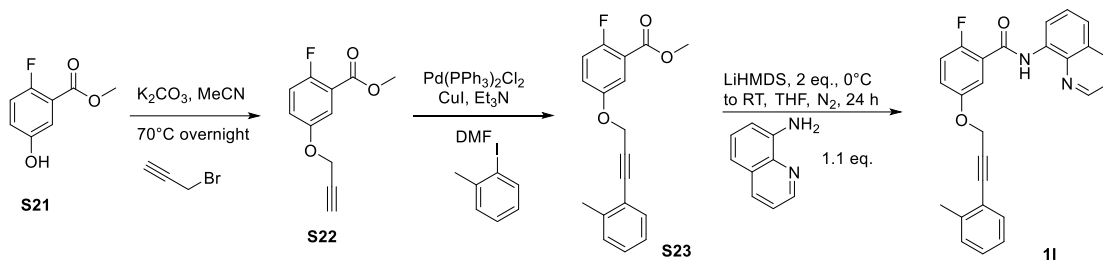


¹H NMR (400 MHz, Chloroform-*d*) δ 10.54 (s, 1H), 8.95 (dd, $J = 7.3, 1.9$ Hz, 1H), 8.74 (dd, $J = 4.1, 1.8$ Hz, 1H), 8.17 (dd, $J = 8.2, 1.9$ Hz, 1H), 7.63 – 7.54 (m, 2H), 7.52 (d, $J = 3.0$ Hz, 1H), 7.47 – 7.37 (m, 3H), 7.21 (t, $J = 7.5$ Hz, 1H), 7.17 – 7.06 (m, 3H), 5.01 (s, 2H), 2.36 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 164.49, 156.51, 148.39, 140.60, 138.62, 136.38, 136.30, 134.38, 132.22, 131.39, 129.44, 128.81, 127.96, 127.37, 125.50, 123.08, 122.17, 121.73, 121.71, 118.76, 116.92, 116.28, 86.88, 86.75, 57.13, 20.65.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{26}H_{20}ClN_2O_2^+$ 427.1208; found: 427.1209.

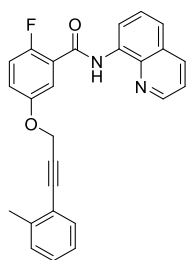
2-Fluoro-*N*-(quinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (**1l**)



Methyl 2-fluoro-5-(prop-2-yn-1-yloxy)benzoate **S22** was prepared according to **General Procedure B** on a 20.0 mmol scale. Purification by flash chromatography (10:90 EA:PE) gave **S22** as an off-white solid (3.05 g, 73%).

methyl 2-fluoro-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzoate **S23** was prepared according to **General Procedure C** on a 10.0 mmol scale. Purification by flash chromatography (7:93 EA:PE) gave **S23** as light yellow liquid (1.47 g, 37%).

2-fluoro-*N*-(quinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide **11** was prepared according to **General Procedure D** on a 4.84 mmol scale. Purification by flash chromatography (3:30:67 EA:DCM:PE) gave **11** as an off-white solid (1.89 g, 95%).



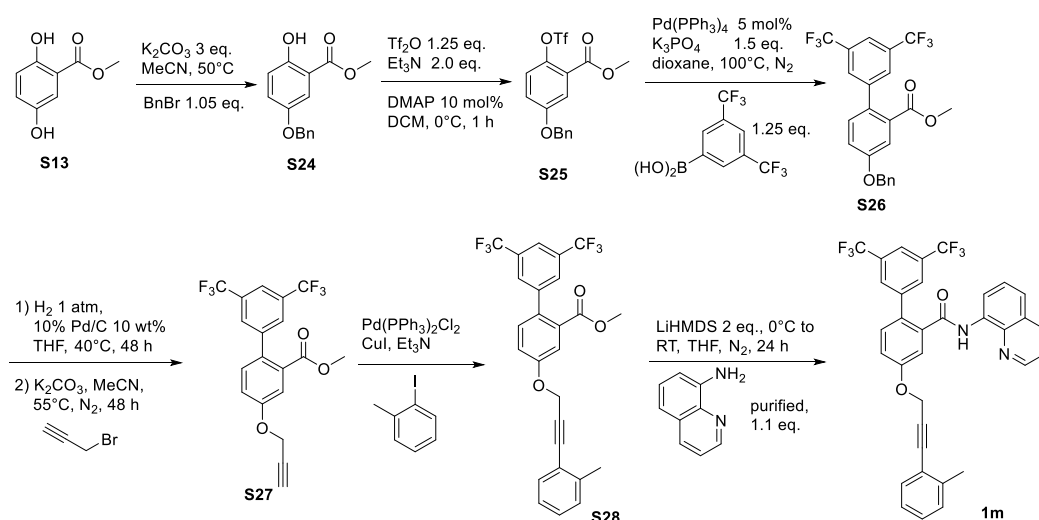
¹H NMR (400 MHz, Chloroform-*d*) δ 11.21 (d, $J = 13.3$ Hz, 1H), 8.98 (dd, $J = 7.2, 1.8$ Hz, 1H), 8.86 (dd, $J = 4.3, 1.7$ Hz, 1H), 8.17 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.89 (ddd, $J = 6.1, 2.4, 1.3$ Hz, 1H), 7.63 – 7.52 (m, 2H), 7.47 (dd, $J = 8.3, 4.2$ Hz, 1H), 7.41 (dd, $J = 7.6, 1.4$ Hz, 1H), 7.23 – 7.07 (m, 5H), 5.03 (s, 2H), 2.38 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 161.24(d, C–F, $^3J_{C-F} = 3.8$ Hz), 155.51 (d, C–F, $^1J_{C-F} = 221.3$ Hz), 154.12 (d, C–F, $^4J_{C-F} = 1.9$ Hz), 148.52, 140.64, 138.79, 136.27, 134.80, 132.22, 129.42, 128.75, 127.97, 127.38, 125.49, 122.34 (d, C–F, $^2J_{C-F} = 13.2$ Hz), 122.10, 121.85, 121.70, 121.11 (d, C–F, $^3J_{C-F} = 8.9$ Hz), 117.29 (d, C–F, $^2J_{C-F} = 26.7$ Hz), 117.25, 116.53 (d, C–F, $^3J_{C-F} = 2.1$ Hz), 87.03, 86.64, 57.38, 20.66.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -121.35.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{26}H_{20}FN_2O_2^+$ 411.1503; found: 411.1504.

***N*-(Quinolin-8-yl)-4-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)-3',5'-bis(trifluoromethyl)-[1,1'-biphenyl]-2-carboxamide (1m)**



Methyl 2,5-dihydroxybenzoate **S13** (13.45 g, 80.00 mmol), potassium carbonate (33.12 g, 0.24 mol), acetonitrile (250 mL) and benzyl bromide (10.0 mL 84 mmol) were added to a 500 mL round-bottom flask heated in an oil bath at 40°C for 18 h under stirring. The mixture was cooled to room temperature and filtered through celite. Solvent was removed by rotary evaporation. Purification by flash chromatography (1:30:69 EA:DCM:PE) and recrystallization in DCM/hexane gave methyl 5-(benzyloxy)-2-hydroxybenzoate **S24** as white crystal (17.58 g, 85%).

S24 (17.04 g, 66.00 mmol), DMAP (6.6 mmol, 740 mg), DCM (250 mL) and triethylamine (18.5 mL, 132 mmol) were added to a 500 mL 3-necked round-bottom flask under nitrogen flow. The mixture was cooled with ice and triflic anhydride was dropped slowly from a pressure-equalizing drop funnel under effective stirring. After 1 h, 8 mL of ethanol was added in order to quench the reaction. The solution was washed with 1 M hydrochloric acid, saturated sodium bicarbonate solution and brine. The organic phase was then dried with anhydrous sodium sulfate and the solvent was removed by rotary evaporation. Purification by flash chromatography (2:30:68 EA:DCM:PE) and recrystallization in DCM/hexane gave methyl 5-(benzyloxy)-2-(((trifluoromethyl)sulfonyl)oxy)benzoate **S25** as white crystal (24.31 g, 94%).

General Procedure F:

S25 (3.90 g, 10.0 mmol), (3,5-bis(trifluoromethyl)phenyl)boronic acid (3.224 g, 12.5 mmol), Pd(PPh₃)₄ (578 mg, 0.5 mmol), potassium phosphate (3.184 g, 15 mmol) and 1,4-dioxane (75 mL) was added into a 250 mL round-bottom flask under nitrogen atmosphere. The mixture was heated to 100 °C overnight. Solvent was removed by rotary evaporation. To the residue, 100 mL of water and 50 mL DCM were added. The aqueous phase was extracted twice with DCM (50 mL). The organic phase was washed with brine then dried with anhydrous sodium sulfate. Solvent was removed by rotary evaporation. Purification by flash chromatography (5: 95 EA: PE) gave methyl 4-(benzyloxy)-3',5'-bis(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylate **S25** as colorless oil (4.24 g, 93%).

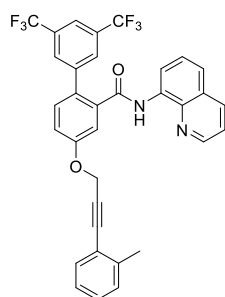
General Procedure G:

S26 (4.07 g, 8.96 mmol), 0.41 g 10% Pd/C and THF (80 mL) was added into a 250 mL round-bottom flask which was flushed with nitrogen and then hydrogen with a balloon filled with hydrogen.

The mixture was heated to 40°C and stirred vigorously for 48 h. the flask was re-flushed with nitrogen and the mixture was filtered through celite into another 250 mL round-bottom flask and washed with DCM. Solvent was removed from the filtrate by rotary evaporation. To the residue, potassium carbonate (3.7 g, 27 mmol), acetonitrile (50 mL) and propargyl bromide (0.8 mL, 10.8 mmol) were added, then stirred and heated in an oil bath at 55°C for 48 h. The mixture was cooled to room temperature and filtered through celite. Solvent was removed by rotary evaporation. Purification by flash chromatography (20:80 EA:PE) gave methyl 4-(prop-2-yn-1-yloxy)-3',5'-bis(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylate **S27** as white solid (3.36 g, 93%).

Methyl 4-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)-3',5'-bis(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylate **S28** was prepared according to **General Procedure C** on a 8.06 mmol scale. Purification by flash chromatography (10:90 EA:PE) gave **S28** as light yellow liquid (2.01 g, 51%).

N-(quinolin-8-yl)-4-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)-3',5'-bis(trifluoromethyl)-[1,1'-biphenyl]-2-carboxamide **1m** was prepared according to **General Procedure D** on a 4.00 mmol scale. Purification by flash chromatography (3:30:67 EA:DCM:PE) gave **1m** as an off-white amorphous solid (2.17 g, 90%).



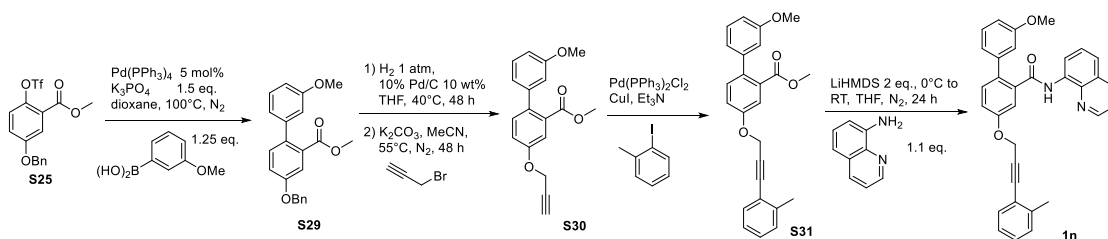
¹H NMR (400 MHz, Chloroform-*d*) δ 9.74 (s, 1H), 8.75 (dd, *J* = 7.3, 1.8 Hz, 1H), 8.43 (dd, *J* = 4.3, 1.6 Hz, 1H), 8.10 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.93 (s, 2H), 7.64 (t, *J* = 2.0 Hz, 1H), 7.60 (s, 1H), 7.56 – 7.41 (m, 4H), 7.33 (ddd, *J* = 15.5, 8.4, 3.5 Hz, 2H), 7.24 – 7.08 (m, 3H), 5.11 (s, 2H), 2.40 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 166.37, 158.27, 147.94, 141.90, 140.66, 138.28, 137.49, 136.21, 133.88, 132.31, 131.81, 131.58 (q, C–F, ²*J*_{C–F} = 33.1 Hz), 130.22, 129.52, 129.26, 128.91, 127.76, 127.25, 125.59, 123.22 (q, C–F, ¹*J*_{C–F} = 271.3 Hz), 122.12, 121.86, 121.54, 120.85 (m), 118.04, 116.49, 115.77, 87.03, 86.96, 57.05, 20.69.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -62.92.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₃₄H₂₁F₆N₂O₂⁺ 603.1502; found: 603.1502.

3'-Methoxy-*N*-(quinolin-8-yl)-4-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)-[1,1'-biphenyl]-2-carboxamide (1n)

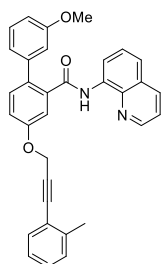


S29 was prepared according to **General Procedure F** on a 10.0 mmol scale. Purification by flash chromatography (2:30:68 EA:DCM:PE) gave **S29** as a colorless oil (3.27 g, 94%).

S30 was prepared according to **General Procedure G** on a 9.34 mmol scale. Purification by flash chromatography (15:85 EA:PE) gave **S30** as a colorless oil (2.71 g, 98%).

S31 was prepared according to **General Procedure C** on an 8.97 mmol scale. Purification by flash chromatography (15:85 EA:PE) gave **S31** as a yellow oil (1.49 g, 43%).

1n was prepared according to **General Procedure D** on a 3.78 mmol scale. Purification by flash chromatography (4:30:66 EA:DCM:PE) gave **1n** as a yellow foam (1.33 g, 71%).

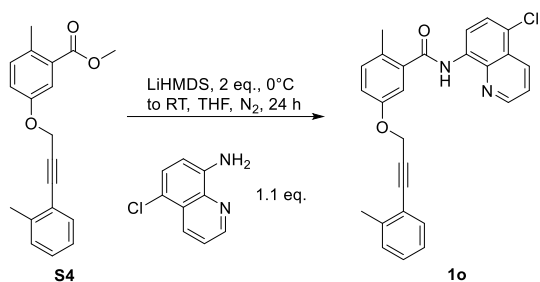


¹H NMR (400 MHz, Chloroform-*d*) δ 9.80 (s, 1H), 8.81 (dd, $J = 7.5, 1.4$ Hz, 1H), 8.48 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.06 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.60 (d, $J = 2.7$ Hz, 1H), 7.51 (t, $J = 7.9$ Hz, 1H), 7.48 – 7.40 (m, 3H), 7.33 (dd, $J = 8.3, 4.2$ Hz, 1H), 7.25 – 7.17 (m, 2H), 7.16 – 7.03 (m, 5H), 6.67 (ddd, $J = 8.2, 2.4, 1.2$ Hz, 1H), 5.07 (s, 2H), 3.68 (s, 3H), 2.39 (s, 3H).

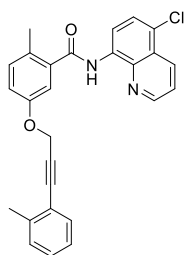
¹³C NMR (101 MHz, Chloroform-*d*) δ 167.35, 159.60, 157.20, 147.75, 141.00, 140.66, 138.41, 137.05, 135.95, 134.54, 133.29, 132.26, 131.77, 129.42, 129.33, 128.72, 127.68, 127.23, 125.48, 121.93, 121.60, 121.56, 121.41, 117.72, 116.23, 115.20, 114.16, 113.48, 87.24, 86.62, 56.98, 55.17, 20.67.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{33}H_{27}N_2O_3^+$ 499.2016; found: 499.2018.

***N*-(5-Chloroquinolin-8-yl)-2-methyl-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (1o)**



1o was prepared according to **General Procedure D** on a 2.27 mmol scale. Purification by flash chromatography (3:30:67 EA:DCM:PE) gave **1o** as an off-white solid (0.849 g, 85%).

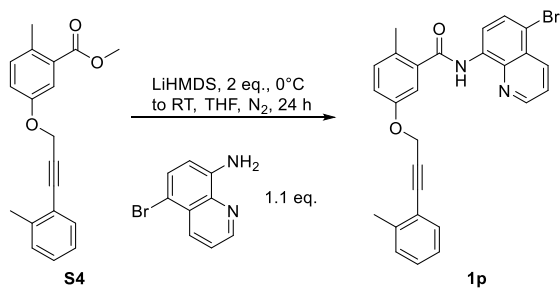


¹H NMR (400 MHz, Chloroform-*d*) δ 10.17 (s, 1H), 8.88 (d, J = 8.4 Hz, 1H), 8.69 (dd, J = 4.2, 1.6 Hz, 1H), 8.57 (dd, J = 8.6, 1.6 Hz, 1H), 7.65 (d, J = 8.4 Hz, 1H), 7.54 (dd, J = 8.5, 4.2 Hz, 1H), 7.42 – 7.35 (m, 2H), 7.27 – 7.18 (m, 3H), 7.17 – 7.06 (m, 3H), 5.01 (s, 2H), 2.53 (s, 3H), 2.35 (s, 3H).

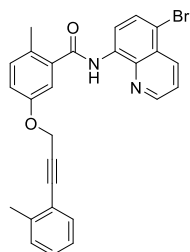
¹³C NMR (101 MHz, Chloroform-*d*) δ 167.73, 155.79, 148.77, 140.57, 139.11, 137.06, 133.89, 133.36, 132.44, 132.19, 129.43, 129.27, 128.72, 127.21, 125.95, 125.49, 124.60, 122.39, 121.92, 117.16, 116.44, 114.07, 87.37, 86.48, 56.99, 20.64, 19.33.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for C₂₇H₂₂ClN₂O₂⁺ 441.1364; found: 441.1365.

***N*-(5-Bromoquinolin-8-yl)-2-methyl-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (**1p**)**



1p was prepared according to **General Procedure D** on a 2.00 mmol scale. Purification by flash chromatography (3:30:67 EA:DCM:PE) gave **1p** as an off-white solid (0.350 g, 40%).

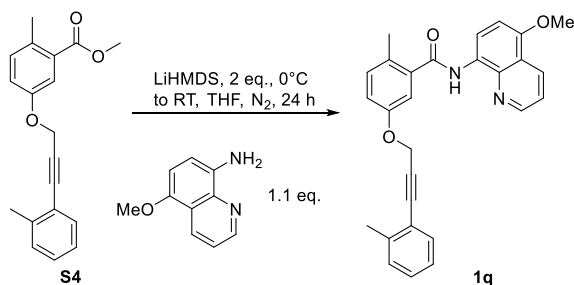


¹H NMR (400 MHz, Chloroform-*d*) δ 10.19 (s, 1H), 8.83 (d, J = 8.3 Hz, 1H), 8.66 (dd, J = 4.2, 1.6 Hz, 1H), 8.53 (dd, J = 8.5, 1.6 Hz, 1H), 7.85 (d, J = 8.3 Hz, 1H), 7.53 (dd, J = 8.5, 4.2 Hz, 1H), 7.43 – 7.34 (m, 2H), 7.27 – 7.17 (m, 3H), 7.17 – 7.05 (m, 3H), 5.01 (s, 2H), 2.53 (s, 3H), 2.35 (s, 3H).

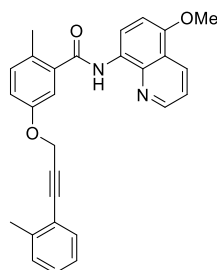
¹³C NMR (101 MHz, Chloroform-*d*) δ 167.73, 155.78, 148.78, 140.56, 139.23, 137.03, 135.92, 134.53, 132.45, 132.19, 130.87, 129.42, 129.27, 128.71, 127.20, 125.48, 122.72, 121.91, 117.16, 116.99, 114.55, 114.06, 87.36, 86.48, 56.98, 20.64, 19.34.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{27}H_{22}BrN_2O_2^+$ 485.0859; found: 485.0861.

***N*-(5-Methoxyquinolin-8-yl)-2-methyl-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (1q)**



1q was prepared according to **General Procedure D** on a 2.00 mmol scale. Purification by flash chromatography (3:30:67 EA:DCM:PE) gave **1q** as an off-white solid (0.350 g, 40%).

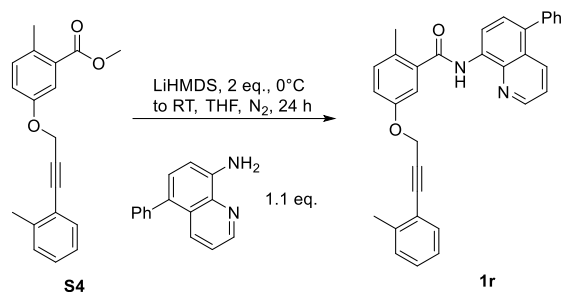


¹H NMR (400 MHz, Chloroform-*d*) δ 9.96 (s, 1H), 8.85 (d, J = 8.5 Hz, 1H), 8.67 (dd, J = 4.3, 1.7 Hz, 1H), 8.58 (dd, J = 8.4, 1.7 Hz, 1H), 7.44 – 7.34 (m, 3H), 7.25 – 7.17 (m, 2H), 7.14 (d, J = 7.5 Hz, 1H), 7.09 (dq, J = 8.5, 2.2 Hz, 2H), 6.89 (d, J = 8.6 Hz, 1H), 5.00 (s, 2H), 4.01 (s, 3H), 2.53 (s, 3H), 2.36 (s, 3H).

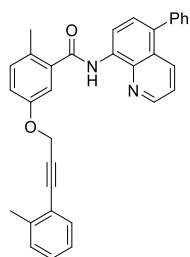
¹³C NMR (101 MHz, Chloroform-*d*) δ 167.45, 155.75, 150.50, 148.74, 140.60, 139.27, 137.63, 132.27, 132.20, 131.20, 129.40, 129.09, 128.67, 128.07, 125.46, 121.96, 120.77, 120.44, 116.83, 116.68, 114.02, 104.24, 87.46, 86.40, 56.97, 55.80, 20.65, 19.31.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{28}H_{25}N_2O_3^+$ 437.1860; found: 437.1861.

2-Methyl-*N*-(5-phenylquinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (1r)



1r was prepared according to **General Procedure D** on a 3.00 mmol scale. Purification by flash chromatography (2:30:68 EA:DCM:PE) gave **1r** as a yellow solid (1.26 g, 87%).

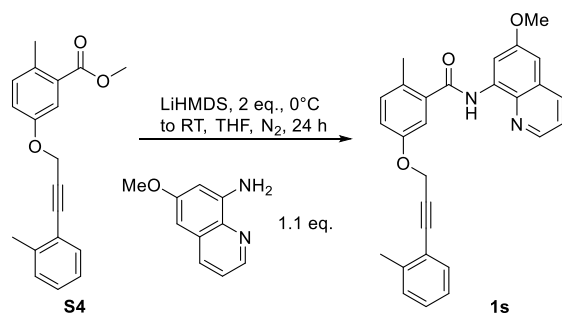


¹H NMR (400 MHz, Chloroform-*d*) δ 10.32 (s, 1H), 8.98 (d, $J = 7.9$ Hz, 1H), 8.67 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.30 (dd, $J = 8.5, 1.7$ Hz, 1H), 7.57 (d, $J = 8.0$ Hz, 1H), 7.54 – 7.36 (m, 8H), 7.28 – 7.18 (m, 3H), 7.17 – 7.07 (m, 3H), 5.02 (s, 2H), 2.56 (s, 3H), 2.37 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.79, 155.79, 148.08, 140.60, 139.16, 138.59, 137.41, 134.72, 134.61, 134.02, 132.38, 132.21, 130.10, 129.42, 129.21, 128.69, 128.52, 127.89, 127.51, 126.30, 125.48, 121.95, 121.59, 117.00, 116.11, 114.11, 87.42, 86.45, 56.98, 20.67, 19.36.

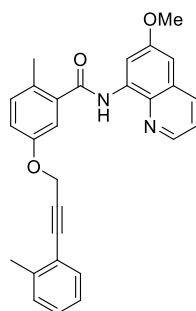
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{33}H_{27}N_2O_2^+$ 483.2067; found: 483.2070.

***N*-(6-Methoxyquinolin-8-yl)-2-methyl-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (1s)**



1s was prepared according to **General Procedure D** on a 2.05 mmol scale. Purification by flash

chromatography (3:30:67 EA:DCM:PE) gave **1s** as a yellow oil (0.672 g, 75%).

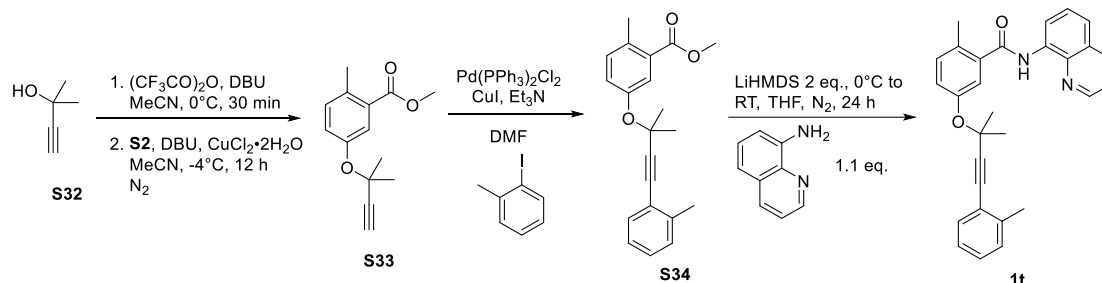


¹H NMR (400 MHz, Chloroform-*d*) δ 10.16 (s, 1H), 8.67 (d, $J = 2.7$ Hz, 1H), 8.49 (dd, $J = 4.2, 1.6$ Hz, 1H), 8.03 (dd, $J = 8.3, 1.6$ Hz, 1H), 7.42 – 7.33 (m, 3H), 7.25 – 7.17 (m, 2H), 7.14 (d, $J = 7.5$ Hz, 1H), 7.10 (dd, $J = 8.5, 2.6$ Hz, 2H), 6.83 (d, $J = 2.7$ Hz, 1H), 5.00 (s, 2H), 3.95 (s, 3H), 2.52 (s, 3H), 2.36 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.78, 158.51, 155.83, 145.71, 140.60, 137.32, 135.54, 135.19, 134.94, 132.37, 132.22, 129.42, 129.21, 128.96, 128.68, 125.48, 122.12, 121.99, 117.14, 114.11, 109.04, 100.05, 87.46, 86.47, 57.03, 55.65, 20.64, 19.30.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{28}H_{25}N_2O_3^+$ 437.1860; found: 437.1863.

2-Methyl-5-((2-methyl-4-(*o*-tolyl)but-3-yn-2-yl)oxy)-*N*-(quinolin-8-yl)benzamide (**1t**)

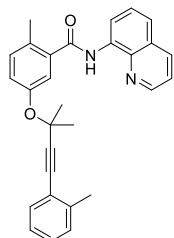


1,1-dimethylprop-3-yn-1-ol **S32** (0.97 mL, 10 mmol), dry acetonitrile (6 mL) and DBU (2.39 mL, 16 mmol) were added to a 50 mL round-bottom flask under nitrogen atmosphere. Then the mixture was cooled with ice. Trifluoroacetic anhydride (1.67 mL, 12 mmol) was added dropwise. The mixture was allowed to react for 30 min.

To another 50 mL round-bottom flask, methyl 2-methyl-5-hydroxybenzoate **S2** (1.66 g, 10.0 mmol) and cupric chloride dihydrate (1.7 mg, 0.01 mmol) were added under nitrogen atmosphere. Then dry acetonitrile (6 mL) and DBU (1.79 mL, 12 mmol) were added via syringe. The mixture was cooled with ice. Using a syringe, the former prepared solution was dropped into this flask. The mixture was stirred in a coolant bath at -4°C overnight. To mixture 50 mL of water and 50 mL ether were added. The aqueous phase was extracted twice with ether (25 mL). The organic phase was washed with brine then dried with anhydrous sodium sulfate. Solvent was removed by rotary evaporation. Purification by flash chromatography (8:92 EA: PE) gave methyl 2-methyl-5-((2-methylbut-3-yn-2-yl)oxy)benzoate **S33** as slightly yellow oil (1.68 g, 72%).

Methyl 2-methyl-5-((2-methyl-4-(*o*-tolyl)but-3-yn-2-yl)oxy)benzoate **S34** was prepared according to **General Procedure C** on a 7.19 mmol scale. Purification by flash chromatography (6:94 EA:PE) gave **S34** as light yellow liquid (1.35 g, 58%).

1t was prepared according to **General Procedure D** on a 4.16 mmol scale. Purification by flash chromatography (20:80 EA:PE) gave **1t** as a yellow viscous oil (1.57 g, 87%).

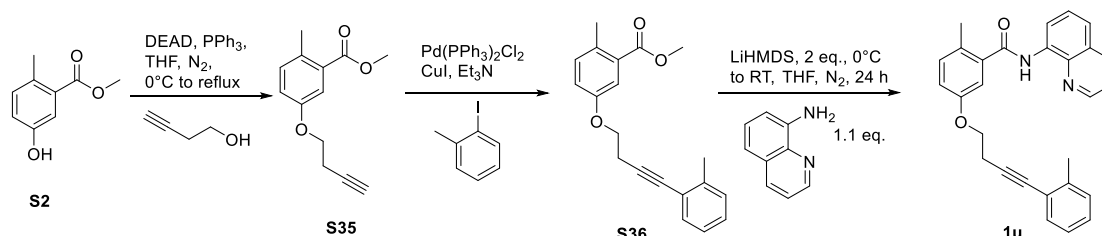


¹H NMR (400 MHz, Chloroform-*d*) δ 10.19 (s, 1H), 8.91 (d, $J = 7.4$ Hz, 1H), 8.66 (dd, $J = 4.2, 1.6$ Hz, 1H), 8.15 (dd, $J = 8.2, 1.7$ Hz, 1H), 7.63 – 7.52 (m, 3H), 7.41 (dd, $J = 8.3, 4.2$ Hz, 1H), 7.37 – 7.28 (m, 2H), 7.21 (d, $J = 8.4$ Hz, 1H), 7.13 – 7.03 (m, 2H), 6.94 (td, $J = 7.4, 1.6$ Hz, 1H), 2.54 (s, 3H), 2.31 (s, 3H), 1.78 (s, 6H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.89, 153.76, 148.25, 140.14, 138.58, 136.93, 136.23, 134.73, 131.90, 131.88, 130.97, 129.30, 128.31, 127.95, 127.39, 125.36, 123.65, 122.25, 121.72, 121.63, 120.54, 116.51, 95.14, 85.07, 73.76, 29.91, 20.54, 19.44.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{29}H_{27}N_2O_2^+$ 435.2067; found: 435.2067.

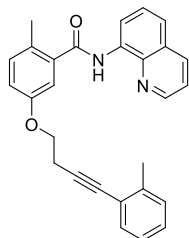
2-Methyl-*N*-(quinolin-8-yl)-5-((4-(*o*-tolyl)but-3-yn-1-yl)oxy)benzamide (**1u**)



S2 (2.49 g, 15.0 mmol) and PPh_3 (5.89 g, 22.5 mmol) were added to a 100 mL 2-necked round-bottom flask. Then the flask was flushed with nitrogen. THF (40 mL) and but-3-yn-1-ol (1.7 mL, 22.5 mmol) were added via syringe. The mixture was cooled to 0°C with ice. Under stirring, DEAD (3.5 mL, 22.5 mmol) was added dropwise with a syringe. The mixture was allowed to turn to room temperature and heated in an oil bath and refluxed for 24 h. The mixture was cooled to room temperature. Solvent was removed by rotary evaporation. Purification by flash chromatography (10:90 EA:PE) gave methyl 5-((but-3-yn-1-yl)oxy)-2-methylbenzoate **S35** as colorless oil (1.25 g, 38%).

Methyl 2-methyl-5-((4-(*o*-tolyl)but-3-yn-1-yl)oxy)benzoate **S36** was prepared according to **General Procedure C** on a 5.65 mmol scale. Purification by flash chromatography (5:95 EA:PE) gave **S36** as light-yellow liquid (1.09 g, 63%).

1u was prepared according to **General Procedure D** on a 3.49 mmol scale. Purification by flash chromatography (2:30:68 EA:DCM:PE) gave **1u** as a white solid (1.10 g, 75%).

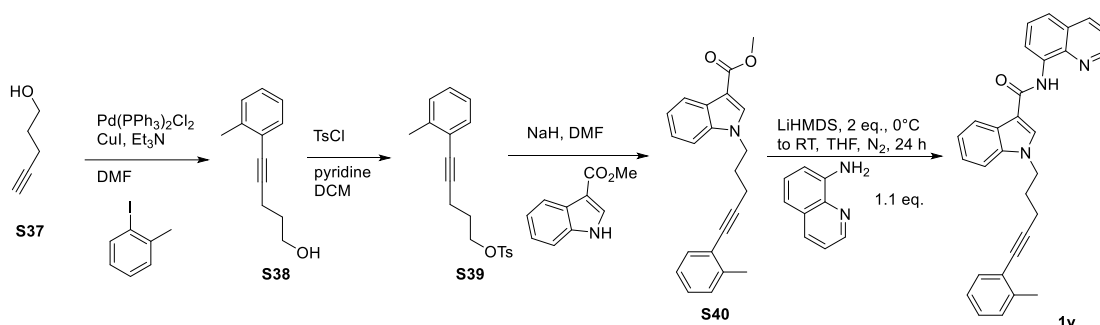


¹H NMR (400 MHz, Chloroform-*d*) δ 10.20 (s, 1H), 8.93 (d, J = 7.4 Hz, 1H), 8.77 (dd, J = 4.3, 1.7 Hz, 1H), 8.18 (dd, J = 8.3, 1.7 Hz, 1H), 7.63 – 7.52 (m, 2H), 7.45 (dd, J = 8.3, 4.2 Hz, 1H), 7.37 (d, J = 7.5 Hz, 1H), 7.28 – 7.14 (m, 4H), 7.09 (td, J = 6.7, 5.7, 2.9 Hz, 1H), 6.99 (dd, J = 8.5, 2.7 Hz, 1H), 4.23 (t, J = 7.0 Hz, 2H), 2.97 (t, J = 7.0 Hz, 2H), 2.53 (s, 3H), 2.41 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.89, 156.63, 148.31, 140.15, 138.59, 137.50, 136.35, 134.62, 132.43, 131.87, 129.31, 128.63, 127.98, 127.86, 127.41, 125.42, 123.12, 121.83, 121.68, 116.81, 116.55, 113.54, 89.59, 80.98, 66.66, 20.72, 20.64, 19.29.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{28}H_{25}N_2O_2^+$ 421.1911; found: 421.1911.

N-(Quinolin-8-yl)-1-(5-(*o*-tolyl)pent-4-yn-1-yl)-1*H*-indole-3-carboxamide (**1v**)



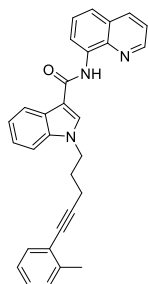
5-(*o*-tolyl)pent-4-yn-1-ol **S38** was prepared according to **General Procedure C** on a 5.65 mmol scale. Purification by flash chromatography (2:98 EA:DCM) gave **S38** as light yellow liquid (2.70 g, 78%).

S39 (2.70 g, 15.5 mmol), pyridine (2.4 mL), DCM (50 mL) and TsCl (3.81 g, 20 mmol) were added to a 100 mL round-bottom flask. The mixture was stirred overnight at room temperature and then washed with saturated sodium bicarbonate and brine. The organic phase was washed with water and brine then dried with anhydrous sodium sulfate. Purification by flash chromatography (10:90 EA:PE) gave 5-(*o*-tolyl)pent-4-yn-1-yl 4-methylbenzenesulfonate **S39** as light yellow oil (3.56 g, 70%).

Methyl 1*H*-indole-3-carboxylate (2.09 g, 12.0 mmol) and dry DMF (50 mL) were added to a 100 mL round-bottom flask. To which was carefully added sodium hydride (0.72 g, 18 mmol) in small portions. After stirring for 30 min, 5-(*o*-tolyl)pent-4-yn-1-yl 4-methylbenzenesulfonate **S39** (10.5 mmol, 3.45 g) was added and the mixture was heated to 50°C in an oil bath and refluxed for 24 h. The mixture was cooled to room temperature. To the mixture were added 200 mL of water and 100

mL of ether. The aqueous phase was extracted twice with ether (50 mL). The organic phase was washed with water and brine then dried with anhydrous sodium sulfate. Purification by flash chromatography (20:80 EA:PE) gave methyl 1-(5-(*o*-tolyl)pent-4-yn-1-yl)-1H-indole-3-carboxylate **S40** as light yellow oil (1.39 g, 40%).

1v was prepared according to **General Procedure D** on a 4.09 mmol scale. Purification by flash chromatography (20:80 EA:PE) gave **1v** as a yellow oil (1.40 g, 77%).

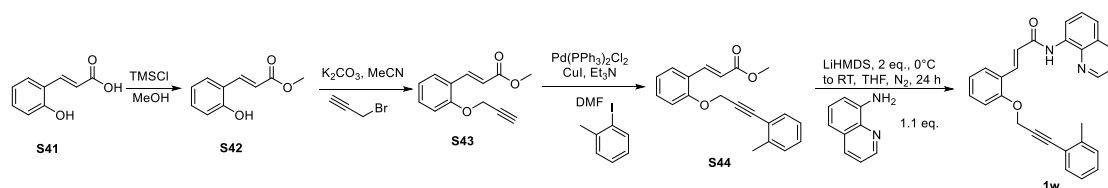


¹H NMR (400 MHz, Chloroform-*d*) δ 10.58 (s, 1H), 8.96 (dd, $J = 7.7, 1.3$ Hz, 1H), 8.84 (dd, $J = 4.2, 1.6$ Hz, 1H), 8.49 (d, $J = 7.8$ Hz, 1H), 8.19 (dd, $J = 8.3, 1.6$ Hz, 1H), 8.04 (s, 1H), 7.60 (t, $J = 7.9$ Hz, 1H), 7.55 – 7.31 (m, 6H), 7.21 (d, $J = 4.2$ Hz, 2H), 7.14 (dt, $J = 8.7, 4.3$ Hz, 1H), 4.46 (t, $J = 6.8$ Hz, 2H), 2.49 (m, 5H), 2.22 (p, $J = 6.7$ Hz, 2H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.25, 148.15, 139.95, 138.62, 136.75, 136.35, 135.30, 132.26, 131.99, 129.42, 128.03, 127.93, 127.60, 125.65, 125.57, 123.20, 122.72, 121.90, 121.52, 120.90, 120.83, 116.26, 112.12, 110.29, 91.83, 81.12, 45.48, 28.91, 20.91, 16.92.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{30}H_{26}N_3O^+$ 444.2070; found: 444.2070.

(*E*)-*N*-(Quinolin-8-yl)-3-(2-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)phenyl)acrylamide (**1w**)

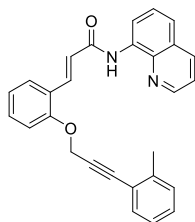


(*E*)-3-(2-hydroxyphenyl)acrylic acid **S41** (5.50 g, 30 mmol) was dissolved in 75 mL of methanol in a 250 mL round-bottom flask, to which TMSCl (7.6 mL, 60 mmol) was added dropwise and the mixture was stirred overnight. The solvent was removed by rotary evaporation and in vacuo giving methyl (*E*)-3-(2-hydroxyphenyl)acrylate **S42** as white solid (5.24 g, 98%).

S43 was prepared according to **General Procedure B** on a 30 mmol scale. Purification by flash chromatography (15:85 EA:PE) gave **S43** as a colorless liquid (5.85 g, 90%).

S44 was prepared according to **General Procedure C** on a 12.0 mmol scale. Purification by flash chromatography (15:85 EA:PE) gave **S44** as a yellow oil (2.18 g, 59%).

1w was prepared according to **General Procedure D** on a 6.75 mmol scale. Purification by flash chromatography (4:50:50 EA:DCM:PE) gave **1w** as a light yellow crystal (2.16 g, 77%).

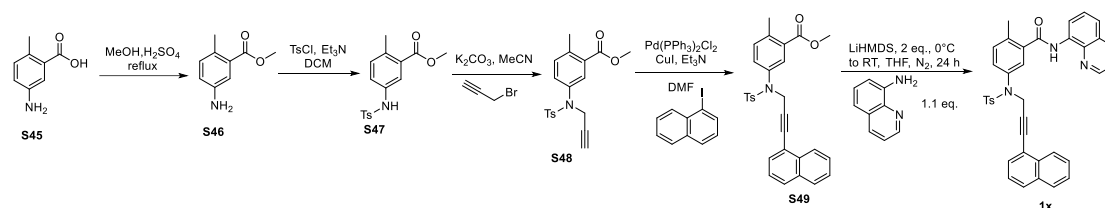


¹H NMR (400 MHz, Chloroform-*d*) δ 10.01 (s, 1H), 8.94 (dd, $J = 7.6, 1.4$ Hz, 1H), 8.77 (dd, $J = 4.3, 1.6$ Hz, 1H), 8.21 – 8.09 (m, 2H), 7.64 (dd, $J = 7.8, 1.6$ Hz, 1H), 7.58 (t, $J = 7.9$ Hz, 1H), 7.52 (dd, $J = 8.4, 1.4$ Hz, 1H), 7.48 – 7.34 (m, 3H), 7.24 – 7.14 (m, 3H), 7.11 (t, $J = 7.5$ Hz, 1H), 7.05 (t, $J = 7.5$ Hz, 1H), 6.97 (d, $J = 15.7$ Hz, 1H), 5.10 (s, 2H), 2.38 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 164.82, 156.62, 148.16, 140.66, 138.52, 137.63, 136.47, 134.87, 132.22, 130.87, 129.50, 129.45, 128.77, 128.02, 127.60, 125.58, 124.51, 122.68, 122.05, 121.67, 121.55, 116.85, 113.18, 87.53, 86.64, 57.15, 20.75.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for C₂₈H₂₃N₂O₂⁺ 419.1754; found: 419.1756.

2-Methyl-5-((4-methyl-N-(3-(naphthalen-1-yl)prop-2-yn-1-yl)phenyl)sulfonamido)-N-(quinolin-8-yl)benzamide (1x)



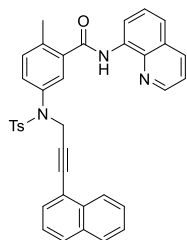
S45 (15.12 g, 100.0 mmol) was dissolved in 200 mL of methanol. Sulfuric acid (12 mL) was dropped slowly. The mixture was refluxed for 4 h and the solvent was removed on a rotavap. The remaining liquid was poured into 150 mL of iced water. Concentrated sodium carbonate solution was added until the pH = 8. The mixture was then extracted with ether three times and the organic phase was washed with brine, dried over anhydrous sodium sulfate and evaporated giving **S46** as a brown liquid (11.79 g, 71%).

S46 (4.13 g, 25.0 mmol), TsCl (5.72 g, 30.0 mmol), triethylamine (5.5 mL, 40 mmol) and 100 mL of DCM were added to a 250 mL round-bottom flask and stirred overnight. The solvent was removed by rotary evaporation. Purification by flash chromatography (DCM) gave **S47** as white solid (5.52 g, 69%).

S48 was prepared according to **General Procedure B** on an 8.00 mmol scale. Purification by flash chromatography (10:90 EA:PE) gave **S48** as an off-white solid (2.88 g, 100%).

S49 was prepared according to **General Procedure C** on a 3.50 mmol scale. Purification by flash chromatography (10:90 EA:PE) gave **S49** as light-yellow liquid (1.10 g, 65%).

1x was prepared according to **General Procedure D** on a 4.84 mmol scale. Purification by flash chromatography (25:25:1 PE:DCM:EA) gave **1x** as an off-white solid (0.686 g, 51%).

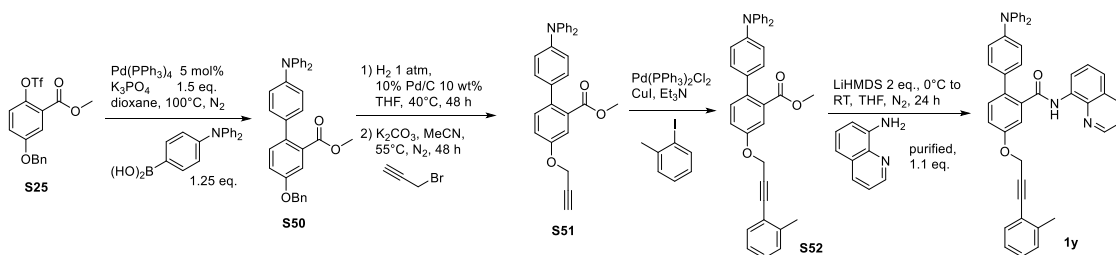


¹H NMR (400 MHz, Chloroform-*d*) δ 10.11 (s, 1H), 8.84 (dd, J = 7.4, 1.6 Hz, 1H), 8.47 (dd, J = 4.2, 1.6 Hz, 1H), 8.10 (dd, J = 8.3, 1.7 Hz, 1H), 7.76 (dd, J = 6.7, 2.1 Hz, 2H), 7.71 – 7.64 (m, 4H), 7.59 – 7.50 (m, 2H), 7.47 (dd, J = 8.2, 2.3 Hz, 1H), 7.39 – 7.28 (m, 5H), 7.19 (dd, J = 8.3, 7.1 Hz, 1H), 7.12 (d, J = 8.0 Hz, 2H), 4.86 (s, 2H), 2.61 (s, 3H), 2.16 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.02, 148.11, 143.79, 138.35, 137.71, 137.25, 136.95, 136.17, 135.53, 134.38, 133.01, 132.83, 132.22, 130.61, 130.41, 129.47, 128.83, 128.06, 127.99, 127.84, 127.25, 126.70, 126.67, 126.24, 125.72, 124.81, 121.95, 121.57, 119.84, 116.61, 87.98, 84.31, 42.17, 21.38, 19.94.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for C₃₇H₃₀N₃O₃S⁺ 596.2002; found: 596.2005.

4'-((Diphenylamino)-*N*-(quinolin-8-yl)-4-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)-[1,1'-biphenyl]-2-carboxamide (**1y**)

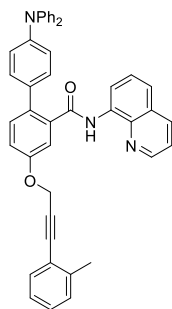


S50 was prepared according to **General Procedure F** on a 10.0 mmol scale. Purification by flash chromatography (1:50:49 EA:DCM:PE) gave **S50** as a yellow oil (4.31 g, 89%).

S51 was prepared according to **General Procedure G** on an 8.85 mmol scale. Purification by flash chromatography (15:85 EA:PE) gave **S51** as white crystal (3.57 g, 93%).

S52 was prepared according to **General Procedure C** on a 5.00 mmol scale. Purification by flash chromatography (15:85 EA:PE) gave **S52** as a yellow oil (1.70 g, 65%).

1y was prepared according to **General Procedure D** on a 3.19 mmol scale. Purification by flash chromatography (4:30:66 EA:DCM:PE) gave **1z** as a yellow foam (0.828 g, 41%).

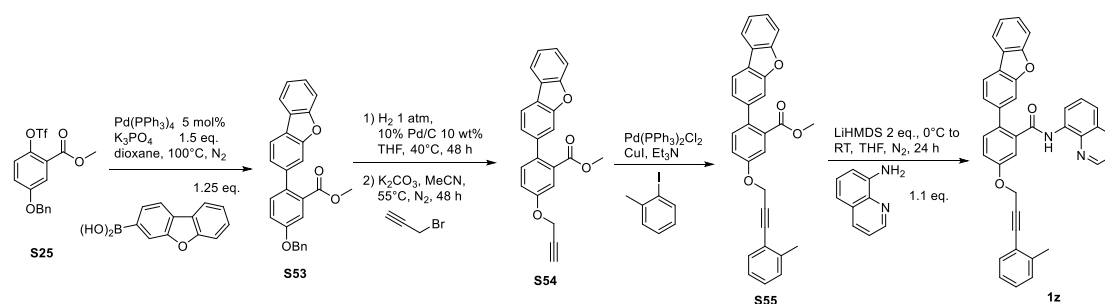


¹H NMR (400 MHz, Chloroform-*d*) δ 9.75 (s, 1H), 8.85 (dd, $J = 7.2, 1.8$ Hz, 1H), 8.56 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.16 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.61 – 7.51 (m, 3H), 7.47 – 7.33 (m, 5H), 7.25 – 7.06 (m, 4H), 7.00 (t, $J = 7.8$ Hz, 4H), 6.94 – 6.87 (m, 4H), 6.62 (dd, $J = 7.3, 1.7$ Hz, 4H), 5.07 (s, 2H), 2.39 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.61, 157.00, 147.90, 147.36, 147.04, 140.66, 138.32, 136.99, 136.03, 134.58, 133.48, 132.97, 132.25, 131.44, 129.85, 129.40, 129.00, 128.69, 127.71, 127.55, 125.46, 123.92, 123.53, 122.63, 121.94, 121.60, 121.31, 118.07, 116.06, 115.28, 87.28, 86.56, 56.96, 20.68.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{44}H_{34}N_3O_2^+$ 636.2646; found: 636.2646.

2-(Dibenzo[*b,d*]furan-3-yl)-*N*-(quinolin-8-yl)-5-((3-(*o*-tolyl)prop-2-yn-1-yl)oxy)benzamide (**1z**)

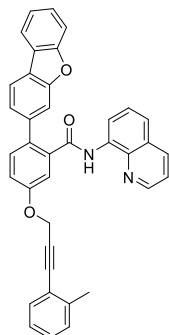


S53 was prepared according to **General Procedure F** on an 8.00 mmol scale. Purification by flash chromatography (1:25:74 to 2:35:63 EA:DCM:PE) gave **S53** as a white amorphous solid (3.04 g, 93%).

S54 was prepared according to **General Procedure G** on a 7.43 mmol scale. Purification by flash chromatography (1:30:69 to 2:30:68 EA:DCM:PE) gave **S54** as white amorphous solid (2.41 g, 91%).

S55 was prepared according to **General Procedure C** on a 6.73 mmol scale. Purification by flash chromatography (2:30:68 EA:DCM:PE) gave **S55** as a yellow oil (1.69 g, 56%).

1z was prepared according to **General Procedure D** on a 3.74 mmol scale. Purification by flash chromatography (1:30:69 EA:DCM:PE) gave **1z** as a yellow foam (1.07 g, 51%).

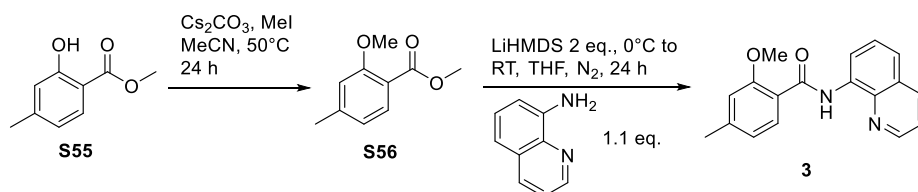


¹H NMR (400 MHz, Chloroform-*d*) δ 9.83 (s, 1H), 8.78 (dd, $J = 7.7, 1.4$ Hz, 1H), 8.18 (dd, $J = 4.2, 1.7$ Hz, 1H), 7.92 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.81 – 7.70 (m, 3H), 7.65 (d, $J = 2.7$ Hz, 1H), 7.54 – 7.36 (m, 7H), 7.31 – 7.05 (m, 6H), 5.09 (s, 2H), 2.40 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.27, 157.36, 156.55, 156.41, 147.64, 140.71, 139.13, 138.31, 137.25, 135.82, 134.43, 133.24, 132.30, 132.20, 129.47, 128.78, 127.65, 127.19, 127.04, 125.53, 124.22, 123.95, 123.37, 122.70, 121.96, 121.64, 121.28, 120.59, 120.43, 117.85, 116.37, 115.43, 112.27, 111.57, 87.24, 86.73, 57.05, 20.71.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{38}H_{27}N_2O_3^+$ 559.2016; found: 559.2019.

2-Methoxy-4-methyl-*N*-(quinolin-8-yl)benzamide (**3**)



S55 was prepared according to **General Procedure E** on a 45.0 mmol scale. Purification by flash chromatography (8:92 to 12:88 EA:PE) gave **S55** as slightly yellow liquid (5.59 g, 72%).

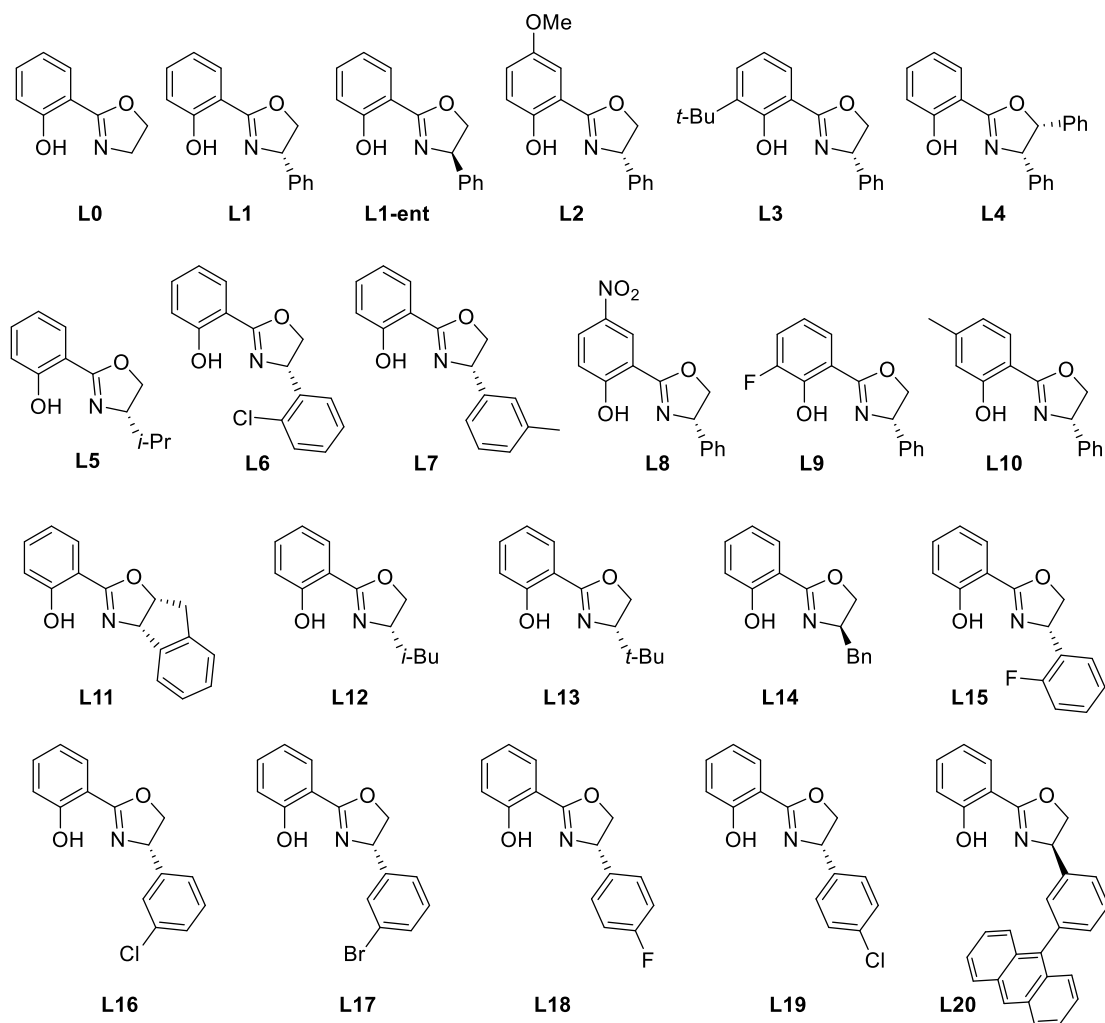
3 was prepared according to **General Procedure D** on a 25.0 mmol scale. Purification by flash chromatography (2:30:68 Acetone:DCM:PE) gave **3** as a slightly yellow solid (7.12 g, 97%).

¹H NMR (400 MHz, Chloroform-*d*) δ 12.33 (s, 1H), 9.03 (dd, $J = 7.6, 1.4$ Hz, 1H), 8.86 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.24 (d, $J = 7.9$ Hz, 1H), 8.15 (dd, $J = 8.2, 1.7$ Hz, 1H), 7.57 (t, $J = 7.9$ Hz, 1H), 7.50 (dd, $J = 8.2, 1.4$ Hz, 1H), 7.44 (dd, $J = 8.2, 4.2$ Hz, 1H), 6.94 (ddd, $J = 8.0, 1.6, 0.8$ Hz, 1H), 6.86 (d, $J = 1.5$ Hz, 1H), 4.18 (s, 3H), 2.42 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.79, 157.71, 148.22, 144.10, 139.29, 136.25, 135.88, 132.33, 128.12, 127.62, 122.18, 121.41, 121.33, 119.63, 117.27, 112.32, 56.08, 21.84.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{18}H_{17}N_2O_2^+$ 293.1285; found: 293.1283.

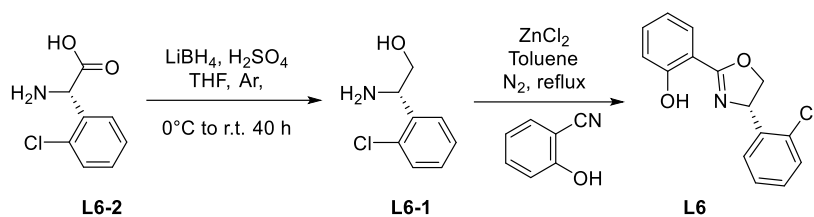
3. Synthesis of Chiral Ligands



L0,¹ L1, L1-ent, L4, L5, L11, L13, L14,² L2, L8,³ L3,⁴ and L12⁵ were known compounds synthesized according to the literatures and used directly.

L6, L7, L9, L10, L15, L16, L17, L18, L19 and L20 were new compounds and synthesized following the steps below.

(*S*)-2-(4-(2-Chlorophenyl)-4,5-dihydrooxazol-2-yl)phenol (L6)



General Procedure H:

L6-2 (4.826 g, 26 mmol) and lithium borohydride (1.76 g, 80 mmol) was added into a 250 mL two-necked flask, in which the gas was replaced with argon. Then 40 mL of dry THF was added and the flask was placed in an ice-water mixture. A solution of sulfuric acid (2.1 mL, > 98%, 40 mmol) in THF (10 mL) was added dropwise. The mixture was let for 40 h. To quench the reaction, 30 mL of MeOH was added, followed by 40 mL of NaOH solution (4 M, aqueous). The organic solvents were evaporated. The resulting liquid was extracted with toluene. Evaporation of toluene gave **L6-1** as a yellow viscous oil, and used without purification.

General Procedure I:

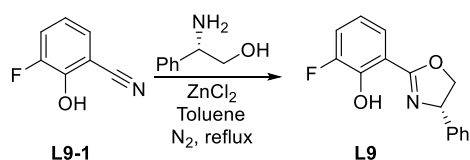
To a 250 mL flask, 2-hydroxybenzonitrile (1.19 g, 10.0 mmol), **L6-1** (2.06 g, 12 mmol), zinc chloride (0.27 g, 2 mmol) were added to a dry flask and flushed with nitrogen. Then 20 mL of toluene was added. The mixture was heated to reflux for 24 h. The solvent was evaporated and the residue was purified by flash chromatography (5:95 EA:PE), giving **L6** as a white solid (1.74 g, 64%).

¹H NMR (400 MHz, DMSO-*d*₆) δ 12.12 (s, 1H), 7.71 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.52 (td, *J* = 8.9, 3.2 Hz, 2H), 7.37 (dq, *J* = 10.1, 5.2 Hz, 3H), 7.06 (d, *J* = 8.4 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 5.82 (dd, *J* = 10.4, 7.8 Hz, 1H), 5.02 (dd, *J* = 10.4, 8.5 Hz, 1H), 4.26 (t, *J* = 8.2 Hz, 1H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ 166.72, 159.78, 139.51, 134.67, 132.04, 129.99, 128.57, 128.23, 128.06, 119.65, 117.10, 110.33, 73.33, 65.91.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₁₅H₁₃ClNO₂⁺ 274.0629; found: 274.0631.

(*S*)-2-Fluoro-6-(4-phenyl-4,5-dihydrooxazol-2-yl)phenol (**L9**)



L9 was prepared according to **General Procedure I** with 3-fluoro-2-hydroxybenzonitrile **L9-1** (1.37 g, 10.0 mmol) and (*S*)-phenylglycinol (1.51 g, 11.0 mmol) as starting materials. Purification by flash chromatography (5:95 EA:PE) gave **L9** as white solid (2.16 g, 84%).

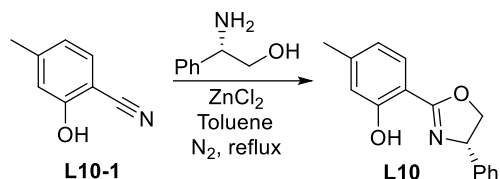
¹H NMR (400 MHz, Chloroform-*d*) δ 13.12 (s, 1H), 7.41 – 7.19 (m, 6H), 6.83 (d, *J* = 8.5 Hz, 1H), 6.61 (dd, *J* = 11.1, 8.3 Hz, 1H), 5.39 (t, *J* = 9.3 Hz, 1H), 4.83 (t, *J* = 9.4 Hz, 1H), 4.29 (t, *J* = 8.5 Hz, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.40 (d, $J = 2.9$ Hz), 161.81 (d, $J = 4.3$ Hz), 161.50 (d, $J = 257.8$ Hz), 141.17, 133.54 (d, $J = 11.7$ Hz), 128.89, 127.99, 126.50, 112.90 (d, $J = 3.2$ Hz), 106.10 (d, $J = 22.1$ Hz), 100.20 (d, $J = 12.7$ Hz), 74.52, 67.20.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.74.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{15}\text{H}_{13}\text{FNO}_2^+$ 258.0925; found: 258.0925.

(*S*)-5-Methyl-2-(4-phenyl-4,5-dihydrooxazol-2-yl)phenol (**L10**)



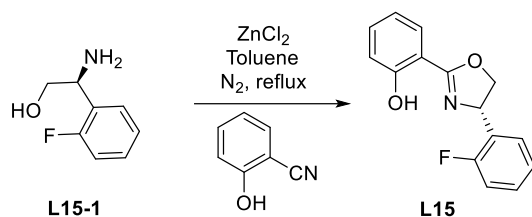
L10 was prepared according to **General Procedure I** with (*S*)-phenylglycinol (1.51 g, 11 mmol) and **L10-1** (1.33 g, 10 mmol) as starting materials. Purification by flash chromatography (5:95 EA:PE) gave **L10** as white solid (2.05 g, 81%).

^1H NMR (400 MHz, Chloroform-*d*) δ 12.08 (s, 1H), 7.59 (d, $J = 8.0$ Hz, 1H), 7.39 – 7.25 (m, 5H), 6.86 (d, $J = 1.6$ Hz, 1H), 6.72 (dd, $J = 8.0, 1.6$ Hz, 1H), 5.43 (dd, $J = 10.0, 8.1$ Hz, 1H), 4.76 (dd, $J = 10.0, 8.4$ Hz, 1H), 4.20 (t, $J = 8.3$ Hz, 1H), 2.35 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.32, 159.98, 144.63, 141.74, 128.81, 127.97, 127.82, 126.49, 119.92, 117.15, 107.86, 73.95, 68.73, 21.84.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{16}\text{H}_{15}\text{NO}_2^+$ 254.1176; found: 254.1175.

(*S*)-2-(4-(2-Fluorophenyl)-4,5-dihydrooxazol-2-yl)phenol (**L15**)



L15 was prepared according to **General Procedure I** with **L15-1** (250 mg, 1.61 mmol) and 2-hydroxybenzonitrile (192 mg, 1.61 mmol) as starting materials. Purification by flash chromatography (5:95 EA:PE) gave **L15** as white solid (356 mg, 86%).

^1H NMR (400 MHz, DMSO-*d*₆) δ 12.08 (s, 1H), 7.72 (dd, $J = 7.9, 1.7$ Hz, 1H), 7.50 (ddd, $J = 8.6, 7.3, 1.7$ Hz, 1H), 7.40 (dddd, $J = 9.5, 7.7, 6.5, 1.8$ Hz, 2H), 7.30 – 7.20 (m, 2H), 7.07 – 6.93 (m, 2H), 5.74 (dd, $J = 10.3, 7.9$ Hz, 1H), 4.94 (dd, $J = 10.3, 8.6$ Hz, 1H), 4.35 (t, $J = 8.2$ Hz, 1H).

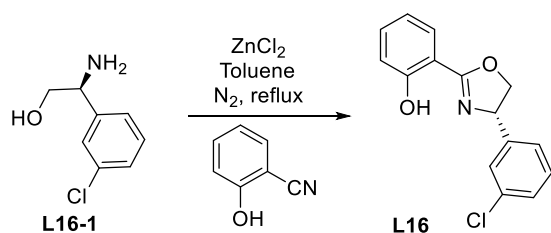
^{13}C NMR (101 MHz, DMSO-*d*₆) δ 166.37, 160.43 (d, $J = 245.2$ Hz), 159.73, 134.61, 130.39 (d, J

= 8.3 Hz), 128.86 (d, $J = 8.0$ Hz), 128.77, 128.59, 125.34 (d, $J = 3.4$ Hz), 119.66, 117.09, 116.13 (d, $J = 20.9$ Hz), 110.39, 73.25, 63.19 (d, $J = 2.4$ Hz).

^{19}F NMR (376 MHz, DMSO- d_6) δ -118.42.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{15}\text{H}_{13}\text{FNO}_2^+$ 258.0925; found: 258.0925.

(*S*)-2-(4-(3-Chlorophenyl)-4,5-dihydrooxazol-2-yl)phenol (**L16**)



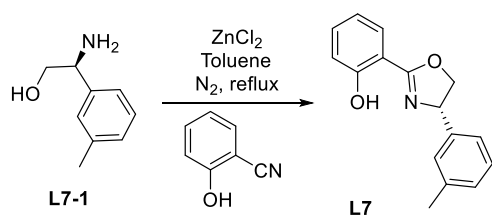
L16 was prepared according to **General Procedure I** with **L16-1** (1.00 g, 5.83 mmol) and 2-hydroxybenzonitrile (694 mg, 5.83 mmol) as starting materials. Purification by flash chromatography (5:95 EA:PE) gave **L16** as white solid (1.26 g, 79%).

^1H NMR (400 MHz, DMSO- d_6) δ 12.09 (s, 1H), 7.71 (dd, $J = 7.8, 1.7$ Hz, 1H), 7.53 – 7.37 (m, 4H), 7.30 (dt, $J = 7.0, 1.8$ Hz, 1H), 7.07 – 6.95 (m, 2H), 5.59 (dd, $J = 10.1, 8.0$ Hz, 1H), 4.92 (dd, $J = 10.1, 8.7$ Hz, 1H), 4.30 (t, $J = 8.4$ Hz, 1H).

^{13}C NMR (101 MHz, DMSO- d_6) δ 166.38, 159.72, 144.51, 134.58, 133.83, 131.19, 128.61, 128.20, 127.04, 125.80, 119.61, 117.05, 110.34, 74.14, 67.67.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{15}\text{H}_{13}\text{ClNO}_2^+$ 274.0629; found: 274.0630.

(*S*)-2-(4-(3-Methylphenyl)-4,5-dihydrooxazol-2-yl)phenol (**L7**)



L7 was prepared according to **General Procedure I** with **L7-1** (250 mg, 1.65 mmol) and 2-hydroxybenzonitrile (197 mg, 1.65 mmol) as starting materials. Purification by flash chromatography (5:95 EA:PE) gave **L7** as white solid (347 mg, 83%).

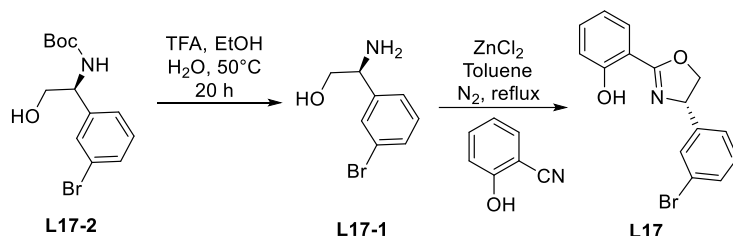
^1H NMR (400 MHz, DMSO- d_6) δ 12.20 (s, 1H), 7.71 (dd, $J = 7.8, 1.7$ Hz, 1H), 7.49 (ddd, $J = 8.8, 7.3, 1.8$ Hz, 1H), 7.31 – 7.24 (m, 1H), 7.16 – 7.08 (m, 3H), 7.05 – 6.94 (m, 2H), 5.51 (dd, $J = 10.1, 8.1$ Hz, 1H), 4.90 (dd, $J = 10.1, 8.5$ Hz, 1H), 4.26 (t, $J = 8.3$ Hz, 1H), 2.31 (s, 3H).

^{13}C NMR (101 MHz, DMSO- d_6) δ 165.89, 159.73, 142.01, 138.48, 134.45, 129.15, 128.86, 128.51,

127.57, 124.18, 119.56, 117.01, 110.43, 74.38, 68.24, 21.49.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{16}H_{16}NO_2^+$ 254.1176; found: 254.1177.

(S)-2-(4-(3-Bromophenyl)-4,5-dihydrooxazol-2-yl)phenol (L17)



L17-2 (500 mg, 1.58 mmol), 5 mL of ethanol, 1 mL of water and 1 mL of trifluoroacetic acid were added to a 50 mL flask. The mixture was refluxed for 24 h. Then solvent was evaporated and water was added. The liquid was extracted with DCM and dried over sodium sulfate anhydrate. Removal of DCM gave **L17-1** as white solid (301 mg, 88%).

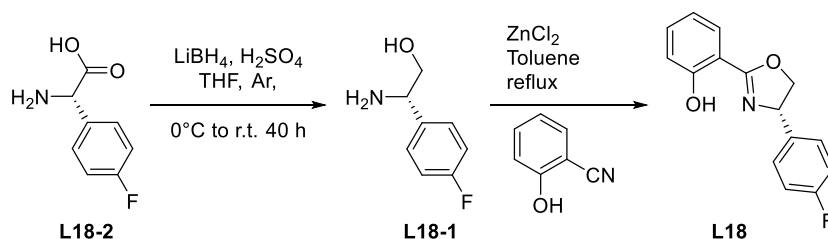
L17 was prepared according to **General Procedure I** with **L17-1** (289 mg, 1.34 mmol) and 2-hydroxybenzonitrile (159 mg, 1.33 mmol) as starting materials. Purification by flash chromatography (5:95 EA:PE) gave **L17** as white solid (362 mg, 85%).

¹H NMR (400 MHz, DMSO-*d*₆) δ 12.08 (s, 1H), 7.71 (dd, J = 7.8, 1.7 Hz, 1H), 7.58 – 7.46 (m, 3H), 7.41 – 7.31 (m, 2H), 7.06 – 6.93 (m, 2H), 5.58 (dd, J = 10.1, 8.1 Hz, 1H), 4.91 (dd, J = 10.1, 8.7 Hz, 1H), 4.29 (t, J = 8.4 Hz, 1H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ 166.37, 159.71, 144.76, 134.59, 131.49, 131.11, 129.91, 128.61, 126.19, 122.45, 119.62, 117.05, 110.33, 74.16, 67.62.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{15}H_{13}BrNO_2^+$ 318.0124; found: 318.0124.

(S)-2-(4-(4-Fluorophenyl)-4,5-dihydrooxazol-2-yl)phenol (L18)



L18-1 was prepared according to **General Procedure H** on a 13.0 mmol scale giving **L18-1** as yellow viscous oil (1.31 g, 65%).

L18 was prepared according to **General Procedure I** with **L18-1** (1.30 g, 8.38 mmol) and 2-hydroxybenzonitrile (907 mg, 7.62 mmol) as starting materials. Purification by flash chromatography (5:95 EA:PE) gave **L18** as white solid (884 mg, 45%).

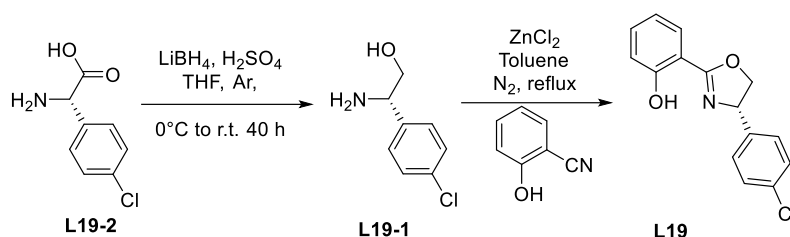
¹H NMR (400 MHz, DMSO-*d*₆) δ 12.13 (s, 1H), 7.71 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.54 – 7.45 (m, 1H), 7.38 (dd, *J* = 8.4, 5.5 Hz, 2H), 7.22 (t, *J* = 8.7 Hz, 2H), 7.05 – 6.94 (m, 2H), 5.58 (dd, *J* = 10.0, 8.0 Hz, 1H), 4.90 (t, *J* = 9.3 Hz, 1H), 4.27 (t, *J* = 8.3 Hz, 1H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ 166.04, 162.11 (d, *J* = 243.5 Hz), 159.72, 138.27 (d, *J* = 3.0 Hz), 134.50, 129.15 (d, *J* = 8.3 Hz), 128.55, 119.58, 117.02, 116.00 (d, *J* = 21.4 Hz), 110.37, 74.34, 67.56.

¹⁹F NMR (376 MHz, DMSO-*d*₆) δ -114.82.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₁₅H₁₃FNO₂⁺ 258.0925; found: 258.0926.

(*S*)-2-(4-(4-Chlorophenyl)-4,5-dihydrooxazol-2-yl)phenol (L19)



L19-1 was prepared according to **General Procedure H** on a 26.0 mmol scale giving L19-1 as yellow viscous oil (3.89 g, 87%).

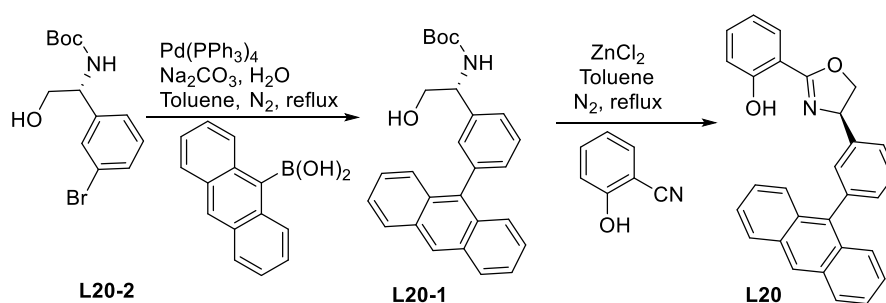
L19 was prepared according to **General Procedure I** with L19-1 (1.76 g, 10.3 mmol) and 2-hydroxybenzonitrile (1.02 g, 8.55 mmol) as starting materials. Purification by flash chromatography (5:95 EA:PE) gave L19 as white solid (548 mg, 17%).

¹H NMR (400 MHz, DMSO-*d*₆) δ 12.10 (s, 1H), 7.71 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.53 – 7.42 (m, 3H), 7.39 – 7.32 (m, 2H), 7.06 – 6.94 (m, 2H), 5.58 (dd, *J* = 10.1, 7.9 Hz, 1H), 4.91 (dd, *J* = 10.1, 8.7 Hz, 1H), 4.27 (t, *J* = 8.3 Hz, 1H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ 166.21, 159.72, 141.06, 134.56, 132.79, 129.21, 129.01, 128.57, 119.61, 117.04, 110.33, 74.23, 67.56.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₁₅H₁₃ClNO₂⁺ 274.0629; found: 274.0634.

(*R*)-2-(4-(3-(Anthracen-9-yl)phenyl)-4,5-dihydrooxazol-2-yl)phenol (L20)



L20-2 (632 mg, 2.00 mmol), anthracene-9-boronic acid (666 mg, 3.00 mmol) Pd(PPh₃)₄ (116 mg, 0.1 mmol), Na₂CO₃ (1.5 g), toluene (12 mL) and water (4.5 mL) was added into a 50 mL flask which was then flushed with nitrogen. The mixture was set to reflux overnight. Then the organic layer was separated and solvent evaporated. Purification by flash chromatography (2:98 MeOH:DCM) gave **L20-1** as yellow solid (707 mg, 85%).

L20 was prepared **General Procedure I** with **L20-1** (413 mg, 1.00 mmol) and 2-hydroxybenzotrile (119 g, 1.00 mmol) as starting materials. Purification by flash chromatography (pure PE to 15:85 EA:PE) gave **L19** as yellow solid (244 mg, 59%).

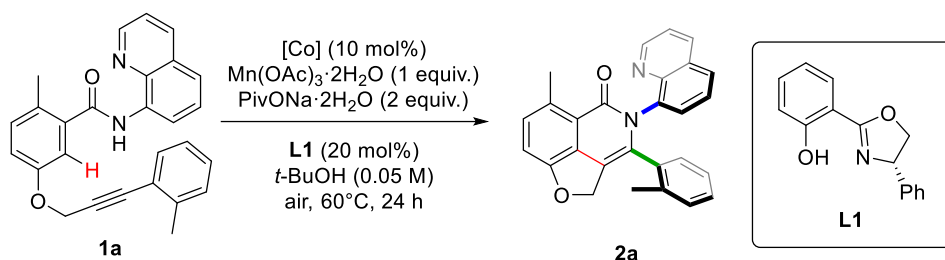
¹H NMR (400 MHz, DMSO-*d*₆) δ 12.20 (s, 1H), 8.69 (s, 1H), 8.16 (d, *J* = 8.4 Hz, 2H), 7.71 – 7.65 (m, 2H), 7.59 – 7.50 (m, 5H), 7.49 – 7.37 (m, 5H), 7.03 – 6.91 (m, 2H), 5.71 (dd, *J* = 10.0, 8.1 Hz, 1H), 4.99 (dd, *J* = 10.1, 8.6 Hz, 1H), 4.42 (t, *J* = 8.3 Hz, 1H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ 166.17, 159.69, 142.52, 138.82, 136.45, 134.47, 131.33, 130.77, 129.91, 129.63, 129.51, 128.92, 128.52, 127.13, 126.49, 126.45, 126.42, 126.31, 125.79, 119.56, 116.99, 110.37, 74.52, 68.17.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₂₉H₂₂NO₂⁺ 416.1645; found: 416.1644.

4. Optimization of Reaction Conditions

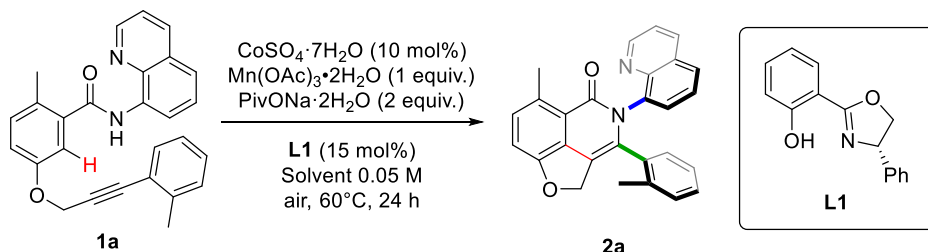
Table S1. Screening of Cobalt Salt^a



Entry	[Co]	yield (%)	ee major (%)	ee minor (%)	dr
1	Co(OAc) ₂ ·4H ₂ O	83	93	19	83/17
2	Co(acac) ₂ ·xH ₂ O	82	81	35	77/23
3	Co(NH ₂ SO ₃) ₂ ·xH ₂ O	68	95	35	82/19
4	Co(SCN) ₂	79	95	22	84/16
5	Co(PPh ₃) ₃ Cl	77	95	29	84/16
6	Co(hfac) ₂ ·xH ₂ O	84	94	13	85/15
7	CoCl ₂	98	94	11	85/15
8	CoCO ₃	0	-	-	-
9	CoSO ₄ ·7H ₂ O	99	95	26	86/14
10	CoC ₂ O ₄	94	94	21	86/14

^aReactions are conducted in 0.05 mmol scale.

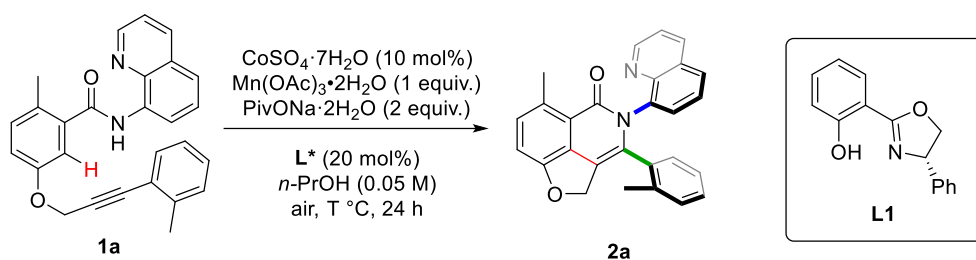
Table S2. Screening of Solvent^a



Entry	Solvent	yield (%)	ee major (%)	ee minor (%)	dr
1	MeOH	32	94	77	9/1
2	EtOH	71	93	27	84/16
3	<i>n</i> -PrOH	99	96	20	87/13
4	<i>i</i> -PrOH	98	94	27	88/12
5	TFE	29	96	92	68/32
6	Et ₂ O	49	96	-4	82/18
7	DCE	75	80	8	83/17
8	toluene	72	82	-15	77/23
9	<i>t</i> -BuOH	82	93	28	87/13
10	1:1 <i>t</i> -BuOH/ <i>n</i> -PrOH	97	95	23	88/12
11	1:1 <i>n</i> -PrOH/ <i>i</i> -PrOH	89	95	34	89/11

^aReactions are conducted in 0.05 mmol scale.

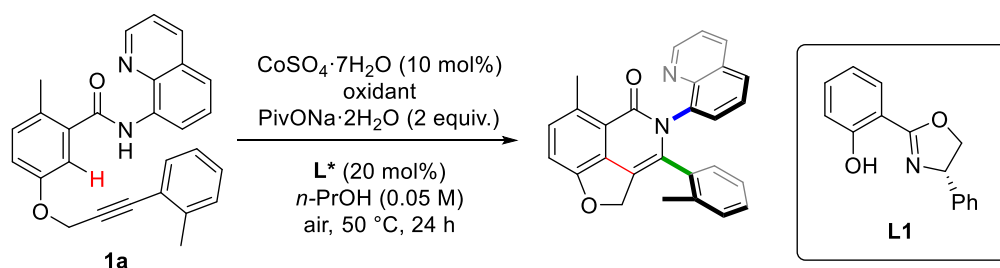
Table S3. Optimization of Temperature^a



entry	T (°C)	yield (%)	ee major (%)	ee minor (%)	dr
1	60	92	96	37	7/1
2	50	95	96	95	23/1
3	40	93	93	87	17/1
4	30 (36 h)	86	97	92	22/1
5	R.T. (36 h)	50	97	95	15/1

^aReactions are conducted in 0.05 mmol scale.

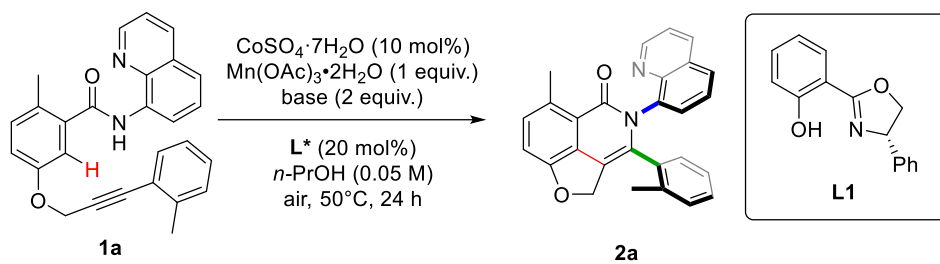
Table S4. Screening of Oxidant^a



Entry	oxidant	equivalent	yield (%)	ee major (%)	ee minor (%)	dr
1	$\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$	1	95	96	95	23/1
2	Mn_2O_3	1	0	-	-	-
3	MnO_2	1	0	-	-	-
4	$\text{Mn}(\text{acac})_3$	2	0	-	-	-
5	$\text{Fe}(\text{OTf})_3$	2	0	-	-	-
6	MnF_3	2	74	95	81	16/1
7	AgOAc	2	20	-	-	-
8	$\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$	0.5	98	83	84	15/1
9	$\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$	0.1	91	97	88	16/1
10	$\text{Mn}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$	2	97	95	90	12/1

^aReactions are conducted in 0.05 mmol scale.

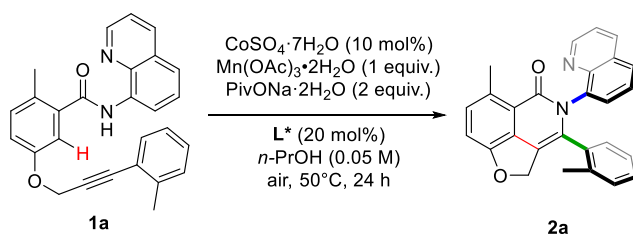
Table S5. Screening of Additive^a



entry	base	yield (%)	ee major (%)	ee minor (%)	dr
1	PivONa·2H ₂ O	95	96	95	96/4
2	AcONa	80	89	73	93/7
3	BzONa	55	97	80	95/5
4	1-AdCO ₂ Na	98	97	82	94/6
5	Na ₂ CO ₃	66	93	86	93/7
6	PivOH	99	92	69	93/7

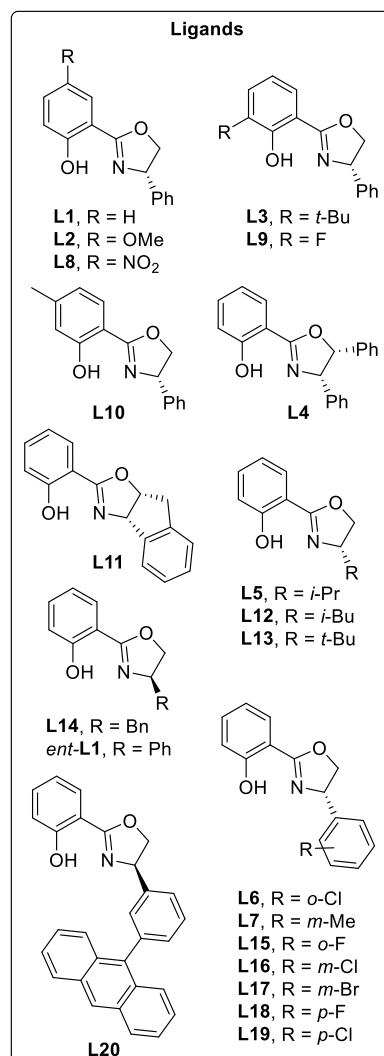
^aReactions are conducted in 0.05 mmol scale.

Table S6. Screening of Chiral Ligand^a



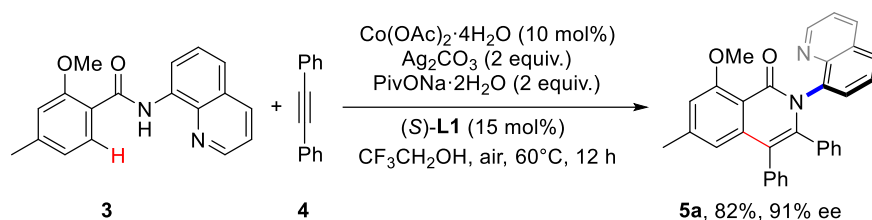
Entry	Ligand	yield (%)	ee major (%)	ee minor (%)	dr
1	L1	95	96	95	96/4
2	<i>ent</i> - L1	91	-96	-77	95/5
3	L2	84	67	78	93/7
4	L3	0	-	-	-
5	L4	45	78	77	91/9
6	L5	53	90	60	94/6
7	L6	93	93	69	96/4
8	L7	71	97	82	95/5
9	L8	71	88	93	4/1
10	L9	56	88	76	92/8
11	L10	88	88	81	86/14
12	L11	21	23	32	94/6
13	L12	41	68	39	94/6
14	L13	trace	-	-	-
15	L14	49	-62	-20	93/7
16	L15	87	96	79	95/5
17	L16	60	94	85	94/6
18	L17	76	97	86	94/6
19	L18	74	97	82	94/6
20	L19	96	94	85	94/6
21	L20	45	-96	21	88/12

^aReactions are conducted in 0.05 mmol scale.



5. General Procedure for Atroposelective C–H Annulation and Characterization of Products

5.1. Synthesis and characterization of 5a



To a 10 mL sealed tube, **3** (58.5 mg, 0.2 mmol), diphenylacetylene **4** (53.5 mg, 0.3 mmol), $\text{Co(OAc)}_2 \cdot 4\text{H}_2\text{O}$ (5.0 mg, 0.02 mmol), **L1** (7.2 mg, 0.03 mmol), $\text{PivONa} \cdot 2\text{H}_2\text{O}$ (64 mg, 0.4 mmol), Ag_2CO_3 (110 mg, 0.4 mmol), a magnetic stir bar and trifluoroethanol (2 mL) were added. Then the tube was sealed and heated on an aluminum heat transfer block at 60°C for 12 h. Upon completion, 5 mL of DCM was added to the tube and the suspension filtered through celite. The filtrate was poured into a separative funnel and washed with 15 mL of 0.25 M NaHCO_3 and 0.05 M EDTANa_2 aqueous solution. The aqueous phase was extracted twice with DCM. The combined organic phase was then vacuum filtered through anhydrous sodium sulfate. The solvent was removed by rotary evaporation. Purification by preparative TLC (eluent: acetone: DCM: PE = 30 : 20: 50) gave **5a** as a yellow oil (77.3 mg, 82%).

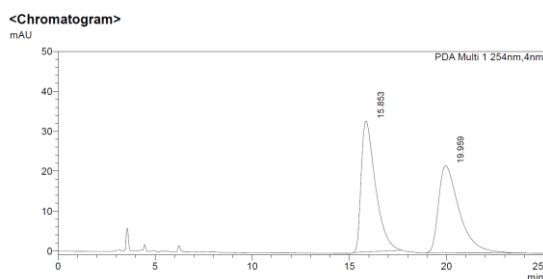
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 8.90 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.00 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.59 (dd, $J = 8.3, 1.4$ Hz, 1H), 7.47 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.36 – 7.28 (m, 2H), 7.23 – 7.09 (m, 5H), 6.95 (dt, $J = 7.7, 1.6$ Hz, 1H), 6.80 (td, $J = 7.6, 1.4$ Hz, 1H), 6.74 (dd, $J = 7.3, 1.6$ Hz, 2H), 6.71 – 6.64 (m, 1H), 6.61 (s, 1H), 6.45 (td, $J = 7.7, 1.4$ Hz, 1H), 3.94 (s, 3H), 2.32 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 161.54, 161.13, 150.64, 145.06, 143.69, 142.80, 141.31, 138.18, 137.41, 135.90, 135.20, 132.07, 131.93, 131.23, 130.67, 129.69, 128.69, 128.22, 127.97, 127.77, 127.05, 126.60, 126.55, 126.34, 125.67, 121.30, 118.04, 117.61, 113.14, 109.78, 56.17, 22.50.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{32}\text{H}_{25}\text{N}_2\text{O}_2^+$ 469.1911; found: 469.1915.

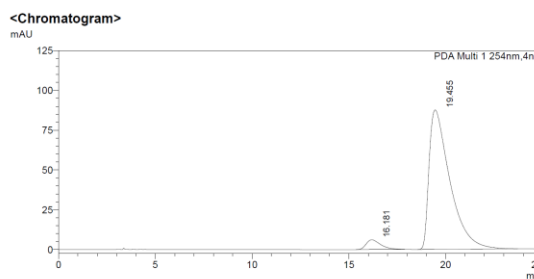
$[\alpha]_{\text{D}}^{20} = -30.2^\circ$ ($c = 0.500$, THF) (91% ee)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 16.2$ min (peak 1), 19.5 min (peak 2): 91% ee.



<Peak Table>

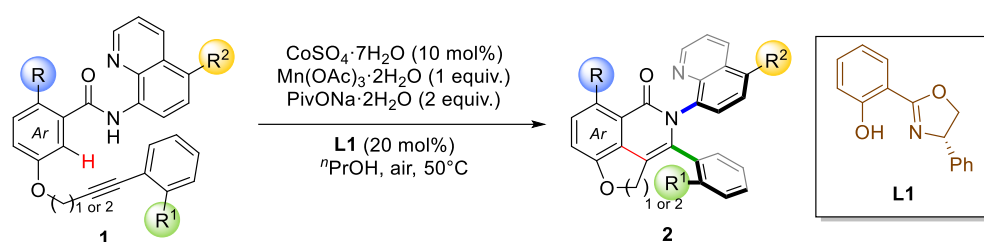
Peak#	Ref. Time	Area	Height	Area%
1	16.853	1673136	32799	50.874
2	19.959	1615663	21813	49.126
Total		3288799	54612	100.000



<Peak Table>

Peak#	Ref. Time	Area	Height	Area%
1	16.181	320719	6140	4.661
2	19.455	6560257	87649	95.339
Total		6880976	93789	100.000

5.2. General Procedure for Intramolecular Atroposelective C–H Annulation

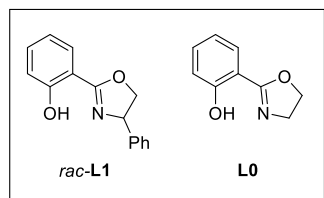


To a 10 mL sealed tube, substrate (0.1 mmol), CoSO₄·7H₂O (2.8 mg, 0.01 mmol), **L1** (4.8 mg, 0.02 mmol), PivONa·2H₂O (32 mg, 0.2 mmol), Mn(OAc)₃·2H₂O (26.8 mg, 0.1 mmol), a magnetic stir bar and *n*-PrOH (2 mL) were added. Then the tube was sealed and heated on an aluminum heat transfer block. The mixture was checked by TLC to monitor the conversion of the substrate. Upon completion, 5 mL of DCM was added to the tube and the suspension was poured into a separative funnel and washed with 15 mL of 0.25 M NaHCO₃ and 0.05 M EDTANa₂ aqueous solution. The aqueous phase was extracted twice with DCM. The combined organic phase was then vacuum filtered through anhydrous sodium sulfate and celite. The solvent was removed by rotary evaporation. Purification by preparative TLC gave the final product.

The ee and dr values were determined by HPLC analysis.

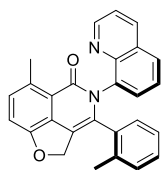
The absolute stereochemistry of **2a**, **2d** and **2m** was determined by XRD and the rest by analogy.

The racemic samples for HPLC analysis were prepared following the General Procedure using *rac*-**L1**- or **L0** as ligand.



5.3. Characterization of Products

6-methyl-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2a)



Following the General Procedure in a 0.05 mmol scale, reacted for 24 h. A purification by preparative TLC (30:70 acetone:PE) gave **2a** as yellow oil (19.2 mg, 95%, 24/1 dr).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.96 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.06 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.67 (dd, $J = 8.2, 1.4$ Hz, 1H), 7.51 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.42 – 7.33 (m, 2H), 7.12 (dd, $J = 7.8, 1.0$ Hz, 1H), 6.99 (d, $J = 7.6$ Hz, 1H), 6.96 – 6.87 (m, 2H), 6.83 (dd, $J = 7.8, 1.4$ Hz, 1H), 6.55 (td, $J = 7.6, 1.4$ Hz, 1H), 5.37 – 5.21 (m, 2H), 2.77 (s, 3H), 2.33 (s, 3H).

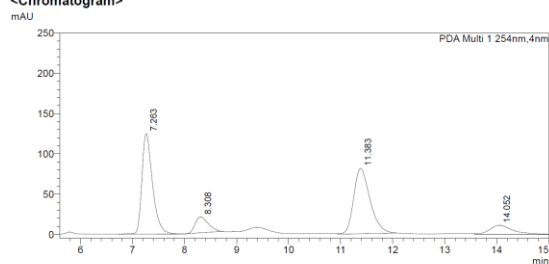
¹³C NMR (101 MHz, Chloroform-*d*) δ 163.37, 158.57, 150.93, 144.89, 137.70, 136.08, 135.51, 134.16, 133.20, 133.12, 130.91, 130.86, 129.63, 129.01, 128.87, 128.84, 128.76, 128.65, 125.80, 124.92, 121.59, 121.02, 115.52, 109.25, 74.93, 20.11, 19.65.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{27}H_{21}N_2O_2^+$ 405.1598; found: 405.1598.

$[\alpha]_D^{20} = -84.6^\circ$ ($c = 0.550$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 7.2$ min (peak 1), 8.3 min (peak 2), 11.4 min (peak 3), 14.0 min (peak 4): 96% ee (major diastereomer), 95% ee (minor diastereomer).

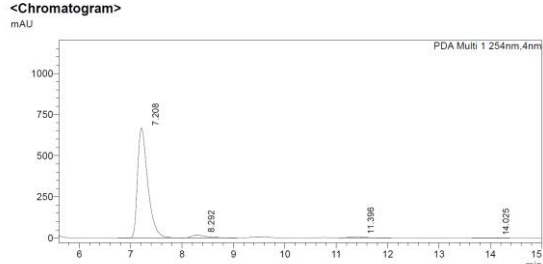
<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Area%
1	7.283	1764622	124834	41.727
2	8.308	348331	19685	8.257
3	11.383	1767347	81086	41.791
4	14.052	348711	11292	8.246
Total		4229011	236897	100.000

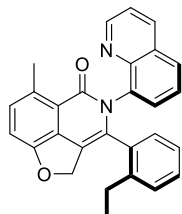
<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Area%
1	7.208	9247209	668116	94.188
2	8.292	390108	18274	3.973
3	11.396	1708591	7632	17.738
4	14.025	9820	476	0.100
Total		9817797	694498	100.000

3-(2-ethylphenyl)-6-methyl-4-(quinolin-8-yl)-2,4-dihydro-5H-furo[4,3,2-de]isoquinolin-5-one (2b)



Following the general procedure. A purification by preparative TLC (30:70 acetone: PE) gave **2b** as light yellow-oil (34.2 mg, 82%, 11/1 dr).

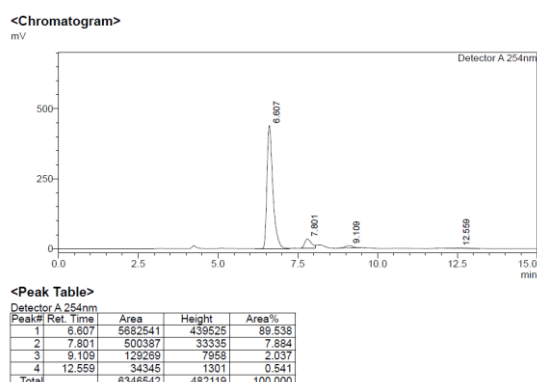
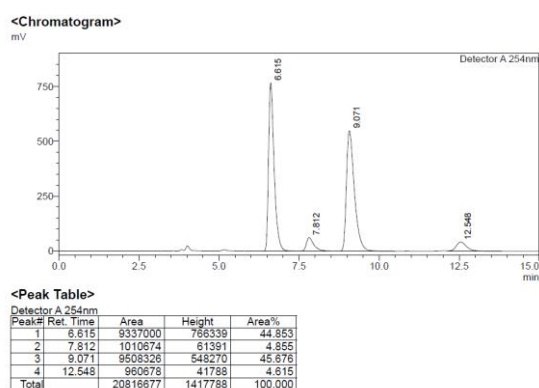
¹H NMR (400 MHz, Chloroform-*d*) δ 8.94 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.03 (dd, $J = 8.3, 1.8$ Hz, 1H), 7.65 (dd, $J = 8.3, 1.4$ Hz, 1H), 7.54 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.41 – 7.34 (m, 2H), 7.12 (d, $J = 7.8$ Hz, 1H), 7.03 (d, $J = 7.8$ Hz, 1H), 6.96 (td, $J = 7.6, 1.5$ Hz, 1H), 6.92 – 6.85 (m, 2H), 6.56 (td, $J = 7.5, 1.4$ Hz, 1H), 5.34 (d, $J = 13.9$ Hz, 1H), 5.26 (d, $J = 13.9$ Hz, 1H), 2.77 (s, 3H), 2.65 (m, 2H), 1.21 (t, $J = 7.6$ Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.48, 158.65, 150.88, 144.79, 141.61, 137.57, 136.17, 134.32, 133.22, 132.48, 130.98, 130.89, 129.61, 129.14, 128.95, 128.91, 128.84, 127.55, 125.76, 124.90, 121.62, 121.13, 115.82, 109.31, 75.11, 25.85, 20.16, 14.99.

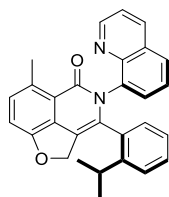
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{28}H_{23}N_2O_2^+$ 419.1754; found: 419.1755.

$[\alpha]_D^{20} = -34.0^\circ$ ($c = 0.610$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 6.6$ min (peak 1), 7.8 min (peak 2), 9.1 min (peak 3), 12.6 min (peak 4): 96% ee (major diastereomer), 87% ee (minor diastereomer).



3-(2-isopropylphenyl)-6-methyl-4-(quinolin-8-yl)-2,4-dihydro-5H-furo[4,3,2-de]isoquinolin-5-one (2c)



Following the general procedure, reacted for 24 h. A purification by preparative TLC (30:70 acetone:PE) gave **2c** as yellow oil (32.4 mg, 75%, 13/1 dr).

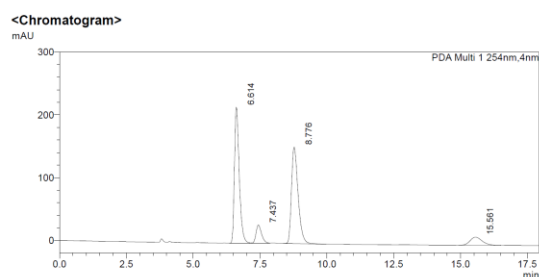
¹H NMR (400 MHz, Chloroform-*d*) δ 8.92 (dd, $J = 4.3, 1.7$ Hz, 1H), 8.02 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.67 (dd, $J = 8.2, 1.4$ Hz, 1H), 7.61 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.45 – 7.39 (m, 1H), 7.35 (dd, $J = 8.3, 4.2$ Hz, 1H), 7.15 – 7.10 (m, 1H), 7.06 – 6.94 (m, 3H), 6.90 (d, $J = 7.8$ Hz, 1H), 6.58 (td, $J = 7.4, 1.4$ Hz, 1H), 5.36 (d, $J = 13.9$ Hz, 1H), 5.29 (d, $J = 13.9$ Hz, 1H), 3.10 (hept, $J = 6.9$ Hz, 1H), 2.77 (s, 3H), 1.21 (d, $J = 6.8$ Hz, 3H), 1.14 (d, $J = 6.7$ Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.43, 158.58, 150.71, 146.73, 144.62, 137.24, 136.07, 134.43, 133.16, 131.57, 130.91, 130.80, 130.50, 129.39, 129.29, 128.92, 128.89, 125.56, 125.00, 124.77, 121.54, 121.06, 116.00, 109.25, 75.17, 30.59, 25.94, 22.68, 20.11.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{29}H_{25}N_2O_2^+$ 433.1911; found: 433.1909.

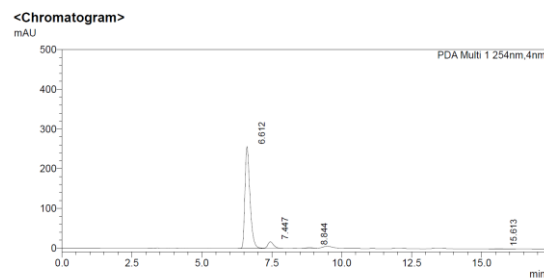
$[\alpha]_D^{20} = -37.7^\circ$ ($c = 0.520$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 6.6$ min (peak 1), 7.4 min (peak 2), 8.8 min (peak 3), 15.6 min (peak 4): 98% ee (major diastereomer), 93% ee (minor diastereomer).



<Peak Table>
PDA Ch1 254nm

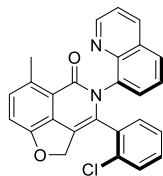
Peak#	Ret. Time	Area	Height	Area%
1	6.614	2696909	216212	43.724
2	7.437	406368	28812	6.588
3	8.776	2654170	153787	43.031
4	15.561	410545	13030	6.656
Total		6167993	411840	100.000



<Peak Table>
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%
1	6.612	3202152	256285	92.206
2	7.447	233423	16459	6.721
3	8.844	29273	2092	0.843
4	15.613	7994	299	0.230
Total		3472842	275136	100.000

3-(2-chlorophenyl)-6-methyl-4-(quinolin-8-yl)-2,4-dihydro-5H-furo[4,3,2-de]isoquinolin-5-one (2d)



Following the general procedure, reacted for 24 h. A purification by preparative TLC (25:75 acetone:PE) gave **2d** as light-yellow oil (30.1 mg, 71%, 70/1 dr).

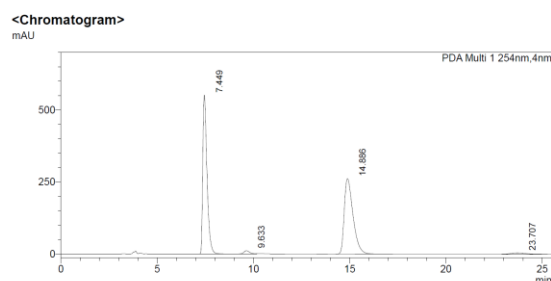
¹H NMR (400 MHz, Chloroform-*d*) δ 8.96 (dd, *J* = 4.3, 1.7 Hz, 1H), 8.08 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.74 – 7.64 (m, 2H), 7.40 (ddd, *J* = 8.5, 5.8, 3.2 Hz, 2H), 7.23 – 7.11 (m, 2H), 7.02 – 6.87 (m, 3H), 6.65 (td, *J* = 7.6, 1.2 Hz, 1H), 5.42 (d, *J* = 13.9 Hz, 1H), 5.29 (d, *J* = 14.0 Hz, 1H), 2.77 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.06, 158.72, 151.02, 144.83, 137.45, 136.21, 133.15, 133.05, 132.63, 131.47, 131.32, 130.98, 130.29, 130.23, 129.55, 129.12, 128.86, 128.77, 126.12, 125.96, 121.59, 121.31, 116.68, 109.42, 74.81, 20.09.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₂₆H₁₈ClN₂O₂⁺ 425.1051; found: 425.1054.

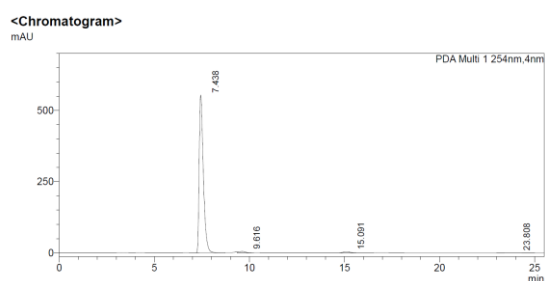
[α]_D²⁰ = -66.1° (*c* = 0.510, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm) with *t*_r = 7.4 min (peak 1), 9.6 min (peak 2), 15.1 min (peak 3), 23.8 min (peak 4): 97% ee (major diastereomer), 75% ee (minor diastereomer).



<Peak Table>
PDA Ch1 254nm

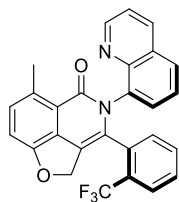
Peak#	Ret. Time	Area	Height	Area%
1	7.449	8396822	551592	49.067
2	9.633	243604	11313	1.424
3	14.896	825832	26204	49.249
4	23.707	215699	4380	1.260
Total		17113008	829369	100.000



<Peak Table>
PDA Ch1 254nm

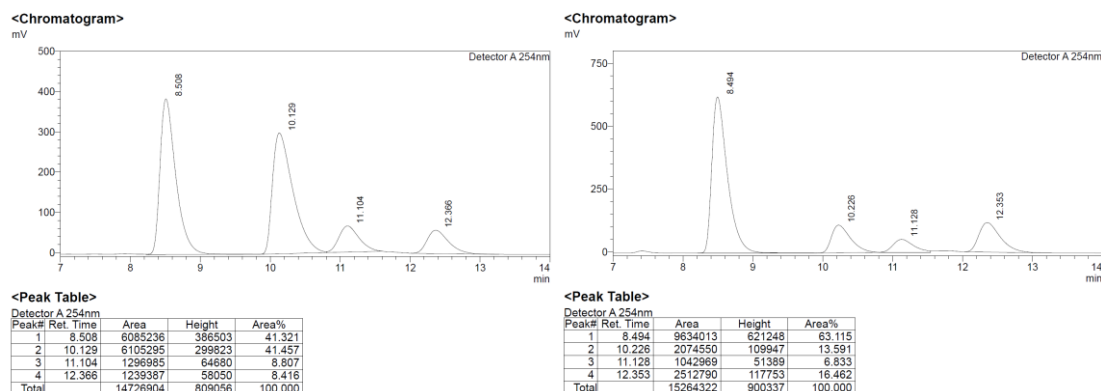
Peak#	Ret. Time	Area	Height	Area%
1	7.438	8389818	553330	97.357
2	9.616	105908	4830	1.229
3	15.091	106846	3441	1.240
4	23.808	15006	300	0.174
Total		8617577	561901	100.000

6-methyl-4-(quinolin-8-yl)-3-(2-(trifluoromethyl)phenyl)-2,4-dihydro-5H-furo[4,3,2-*de*]isoquinolin-5-one (2e)



Following the general procedure, in a 0.5 mmol scale, reacted for 40 h. A purification by preparative TLC (25:75 acetone:PE) gave **2e** as light-yellow foam (220 mg, 96%, 3.3/1 dr).

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 80/20, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 8.5$ min (peak 1), 10.1 min (peak 2), 11.1 min (peak 3), 12.4 min (peak 4): 65% ee (major diastereomer), 41% ee (minor diastereomer).



The major diastereomers (peaks 1 and 2 of the chromatogram above) could be separated by preparative TLC. The following data are of the major diastereomers.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.98 – 8.89 (m, 1H), 8.07 (d, $J = 8.3$ Hz, 1H), 7.66 (d, $J = 8.2$ Hz, 1H), 7.60 (d, $J = 7.3$ Hz, 1H), 7.49 (d, $J = 8.0$ Hz, 1H), 7.43 – 7.33 (m, 2H), 7.15 (d, $J = 8.0$ Hz, 2H), 7.09 (d, $J = 7.8$ Hz, 1H), 6.91 (dt, $J = 7.9, 3.9$ Hz, 2H), 5.37 (d, $J = 13.9$ Hz, 1H), 5.24 (d, $J = 13.9$ Hz, 1H), 2.76 (s, 3H).

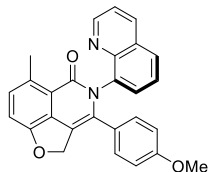
¹³C NMR (¹³C NMR (101 MHz, Chloroform-*d*) δ 163.14, 158.77, 150.86, 145.00, 137.39, 136.32, 132.89, 131.46, 131.31(q, $J_{C-F} = 2.2$), 130.97, 130.92, 130.68(q, $J_{C-F} = 2.3$), 129.38, 128.92, 128.85, 128.79(q, $J_{C-F} = 30.0$), 126.34(q, $J_{C-F} = 4.8$), 126.21, 123.84(q, $J_{C-F} = 272.1$), 121.67, 121.34, 116.56, 109.53, 74.75, 20.08.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -59.07.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{27}H_{18}F_3N_2O_2^+$ 459.1315; found: 459.1314.

$[\alpha]_D^{20} = -131.6^\circ$ ($c = 0.475$, THF)

3-(4-methoxyphenyl)-6-methyl-4-(quinolin-8-yl)-2,4-dihydro-5H-furo[4,3,2-de]isoquinolin-5-one (2f)



Following the general procedure on a 0.5 mmol scale, reacted for 24 h. A purification by column chromatography (25:75 acetone:PE) gave **2f** as light-yellow amorphous solid (189 mg, 90%).

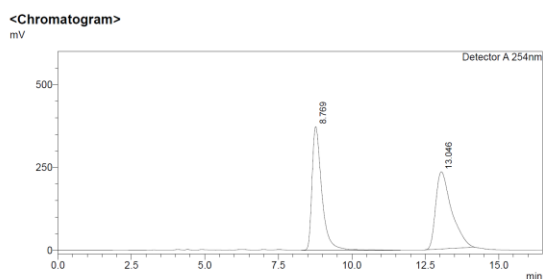
¹H NMR (400 MHz, Chloroform-*d*) δ 8.91 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.08 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.71 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.51 (dd, *J* = 7.3, 1.5 Hz, 1H), 7.47 – 7.40 (m, 1H), 7.36 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.09 (dd, *J* = 7.8, 1.0 Hz, 1H), 6.96 – 6.89 (m, 2H), 6.87 (d, *J* = 7.8 Hz, 1H), 6.51 – 6.43 (m, 2H), 5.46 (d, *J* = 3.3 Hz, 2H), 3.61 (s, 3H), 2.75 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.29, 159.08, 158.52, 150.94, 144.94, 137.77, 136.19, 134.98, 133.29, 131.09, 130.77, 129.62, 128.90, 128.53, 126.67, 125.94, 121.52, 120.78, 115.68, 113.23, 109.15, 75.15, 54.99, 20.14.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₂₇H₂₁N₂O₃⁺ 421.1547; found: 421.1544.

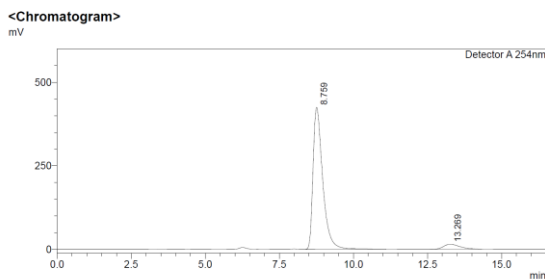
[α]_D²⁰ = -76.8° (*c* = 0.525, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 55/45, flow rate = 1.0 mL/min, λ = 254 nm) with *t*_r = 8.8 min (peak 1), 13.3 min (peak 2): 89% ee.



<Peak Table>
Detector A 254nm

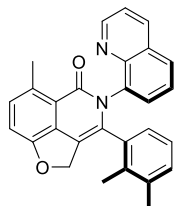
Peak#	Ret. Time	Area	Height	Area%
1	8.769	8640412	372949	49.712
2	13.046	8740439	232994	50.288
Total		17380851	605943	100.000



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	8.759	9680671	424843	94.323
2	13.269	582653	15170	5.677
Total		10263324	440013	100.000

3-(2,3-dimethylphenyl)-6-methyl-4-(quinolin-8-yl)-2,4-dihydro-5H-furo[4,3,2-de]isoquinolin-5-one (2g)



Following the general procedure. A purification by preparative TLC (30:70 acetone: PE) gave **2g** as light yellow-oil (40.5 mg, 97%, 9/1 dr).

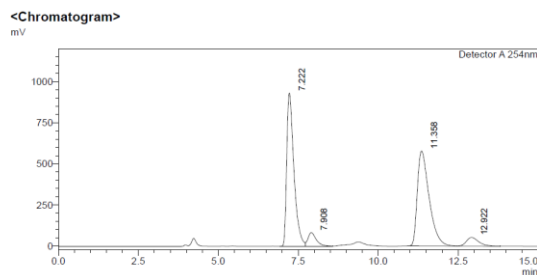
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 8.94 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.05 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.65 (dd, $J = 8.3, 1.4$ Hz, 1H), 7.48 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.39 – 7.32 (m, 2H), 7.14 – 7.08 (m, 1H), 6.89 (d, $J = 7.8$ Hz, 1H), 6.79 (d, $J = 7.5$ Hz, 1H), 6.71 (d, $J = 7.7$ Hz, 1H), 6.46 (t, $J = 7.6$ Hz, 1H), 5.31 (d, $J = 13.9$ Hz, 1H), 5.24 (d, $J = 13.8$ Hz, 1H), 2.77 (s, 3H), 2.23 (s, 3H), 2.13 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 163.44, 158.63, 150.94, 144.95, 137.82, 136.73, 136.09, 134.84, 134.08, 133.32, 130.94, 130.81, 130.23, 129.16, 128.91, 128.77, 126.44, 125.75, 124.72, 121.60, 121.04, 115.57, 109.23, 75.06, 20.26, 20.16, 16.84.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{28}\text{H}_{23}\text{N}_2\text{O}_2^+$ 419.1754; found: 419.1755.

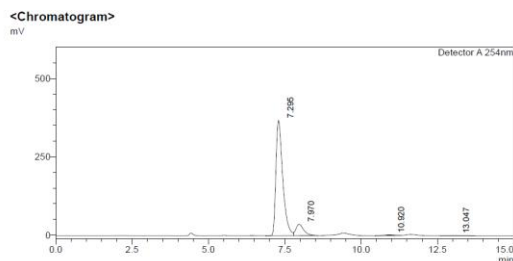
$[\alpha]_{\text{D}}^{20} = +11.9^\circ$ ($c = 0.495$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_{\text{r}} = 7.3$ min (peak 1), 8.0 min (peak 2), 10.9 min (peak 3), 13.0 min (peak 4): 98% ee (major diastereomer), 94% ee (minor diastereomer).



<Peak Table>
Detector A 254nm

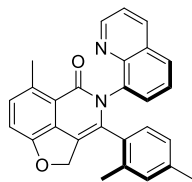
Peak#	Ret. Time	Area	Height	Area%
1	7.222	14806984	933392	45.074
2	7.908	1527403	83654	4.713
3	11.368	14847965	578269	45.818
4	12.922	1424074	52946	4.394
Total		32406426	1648161	100.000



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	7.296	5747509	381198	89.231
2	7.970	627078	36275	9.739
3	10.920	44856	1796	0.697
4	13.047	19516	702	0.303
Total		6438959	406971	100.000

3-(2,4-dimethylphenyl)-6-methyl-4-(quinolin-8-yl)-2,4-dihydro-5H-furo[4,3,2-de]isoquinolin-5-one (2h)



Following the general procedure. A purification by preparative TLC (30:70 acetone: PE) gave **2h** as light yellow-oil (41.4 mg, 99%, 14/1 dr).

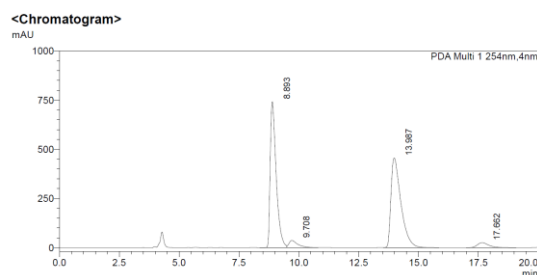
¹H NMR (400 MHz, Chloroform-*d*) δ 8.96 (dd, $J = 4.3, 1.7$ Hz, 1H), 8.07 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.68 (dd, $J = 8.2, 1.5$ Hz, 1H), 7.50 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.43 – 7.33 (m, 2H), 7.11 (d, $J = 7.8$ Hz, 1H), 6.89 (d, $J = 7.8$ Hz, 1H), 6.80 (s, 1H), 6.70 (d, $J = 7.8$ Hz, 1H), 6.35 (d, $J = 7.8$ Hz, 1H), 5.31 (d, $J = 13.7$ Hz, 1H), 5.25 (d, $J = 13.9$ Hz, 1H), 2.76 (s, 3H), 2.28 (s, 3H), 2.05 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.49, 158.58, 150.94, 144.94, 138.57, 137.81, 136.19, 135.25, 134.37, 133.27, 130.88, 130.76, 130.39, 130.29, 129.06, 128.91, 128.73, 128.47, 125.90, 125.78, 121.59, 121.00, 115.70, 109.18, 75.04, 21.03, 20.15, 19.59.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for C₂₈H₂₃N₂O₂⁺ 419.1754; found: 419.1754.

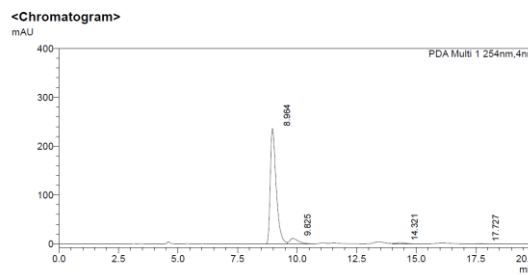
$[\alpha]_D^{20} = -0.9^\circ$ ($c = 0.675$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 80/20, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 9.0$ min (peak 1), 9.8 min (peak 2), 14.3 min (peak 3), 17.7 min (peak 4): 96% ee (major diastereomer), 91% ee (minor diastereomer).



<Peak Table>

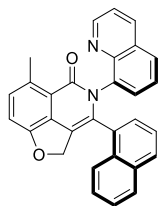
Peak#	Rel. Time	Area	Height	Area%
1	8.893	12835196	741921	46.219
2	9.708	935321	36954	3.368
3	13.987	13154671	456143	47.370
4	17.662	845064	25282	3.043
Total		27770252	1260300	100.000



<Peak Table>

Peak#	Rel. Time	Area	Height	Area%
1	8.964	4066017	236165	91.538
2	9.825	285914	11356	6.437
3	14.321	75660	2544	1.703
4	17.727	14323	516	0.322
Total		4441914	250581	100.000

6-methyl-3-(naphthalen-1-yl)-4-(quinolin-8-yl)-2,4-dihydro-5H-furo[4,3,2-de]isoquinolin-5-one (2i)



Following the general procedure, reacted for 24 h. A purification by preparative TLC (25:75 acetone:PE) gave **2i** as light-yellow oil (35.2 mg, 80%, 7.7/1 dr).

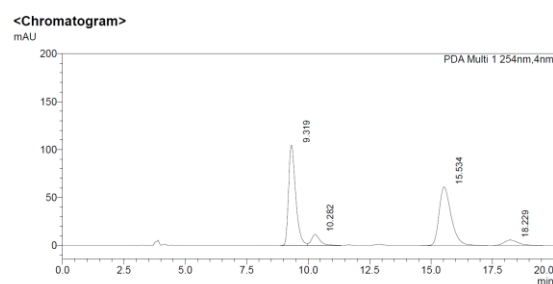
¹H NMR (400 MHz, Chloroform-*d*) δ 9.00 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.03 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.94 (d, $J = 8.4$ Hz, 1H), 7.73 (d, $J = 8.1$ Hz, 1H), 7.51 (ttdd, $J = 16.3, 8.1, 6.8, 1.3$ Hz, 4H), 7.39 (dd, $J = 8.3, 4.2$ Hz, 1H), 7.29 – 7.26 (m, 1H), 7.17 (d, $J = 7.9$ Hz, 1H), 7.09 – 6.98 (m, 2H), 6.92 (d, $J = 7.8$ Hz, 1H), 6.86 (dd, $J = 8.2, 7.1$ Hz, 1H), 5.24 (d, $J = 14.0$ Hz, 1H), 5.18 (d, $J = 14.1$ Hz, 1H), 2.81 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.38, 158.69, 150.98, 144.91, 137.50, 136.13, 133.16, 133.06, 132.64, 131.12, 130.97, 130.89, 130.53, 129.45, 129.12, 128.68, 128.60, 128.53, 127.13, 126.90, 126.08, 125.64, 124.61, 124.47, 121.55, 121.24, 116.86, 109.36, 74.96, 20.14.

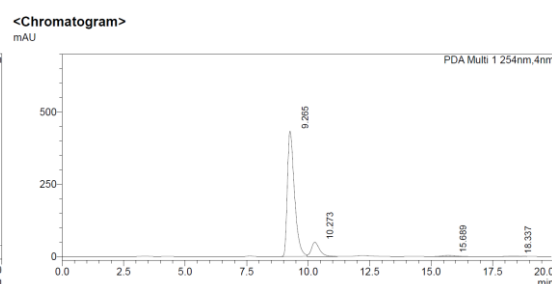
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{30}H_{20}N_2O_2^+$ 441.1598; found: 441.1598.

$[\alpha]_D^{20} = +84.7^\circ$ ($c = 0.450$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 9.3$ min (peak 1), 10.3 min (peak 2), 15.7 min (peak 3), 18.3 min (peak 4): 97% ee (major diastereomer), 96% ee (minor diastereomer).

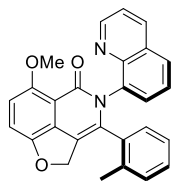


Peak#	Ret. Time	Area	Height	Area%
1	9.319	2100863	104628	44.847
2	10.282	281921	11564	6.018
3	15.534	2077856	61042	44.351
4	18.229	224098	5612	4.784
Total		4684537	182846	100.000



Peak#	Ret. Time	Area	Height	Area%
1	9.265	8722925	433798	87.211
2	10.273	1125570	49305	11.253
3	15.689	133087	3863	1.331
4	18.337	20518	618	0.205
Total		10002100	487583	100.000

6-methoxy-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5H-furo[4,3,2-*de*]isoquinolin-5-one (2j)



Following the general procedure, reacted for 48 h. A purification by preparative TLC (50:50 acetone:PE) gave **2j** as light-yellow oil (10.1 mg, 24%, 20/1 dr).

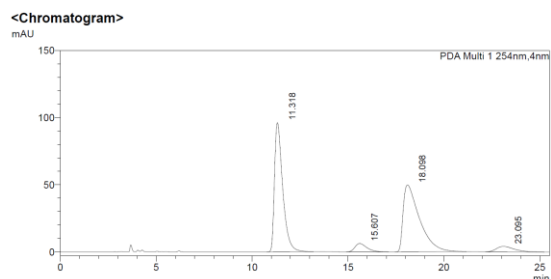
¹H NMR (400 MHz, Chloroform-*d*) δ 8.94 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.05 (dd, $J = 8.3, 1.8$ Hz, 1H), 7.66 (dd, $J = 8.3, 1.4$ Hz, 1H), 7.47 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.35 (ddd, $J = 9.8, 7.5, 5.7$ Hz, 2H), 7.03 – 6.98 (m, 1H), 6.96 – 6.89 (m, 2H), 6.84 (dd, $J = 7.7, 1.4$ Hz, 1H), 6.76 (d, $J = 8.4$ Hz, 1H), 6.59 – 6.52 (m, 1H), 5.35 – 5.22 (m, 2H), 3.90 (s, 3H), 2.33 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 160.96, 153.87, 153.12, 150.83, 144.94, 137.49, 136.01, 135.43, 135.06, 134.15, 133.05, 129.65, 129.06, 128.86, 128.75, 128.73, 128.55, 125.68, 124.98, 121.43, 115.06, 112.57, 110.09, 109.70, 75.05, 56.92, 19.63.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{27}H_{21}N_2O_3^+$ 421.1547; found: 421.1544.

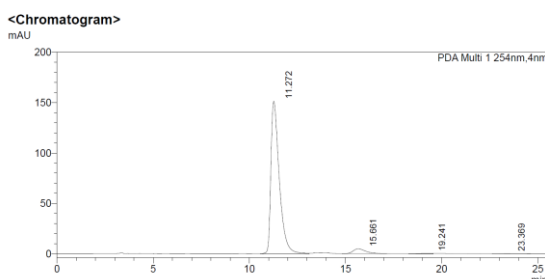
$[\alpha]_D^{20} = -105.4^\circ$ ($c = 0.475$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 60/40, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 11.3$ min (peak 1), 15.7 min (peak 2), 19.2 min (peak 3), 23.4 min (peak 4): >99% ee (major diastereomer), 94% ee (minor diastereomer).



<Peak Table>
PDA Ch1 254nm

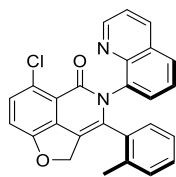
Peak#	Ret. Time	Area	Height	Area%
1	11.318	2866718	96198	45.051
2	15.607	273685	6298	4.301
3	18.098	2958663	49934	46.496
4	23.095	264194	4119	4.152
Total		6363260	156548	100.000



<Peak Table>
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%
1	11.272	4575778	151246	95.148
2	15.661	214704	4797	4.465
3	19.241	11939	240	0.246
4	23.369	6891	113	0.139
Total		4809112	156396	100.000

6-chloro-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2k)



Following the general procedure, reacted for 24 h. A purification by preparative TLC (30:70 acetone:PE) gave **2k** as light-yellow oil (40.4 mg, 95%, 28/1 dr).

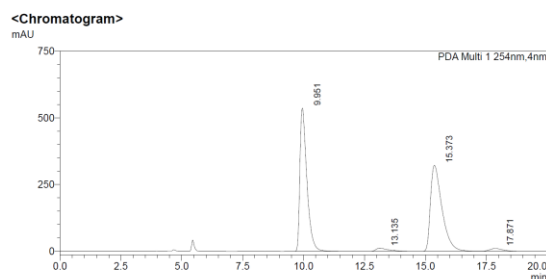
¹H NMR (400 MHz, Chloroform-*d*) δ 8.94 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.06 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.67 (dd, $J = 8.2, 1.4$ Hz, 1H), 7.51 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.40 – 7.31 (m, 3H), 7.01 (d, $J = 7.7$ Hz, 1H), 6.96 – 6.87 (m, 2H), 6.84 (dd, $J = 7.8, 1.4$ Hz, 1H), 6.57 (t, $J = 7.5$ Hz, 1H), 5.36 (d, $J = 13.9$ Hz, 1H), 5.30 (d, $J = 14.0$ Hz, 1H), 2.33 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 160.78, 159.18, 150.94, 144.71, 137.12, 136.06, 135.73, 135.34, 134.47, 132.69, 130.89, 129.74, 129.10, 128.97, 128.84, 128.44, 125.72, 125.05, 123.56, 121.62, 119.23, 114.61, 110.02, 75.61, 19.63.

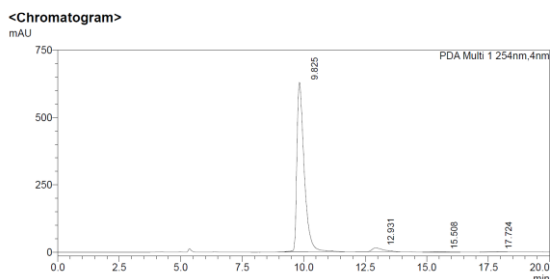
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{26}H_{18}ClN_2O_2^+$ 425.1051; found: 425.1050.

$[\alpha]_D^{20} = -86.1^\circ$ ($c = 0.590$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 9.8$ min (peak 1), 12.9 min (peak 2), 15.5 min (peak 3), 17.7 min (peak 4): >99% ee (major diastereomer), 83% ee (minor diastereomer).

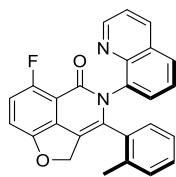


<Peak Table>				
PDA Ch1 254nm				
Peak#	Ret. Time	Area	Height	Area%
1	9.951	10688536	536546	48.454
2	13.135	397226	11156	1.604
3	15.373	10556970	321882	47.961
4	17.871	392314	10446	1.782
Total		22018046	880029	100.000



<Peak Table>				
PDA Ch1 254nm				
Peak#	Ret. Time	Area	Height	Area%
1	9.825	12984448	626846	96.181
2	12.931	427804	13446	3.169
3	15.508	47953	1360	0.355
4	17.724	39780	1258	0.295
Total		13499984	644930	100.000

6-fluoro-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5H-furo[4,3,2-*de*]isoquinolin-5-one (21)



Following the general procedure, reacted for 48 h. A purification by preparative TLC (25:75 acetone:PE) gave **21** as light-yellow oil (39.6 mg, 97%, 26/1 dr).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.96 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.07 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.67 (dd, $J = 8.3, 1.4$ Hz, 1H), 7.48 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.41 – 7.31 (m, 2H), 7.04 – 6.85 (m, 4H), 6.82 (dd, $J = 7.8, 1.4$ Hz, 1H), 6.61 – 6.51 (m, 1H), 5.39 – 5.27 (m, 2H), 2.34 (s, 3H).

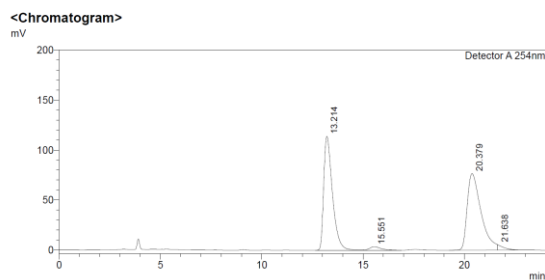
¹³C NMR (101 MHz, Chloroform-*d*) δ 159.61 (d, $J = 4.4$ Hz), 155.94 (d, $J = 2.7$ Hz), 154.52 (d, $J = 254.9$ Hz), 150.92, 144.66, 136.88, 136.18, 135.52, 135.37, 133.80 (d, $J = 3.8$ Hz), 132.69, 129.73, 129.06, 129.01, 128.81, 128.46, 125.73, 125.05, 121.61, 114.94 (d, $J = 2.4$ Hz), 114.75 (d, $J = 23.4$ Hz), 111.68 (d, $J = 13.1$ Hz), 109.71 (d, $J = 7.6$ Hz), 75.73, 26.97, 19.63.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -125.80.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{26}H_{18}FN_2O_2^+$ 409.1347; found: 409.1345.

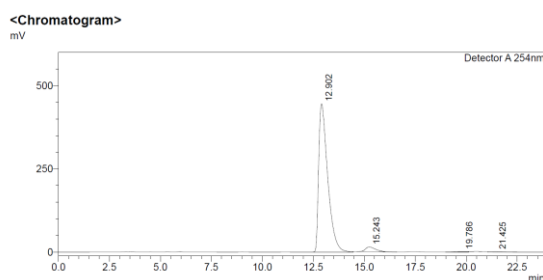
$[\alpha]_D^{20} = -23.6^\circ$ ($c = 0.570$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 12.9$ min (peak 1), 15.2 min (peak 2), 19.8 min (peak 3), 21.4 min (peak 4): 99% ee (major diastereomer), 99% ee (minor diastereomer).



<Peak Table>
Detector A 254nm

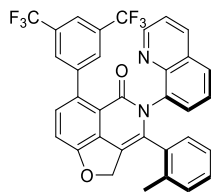
Peak#	Ret. Time	Area	Height	Area%
1	13.214	3410933	113910	46.822
2	15.551	135590	3525	1.861
3	20.379	3623155	76637	49.736
4	21.638	115195	5464	1.581
Total		7284833	199536	100.000



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	12.902	13742771	445764	95.792
2	15.243	477189	13900	3.326
3	19.786	69294	1823	0.483
4	21.425	57155	1245	0.398
Total		14346399	462732	100.000

6-(3,5-bis(trifluoromethyl)phenyl)-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2m)



Following the general procedure, reacted for 24 h. A purification by preparative TLC (5:30:65 acetone:DCM:PE) gave **2m** as light-yellow oil (50.5 mg, 84%, 13/1 dr).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.93 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.04 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.71 (s, 1H), 7.63 (dd, $J = 8.3, 1.4$ Hz, 1H), 7.42 (dd, $J = 7.4, 1.4$ Hz, 1H), 7.37 (dd, $J = 8.3, 4.3$ Hz, 1H), 7.33 – 7.27 (m, 1H), 7.23 (d, $J = 7.9$ Hz, 1H), 7.05 (dd, $J = 10.4, 7.7$ Hz, 2H), 6.95 (td, $J = 7.5, 1.4$ Hz, 1H), 6.78 (dd, $J = 7.8, 1.4$ Hz, 1H), 6.61 – 6.52 (m, 1H), 5.40 (d, $J = 1.4$ Hz, 2H), 2.38 (s, 3H).

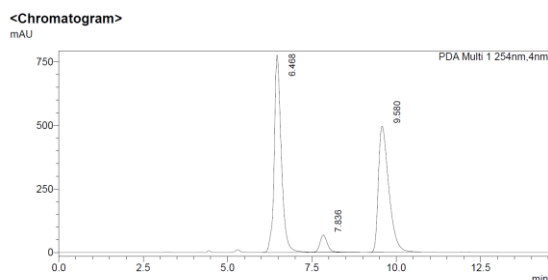
¹³C NMR (101 MHz, Chloroform-*d*) δ 161.41, 161.04, 150.80, 144.54, 142.27, 137.28, 136.16, 135.54, 135.36, 133.73, 132.85, 132.67, 130.88, 130.09 (q, $J = 32.9$ Hz), 129.97, 129.81, 129.06, 128.93, 128.90, 128.89, 128.46, 125.71, 125.10, 123.56 (q, $J = 271.0$ Hz), 121.62, 120.41 (m), 119.38, 114.77, 109.16, 75.62, 19.66.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -62.57.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{34}H_{21}F_6N_2O_2^+$ 603.1502; found: 603.1502.

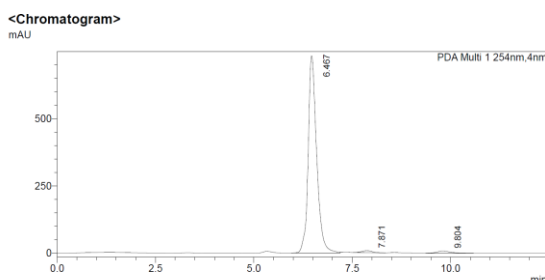
$[\alpha]_D^{20} = -157.2^\circ$ ($c = 0.490$, THF)

HPLC (Daicel Chiralpak IE column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 6.5$ min (peak 1, contains 2 isomers), 7.9 min (peak 2), 9.8 min (peak 3): 97% ee (major diastereomer), 58% ee (minor diastereomer) (dr was determined by ¹H NMR, ee major and ee minor were calculated).



<Peak Table>
PDA Ch1 254nm

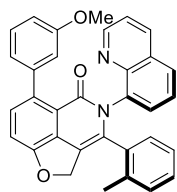
Peak#	Ret. Time	Area	Height	Area%
1	6.468	11332644	778634	49.206
2	7.806	1071376	69290	4.652
3	9.800	10627175	496547	46.143
Total		23031194	1341472	100.000



<Peak Table>
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%
1	6.467	11003958	732754	97.235
2	7.871	137458	7516	1.215
3	9.804	175504	8110	1.551
Total		11316920	748380	100.000

6-(3-methoxyphenyl)-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5H-furo[4,3,2-*de*]isoquinolin-5-one (2n)



Following the general procedure, reacted for 36 h. A purification by preparative TLC (5:40:55 acetone:DCM:PE) gave **2n** as light-yellow oil (44.7 mg, 90%, 12/1 dr).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.93 (dd, $J = 4.3, 1.7$ Hz, 1H), 8.01 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.59 (dd, $J = 8.3, 1.4$ Hz, 1H), 7.47 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.38 – 7.25 (m, 3H), 7.19 (t, $J = 7.9$ Hz, 1H), 7.08 – 6.95 (m, 4H), 6.92 (td, $J = 7.5, 1.4$ Hz, 1H), 6.84 (dd, $J = 7.8, 1.4$ Hz, 1H), 6.76 (ddd, $J = 8.2, 2.6, 1.0$ Hz, 1H), 6.55 (t, $J = 7.6$ Hz, 1H), 5.46 – 5.28 (m, 2H), 3.73 (s, 3H), 2.34 (s, 3H).

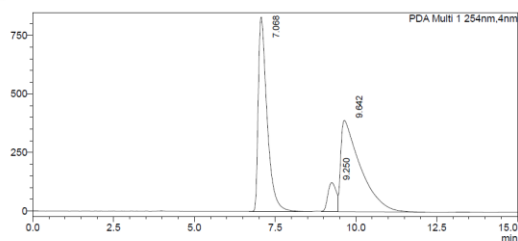
¹³C NMR (101 MHz, Chloroform-*d*) δ 161.57, 160.05, 158.45, 150.58, 144.62, 141.85, 137.50, 136.23, 135.43, 134.79, 134.23, 133.25, 133.08, 132.46, 129.66, 129.31, 128.88, 128.68, 128.56, 128.00, 125.77, 124.96, 122.52, 121.49, 119.70, 115.39, 114.86, 112.13, 109.02, 75.21, 55.03, 19.68.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{33}H_{25}N_2O_3^+$ 497.1860; found: 497.1858.

$[\alpha]_D^{20} = -190.8^\circ$ ($c = 0.500$, THF).

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 6.9$ min (peak 1), 9.0 min (peak 2, containing two enantiomers of the minor diastereomer), 10.2 min (peak 3): 99% ee (major diastereomer).

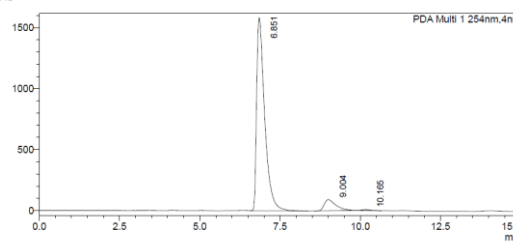
<Chromatogram>
mAU



<Peak Table>

Peak#	Ret. Time	Area	Height	Area%
1	7.068	15834348	830035	45.796
2	9.250	2249451	123924	6.506
3	9.642	16491729	389639	47.698
Total		34575527	1343598	100.000

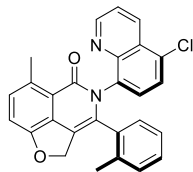
<Chromatogram>
mAU



<Peak Table>

Peak#	Ret. Time	Area	Height	Area%
1	6.851	27749595	1585203	91.746
2	9.004	2339061	91282	7.733
3	10.165	157466	7450	0.521
Total		30246122	1683934	100.000

4-(5-chloroquinolin-8-yl)-6-methyl-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2o)



Following the general procedure, reacted for 36 h. A purification by preparative TLC (25:75 acetone:PE) gave **2o** as light-yellow oil (33.4mg, 76%, 56/1 dr).

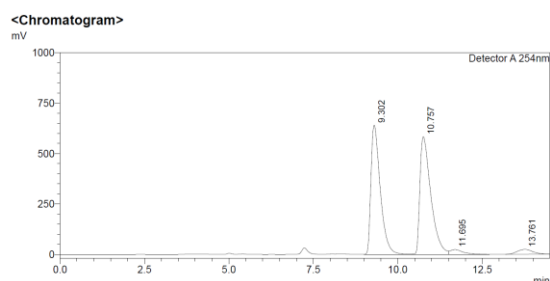
¹H NMR (400 MHz, Chloroform-*d*) δ 8.99 (dd, $J = 4.3, 1.6$ Hz, 1H), 8.47 (dd, $J = 8.5, 1.7$ Hz, 1H), 7.58 – 7.40 (m, 3H), 7.13 (d, $J = 7.8$ Hz, 1H), 7.05 – 6.88 (m, 3H), 6.82 (d, $J = 7.7$ Hz, 1H), 6.58 (t, $J = 7.5$ Hz, 1H), 5.37 – 5.22 (m, 2H), 2.75 (s, 3H), 2.32 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.36, 158.58, 151.42, 145.38, 136.99, 135.49, 133.97, 133.12, 132.92, 131.83, 131.02, 130.91, 129.82, 129.06, 128.88, 128.65, 126.87, 125.89, 125.15, 122.35, 120.91, 115.71, 109.45, 74.88, 20.06, 19.64.

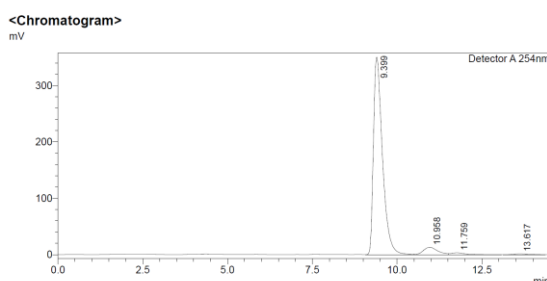
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{27}H_{20}ClN_2O_2^+$ 439.1208; found: 439.1209.

$[\alpha]_D^{20} = -28.2^\circ$ ($c = 0.500$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 85/15, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 9.4$ min (peak 1), 11.0 min (peak 2), 11.8 min (peak 3), 13.6 min (peak 4): 89% ee (major diastereomer), 29% ee (minor diastereomer).

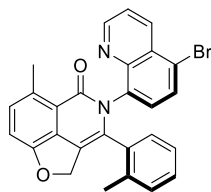


<Peak Table>				
Detector A 254nm				
Peak#	Ret. Time	Area	Height	Area%
1	9.302	12324204	640329	45.926
2	10.757	13099284	583184	48.815
3	11.665	624420	24121	2.327
4	13.761	786860	24562	2.932
Total		26834767	1272175	100.000



<Peak Table>				
Detector A 254nm				
Peak#	Ret. Time	Area	Height	Area%
1	9.399	6463192	350336	92.501
2	10.958	383118	13008	5.483
3	11.759	93614	3402	1.340
4	13.617	47237	1466	0.676
Total		6987161	368212	100.000

4-(5-bromoquinolin-8-yl)-6-methyl-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2p)



Following the general procedure, reacted for 36 h. A purification by preparative TLC (25:75 acetone:PE) gave **2p** as light-yellow oil (47.4 mg, 98%, 22/1 dr).

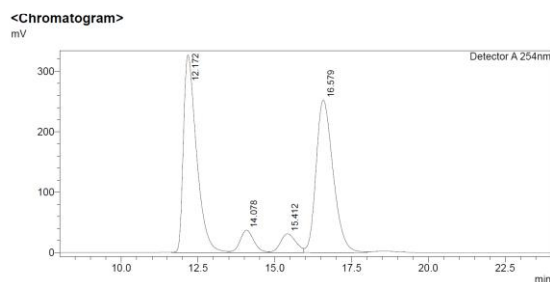
¹H NMR (400 MHz, Chloroform-*d*) δ 8.96 (dd, *J* = 4.3, 1.6 Hz, 1H), 8.43 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.48 (dd, *J* = 8.6, 4.2 Hz, 1H), 7.38 (d, *J* = 7.9 Hz, 1H), 7.13 (d, *J* = 7.9 Hz, 1H), 7.02 (d, *J* = 7.7 Hz, 1H), 6.98 – 6.87 (m, 2H), 6.82 (d, *J* = 7.7 Hz, 1H), 6.58 (t, *J* = 7.5 Hz, 1H), 5.36 – 5.21 (m, 2H), 2.75 (s, 3H), 2.32 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.30, 158.56, 151.44, 145.49, 137.71, 135.72, 135.47, 133.90, 133.11, 132.89, 131.01, 130.89, 129.82, 129.54, 129.34, 129.07, 128.63, 128.18, 125.15, 122.70, 122.42, 120.89, 115.70, 109.44, 74.86, 20.04, 19.63.

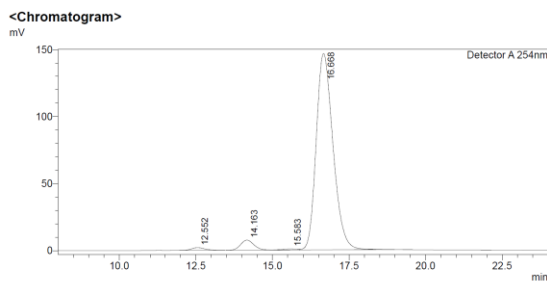
HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₂₇H₂₀BrN₂O₂⁺ 483.0703; found: 483.0703.

[α]_D²⁰ = +7.0° (*c* = 0.487, THF)

HPLC (Daicel Chiralpak IG column, eluent hexane/isopropanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm) with *t*_r = 12.2 min (peak 1), 14.1 min (peak 2), 15.4 min (peak 3), 16.6 min (peak 4): 98% ee (major diastereomer), 78% ee (minor diastereomer).

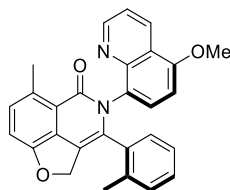


Peak#	Ret. Time	Area	Height	Area%
1	12.172	9679035	326487	44.736
2	14.078	1140270	36813	5.270
3	15.412	1076514	30931	4.976
4	16.579	9740194	251952	45.018
Total		21636013	646183	100.000



Peak#	Ret. Time	Area	Height	Area%
1	12.552	61310	2040	1.037
2	14.163	227508	7532	3.846
3	15.583	28479	840	0.481
4	16.668	5597768	146595	94.636
Total		5915064	157007	100.000

4-(5-methoxyquinolin-8-yl)-6-methyl-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2q)



Following the general procedure, reacted for 48 h. A purification by preparative TLC (4:40:56 acetone:DCM:PE) gave **2q** as light-yellow oil (28.5 mg, 66%, 14/1 dr).

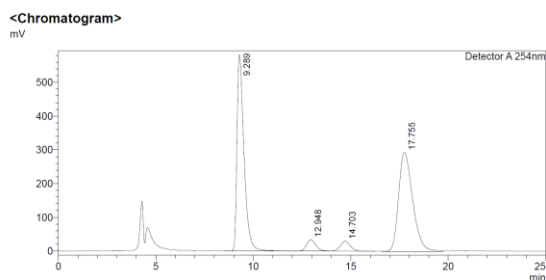
¹H NMR (400 MHz, Chloroform-*d*) δ 8.96 (dd, $J = 4.3, 1.7$ Hz, 1H), 8.46 (dd, $J = 8.5, 1.8$ Hz, 1H), 7.42 (d, $J = 8.2$ Hz, 1H), 7.35 (dd, $J = 8.5, 4.2$ Hz, 1H), 7.11 (dd, $J = 7.8, 1.0$ Hz, 1H), 7.01 (d, $J = 7.6$ Hz, 1H), 6.97 – 6.85 (m, 3H), 6.65 (d, $J = 8.3$ Hz, 1H), 6.59 (td, $J = 7.5, 1.4$ Hz, 1H), 5.36 – 5.20 (m, 2H), 3.90 (s, 3H), 2.80 – 2.72 (m, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.62, 158.52, 155.20, 151.03, 145.18, 135.38, 134.59, 133.35, 133.19, 131.01, 130.87, 130.69, 130.05, 129.58, 128.96, 128.75, 128.67, 125.03, 124.76, 121.20, 121.06, 120.63, 115.32, 109.09, 103.32, 103.12, 74.96, 55.72, 20.11, 19.66.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for C₂₈H₂₃N₂O₃⁺ 435.1703; found: 435.1702.

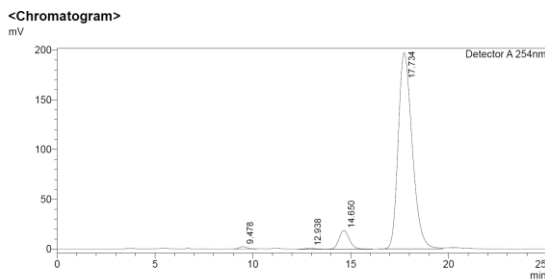
$[\alpha]_D^{20} = -15.0^\circ$ ($c = 0.550$, THF)

HPLC (Daicel Chiralpak IG column, eluent hexane/isopropanol = 65/35, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 9.5$ min (peak 1), 12.9 min (peak 2), 14.7 min (peak 3), 17.7 min (peak 4): 99% ee (major diastereomer), 94% ee (minor diastereomer).



<Peak Table>
Detector A 254nm

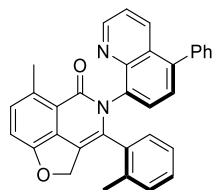
Peak#	Ret. Time	Area	Height	Area%
1	9.289	14608968	581503	46.455
2	12.948	1146096	34329	3.644
3	14.703	1074049	29219	3.415
4	17.755	14618341	292664	46.485
Total		31447454	937716	100.000



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	9.478	64063	2329	0.605
2	12.938	21223	636	0.200
3	14.650	673678	18567	6.362
4	17.734	9830016	197236	92.833
Total		10588981	218768	100.000

4-(5-phenylquinolin-8-yl)-6-methyl-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2r)



Following the general procedure, reacted for 42 h. A purification by preparative TLC (4:40:56 acetone:DCM:PE) gave **2r** as light-yellow oil (44.8 mg, 93%, 19/1 dr).

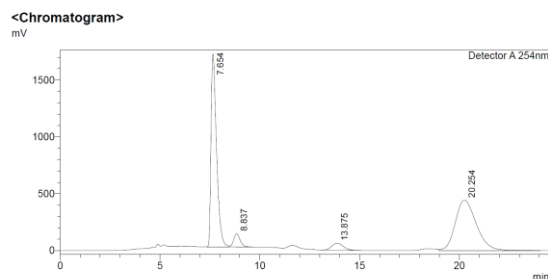
¹H NMR (400 MHz, Chloroform-*d*) δ 8.95 (dd, *J* = 4.1, 1.7 Hz, 1H), 8.12 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.48 – 7.38 (m, 3H), 7.32 (dd, *J* = 8.2, 3.4 Hz, 4H), 7.13 (d, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 7.7 Hz, 1H), 6.98 – 6.86 (m, 3H), 6.59 (t, *J* = 7.5 Hz, 1H), 5.40 – 5.24 (m, 2H), 2.79 (s, 3H), 2.35 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.53, 158.64, 150.65, 145.09, 141.33, 138.89, 137.04, 135.60, 134.61, 134.34, 133.29, 133.24, 130.99, 130.91, 130.02, 129.78, 128.90, 128.75, 128.50, 128.46, 127.85, 127.32, 126.47, 125.05, 121.50, 121.10, 115.60, 109.31, 75.02, 20.19, 19.75.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₃₃H₂₅N₂O₂⁺ 481.1911; found: 481.1908.

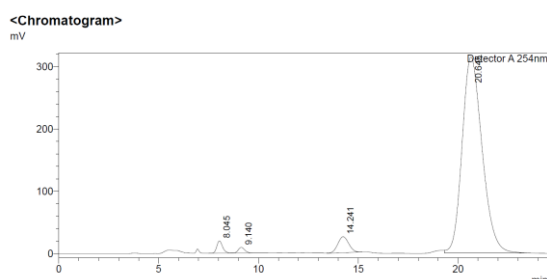
[α]_D²⁰ = +8.1° (*c* = 0.610, THF)

HPLC (Daicel Chiralpak IG column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm) with *t_r* = 8.0 min (peak 1), 9.1 min (peak 2), 14.2 min (peak 3), 20.6 min (peak 4): 96% ee (major diastereomer), 65% ee (minor diastereomer).



<Peak Table>
Detector A 254nm

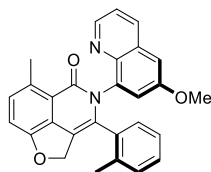
Peak#	Ret. Time	Area	Height	Area%
1	7.654	32514887	1695906	46.439
2	8.837	2613047	115973	3.732
3	13.875	2447157	61981	3.495
4	20.254	32440558	443616	46.333
Total		70015649	2317476	100.000



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	8.045	399178	19723	1.703
2	9.140	208926	9181	0.891
3	14.241	981591	25699	4.188
4	20.645	21850261	314237	93.218
Total		23439955	368840	100.000

4-(6-methoxyquinolin-8-yl)-6-methyl-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2s)



Following the general procedure. A purification by preparative TLC (30:70 acetone: PE) gave **2s** as light yellow-oil (32.5 mg, 75%, 21/1 dr).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.80 (dd, *J* = 4.3, 1.7 Hz, 1H), 7.93 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.32 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.20 (d, *J* = 2.7 Hz, 1H), 7.14 – 7.09 (m, 1H), 7.02 (d, *J* = 7.7 Hz, 1H), 6.98 – 6.84 (m, 4H), 6.58 (t, *J* = 7.5 Hz, 1H), 5.30 (d, *J* = 13.8 Hz, 1H), 5.25 (d, *J* = 13.9 Hz, 1H), 3.79 (s, 3H), 2.76 (s, 3H), 2.33 (s, 3H).

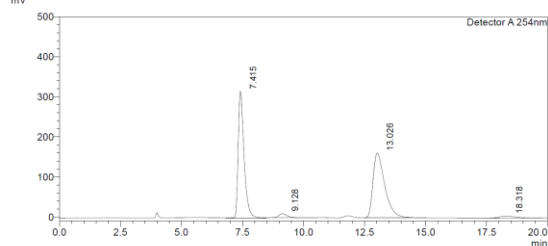
¹³C NMR (101 MHz, Chloroform-*d*) δ 163.28, 158.62, 156.78, 148.44, 141.15, 138.79, 135.63, 134.92, 134.07, 133.22, 133.07, 130.97, 130.93, 129.78, 129.66, 128.96, 128.77, 125.01, 122.11, 121.94, 121.08, 115.60, 109.34, 106.32, 74.97, 55.60, 20.13, 19.70.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₂₈H₂₃N₂O₃⁺ 435.1703; found: 435.1705.

[α]_D²⁰ = -26.2° (*c* = 0.490, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm) with *t*_r = 7.4 min (peak 1), 9.2 min (peak 2), 13.3 min (peak 3), 18.4 min (peak 4): 96% ee (major diastereomer), 59% ee (minor diastereomer).

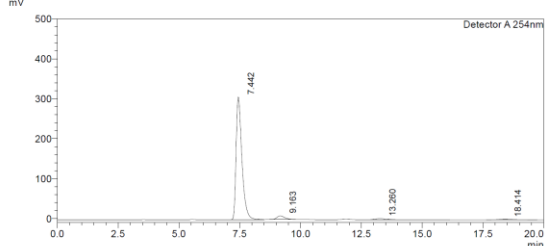
<Chromatogram>
mV



<Peak Table>

Peak#	Ret. Time	Area	Height	Area%
1	7.415	5298717	316257	47.367
2	9.128	224757	9685	2.009
3	13.026	5449481	161792	48.715
4	18.318	213588	4768	1.909
Total		11186542	492501	100.000

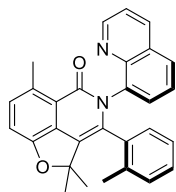
<Chromatogram>
mV



<Peak Table>

Peak#	Ret. Time	Area	Height	Area%
1	7.442	5158440	307083	93.560
2	9.163	203017	8905	3.682
3	13.260	99681	2862	1.808
4	18.414	52398	1161	0.950
Total		5513535	320010	100.000

2,2,6-trimethyl-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2t)



Following the general procedure, reacted for 30 h. A purification by preparative TLC (25:75 acetone: PE) gave **2t** as light-yellow oil (37.2mg, 86%, 1.2/1 dr).

Mixture of two diastereomers (ratio 1.2/1)

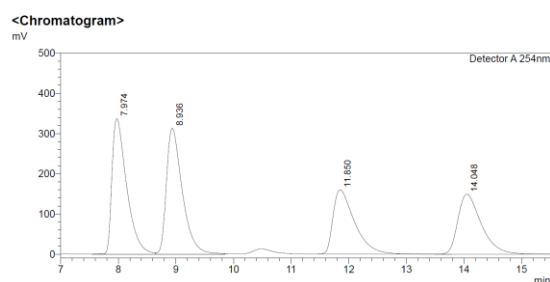
¹H NMR (400 MHz, Chloroform-*d*) δ 8.89 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.03 (dd, $J = 8.3, 1.8$ Hz, 1H), 7.70 – 7.58 (m, 1.5H), 7.43 – 7.23 (m, 3H), 7.15 (ddd, $J = 7.9, 4.1, 1.0$ Hz, 1H), 7.08 – 6.93 (m, 1.57H), 6.92 – 6.83 (m, 2H), 6.74 (dd, $J = 7.5, 1.5$ Hz, 1H), 6.56-6.52 (m, 0.49H), 2.77 (s, 3H), 2.28 (s, 1.47H), 1.83 (s, 1.53H), 1.47 (d, $J = 5.9$ Hz, 2.99H), 1.35 (d, $J = 9.8$ Hz, 3.01H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.49, 163.12, 155.73, 155.69, 150.57, 150.50, 144.61, 144.59, 138.39, 137.54, 137.33, 136.68, 136.09, 135.95, 135.20, 135.08, 132.78, 132.63, 132.37, 131.67, 131.54, 131.12, 130.98, 130.60, 130.44, 130.42, 129.99, 129.22, 129.00, 128.92, 128.81, 128.76, 128.21, 125.59, 125.49, 124.22, 123.70, 122.57, 122.00, 121.53, 121.47, 121.28, 121.23, 109.15, 92.13, 92.07, 28.11, 28.02, 26.36, 26.21, 20.55, 20.38, 20.35, 20.24.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{29}H_{25}N_2O_2^+$ 433.1911; found: 433.1913.

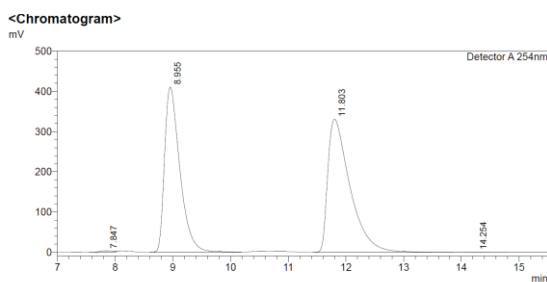
$[\alpha]_D^{20} = -52.9^\circ$ ($c = 0.610$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 85/15, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 7.8$ min (peak 1), 9.0 min (peak 2), 11.8 min (peak 3), 14.3 min (peak 4): >99% ee (major diastereomer), 99% ee (minor diastereomer).



<Peak Table>
Detector A 254nm

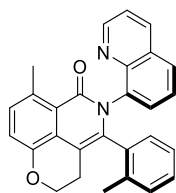
Peak#	Ret. Time	Area	Height	Area%
1	7.974	5974449	337279	29.363
2	8.936	6017984	313184	29.577
3	11.850	4134395	159260	20.319
4	14.048	4220244	149221	20.741
Total		20347071	958944	100.000



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	7.847	56292	3483	0.343
2	8.955	7564660	410529	46.041
3	11.803	8794172	330655	53.524
4	14.254	15222	568	0.093
Total		16430345	745235	100.000

7-methyl-5-(quinolin-8-yl)-4-(*o*-tolyl)-3,5-dihydropyrano[4,3,2-*de*]isoquinolin-6(2*H*)-one (2u)



Following the general procedure, reacted for 48 h. A purification by preparative TLC (10:40:50 acetone:DCM:PE) gave **2u** as light-yellow oil (39.3mg, 94%, 1.4/1 dr).

Mixture of two diastereomers (ratio 1.4/1)

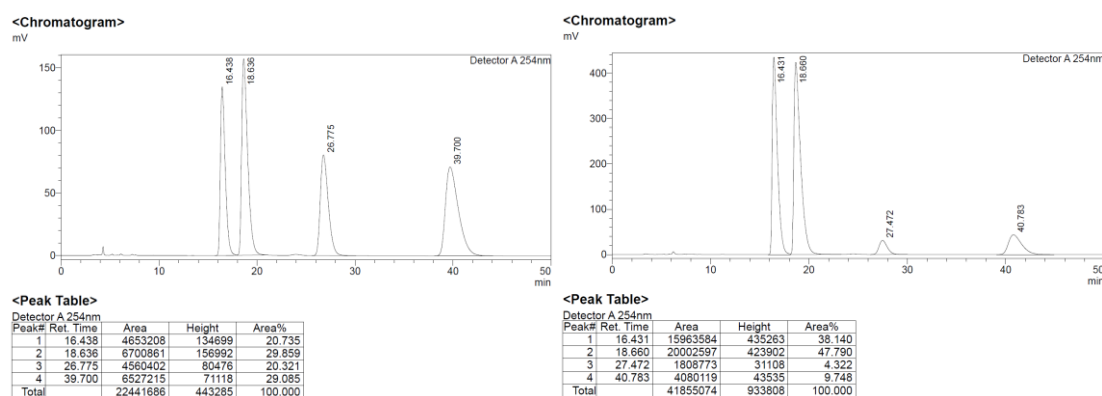
¹H NMR (400 MHz, Chloroform-*d*) δ 8.87 (ddd, $J = 60.2, 4.2, 1.7$ Hz, 1H), 8.03 (ddd, $J = 11.7, 8.3, 1.7$ Hz, 1H), 7.64 (ddd, $J = 8.3, 5.9, 1.4$ Hz, 1H), 7.53 (ddd, $J = 15.6, 7.4, 1.4$ Hz, 1H), 7.43 – 7.28 (m, 2H), 7.18 (ddd, $J = 8.1, 3.6, 0.8$ Hz, 1H), 7.14 – 7.07 (m, 1.36H), 6.93 (dtd, $J = 23.0, 9.0, 8.4, 7.0$ Hz, 2H), 6.79 (ddd, $J = 19.2, 7.5, 1.6$ Hz, 0.59H), 6.56 – 6.48 (m, 1H), 4.29 – 4.18 (m, 2H), 2.83 (s, 3H), 2.50 (dtd, $J = 8.3, 6.7, 5.9, 3.9$ Hz, 2H), 2.27 (s, 1.73H), 2.04 (s, 1.27H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.47, 150.92, 150.87, 150.81, 150.44, 144.72, 144.50, 137.93, 137.79, 137.45, 137.27, 136.03, 135.96, 135.92, 134.63, 133.33, 132.94, 131.68, 131.41, 130.24, 130.20, 129.89, 129.35, 128.97, 128.88, 128.80, 128.66, 128.59, 128.48, 128.25, 128.12, 125.80, 125.63, 125.54, 125.40, 124.75, 124.72, 124.27, 124.23, 121.55, 121.48, 118.09, 118.07, 106.45, 106.11, 65.73, 65.67, 26.10, 25.98, 23.40, 23.34, 19.78, 19.64.

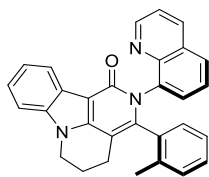
HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{28}H_{23}N_2O_2^+$ 419.1754; found: 419.1754.

$[\alpha]_D^{20} = -46.5^\circ$ ($c = 0.500$, THF)

HPLC (Daicel Chiralpak IE column, eluent hexane/isopropanol = 60/40, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 16.4$ min (peak 1), 18.7 min (peak 2), 27.5 min (peak 3), 40.8 min (peak 4): 66% ee (major diastereomer), 80% ee (minor diastereomer).



2-(quinolin-8-yl)-3-(*o*-tolyl)-2,4,5,6-tetrahydro-1*H*-indolo[3,2-*ij*][1,6]naphthyridin-1-one (2v)



Following the general procedure, reacted for 48 h. A purification by preparative TLC (10:40:50 acetone:DCM:PE) gave **2v** as light yellow-oil (41.8 mg, 95%, 1.3/1 dr).

Mixture of two diastereomers (ratio 1.3/1)

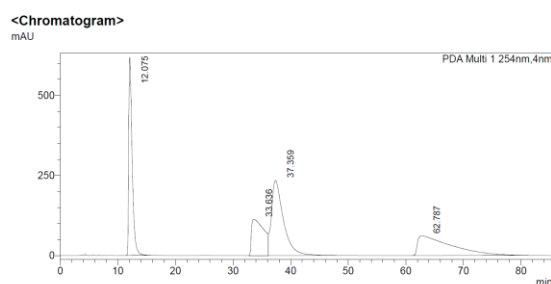
¹H NMR (400 MHz, Chloroform-*d*) δ 8.93 (dd, $J = 4.2, 1.7$ Hz, 0.55H), 8.77 (dd, $J = 4.2, 1.7$ Hz, 0.43H), 8.38 – 8.29 (m, 1H), 8.03 (ddd, $J = 15.7, 8.3, 1.7$ Hz, 1H), 7.69 – 7.52 (m, 2H), 7.45 – 7.26 (m, 5H), 7.17 – 6.85 (m, 3H), 6.82 – 6.52 (m, 1H), 4.28 – 4.14 (m, 2H), 2.55 – 2.35 (m, 2H), 2.30 – 2.05 (m, 5H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 160.31, 160.25, 150.84, 150.43, 145.22, 144.99, 143.29, 143.08, 142.14, 141.86, 138.37, 137.83, 137.68, 137.37, 135.96, 135.85, 135.79, 133.49, 133.08, 132.20, 131.38, 129.82, 129.30, 129.10, 128.86, 128.75, 128.67, 128.59, 128.45, 128.18, 128.08, 125.70, 125.40, 124.92, 124.63, 124.59, 123.67, 123.64, 122.22, 122.17, 121.38, 121.29, 121.26, 108.44, 104.63, 103.67, 103.36, 41.08, 41.03, 22.76, 22.66, 21.95, 21.82, 19.77, 19.71.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{30}H_{24}N_3O^+$ 464.1733; found: 464.1730.

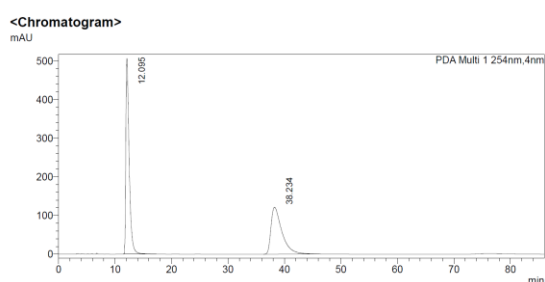
$[\alpha]_D^{20} = -53.4^\circ$ ($c = 0.530$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 60/40, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 12.1$ min (peak 1), 33.6 min (peak 2, not detected in chiral sample), 38.2min (peak 3), 62.8 min (peak 4, not detected in chiral sample): >99% ee (major diastereomer), >99% ee (minor diastereomer).



<Peak Table>
PDA Ch1 254nm

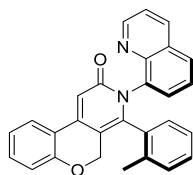
Peak#	Ret. Time	Area	Height	Area%
1	12.075	25332765	617726	25.103
2	33.836	16772208	113035	16.620
3	37.359	33900907	234772	33.593
4	62.787	24910036	61048	24.684
Total		100915915	1026581	100.000



<Peak Table>
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%
1	12.095	20753689	506188	55.932
2	38.234	16351807	121666	44.068
Total		37105496	627853	100.000

3-(quinolin-8-yl)-4-(*o*-tolyl)-3,5-dihydro-2*H*-chromeno[3,4-*c*]pyridin-2-one (2w)



Following the general procedure, reacted for 48 h. A purification by preparative TLC (10:40:50 acetone:DCM:PE) gave **2u** as light yellow-oil (35.7 mg, 86%, 1.2/1 dr).

Mixture of two diastereomers (ratio 1.2/1)

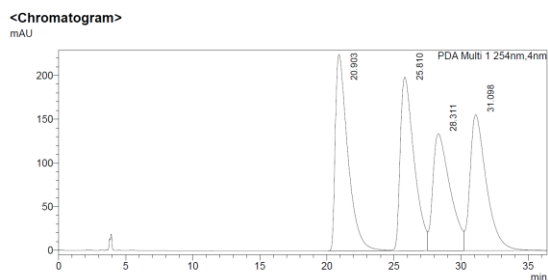
¹H NMR (400 MHz, Chloroform-*d*) δ 8.97 (dd, $J = 4.2, 1.7$ Hz, 0.56H), 8.83 (dd, $J = 4.2, 1.7$ Hz, 0.43H), 8.04 (ddd, $J = 12.6, 8.3, 1.7$ Hz, 1H), 7.84 (ddd, $J = 7.6, 5.4, 1.6$ Hz, 1H), 7.67 (ddd, $J = 8.3, 5.8, 1.4$ Hz, 1H), 7.53 (ddd, $J = 21.7, 7.3, 1.4$ Hz, 1H), 7.44 – 7.30 (m, 3H), 7.16 – 7.07 (m, 2.45H), 7.05 – 6.90 (m, 3H), 6.79 (dt, $J = 6.8, 1.8$ Hz, 1H), 6.56 (td, $J = 7.6, 1.4$ Hz, 0.55H), 4.59 – 4.45 (m, 2H), 2.31 (s, 1.67H), 2.05 (s, 1.33H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.67, 163.64, 156.33, 156.31, 151.01, 150.63, 144.27, 144.00, 143.99, 142.06, 141.75, 137.49, 136.74, 136.23, 136.07, 135.97, 135.41, 132.06, 132.03, 131.89, 131.45, 131.23, 130.74, 130.19, 129.68, 129.21, 129.19, 128.86, 128.82, 128.79, 128.37, 128.13, 125.76, 125.49, 125.10, 125.08, 125.01, 124.97, 122.56, 122.53, 121.75, 121.67, 120.55, 120.50, 118.00, 117.98, 111.37, 111.29, 110.08, 109.81, 65.29, 65.18, 19.85, 19.66.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{28}H_{21}N_2O_2^+$ 417.1598; found: 417.1594.

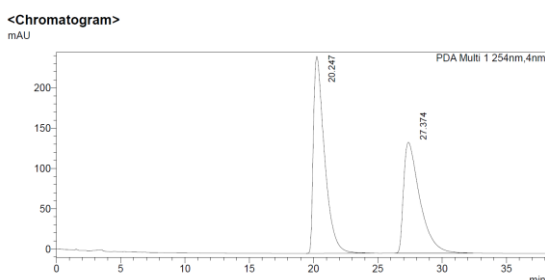
$[\alpha]_D^{20} = +48.5^\circ$ ($c = 0.550$, THF) ($>99\%$ ee (major diastereomer), $>99\%$ ee (minor diastereomer), 1.2/1 dr).

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 20.2$ min (peak 1), 25.8 min (peak 2, not detected in chiral sample), 27.3 min (peak 3), 31.1 min (peak 4, not detected in chiral sample): ($>99\%$ ee (major diastereomer), $>99\%$ ee (minor diastereomer)).



<Peak Table>
PDA Ch1 254nm

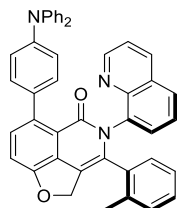
Peak#	Ret. Time	Area	Height	Area%
1	20.903	14594330	224696	26.972
2	28.810	14335898	18636	26.494
3	28.311	11960859	133580	22.105
4	31.088	13218563	155347	24.429
Total		54109650	712259	100.000



<Peak Table>
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%
1	20.247	14750018	244311	54.989
2	27.374	12073475	137609	45.011
Total		26823493	381921	100.000

6-(4-(diphenylamino)phenyl)-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5H-furo[4,3,2-*de*]isoquinolin-5-one (2y)



Following the general procedure on a 0.539 mmol scale, reacted for 36 h. A purification by preparative TLC (2:40:50 acetone:DCM:PE). Then the solid was recrystallized in acetone and washed with ether, giving **2y** as light-yellow solid (148 mg, 43%, 50/1 dr).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.93 (dd, $J = 4.3, 1.7$ Hz, 1H), 8.01 (dd, $J = 8.3, 1.7$ Hz, 1H), 7.61 (dd, $J = 8.3, 1.4$ Hz, 1H), 7.51 (dd, $J = 7.3, 1.4$ Hz, 1H), 7.38 – 7.26 (m, 5H), 7.21 – 7.14 (m, 4H), 7.10 – 6.88 (m, 11H), 6.82 (dd, $J = 7.8, 1.4$ Hz, 1H), 6.54 (td, $J = 7.6, 1.4$ Hz, 1H), 5.44 – 5.26 (m, 2H), 2.16 (s, 3H). (50/1 dr)

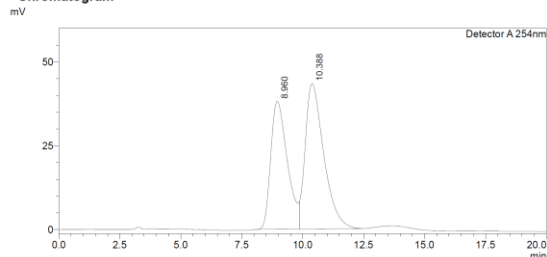
¹³C NMR (101 MHz, Chloroform-*d*) δ 161.89, 159.84, 150.75, 147.82, 146.12, 144.78, 137.61, 136.05, 135.44, 134.73, 134.56, 134.21, 133.38, 133.09, 133.00, 130.73, 129.62, 129.28, 129.07, 128.93, 128.86, 128.76, 128.57, 125.71, 124.89, 124.48, 122.51, 122.32, 121.53, 119.55, 114.93, 109.22, 75.12, 19.68.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{44}H_{32}N_3O_2^+$ 634.2489; found: 634.2486.

$[\alpha]_D^{20} = -238.5^\circ$ ($c = 0.550$, THF)

HPLC (Daicel Chiralpak IG column, eluent hexane/isopropanol = 60/40, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 9.0$ min (peak 1), 9.9 min (peak 2): 95% ee (major diastereomer).

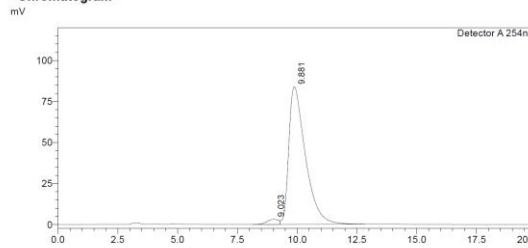
<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Area%
1	8.960	1814150	38164	44.146
2	10.388	2295312	43412	55.854
Total		4109463	81577	100.000

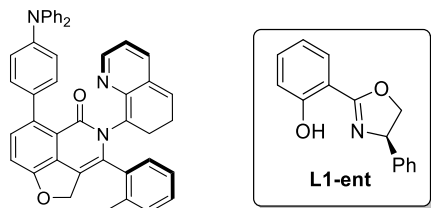
<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Area%
1	9.023	106527	3132	2.543
2	9.881	4043740	83877	97.457
Total		4149267	87009	100.000

6-(4-(diphenylamino)phenyl)-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2y-ent)

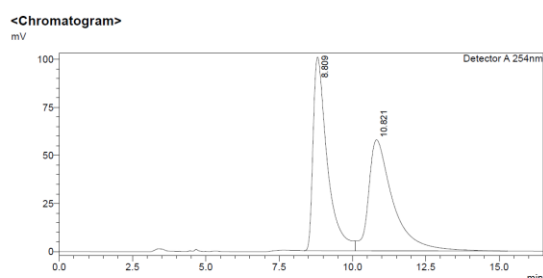


2y-ent was prepared using the same method as **2y** on a 0.5 mmol scale using **L1-ent** as ligand giving **2y-ent** as light-yellow solid (178 mg, 56%, 17/1 dr).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.93 (dd, *J* = 4.3, 1.7 Hz, 1H), 8.01 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.61 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.51 (dd, *J* = 7.3, 1.4 Hz, 1H), 7.38 – 7.26 (m, 5H), 7.21 – 7.14 (m, 4H), 7.10 – 6.88 (m, 11H), 6.82 (dd, *J* = 7.8, 1.4 Hz, 1H), 6.54 (td, *J* = 7.6, 1.4 Hz, 1H), 5.44 – 5.26 (m, 2H), 2.16 (s, 3H). (17/1 dr)

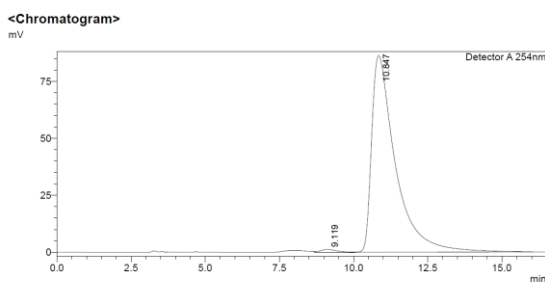
$[\alpha]_D^{20} = +236.6^\circ$ (*c* = 0.520, THF)

HPLC (Daicel Chiralpak ID column, eluent hexane/isopropanol = 60/40, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with *t_r* = 8.8 min (peak 1), 10.8 min (peak 2): 98% ee (major diastereomer).



<Peak Table>
Detector A 254nm

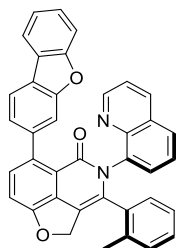
Peak#	Ret. Time	Area	Height	Area%
1	8.809	3385514	100734	50.257
2	10.821	3350895	57758	49.743
Total		6736410	158492	100.000



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	9.119	48432	1261	0.995
2	10.847	4819429	86228	99.005
Total		4867861	87489	100.000

6-(dibenzo[*b,d*]furan-3-yl)-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3-*de*]isoquinolin-5-one (2z)



Following the general procedure on a 0.6 mmol scale, reacted for 48 h. A purification by preparative TLC (2:40:50 acetone:DCM:PE). Then the solid was recrystallized in acetone and washed with ether, giving **2z** as off-white solid (171 mg, 51%, 37/1 dr).

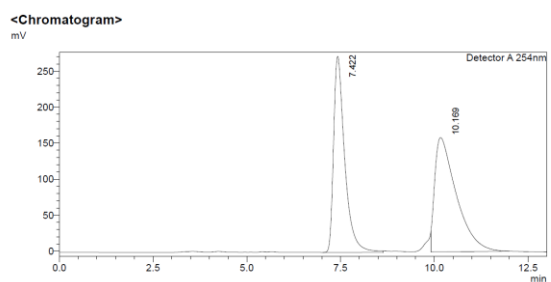
¹H NMR (400 MHz, Chloroform-*d*) δ 8.94 (dd, $J = 4.3, 1.7$ Hz, 1H), 7.99 (dd, $J = 8.3, 1.8$ Hz, 1H), 7.84 (dd, $J = 7.9, 4.6$ Hz, 2H), 7.64 (d, $J = 1.4$ Hz, 1H), 7.57 (dd, $J = 8.2, 1.4$ Hz, 1H), 7.51 – 7.44 (m, 3H), 7.39 – 7.31 (m, 3H), 7.30 – 7.22 (m, 2H), 7.07 (d, $J = 7.9$ Hz, 1H), 7.00 (d, $J = 7.7$ Hz, 1H), 6.92 (td, $J = 7.5, 1.4$ Hz, 1H), 6.85 (d, $J = 7.7$ Hz, 1H), 6.56 (t, $J = 7.5$ Hz, 1H), 5.44 – 5.32 (m, 2H), 2.35 (s, 3H). (37/1 dr)

¹³C NMR (101 MHz, Chloroform-*d*) δ 161.70, 160.28, 156.41, 155.62, 150.80, 144.80, 139.98, 137.56, 136.05, 135.49, 135.03, 134.15, 133.45, 133.07, 132.83, 129.71, 129.17, 128.96, 128.92, 128.74, 128.59, 126.58, 125.73, 125.20, 124.99, 124.47, 122.67, 122.45, 121.56, 120.45, 119.77, 119.09, 114.90, 112.94, 111.48, 109.13, 75.34, 19.75.

HRMS (ESI) m/z : $[M+H]^+$ Calculated for $C_{38}H_{25}N_2O_3^+$ 557.1860; found: 557.1862.

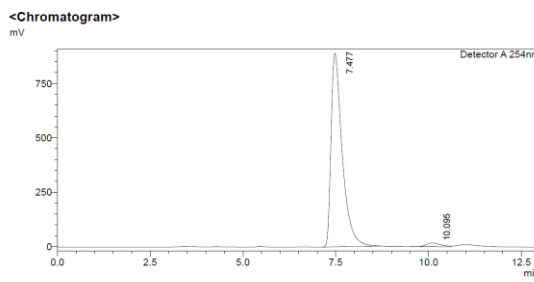
$[\alpha]_D^{20} = -258.3^\circ$ ($c = 0.540$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 60/40, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 7.5$ min (peak 1), 10.1 min (peak 2): 95% ee (major diastereomer).



<Peak Table>
Detector A 254nm

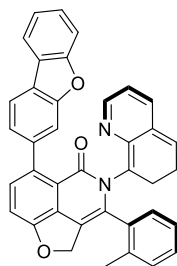
Peak#	Ret. Time	Area	Height	Area%
1	7.422	5626342	272239	47.096
2	10.169	6320322	158594	52.904
Total		11946665	430832	100.000



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	7.477	18635438	891030	97.507
2	10.095	476537	17308	2.493
Total		19111975	908338	100.000

6-(dibenzo[*b,d*]furan-3-yl)-4-(quinolin-8-yl)-3-(*o*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one (2*z*-ent)

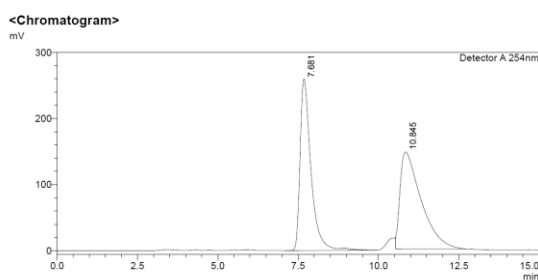


2z-ent was prepared using the same method as **2z** on a 0.5 mmol scale using **L1-ent** as ligand giving **2z-ent** as off-white solid (161 mg, 57%, 63/1 dr).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.94 (dd, $J = 4.3, 1.7$ Hz, 1H), 7.99 (dd, $J = 8.3, 1.8$ Hz, 1H), 7.84 (dd, $J = 7.9, 4.6$ Hz, 2H), 7.64 (d, $J = 1.4$ Hz, 1H), 7.57 (dd, $J = 8.2, 1.4$ Hz, 1H), 7.51 – 7.44 (m, 3H), 7.39 – 7.31 (m, 3H), 7.30 – 7.22 (m, 2H), 7.07 (d, $J = 7.9$ Hz, 1H), 7.00 (d, $J = 7.7$ Hz, 1H), 6.92 (td, $J = 7.5, 1.4$ Hz, 1H), 6.85 (d, $J = 7.7$ Hz, 1H), 6.56 (t, $J = 7.5$ Hz, 1H), 5.44 – 5.32 (m, 2H), 2.35 (s, 3H). (63/1 dr)

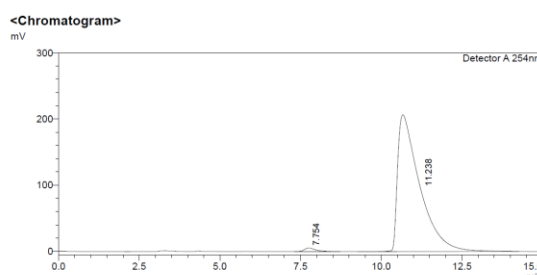
$[\alpha]_D^{20} = +250.7^\circ$ ($c = 0.485$, THF)

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 60/40, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 7.5$ min (peak 1), 11.2 min (peak 2): 97% ee (major diastereomer).



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	7.681	6141367	259927	47.918
2	10.845	6674978	146722	52.082
Total		12816345	406649	100.000



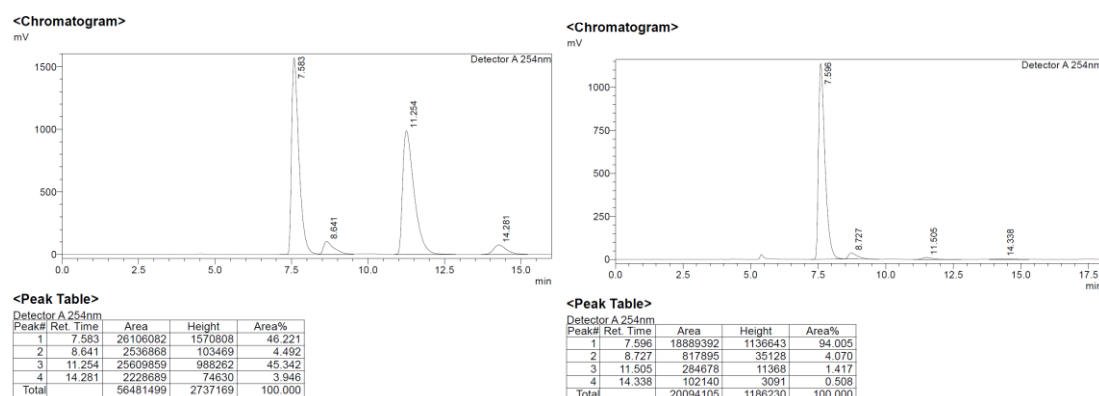
<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%
1	7.754	129154	5303	1.297
2	11.238	9831649	92192	98.703
Total		9960803	97495	100.000

5.4. Gram-Scale Synthesis of 2a

To a 250 mL round-bottom flask, substrate **1a** (1.626 g, 4.0 mmol), $\text{CoSO}_4 \cdot 7\text{H}_2\text{O}$ (112 mg, 0.4 mmol), **L1** (191 mg, 0.8 mmol), $\text{PivONa} \cdot x\text{H}_2\text{O}$ (1.28 g, 8 mmol. Suppose that $x = 2$), $\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$ (1.072 g, 4 mmol), a magnetic stir bar and *n*-PrOH (80 mL) were added. The flask was capped with a septum with an air balloon and heated to 50°C in an oil bath for 36 h. Then the mixture was filtered through a celite pad and washed with ethyl acetate and the filtrate was evaporated. DCM (200 mL) was added to the residue and washed with 200 mL of 0.25 M NaHCO_3 and 0.05 M EDTANa_2 aqueous solution. The aqueous phase was extracted twice with DCM. Combined organic phase was then dried with anhydrous sodium sulfate and vacuum filtered through celite. The solvent was removed by rotary evaporation. Purification by flash chromatography (15:85 acetone:PE) gave **2a** as a yellow solid (1.487 g, 92%, 21/1 dr).

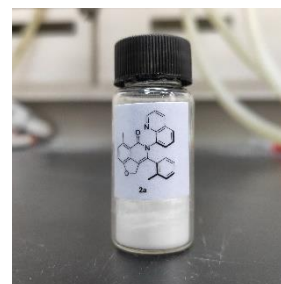
HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 7.6$ min (peak 1), 8.6 min (peak 2), 11.2 min (peak 3), 14.3 min (peak 4): 97% ee (major diastereomer), 78% ee (minor diastereomer).



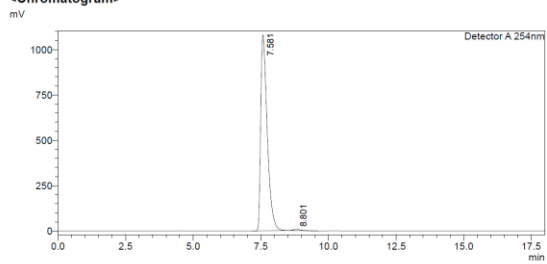
Further purification of 2a

Then the product was triturated in acetone:ether 1:2 (5 mL) at room temperature for 1 h. Filtration was done by vacuum with Büchner funnel. The solid was successively washed with ether and pentane. The remaining solvent was removed *in vacuo* to give white solid (1.231 g, 76% overall yield, > 100/1 dr).

HPLC (Daicel Chiralpak IB N-5 column, eluent hexane/isopropanol = 70/30, flow rate = 1.0 mL/min, $\lambda = 254$ nm) with $t_r = 7.6$ min (peak 1), 8.8 min (peak 2): >99.9% ee.



<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Area%
1	7.581	18097908	1080927	99.135
2	8.801	157980	7218	0.865
Total		18255888	1088145	100.000

6. Optical Properties

6.1. Uv-vis and CD spectra

Solutions of **2y** and **2y-ent** (DCM, 1.0 mM), 1.000 mm path quartz cell. The “average molar absorption coefficient” (ϵ_{avg}) is the average of molar absorption coefficients of **2y** and **2y-ent**.

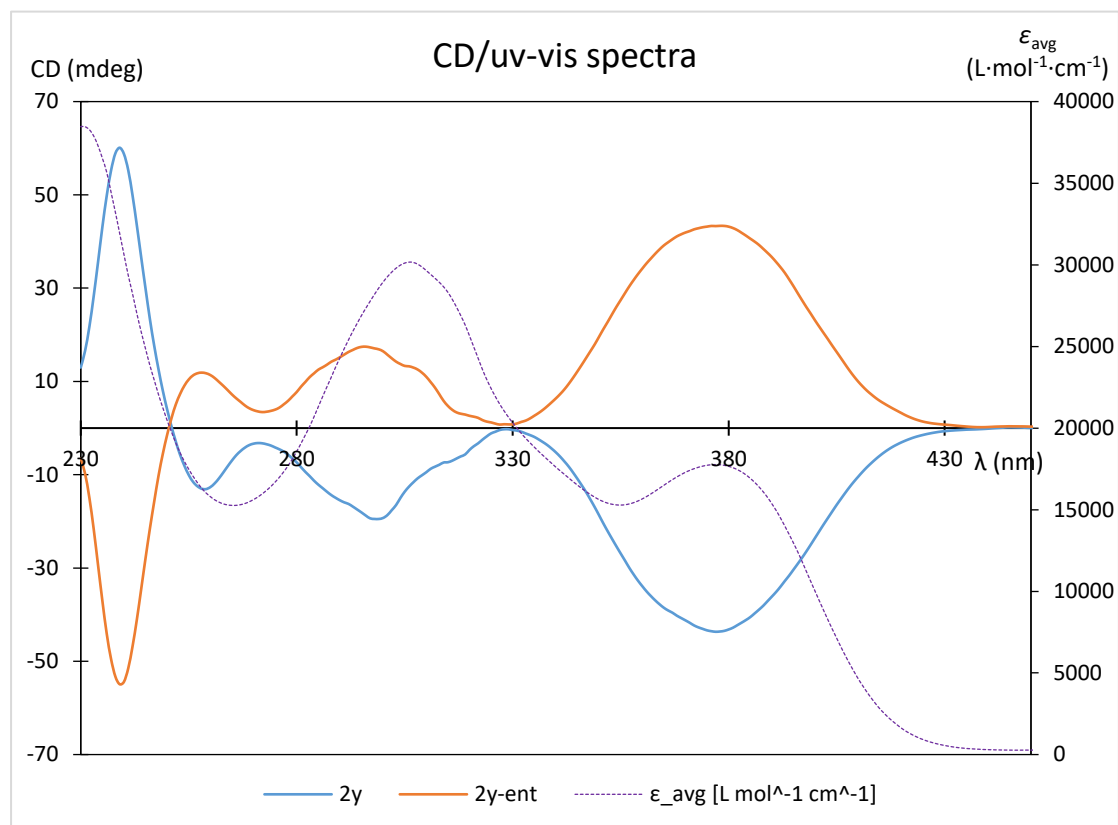


Figure S1. UV-Vis and CD Spectra of **2y** and **2y-ent**

Solutions of **2z** and **2z-ent** (DCM, 1.0 mM), 1.000 mm path quartz cell. The “average molar absorption coefficient” (ϵ_{avg}) is the average of molar absorption coefficients of **2z** and **2z-ent**.

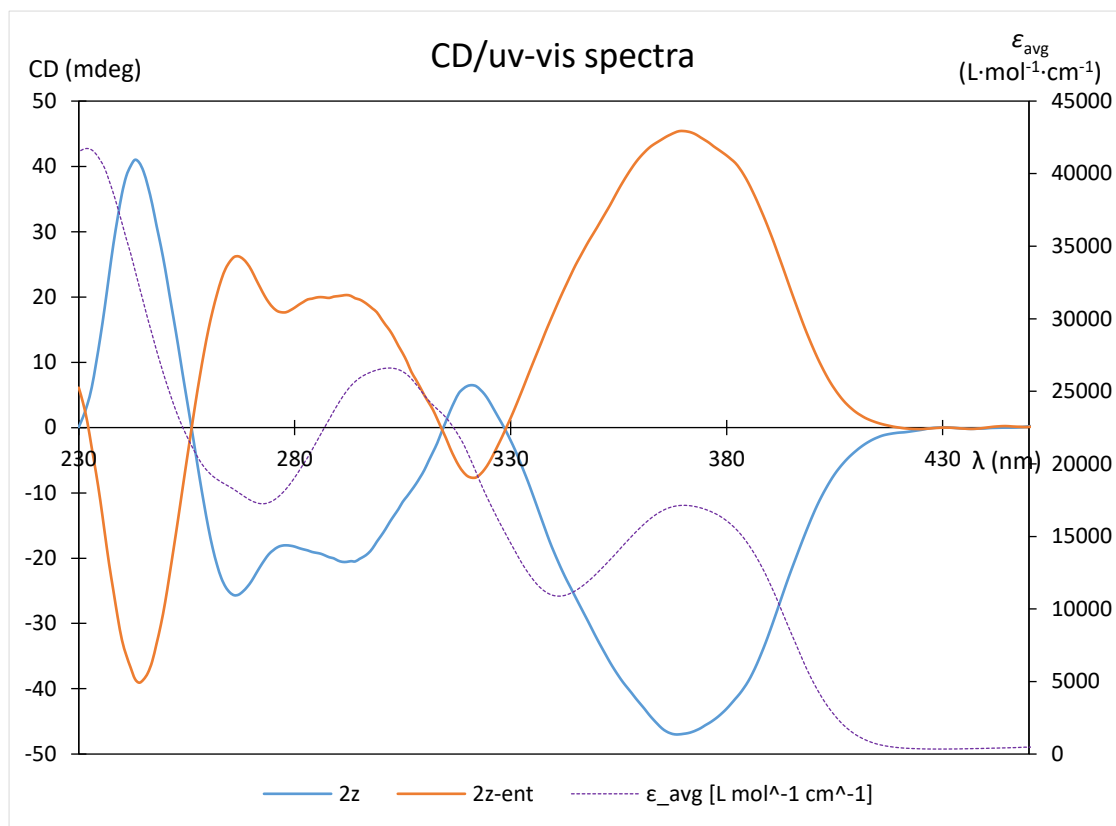


Figure S2. UV-Vis and CD Spectra of 2z and 2z-ent

6.2. Fluorescence Spectra

Solutions of **2y** and **2z** (20 μM), 10 mm \times 10 mm quartz cell. The relative intensity of emission for both **2y** and **2z** solutions are: DCM > THF \gg MeOH.

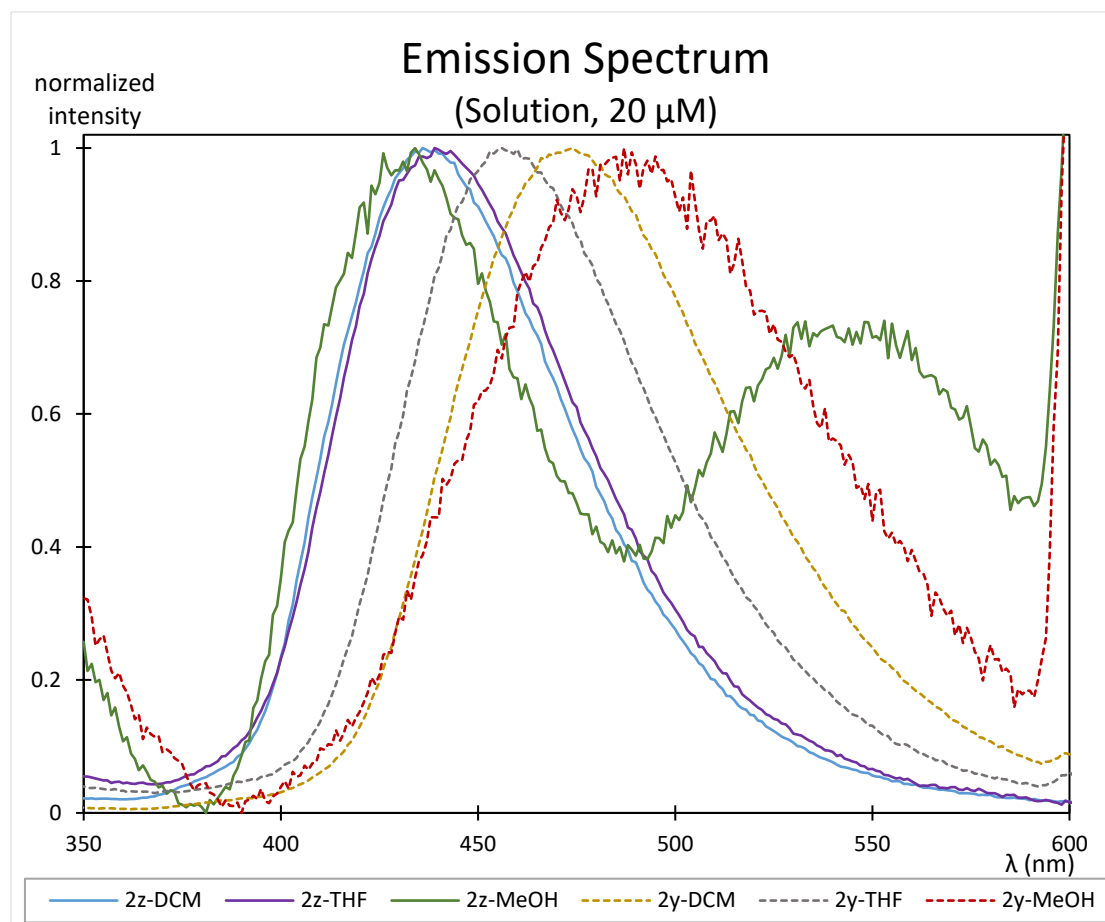


Figure S3. Fluorescence Spectra of **2y** and **2z** in Different Solvents

6.3. Circular polarized luminescence (CPL) spectra

Solutions of **2y** and **2z** (20 μM in DCM), 10 mm \times 10 mm quartz cell.

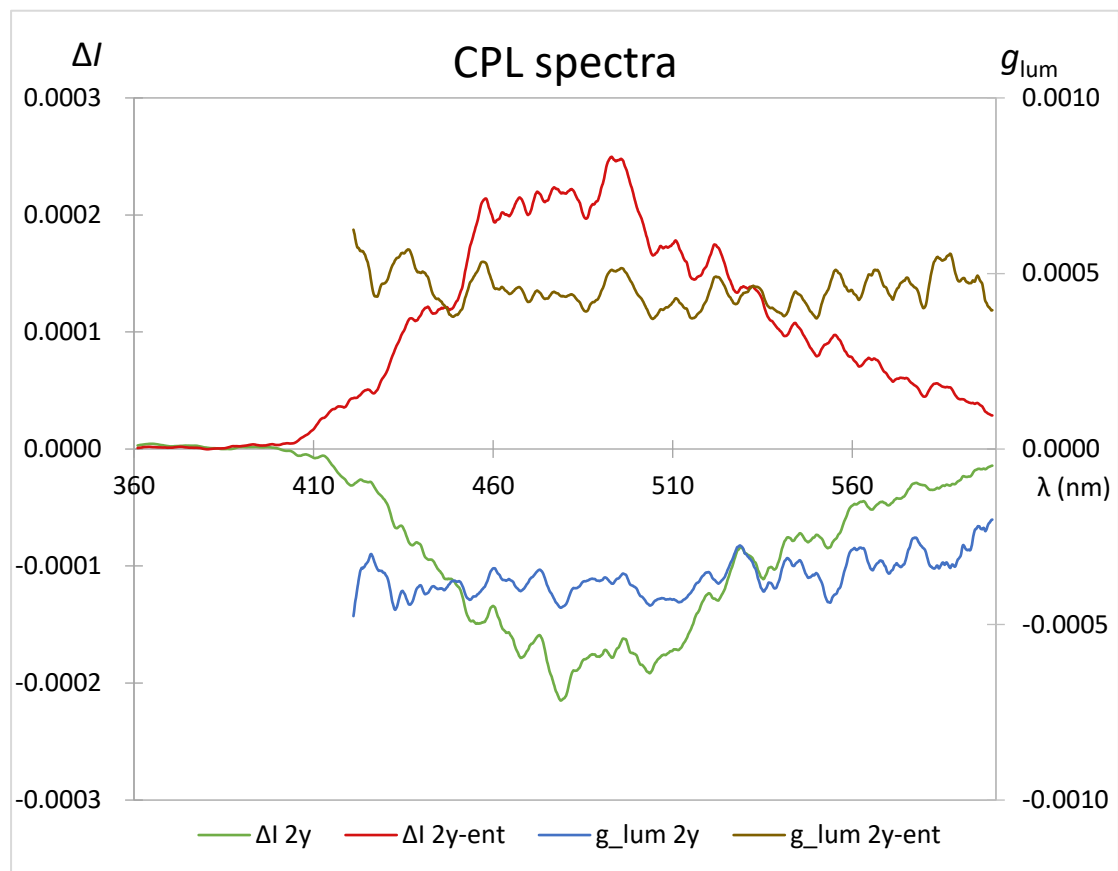


Figure S4. Circular Polarized Luminescence (CPL) Spectra of **2y** and **2y-ent**

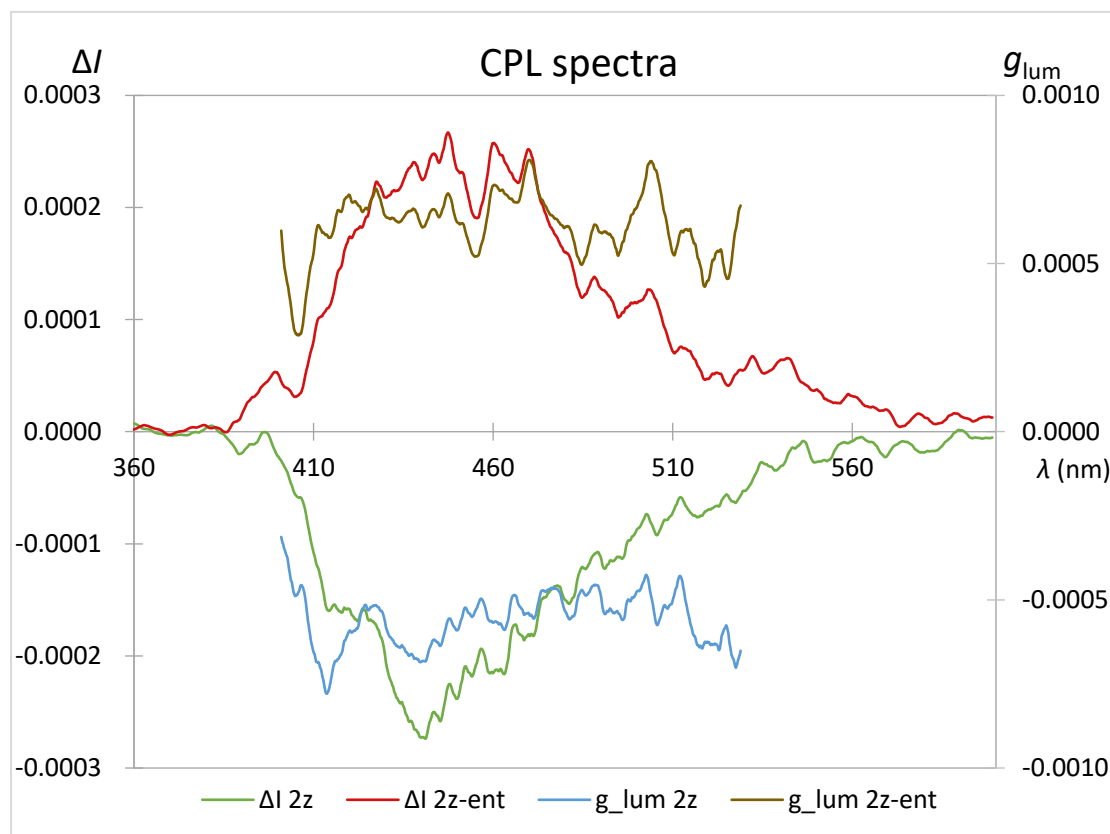


Figure S5. Circular Polarized Luminescence (CPL) Spectra of 2z and 2z-ent

Table S7. Asymmetric Factors of 2y and 2z

Compound	Excitation wavelength (nm)	g_{lum} (range/nm)
2y	290	-4×10^{-4} (423 ~ 453)
2y-ent	290	5×10^{-4} (423 ~ 453)
2z	300	-6×10^{-4} (460 ~ 490)
2z-ent	300	7×10^{-4} (460 ~ 490)

For each compound, the corresponding g_{lum} value in the table is the average of g_{lum} values within the giving range of wavelength indicated in the parentheses.

6.4. Photoluminescence Quantum Yield (PLQY)

The PLQY was measured in an integrating sphere. The sample solution (about 2 mL) was contained in a 10×10 mm quartz cell with a long neck.

Table S8. Photoluminescence quantum yield (PLQY) of 2y and 2z

Compound	Condition	Excitation wavelength (nm)	Integral interval of excitation light (nm)	Integral interval of emission light (nm)	PLQY
2y	5 μ M, DCM	350	330 ~ 364	365 ~ 700	0.29
2z	8 μ M, DCM				0.09

7. Measurements of Rotation Barriers of 5a and 2f

7.1. Experimental Procedure

Analyte (0.1 mmol) and a magnetic stir bar were added into a short test tube to which a rubber septum was mounted. The air in the tube was then carefully flushed with argon via a syringe needle and an argon balloon is remained to equalize the pressure during the following process. Solvent (5 mL) was added to dissolve the solid. The test tube was submerged into an oil bath preheated to the desired temperature. About 3 minutes later, 0.1 mL of solution was extracted via a long needle, transferred into a small vial and dissolved in 1.5 mL of HPLC grade isopropanol. The solution was filtered before HPLC analysis. The time of each extraction was precisely recorded.

7.2. Data processing

According to the reversible first-order reaction dynamics, the rate constant of racemization k_{rac} is the slope of the function of $-\ln ee$ to time

$$-\ln ee = k_{\text{rac}} t + C$$

where C is a constant.

The Gibbs free energy is degenerated in an achiral environment for a pair of enantiomers. Therefore, the forward rate constant is equal to the backward one.

$$k_{\text{atrp}}^+ = k_{\text{atrp}}^-$$

Since an atropisomerization of one molecule eliminates a molecule of one configuration and adds one molecule to the other configuration, the rate constant of atropisomerization k_{atrp} is half of k_{rac} .

$$k_{\text{atrp}} = 1/2 k_{\text{rac}}$$

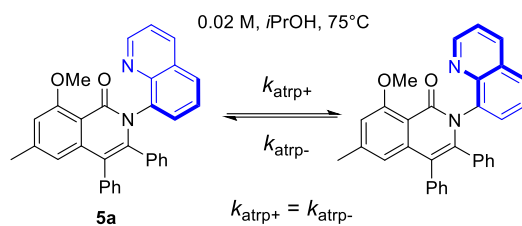
The energy barrier of atropisomerization can be calculated by Eyring equation

$$\Delta G_{\text{atrp}}^\ddagger = -RT \ln \frac{k_{\text{atrp}} h}{k_B T}$$

where R is ideal gas constant, T is absolute temperature, h is Planck constant, k_B is Boltzmann constant.

Data for 5a in *i*PrOH

Table S9. Atropisomerization of 5a in *i*PrOH



N°	$\Delta t/s$	ee/%	$-\ln ee$
1	0	84.1	0.1727
2	108	78.6	0.2413
3	265	71.1	0.3409
4	419	64.6	0.4371
5	683	54.6	0.6051
6	954	45.7	0.7823
7	1480	32.9	1.1113
8	2093	23.2	1.4608
9	2869	15.3	1.8760

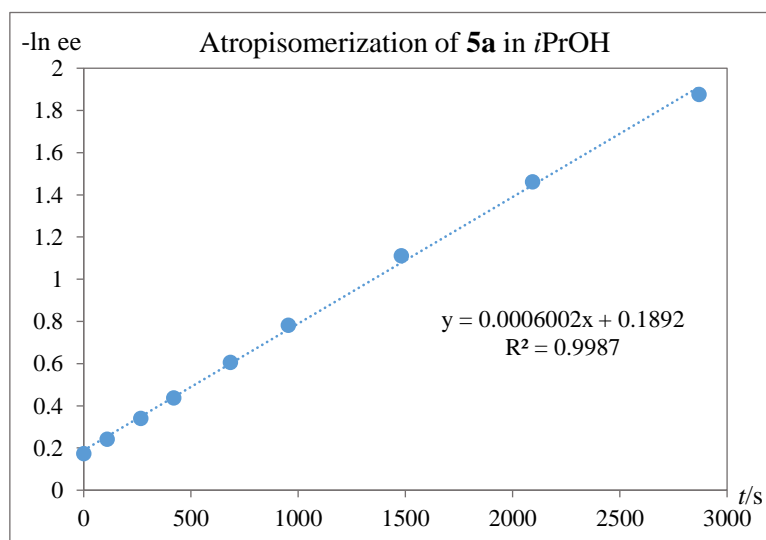


Figure S6. Atropisomerization of 5a in *i*PrOH

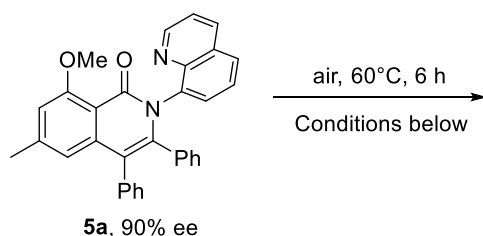
$$k_{\text{rac}} = 0.0006002 \text{ s}^{-1}$$

$$\Delta G_{\text{atrp}}^{\ddagger} = 109.2 \text{ kJ/mol}$$

At reaction temperature of **3** to **5a** (60°C), the half-life of racemization was calculated to be 1.8 h, which contradicted with the high enantioselectivity, high yield and a relatively long reaction time (91% ee, 82%, 12 h). If the energy barrier of atropisomerization of **5a** in the reaction were the same as the result above measured, the product **5a** would have already nearly completely racemized after the reaction. We supposed that the solvent, the metal compounds, the ligand and/or the base presenting in the reaction might affect the energy barrier of atropisomerization of **5a**. Therefore, we conducted a series of control experiments.

These experiments were done on a 20 μmol scale in 1 mL of solvent. After the reaction, **5a** was separated by preparative TLC and analyzed by HPLC as soon as possible to prevent racemization at room temperature.

Table S10. Atropisomerization of 5a in different conditions

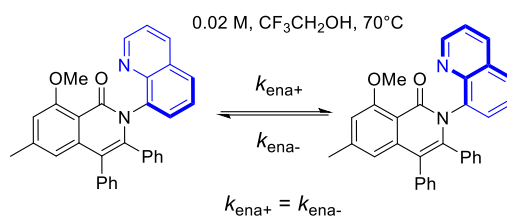


No.	Solvent	Ag ₂ CO ₃ (2 eq.)	Co(OAc) ₂ ·4H ₂ O (1 eq.)	L1 (2 eq.)	PivONa·xH ₂ O (2 eq.)	ee/%
1	<i>i</i> PrOH	0	0	0	0	4
2	TFE	0	0	0	0	86
3	TFE	1	0	0	0	86
4	TFE	1	1	0	0	84
5	TFE	0	1	0	0	84
6	TFE	1	1	1	0	85
7	TFE	1	1	1	1	86

5a in isopropanol almost fully racemized (90% to 4% ee), well corresponding to the energy barrier of atropisomerization measured in isopropanol; while in TFE (CF₃CH₂OH), the enantiomer excess only reduced slightly (90% to 84-86% ee). Also, the racemization was irrelevant to oxidant, catalyst, ligand and base. Then an atropisomerization experiment was conducted in TFE in order to determine the energy barrier more precisely.

Data for **5a** in TFE

Table S11 Atropisomerization of **5a** in TFE



N°	$\Delta t/s$	ee/%	$-\ln ee$
1	0	90.7	0.0978
2	15118	80.6	0.2152
3	22248	76.4	0.2694
4	33926	69.7	0.3614
5	83880	47.9	0.7351
6	90675	44.7	0.8052
7	113780	37.9	0.9690
8	125900	34.2	1.0736

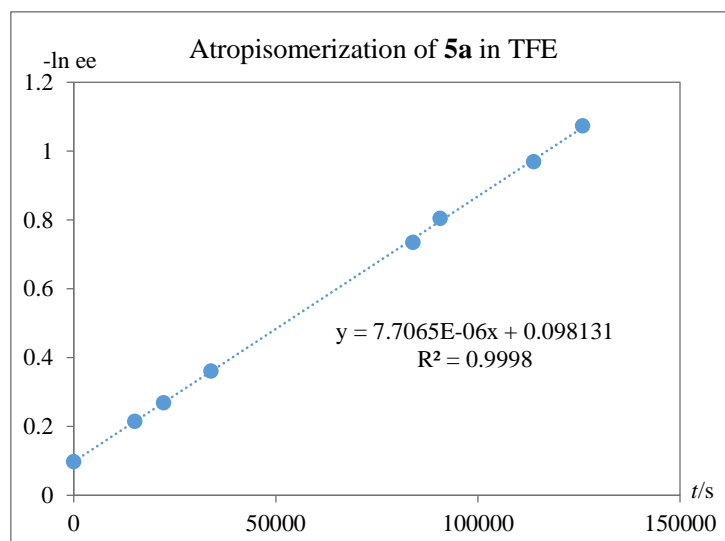


Figure S7. Atropisomerization of **5a** in TFE

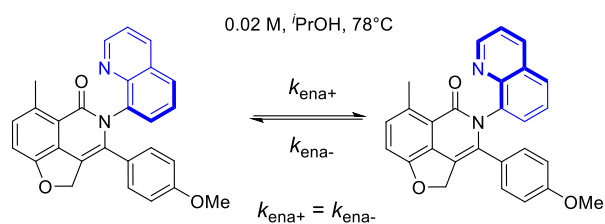
$$k_{\text{rac}} = 7.7065 \times 10^{-6} \text{ s}^{-1}$$

$$\Delta G_{\text{atrp}}^{\ddagger} = 120.0 \text{ kJ/mol}$$

The energy barrier of atropisomerization of **5a** in TFE is significantly higher than that in isopropanol by 10.8 kJ/mol, giving support to the good enantiocontrol of the reaction from **3** to **5a**.

Data for 2f

Table S12 Atropisomerization of 2f in *i*PrOH



N°	<i>t</i> /s	ee/%	-ln ee
1	0	87.3	0.1358
2	360	83.2	0.1839
3	742	78.3	0.2446
4	1060	74.5	0.2944
5	1576	68.6	0.3769
6	2187	61.5	0.4861
7	3213	51.8	0.6578
8	4393	42.4	0.8580
9	6000	32.0	1.1394
10	10344	15.3	1.8773

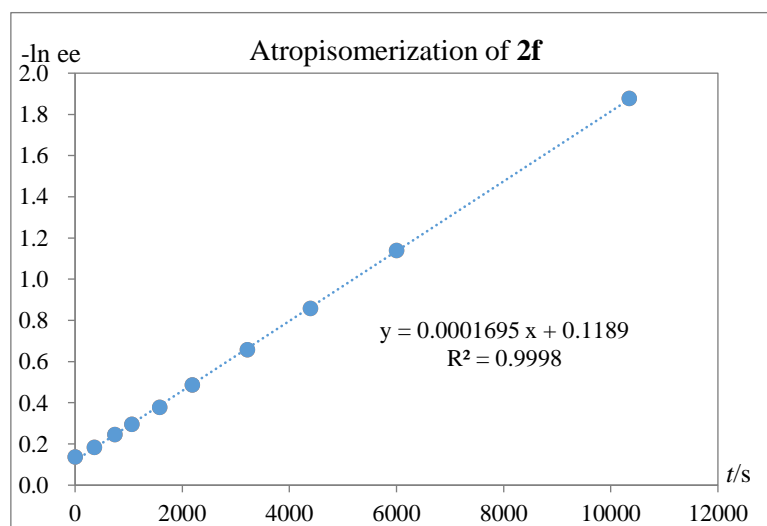


Figure S8. Atropisomerization of 2f in *i*PrOH

$$k_{\text{rac}} = 0.0001695 \text{ s}^{-1}$$

$$\Delta G_{\text{atrp}}^{\ddagger} = 113.9 \text{ kJ/mol}$$

8. Computational Studies of Atropisomerization of 2a, 2c, 2d, 2e, 2f, 5a and 6

8.1. Computational Details

All density functional theory (DFT) calculations were performed using Gaussian 16 program.⁶

Geometry optimizations and solvent effects at *o*-xylene were employed with B3LYP functional,⁷ with the D3 version of Grimme's dispersion corrections⁸ and Becke-Johnson damping.⁹ And 6-31G* basis set was used for all atoms. The solvation energies were calculated with a self-consistent reaction field (SCRF) using the SMD implicit solvent model.¹⁰ Frequency analysis was also performed at the same level of theory as geometry optimization to confirm optimized stationary points were either local minimum or transition state, as well as to evaluate zero-point vibrational energies and thermal corrections for enthalpies and free energies at 298.15 K.

Single-point energies and solvent effects at *o*-xylene were evaluated with B3LYP functional⁷ with D3 version of Grimme's dispersion corrections⁸ with Becke-Johnson damping.⁹ 6-311+G(d,p) basis set was used for all atoms. The solvation energies were calculated with a self-consistent reaction field (SCRF) using the SMD implicit solvent model.¹⁰

To correct the Gibbs free energies under 1 atm to the standard state in solution (1 mol/L), a correction of $RT\ln(c_s/c_g)$ is added to the energies of all species. c_s stands for the standard molar concentration in solution (1 mol/L), c_g stands for the standard molar concentration in gas phase (about 0.040876 mol/L), and R is the gas constant. For calculated intermediates at the standard state of 1 mol/L at 298.15 K, the correction value equaling to 7.9 kJ/mol was used.

The 3D diagrams of optimized structures shown in supplementary information for computations were generated with CYLview software.¹⁰

8.2. Diagrams of Atropisomerization

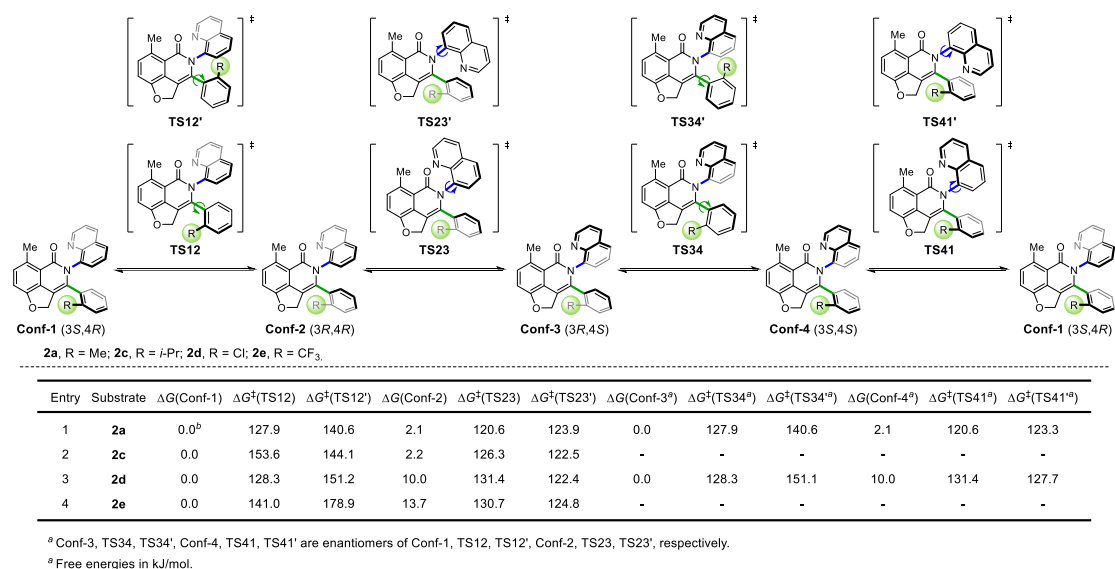


Figure S9. Diagram of single-axis rotation pathways of **2a**, **2c**, **2e**, and **2d**. All energies were calculated at the B3LYP-D3(BJ)/6-311+G(d, p)-SMD(o-xylene)// B3LYP-D3(BJ)/6-31G(d)-SMD(o-xylene) level of theory.

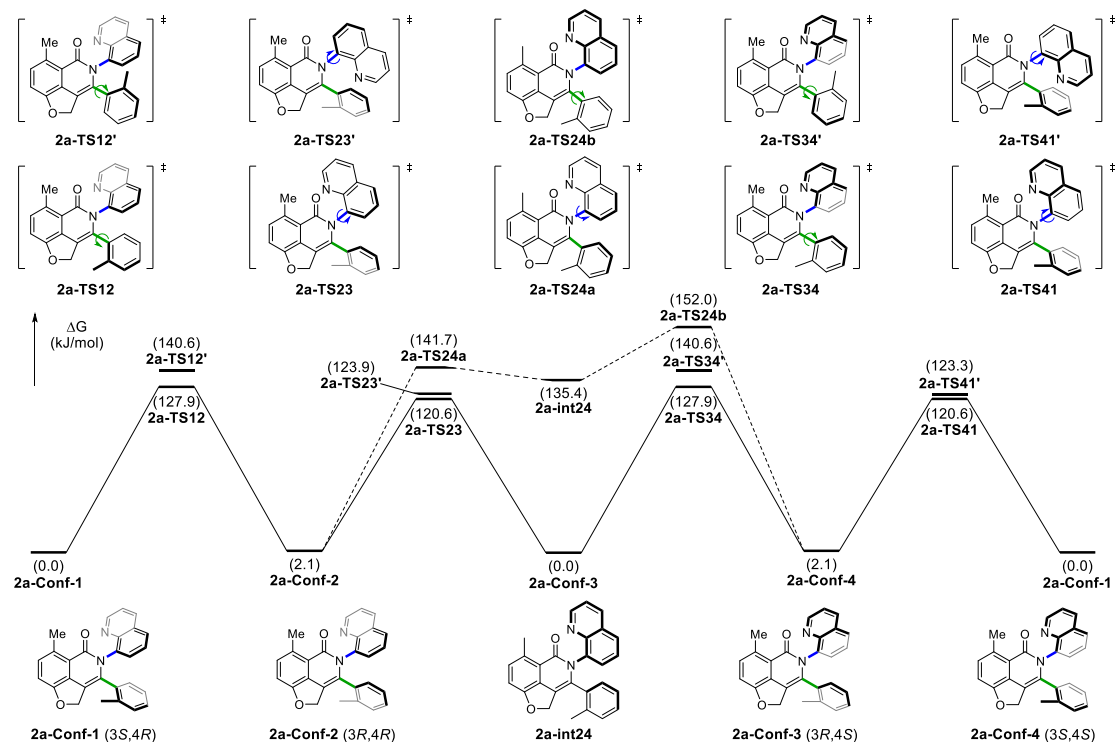


Figure S10. Free energy profile of configuration inversion pathways of **2a**. Solid curve: single-axis rotation pathways. Dashed curve: the stepwise, high-energy but straight inversion pathway between **2a-Conf-2** and **2a-Conf-4**. All energies were calculated at the B3LYP-D3(BJ)/6-311+G(d, p)-SMD(o-xylene)// B3LYP-D3(BJ)/6-31G(d)-SMD(o-xylene) level of theory.

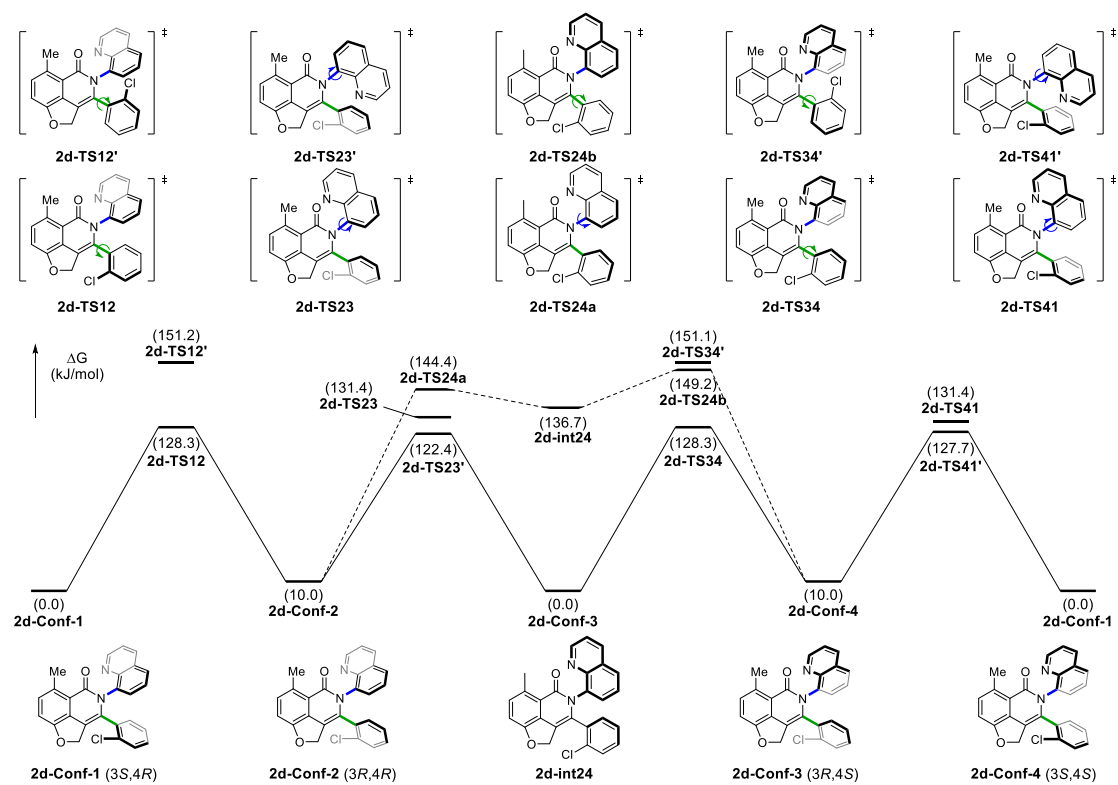


Figure S11. Free energy profile of configuration inversion pathways of **2d**. Solid curve: single-axis rotation pathways. Dashed curve: the stepwise, high-energy but straight inversion pathway between **2d-Conf-2** and **2d-Conf-4**. All energies were calculated at the B3LYP-D3(BJ)/6-311+G(d, p)-SMD(o-xylene)// B3LYP-D3(BJ)/6-31G(d)-SMD(o-xylene) level of theory.

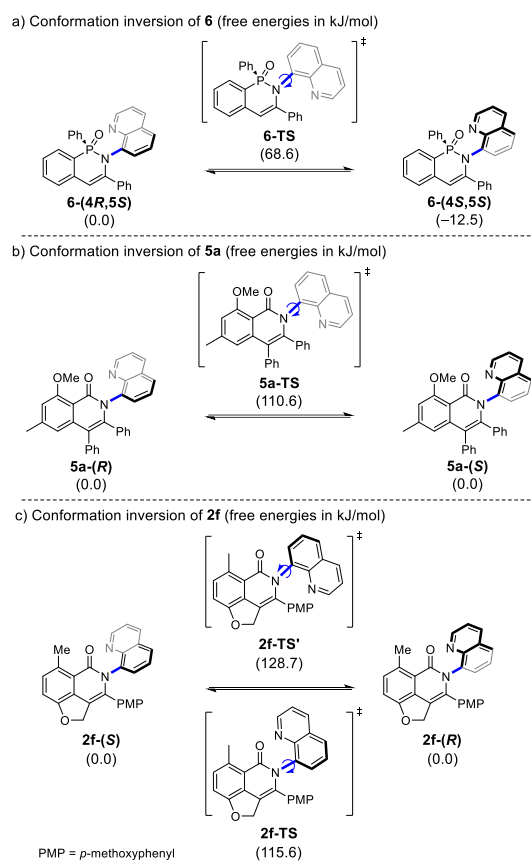


Figure S12. Free energy profile of atropisomerizations of **6**, **5a** and **2f**. a) All energies were calculated at the B3LYP-D3(BJ)/6-311+G(d, p)-SMD(DMSO)// B3LYP-D3(BJ)/6-31G(d)-SMD(DMSO) level of theory. b) All energies were calculated at the B3LYP-D3(BJ)/6-311+G(d, p)-SMD(2-propanol)// B3LYP-D3(BJ)/6-31G(d)-SMD(2-propanol) level of theory. c) All energies were calculated at the B3LYP-D3(BJ)/6-311+G(d, p)-SMD(2-propanol)// B3LYP-D3(BJ)/6-31G(d)-SMD(2-propanol) level of theory.

8.3. Structures of Transition States

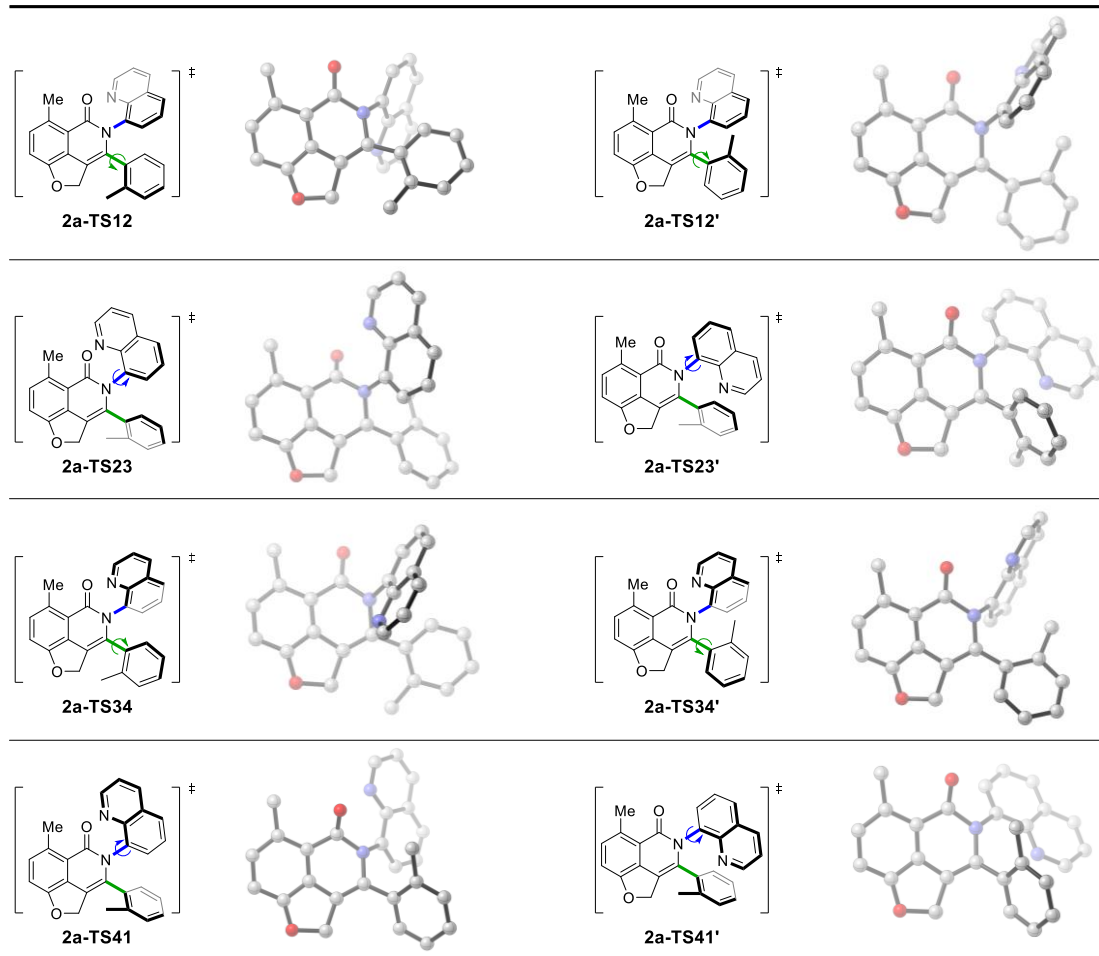


Figure S13. Structures of Transition States of 2a

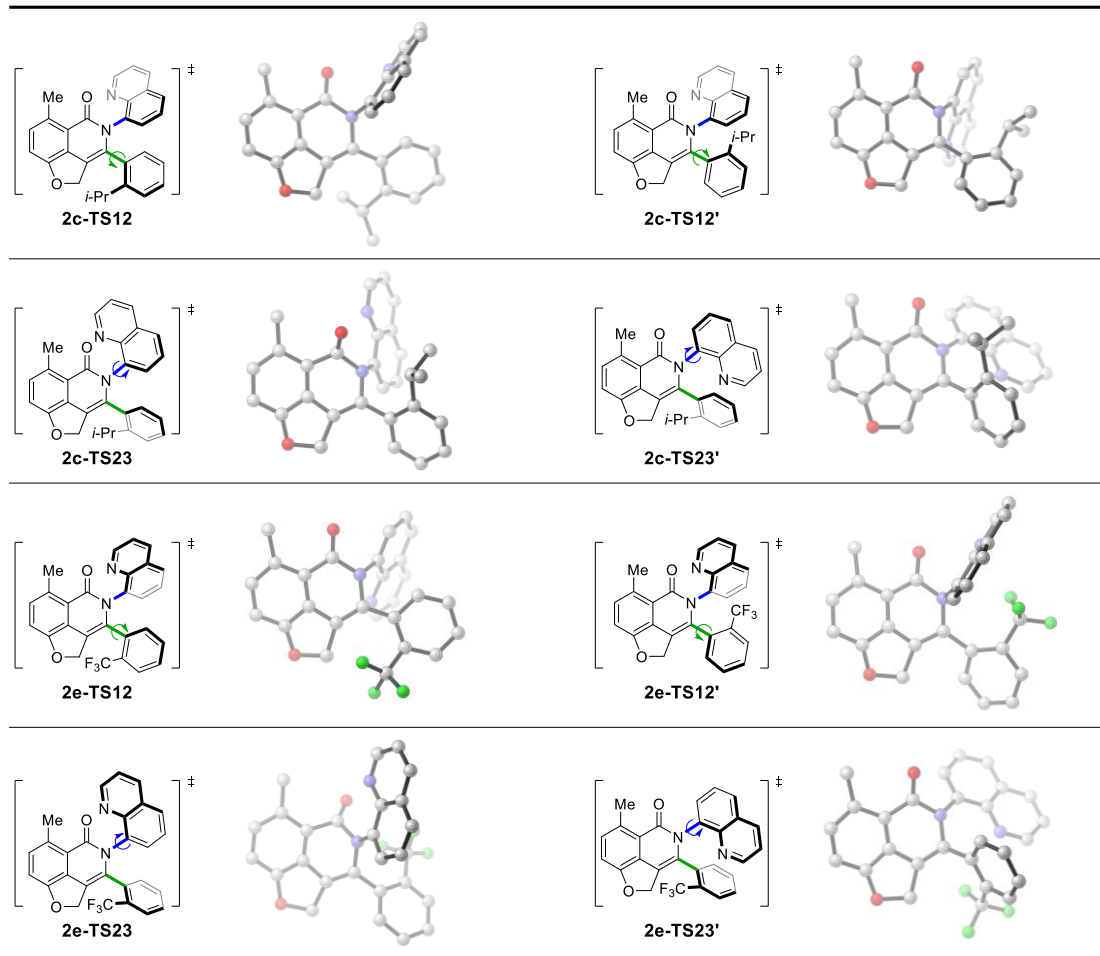


Figure S14. Structures of Transition States of 2c

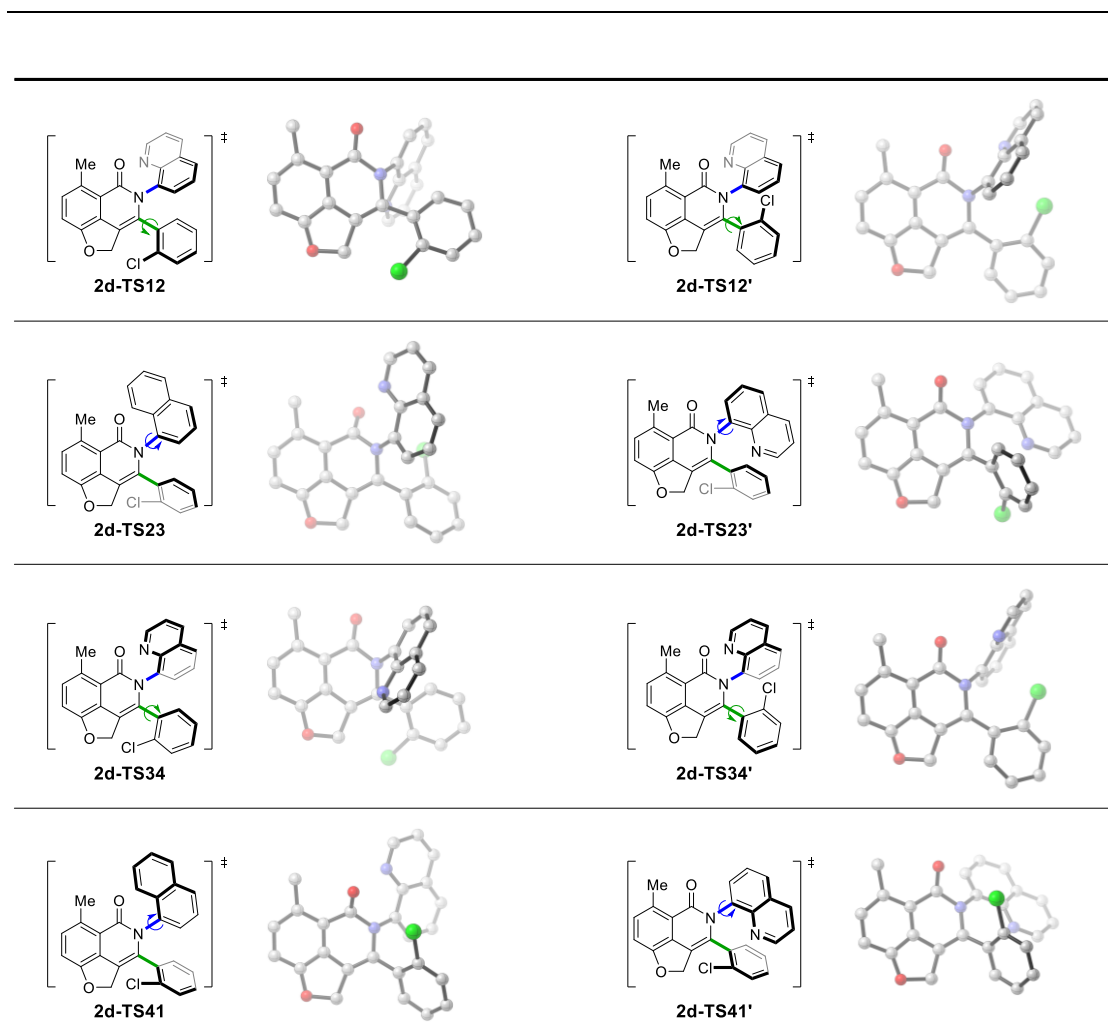


Figure S15. Structures of Transition States of 2d

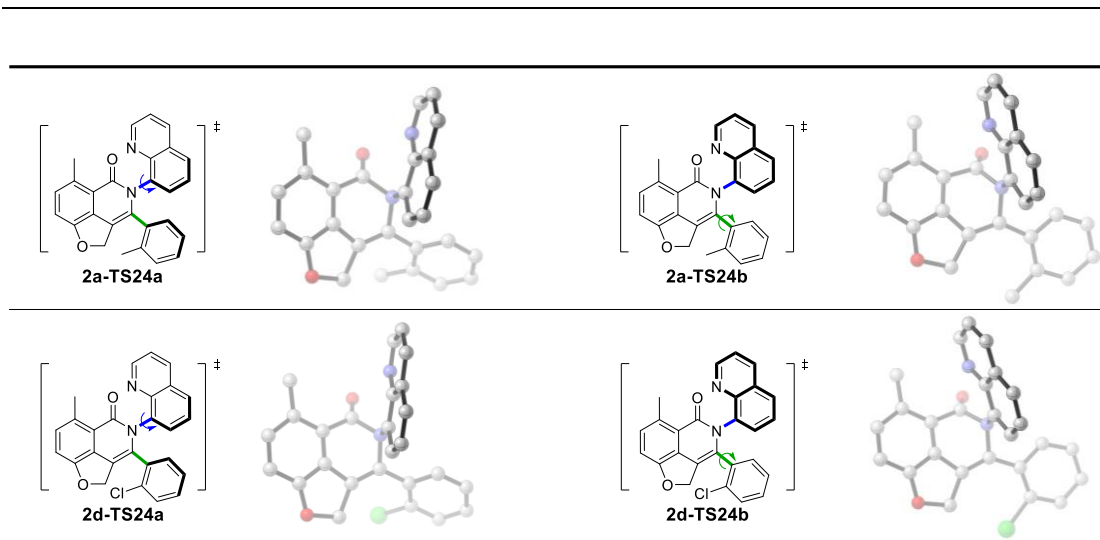


Figure S16. Structures of TS24a and TS24b of 2a and 2d

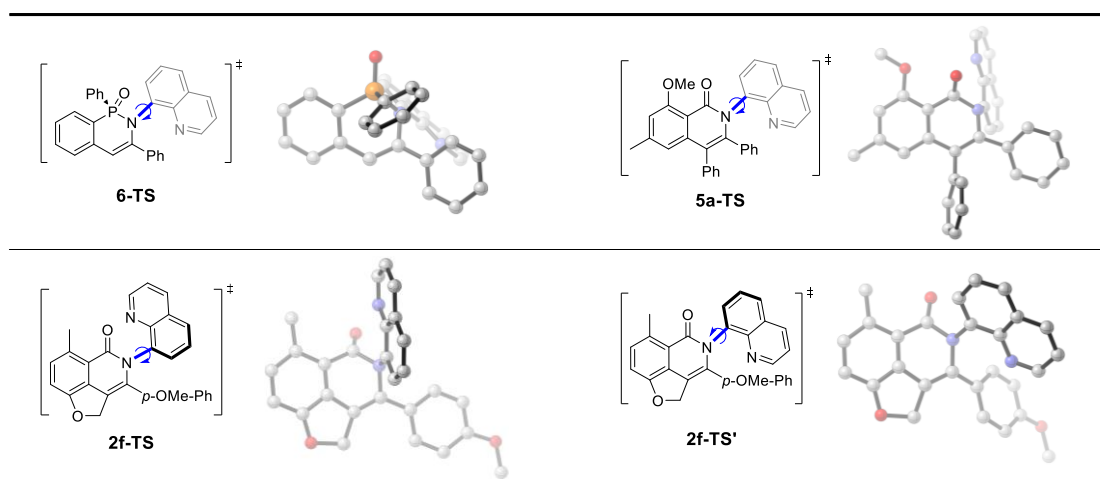


Figure S17. Structures of transition states of 5, 6a and 2f

8.4. Computational Research on Concerted Rotation Pathways

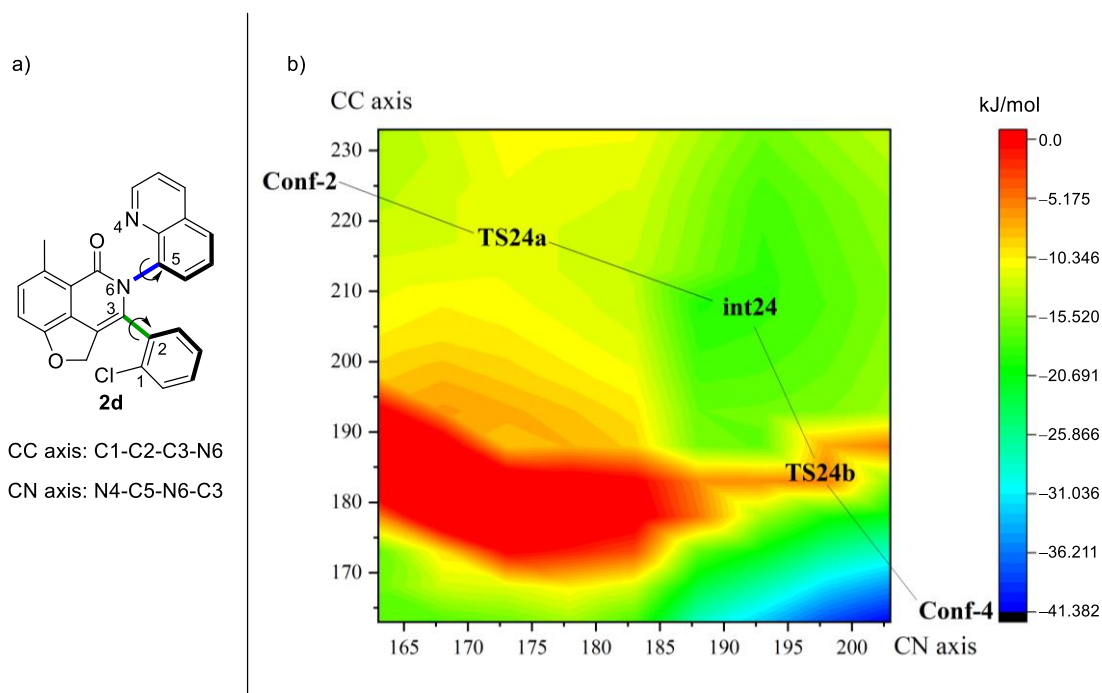


Figure S18. a) Two dihedral angles in **2d**; b) Free energy surface of **2d**. a) Two dihedral angles in **2d** (N4-C5-N6-C3 as the CN axis and C1-C2-C3-N6 as the CC axis) were set as modredundants to investigate the free energy surface of configuration inversion of **2d**. b) Free energy surface of **2d**. The free energy of structure CN_173_CC_173 is set as the zero point of the color bar.

We conducted our investigations on concerted rotation with the disrotatory pathway of **2d**. The free energy surface diagram indicates the inexistence of the concerted rotation pathway. However, we have located a stepwise, high-energy but straight inversion pathway between **2d-Conf-2** and **2d-Conf-4** (TS24a-int24-TS24b).

8.5. Table of Energies

Table S13. Energies in Figure S9, Figure S10 and Figure S11.

Zero-point correction (**ZPE**), thermal correction to enthalpy (**TCH**), thermal correction to Gibbs free energy (**TCG**), energies (**E**), enthalpies (**H**), and Gibbs free energies (**G**) (in Hartree) of the structures calculated at B3LYP-D3(BJ)/6-311+G(d,p)(o-xylene)//B3LYP-D3(BJ)/6-31G(d)(o-xylene) level of theory.

Structure	ZPE	TCH	TCG	E	H	G	Imaginary Frequency
2a-Conf-1	0.404876	0.430112	0.350412	-1301.375883	-1300.945771	-1301.022459	
2a-Conf-2	0.405208	0.430225	0.351384	-1301.376063	-1300.945838	-1301.021667	
2a-Conf-3	0.404656	0.429925	0.350027	-1301.375487	-1300.945562	-1301.022448	
2a-Conf-4	0.405208	0.430225	0.351384	-1301.376063	-1300.945838	-1301.021667	
2a-TS12	0.405575	0.429392	0.354024	-1300.554221	-1300.124829	-1300.197185	62.6i
2a-TS12'	0.405607	0.429281	0.354508	-1300.550709	-1300.121428	-1300.193189	45.3i
2a-TS23	0.403971	0.428399	0.351164	-1300.554997	-1300.126598	-1300.200821	42.4i
2a-TS23'	0.404109	0.428333	0.352493	-1300.555158	-1300.126825	-1300.199653	34.4i
2a-TS34	0.405576	0.429392	0.354026	-1300.554220	-1300.124828	-1300.197182	62.6i
2a-TS34'	0.405609	0.429282	0.354511	-1300.550709	-1300.121427	-1300.193186	45.3i
2a-TS41	0.403972	0.428399	0.351165	-1300.554996	-1300.126597	-1300.200819	42.4i
2a-TS41'	0.404163	0.428365	0.352466	-1300.556089	-1300.127724	-1300.200611	45.3i
2a-TS24a	0.403927	0.428269	0.351669	-1301.323189	-1300.894920	-1300.968508	40.1i
2a-int24	0.404516	0.429370	0.351811	-1301.325725	-1300.896355	-1300.970902	
2a-TS24b	0.404837	0.428864	0.353636	-1301.321258	-1300.892394	-1300.964610	46.9i
2c-Conf-1	0.462105	0.489942	0.404864	-1380.037314	-1379.547372	-1379.629438	
2c-Conf-2	0.462151	0.489914	0.405573	-1380.037172	-1379.547258	-1379.628587	
2c-Conf-3	0.462104	0.489942	0.404861	-1380.037314	-1379.547372	-1379.629441	
2c-Conf-4	0.462151	0.489914	0.405573	-1380.037172	-1379.547258	-1379.628587	
2c-TS12	0.462721	0.489227	0.408360	-1379.982317	-1379.493090	-1379.570945	63.6i
2c-TS12'	0.462219	0.488943	0.407691	-1379.985269	-1379.496326	-1379.574566	35.9i
2c-TS23	0.461009	0.488278	0.404683	-1379.990506	-1379.502228	-1379.582811	40.5i
2c-TS23'	0.461259	0.488325	0.405695	-1379.990057	-1379.501732	-1379.581350	43.0i
2e-Conf-1	0.381857	0.408972	0.324804	-1599.195042	-1598.786070	-1598.867226	
2e-Conf-2	0.381807	0.408775	0.325660	-1599.190676	-1598.781901	-1598.862004	
2e-Conf-3	0.381857	0.408973	0.324806	-1599.195042	-1598.786069	-1598.867224	
2e-Conf-4	0.381807	0.408776	0.325660	-1599.190675	-1598.781899	-1598.862003	
2e-TS12	0.381605	0.407496	0.327419	-1599.143995	-1598.736499	-1598.813564	
2e-TS12'	0.381586	0.407256	0.328520	-1599.130642	-1598.723386	-1598.799110	
2e-TS23	0.380734	0.407051	0.325600	-1599.146062	-1598.739011	-1598.817450	
2e-TS23'	0.380993	0.407124	0.326987	-1599.149702	-1598.742578	-1598.819703	
2d-Conf-1	0.367182	0.392072	0.312132	-1721.670217	-1721.278145	-1721.355073	

2d-Conf-2	0.367408	0.392091	0.313753	-1721.668018	-1721.275927	-1721.351253	
2d-Conf-3	0.367182	0.392072	0.312131	-1721.670217	-1721.278145	-1721.355074	
2d-Conf-4	0.367408	0.392091	0.313749	-1721.668020	-1721.275929	-1721.351259	
2d-TS12	0.367168	0.390867	0.315353	-1721.624595	-1721.233728	-1721.306230	46.8 <i>i</i>
2d-TS12'	0.367180	0.390731	0.315676	-1721.616214	-1721.225483	-1721.297526	42.5 <i>i</i>
2d-TS23	0.366128	0.390231	0.313383	-1721.621449	-1721.231218	-1721.305054	38.3 <i>i</i>
2d-TS23'	0.366532	0.390393	0.314888	-1721.626383	-1721.235990	-1721.308483	32.6 <i>i</i>
2d-TS34	0.367169	0.390868	0.315355	-1721.624595	-1721.233727	-1721.306228	46.9 <i>i</i>
2d-TS34'	0.367180	0.390731	0.315674	-1721.616214	-1721.225483	-1721.297528	42.5 <i>i</i>
2d-TS41	0.366126	0.390230	0.313381	-1721.621449	-1721.231219	-1721.305056	38.3 <i>i</i>
2d-TS41'	0.366470	0.390358	0.314590	-1721.624039	-1721.233681	-1721.306437	42.6 <i>i</i>
2d-TS24a	0.366166	0.390222	0.313753	-1720.858025	-1720.467803	-1720.541260	25.7 <i>i</i>
2d-int24	0.366437	0.391155	0.313052	-1720.859578	-1720.468423	-1720.543514	
2d-TS24b	0.366718	0.390456	0.315404	-1720.858276	-1720.467820	-1720.539860	29.0 <i>i</i>

Table S14. Energies in Figure S12.

Zero-point correction (**ZPE**), thermal correction to enthalpy (**TCH**), thermal correction to Gibbs free energy (**TCG**), energies (**E**), enthalpies (**H**), and Gibbs free energies (**G**) (in Hartree) of the structures calculated at B3LYP-D3(BJ)/6-311+G(d,p)(solvent)//B3LYP-D3(BJ)/6-31G(d)(solvent) level of theory. For substrate **6**, the solvent is DMSO. For substrates **5a** and **2f**, the solvent is 2-propanol.

Structure	ZPE	TCH	TCG	E	H	G	Imaginary Frequency
6-(4R,5S)	0.425263	0.451791	0.367574	-1644.387412	-1643.935621	-1644.016826	
6-(4S,5S)	0.425320	0.451838	0.368166	-1644.392747	-1643.940909	-1644.021569	
6-TS	0.424947	0.450499	0.370595	-1644.364328	-1643.913829	-1643.990721	16.9 <i>i</i>
5a-(R)	0.478966	0.508988	0.416987	-1494.399491	-1493.890503	-1493.979492	
5a-(S)	0.479052	0.509065	0.417333	-1494.399388	-1493.890323	-1493.979043	
5a-TS	0.478152	0.507427	0.418225	-1494.358624	-1493.851197	-1493.937387	42.9 <i>i</i>
2f-(S)	0.409747	0.435826	0.353876	-1376.612068	-1376.176242	-1376.255180	
2f-(R)	0.409745	0.435841	0.353784	-1376.611747	-1376.175906	-1376.254951	
2f-TS	0.408562	0.433979	0.354242	-1376.568411	-1376.134432	-1376.211157	42.2 <i>i</i>
2f-TS'	0.408546	0.433817	0.354777	-1376.563984	-1376.130167	-1376.206195	39.6 <i>i</i>

Table S15 Energies in Figure S18

Zero-point correction (**ZPE**), thermal correction to enthalpy (**TCH**), thermal correction to Gibbs free energy (**TCG**), energies (**E**), enthalpies (**H**), and Gibbs free energies (**G**) (in Hartree) of the structures calculated at B3LYP-D3(BJ)/ 6-311+G(d,p)(o-xylene)// B3LYP-D3(BJ)/6-31G(d) level of theory.

Structure	ZPE	TCH	TCG	E	H	G	Imaginary Frequency
CN_163_CC_233	0.366081	0.390088	0.313633	-1721.618166	-1721.228078	-1721.301521	38.5i
CN_163_CC_223	0.366051	0.390076	0.313564	-1721.617799	-1721.227723	-1721.301223	35.7i
CN_163_CC_213	0.366004	0.390053	0.313343	-1721.617095	-1721.227042	-1721.300740	33.9i
CN_163_CC_208	0.365998	0.390057	0.313159	-1721.616617	-1721.226560	-1721.300446	33.0i
CN_163_CC_203	0.366025	0.390084	0.312900	-1721.616032	-1721.225948	-1721.300120	32.2i
CN_163_CC_198	0.366095	0.390135	0.312703	-1721.615335	-1721.225200	-1721.299620	31.9i
CN_163_CC_193	0.366161	0.389245	0.315821	-1721.614616	-1721.225371	-1721.295783	32.6i
CN_163_CC_188	0.366266	0.389314	0.315987	-1721.613850	-1721.224536	-1721.294851	34.3i
CN_163_CC_183	0.366386	0.389401	0.316146	-1721.613088	-1721.223687	-1721.293930	37.0i
CN_168_CC_208	0.365964	0.390065	0.313093	-1721.616276	-1721.226211	-1721.300171	34.6i
CN_168_CC_203	0.365987	0.390084	0.312974	-1721.615824	-1721.225740	-1721.299838	34.2i
CN_168_CC_198	0.366048	0.390124	0.312966	-1721.615214	-1721.225090	-1721.299236	34.2i
CN_168_CC_193	0.366119	0.390174	0.312833	-1721.614597	-1721.224423	-1721.298752	34.8i
CN_168_CC_188	0.366193	0.389294	0.315772	-1721.613864	-1721.224570	-1721.295080	35.7i
CN_168_CC_183	0.366293	0.389368	0.315900	-1721.613120	-1721.223752	-1721.294208	37.0i
CN_168_CC_178	0.366298	0.389380	0.315756	-1721.612856	-1721.223476	-1721.294088	44.0i
CN_168_CC_173	0.366266	0.390286	0.312152	-1721.615054	-1721.224768	-1721.299890	47.4i
CN_168_CC_168	0.366256	0.390267	0.313285	-1721.617283	-1721.227016	-1721.300986	50.4i
CN_168_CC_163	0.366263	0.390270	0.313533	-1721.619390	-1721.229120	-1721.302845	52.7i
CN_173_CC_233	0.365918	0.390049	0.313052	-1721.616386	-1721.226337	-1721.300322	37.8i
CN_173_CC_223	0.365917	0.390048	0.313120	-1721.616687	-1721.226639	-1721.300555	36.9i
CN_173_CC_213	0.365929	0.390054	0.313114	-1721.616686	-1721.226632	-1721.300560	35.0i
CN_173_CC_208	0.365941	0.390062	0.313089	-1721.616469	-1721.226407	-1721.300368	34.2i
CN_173_CC_203	0.365973	0.390088	0.313033	-1721.616081	-1721.225993	-1721.300036	33.5i
CN_173_CC_198	0.366017	0.390122	0.312951	-1721.615591	-1721.225469	-1721.299628	33.0i
CN_173_CC_193	0.366079	0.390165	0.312924	-1721.614995	-1721.224830	-1721.299059	33.1i
CN_173_CC_188	0.366140	0.390220	0.311915	-1721.614319	-1721.224099	-1721.299392	33.6i
CN_173_CC_183	0.366227	0.389347	0.315679	-1721.613562	-1721.224215	-1721.294871	34.3i
CN_173_CC_178	0.366285	0.389412	0.315639	-1721.612831	-1721.223419	-1721.294180	39.5i
CN_173_CC_173	0.366171	0.389326	0.315415	-1721.614642	-1721.225316	-1721.296215	42.2i
CN_173_CC_168	0.366195	0.390264	0.312855	-1721.616636	-1721.226372	-1721.300769	42.8i
CN_173_CC_163	0.366189	0.390256	0.313188	-1721.618641	-1721.228385	-1721.302441	43.0i
CN_178_CC_208	0.365965	0.390083	0.313163	-1721.616835	-1721.226752	-1721.300660	27.7i

CN_178_CC_203	0.366004	0.390108	0.313167	-1721.616581	-1721.226473	-1721.300402	26.2i
CN_178_CC_198	0.366053	0.390140	0.313139	-1721.616192	-1721.226052	-1721.300041	25.2i
CN_178_CC_193	0.366127	0.390188	0.313162	-1721.615634	-1721.225446	-1721.299460	24.8i
CN_178_CC_188	0.366185	0.390232	0.312820	-1721.614973	-1721.224741	-1721.299141	24.9i
CN_178_CC_183	0.366238	0.389342	0.315785	-1721.614247	-1721.224905	-1721.295450	25.7i
CN_178_CC_178	0.366301	0.389408	0.315787	-1721.613587	-1721.224179	-1721.294788	29.9i
CN_178_CC_173	0.366114	0.389310	0.315203	-1721.614982	-1721.225672	-1721.296767	37.2i
CN_178_CC_168	0.366219	0.390232	0.313518	-1721.616641	-1721.226409	-1721.300111	32.6i
CN_178_CC_163	0.366238	0.390235	0.313900	-1721.618593	-1721.228358	-1721.301681	29.8i
CN_183_CC_233	0.365936	0.390056	0.313136	-1721.616558	-1721.226502	-1721.300410	24.8i
CN_183_CC_223	0.365979	0.390071	0.313387	-1721.617284	-1721.227213	-1721.300885	21.0i
CN_183_CC_213	0.365987	0.390081	0.313326	-1721.617538	-1721.227457	-1721.301200	18.7i
CN_183_CC_208	0.366018	0.390100	0.313356	-1721.617450	-1721.227350	-1721.301082	16.7i
CN_183_CC_203	0.366073	0.390131	0.313457	-1721.617228	-1721.227097	-1721.300759	13.8i
CN_183_CC_198	0.366124	0.390162	0.313467	-1721.616896	-1721.226734	-1721.300417	11.3i
CN_183_CC_193	0.366181	0.390200	0.313399	-1721.616403	-1721.226203	-1721.299992	10.2i
CN_183_CC_188	0.366246	0.390246	0.313187	-1721.615787	-1721.225541	-1721.299588	9.9i
CN_183_CC_183	0.366288	0.389349	0.316029	-1721.615086	-1721.225737	-1721.296045	15.2i
CN_183_CC_178	0.366327	0.389402	0.315943	-1721.614501	-1721.225099	-1721.295546	29.2i
CN_183_CC_173	0.366094	0.389293	0.315155	-1721.615750	-1721.226457	-1721.297583	26.6i
CN_183_CC_168	0.366265	0.390218	0.314115	-1721.618018	-1721.227800	-1721.300891	10.5i
CN_183_CC_163	0.366282	0.390239	0.314192	-1721.620113	-1721.229874	-1721.302909	7.6i
CN_188_CC_208	0.366186	0.391076	0.311672	-1721.618191	-1721.227115	-1721.303507	
CN_188_CC_203	0.366231	0.391101	0.311787	-1721.618020	-1721.226919	-1721.303221	
CN_188_CC_198	0.366277	0.391127	0.311818	-1721.617706	-1721.226579	-1721.302876	
CN_188_CC_193	0.366339	0.391164	0.311783	-1721.617258	-1721.226094	-1721.302463	
CN_188_CC_188	0.366406	0.391210	0.311431	-1721.616677	-1721.225467	-1721.302234	
CN_188_CC_183	0.366466	0.390322	0.314531	-1721.616037	-1721.225715	-1721.298494	15.3i
CN_188_CC_178	0.366494	0.390372	0.314356	-1721.615499	-1721.225127	-1721.298131	30.1i
CN_188_CC_173	0.366360	0.391180	0.311844	-1721.617390	-1721.226210	-1721.302534	
CN_188_CC_168	0.366383	0.391202	0.312011	-1721.619844	-1721.228642	-1721.304821	
CN_188_CC_163	0.366379	0.391214	0.312018	-1721.621985	-1721.230771	-1721.306955	
CN_193_CC_233	0.366231	0.391059	0.312064	-1721.617451	-1721.226392	-1721.302375	
CN_193_CC_223	0.366262	0.391067	0.312370	-1721.618396	-1721.227329	-1721.303014	
CN_193_CC_213	0.366304	0.391087	0.312567	-1721.618825	-1721.227738	-1721.303246	
CN_193_CC_208	0.366328	0.391102	0.312593	-1721.618829	-1721.227727	-1721.303224	
CN_193_CC_203	0.366358	0.391121	0.312619	-1721.618663	-1721.227542	-1721.303032	
CN_193_CC_198	0.366394	0.391145	0.312560	-1721.618339	-1721.227194	-1721.302767	
CN_193_CC_193	0.366451	0.391182	0.312480	-1721.617887	-1721.226705	-1721.302395	
CN_193_CC_188	0.366506	0.391227	0.311793	-1721.617331	-1721.226104	-1721.302526	
CN_193_CC_183	0.366575	0.390343	0.315192	-1721.616718	-1721.226375	-1721.298514	16.7i

CN_193_CC_178	0.366393	0.391197	0.311757	-1721.616361	-1721.225164	-1721.301592	
CN_193_CC_173	0.366419	0.391214	0.312065	-1721.619173	-1721.227959	-1721.304096	
CN_193_CC_168	0.366431	0.391233	0.312155	-1721.621682	-1721.230449	-1721.306515	
CN_193_CC_163	0.366427	0.391249	0.312109	-1721.623858	-1721.232609	-1721.308737	
CN_193_CC_163	0.366427	0.391249	0.312109	-1721.623858	-1721.232609	-1721.308737	
CN_198_CC_208	0.366451	0.391126	0.313189	-1721.618986	-1721.227860	-1721.302785	
CN_198_CC_203	0.366471	0.391144	0.313152	-1721.618817	-1721.227673	-1721.302653	
CN_198_CC_198	0.366503	0.391172	0.313053	-1721.618500	-1721.227328	-1721.302435	
CN_198_CC_193	0.366547	0.391207	0.312867	-1721.618038	-1721.226831	-1721.302159	
CN_198_CC_188	0.366585	0.390305	0.315494	-1721.617501	-1721.227196	-1721.298995	5.3i
CN_198_CC_183	0.366660	0.390362	0.315566	-1721.616913	-1721.226551	-1721.298335	19.4i
CN_198_CC_178	0.366441	0.391236	0.311427	-1721.618021	-1721.226785	-1721.303582	
CN_198_CC_173	0.366472	0.391255	0.311897	-1721.620928	-1721.229673	-1721.306019	
CN_198_CC_168	0.366485	0.391273	0.312040	-1721.623506	-1721.232233	-1721.308454	
CN_198_CC_163	0.366479	0.391288	0.312003	-1721.625714	-1721.234426	-1721.310699	
CN_203_CC_233	0.366406	0.391084	0.312892	-1721.617065	-1721.225981	-1721.301161	
CN_203_CC_223	0.366462	0.391102	0.313289	-1721.618097	-1721.226995	-1721.301796	
CN_203_CC_213	0.366500	0.391119	0.313472	-1721.618569	-1721.227450	-1721.302085	
CN_203_CC_208	0.366504	0.391128	0.313429	-1721.618530	-1721.227402	-1721.302089	
CN_203_CC_203	0.366518	0.391148	0.313363	-1721.618347	-1721.227199	-1721.301972	
CN_203_CC_198	0.366529	0.391168	0.313169	-1721.617987	-1721.226819	-1721.301806	
CN_203_CC_193	0.366576	0.391210	0.312851	-1721.617521	-1721.226311	-1721.301658	
CN_203_CC_188	0.366640	0.390322	0.315683	-1721.617012	-1721.226690	-1721.298317	11.0i
CN_203_CC_183	0.366485	0.391230	0.311610	-1721.616509	-1721.225279	-1721.301887	
CN_203_CC_178	0.366554	0.391263	0.312388	-1721.619659	-1721.228396	-1721.304259	
CN_203_CC_173	0.366580	0.391286	0.312540	-1721.622604	-1721.231318	-1721.307052	
CN_203_CC_168	0.366586	0.391304	0.312562	-1721.625200	-1721.233896	-1721.309626	
CN_203_CC_163	0.366585	0.391326	0.312495	-1721.627444	-1721.236118	-1721.311937	

8.6. Cartesian Coordinates of Computed Species

2a-Conf-1

Charge = 0, Multiplicity = 1

O	3.76140200	2.10926800	-1.03705800
O	0.79210100	-2.49776700	1.04780800
N	0.16504400	-0.37041900	0.46601200
N	-1.43183800	-1.65762100	-1.41032400
C	3.60317600	-3.28179300	0.79201900
H	3.22750500	-3.34536000	1.81850300
H	4.59767000	-3.73885800	0.75605700
H	2.92061800	-3.88221000	0.18192900
C	3.90333100	0.81406900	-0.62043300
C	5.03708600	0.02932800	-0.56866800
H	6.01014300	0.39800600	-0.87557100
C	4.87877200	-1.29741200	-0.09653400
H	5.76519400	-1.92468900	-0.05233700
C	3.66317100	-1.85469800	0.31154300
C	2.50907100	-1.02345400	0.24924700
C	2.68076900	0.27683700	-0.21018800
C	1.66532800	1.25284200	-0.35987000
C	2.34805400	2.48495900	-0.90859400
H	1.98934900	2.78412800	-1.89941800
H	2.29802900	3.35454400	-0.24342300
C	0.39251800	0.92614500	-0.03372800
C	1.13892200	-1.40004900	0.61798400
C	-0.76035600	1.85401500	-0.18286300
C	-0.97966700	2.87540500	0.76304100
C	-2.06155200	3.74141700	0.56545200
H	-2.24371700	4.52977100	1.29144900
C	-2.90604100	3.60803200	-0.53695100
H	-3.73956000	4.29327700	-0.66455400
C	-2.67879200	2.59651600	-1.47045300
H	-3.33037400	2.48576900	-2.33240200
C	-1.60632900	1.72486300	-1.29151400
H	-1.41895900	0.92674500	-2.00225500
C	-0.07820100	3.03487900	1.96186600
H	0.06735200	2.08474200	2.48744000
H	-0.49641400	3.75527500	2.67148900
H	0.91850200	3.39211000	1.67442600
C	-1.17882400	-0.75400100	0.79898300
C	-1.69170100	-0.47765100	2.04364200
H	-1.06405800	0.02054300	2.77517400
C	-3.01885900	-0.84033200	2.37279100

H	-3.40399500	-0.60754200	3.36072000
C	-3.81052200	-1.48705500	1.45227300
H	-4.82952800	-1.77288300	1.69878000
C	-3.30586200	-1.79139300	0.16147000
C	-1.96854100	-1.41950100	-0.18154900
C	-2.18199700	-2.27648600	-2.30118300
H	-1.72653000	-2.45551100	-3.27408200
C	-3.51190300	-2.70157600	-2.06228200
H	-4.06696600	-3.20690900	-2.84611100
C	-4.07160400	-2.45290500	-0.83166000
H	-5.09140600	-2.75267700	-0.60469600

2a-Conf-2

Charge = 0, Multiplicity = 1

O	-3.58402300	2.54029000	0.26810700
O	-1.12427300	-2.72951600	-0.45200600
N	-0.27348300	-0.59489300	-0.50258500
N	1.49941600	-0.74890300	1.64298500
C	-3.98963700	-3.12868900	-0.06258300
H	-3.62394100	-3.49232800	-1.02840100
H	-5.02738300	-3.45515200	0.06232700
H	-3.37517000	-3.62010100	0.69861400
C	-3.85475400	1.20111700	0.23197900
C	-5.06399500	0.54904600	0.36199300
H	-5.99334700	1.08303700	0.52961600
C	-5.04565100	-0.86388500	0.26241500
H	-5.99207700	-1.38824300	0.36480300
C	-3.89659900	-1.62778300	0.03567700
C	-2.66345600	-0.92935200	-0.09858900
C	-2.69327800	0.45464500	0.01839400
C	-1.58447100	1.32903400	-0.09417400
C	-2.14083400	2.72535000	0.07577400
H	-1.76192300	3.24899900	0.95917200
H	-1.99785600	3.36783900	-0.79983200
C	-0.36100900	0.80782000	-0.35868500
C	-1.34730300	-1.52501700	-0.35490900
C	0.85659500	1.62898800	-0.57923500
C	1.41931200	2.40710500	0.45377800
C	2.55967100	3.16995400	0.16147300
H	3.00710000	3.76266800	0.95570100
C	3.13175100	3.17679100	-1.10756700
H	4.01770400	3.77562800	-1.30003300
C	2.56478400	2.41010600	-2.12802000

H	2.99740500	2.40978600	-3.12423800
C	1.43664000	1.64359500	-1.85879500
H	0.98693900	1.04688800	-2.64559400
C	0.84811800	2.44467600	1.84948700
H	0.18890100	3.31252000	1.98568300
H	1.65132000	2.53989500	2.58787200
H	0.27988700	1.54207800	2.07801200
C	1.02334400	-1.19005200	-0.66915700
C	1.39490700	-1.71407800	-1.88563600
H	0.69272100	-1.67749500	-2.71178200
C	2.67365800	-2.28792600	-2.06456100
H	2.94444200	-2.69013400	-3.03589100
C	3.56878400	-2.33060500	-1.01988700
H	4.55706300	-2.76306300	-1.15080700
C	3.20873700	-1.81469300	0.25072300
C	1.91034600	-1.24451900	0.44328500
C	2.34235000	-0.80011800	2.65516000
H	1.98373800	-0.39797400	3.60152700
C	3.65179500	-1.33316900	2.57230900
H	4.29087700	-1.33725900	3.44950200
C	4.08059100	-1.83936800	1.36861000
H	5.07605400	-2.26106500	1.25658900

2a-Conf-3

Charge = 0, Multiplicity = 1

O	-3.51217700	2.50661900	-0.81505900
O	-1.15615800	-2.62721700	0.75168600
N	-0.26065500	-0.52789800	0.45383200
N	1.45756600	-0.85144400	-1.71913600
C	-4.01389600	-3.04207500	0.37555900
H	-3.38910900	-3.64623100	-0.28942800
H	-5.05300300	-3.37414300	0.28280400
H	-3.66428400	-3.25620900	1.39033600
C	-3.80936200	1.19070000	-0.57534600
C	-5.02684000	0.54304900	-0.62501800
H	-5.94361500	1.05830800	-0.89030100
C	-5.03289400	-0.83793500	-0.30904300
H	-5.98582300	-1.35915800	-0.34644000
C	-3.90039200	-1.57419700	0.05207200
C	-2.65926500	-0.88065300	0.09883500
C	-2.66627800	0.46896000	-0.22758200
C	-1.54503200	1.33452600	-0.22675700
C	-2.07514800	2.70043500	-0.60741900

H	-1.94786800	3.45732100	0.17478200
H	-1.65502300	3.09184500	-1.53983500
C	-0.33456200	0.83973800	0.12111700
C	-1.35633900	-1.45329500	0.45862400
C	0.88307700	1.68785200	0.20954300
C	1.41335300	2.08877000	1.45189200
C	2.53465000	2.92780900	1.45552100
H	2.94871200	3.24446700	2.40980000
C	3.11498100	3.37370000	0.26985800
H	3.98410700	4.02477300	0.30418800
C	2.56767800	2.99465800	-0.95663300
H	3.00544600	3.34484000	-1.88693300
C	1.45449400	2.15928200	-0.98077300
H	1.02621400	1.83493900	-1.92235700
C	0.80115600	1.65255300	2.75965800
H	-0.26361000	1.42659200	2.65254500
H	0.91288100	2.43255700	3.51965100
H	1.29142000	0.74927100	3.14064200
C	1.03462300	-1.11492900	0.63236300
C	1.41935700	-1.59139700	1.86491900
H	0.72299000	-1.52575100	2.69272400
C	2.69545600	-2.16838000	2.05200300
H	2.97649500	-2.52850200	3.03682700
C	3.57280800	-2.27233600	0.99716100
H	4.55867500	-2.70877300	1.13405200
C	3.19224000	-1.82735000	-0.29371500
C	1.89599400	-1.25528100	-0.49513800
C	2.27322900	-0.98886900	-2.74422300
H	1.89032100	-0.66291800	-3.71065400
C	3.58298600	-1.52106200	-2.65407800
H	4.20065000	-1.59570300	-3.54339000
C	4.03735000	-1.93876000	-1.42640800
H	5.03218200	-2.36042000	-1.30686200

2a-Conf-4

Charge = 0, Multiplicity = 1

O	3.58402100	2.54029100	0.26810700
O	1.12427500	-2.72951700	-0.45199900
N	0.27348300	-0.59489600	-0.50258200
N	-1.49942000	-0.74889600	1.64298600
C	3.98963900	-3.12868800	-0.06258300
H	3.37518400	-3.62010000	0.69862500
H	5.02738700	-3.45514900	0.06231300

H	3.62392900	-3.49232900	-1.02839400
C	3.85475300	1.20111800	0.23198000
C	5.06399500	0.54904900	0.36199100
H	5.99334800	1.08304000	0.52961100
C	5.04565200	-0.86388300	0.26241300
H	5.99207900	-1.38824000	0.36479900
C	3.89660000	-1.62778200	0.03567800
C	2.66345700	-0.92935200	-0.09858500
C	2.69327700	0.45464500	0.01839900
C	1.58447000	1.32903300	-0.09417100
C	2.14083100	2.72535000	0.07577400
H	1.99785200	3.36783700	-0.79983200
H	1.76192100	3.24900000	0.95917200
C	0.36100900	0.80781900	-0.35868300
C	1.34730300	-1.52501800	-0.35490400
C	-0.85659500	1.62898600	-0.57923800
C	-1.41931300	2.40710800	0.45377100
C	-2.55967100	3.16995600	0.16146100
H	-3.00710000	3.76267400	0.95568700
C	-3.13174900	3.17678700	-1.10757900
H	-4.01770200	3.77562300	-1.30004900
C	-2.56478200	2.41009800	-2.12802800
H	-2.99740200	2.40977300	-3.12424600
C	-1.43663800	1.64358700	-1.85879900
H	-0.98693700	1.04687600	-2.64559400
C	-0.84812000	2.44468500	1.84948000
H	-0.27988900	1.54208800	2.07801000
H	-1.65132200	2.53990800	2.58786500
H	-0.18890300	3.31253000	1.98567300
C	-1.02334300	-1.19005600	-0.66915300
C	-1.39490400	-1.71408900	-1.88563000
H	-0.69271500	-1.67751000	-2.71177400
C	-2.67365300	-2.28793900	-2.06455400
H	-2.94443500	-2.69015200	-3.03588200
C	-3.56878100	-2.33061200	-1.01988200
H	-4.55706000	-2.76307100	-1.15080100
C	-3.20873700	-1.81469300	0.25072600
C	-1.91034700	-1.24451700	0.44328800
C	-2.34235500	-0.80010500	2.65516000
H	-1.98374500	-0.39795700	3.60152500
C	-3.65180000	-1.33315700	2.57230900
H	-4.29088300	-1.33724300	3.44950000
C	-4.08059300	-1.83936200	1.36861100
H	-5.07605600	-2.26106000	1.25659100

2a-int24

Charge = 0, Multiplicity = 1

O	-0.97035200	3.17286300	1.94579900
O	0.48195600	0.53977900	-2.67171200
N	-0.22324600	-0.49499500	-0.67053400
N	2.43290300	-1.11561900	-1.11767500
C	3.27249200	2.13142200	-1.68542700
H	3.99992500	1.40693200	-1.29928700
H	3.81472100	3.04899800	-1.93536000
H	2.84712100	1.71290300	-2.60082400
C	0.16861900	3.00812300	1.20964400
C	1.30432400	3.81116100	1.17500800
H	1.41290100	4.67497100	1.82162900
C	2.29403500	3.47676900	0.23593000
H	3.18353200	4.09987400	0.18746000
C	2.18996100	2.40308400	-0.67270200
C	1.05412600	1.58832100	-0.57725600
C	0.08493900	1.90552100	0.37362900
C	-1.21861800	1.29432300	0.49909900
C	-1.95349400	2.19562600	1.47668500
H	-2.77747700	2.76652200	1.04209200
H	-2.32713000	1.64781000	2.34733100
C	-1.45524000	0.11909300	-0.14681400
C	0.55079400	0.49471300	-1.47240700
C	-2.69899800	-0.64308700	-0.32123200
C	-3.96730100	-0.03535500	-0.50167400
C	-5.09774000	-0.85776700	-0.61213400
H	-6.06697700	-0.38601800	-0.75543800
C	-5.00856300	-2.24479700	-0.58389700
H	-5.90523300	-2.85109900	-0.67540600
C	-3.75165600	-2.84503900	-0.48270500
H	-3.65365800	-3.92656500	-0.50091300
C	-2.61879800	-2.05260400	-0.36936500
H	-1.64585300	-2.52275000	-0.31279700
C	0.51734000	-1.20577700	0.30646400
C	-0.02876500	-1.61294900	1.51696300
H	-1.03902000	-1.32465800	1.77566100
C	0.70114200	-2.41208000	2.42358900
H	0.22014400	-2.71158800	3.35042700
C	1.99164200	-2.80751300	2.15836000
H	2.54985600	-3.42343900	2.85740100
C	2.60455100	-2.38742400	0.95283300

C	1.87518800	-1.57734200	0.02682800
C	3.67605100	-1.43900600	-1.40871400
H	4.07442800	-1.04227600	-2.34067100
C	4.47712600	-2.25342100	-0.57477300
H	5.49491100	-2.49344400	-0.86555800
C	3.93862200	-2.71695300	0.60335900
H	4.52314500	-3.33406400	1.28108000
C	-4.16459200	1.44880400	-0.68709500
H	-4.43993300	1.95482700	0.24732200
H	-3.26635200	1.93096700	-1.08113900
H	-4.98260000	1.63017700	-1.39141400

2a-TS12'

Charge = 0, Multiplicity = 1

O	4.26959000	0.86065400	0.90057300
O	-0.13770200	-2.41550000	-1.02464100
N	-0.05495700	-0.19166300	-0.36164800
N	-2.57873200	-1.10284300	-1.34261000
C	2.20184000	-4.08777700	-0.97498200
H	1.36968700	-4.42822700	-0.35028500
H	2.97883000	-4.85922000	-0.97198600
H	1.80255400	-3.99807800	-1.99024300
C	3.92431800	-0.39155400	0.49039400
C	4.69327200	-1.54018700	0.47461800
H	5.72116300	-1.54681900	0.82103700
C	4.08443300	-2.71263400	-0.02186200
H	4.67949700	-3.62144300	-0.04867200
C	2.76228900	-2.77994800	-0.48019900
C	1.99794900	-1.58358100	-0.43645900
C	2.60402200	-0.43190800	0.04109100
C	2.02185900	0.86795500	0.10276500
C	3.19338700	1.76455900	0.49710400
H	3.61118700	2.35219500	-0.32725900
H	2.97334500	2.43704200	1.33107300
C	0.68466400	1.03310000	-0.16733300
C	0.56133200	-1.46885300	-0.70152000
C	0.09011400	2.40601000	-0.33956800
C	-1.26322600	2.85988300	-0.27098200
C	-1.51069900	4.24356800	-0.31497500
H	-2.54410100	4.56814100	-0.23035200
C	-0.52125200	5.20230700	-0.48935200
H	-0.77366200	6.25837700	-0.51401000
C	0.78175200	4.76292000	-0.69236800

H	1.58381800	5.45973600	-0.91797800
C	1.05389700	3.40397100	-0.62886100
H	2.05664200	3.10345400	-0.87676900
C	-2.50853300	2.01187900	-0.24321000
H	-3.37509600	2.64090000	-0.46848900
H	-2.69176600	1.54590000	0.72753000
H	-2.47059100	1.22936800	-1.00100000
C	-1.17792700	-0.44910900	0.50860300
C	-1.02775700	-0.22719700	1.86269400
H	-0.09900600	0.19932400	2.22690000
C	-2.05596200	-0.55692700	2.77334000
H	-1.90942900	-0.36477900	3.83196900
C	-3.21532000	-1.14776500	2.32508700
H	-4.00266400	-1.42924200	3.01920200
C	-3.40178600	-1.38999300	0.94021300
C	-2.38797800	-1.01567200	0.00337700
C	-3.70489900	-1.62428400	-1.77922200
H	-3.82965300	-1.66703400	-2.86046400
C	-4.73941600	-2.10455300	-0.93618300
H	-5.63409600	-2.54036400	-1.36943700
C	-4.58996900	-1.96945800	0.42136000
H	-5.36839200	-2.28742700	1.11014500

2a-TS12

Charge = 0, Multiplicity = 1

O	-2.83772400	2.29919700	1.60295900
O	-1.41154200	-2.03138700	-2.02941700
N	-0.14340400	-0.41671700	-0.95144000
N	0.92706400	-0.55106900	1.66784600
C	-4.20254700	-2.32970200	-1.37863800
H	-4.04360700	-2.18449000	-2.45199500
H	-5.25062100	-2.60050200	-1.21418900
H	-3.57498800	-3.17936700	-1.09045000
C	-3.30562800	1.20222400	0.95593500
C	-4.56794000	0.64241500	1.02924300
H	-5.34076700	1.06106500	1.66501100
C	-4.81202400	-0.49959400	0.23969300
H	-5.80024300	-0.94939500	0.28346600
C	-3.85432200	-1.09302200	-0.59142400
C	-2.56568800	-0.49844800	-0.62797300
C	-2.32827400	0.63917600	0.13441800
C	-1.13703900	1.43170700	0.15508400
C	-1.49347000	2.57661200	1.10365500

H	-0.82089000	2.60652600	1.96639400
H	-1.55793400	3.56666800	0.66119800
C	-0.01775200	0.95308900	-0.48343300
C	-1.39308700	-1.04148100	-1.30837300
C	1.28669500	1.62251700	-0.78967000
C	1.62078800	2.98845800	-0.53300000
C	2.94004200	3.42217100	-0.73451300
H	3.16908700	4.45933700	-0.50366500
C	3.93696000	2.61108000	-1.26195900
H	4.94499200	2.99123000	-1.39990900
C	3.57945600	1.33287100	-1.67597400
H	4.29288800	0.68521300	-2.17737300
C	2.28810000	0.87411600	-1.45500000
H	2.06016000	-0.10638000	-1.82768300
C	0.64989700	4.09161100	-0.19455300
H	-0.27271800	3.99677600	-0.77150600
H	1.09446700	5.05479100	-0.46091500
H	0.40366500	4.14817500	0.86900200
C	0.85543300	-1.39366000	-0.59823400
C	1.27375600	-2.33513100	-1.52207000
H	0.88154800	-2.29084400	-2.52765400
C	2.21350000	-3.33117200	-1.17901000
H	2.51535600	-4.04959900	-1.93520400
C	2.75604400	-3.38047000	0.08336500
H	3.49197100	-4.13419300	0.34970600
C	2.34991500	-2.43864900	1.06047200
C	1.37219100	-1.44037400	0.73897600
C	1.42626500	-0.60294600	2.88525900
H	1.03701800	0.12348800	3.59767800
C	2.41105000	-1.53171600	3.29850300
H	2.78411200	-1.51241900	4.31748100
C	2.86467500	-2.44895000	2.38214700
H	3.61302600	-3.19044400	2.64988200

2a-TS23'

Charge = 0, Multiplicity = 1

O	-3.16647400	-2.38504500	-1.47718400
O	-1.46450700	2.04640500	1.80113000
N	-0.21471800	0.66230500	0.41230700
N	2.57743300	0.07325400	-0.29594400
C	-4.28531100	2.50835800	1.16153100
H	-4.02536000	2.38660500	2.21797200
H	-5.34728100	2.76358900	1.08965400

H	-3.70226300	3.36224100	0.79928700
C	-3.57891800	-1.16754900	-1.02457400
C	-4.86903600	-0.67369800	-0.92039000
H	-5.72481200	-1.21898200	-1.30398900
C	-5.03470000	0.55265500	-0.24323900
H	-6.04145600	0.95162700	-0.15403100
C	-3.99184100	1.25713400	0.37583400
C	-2.68092900	0.73460600	0.23124800
C	-2.51386700	-0.41604600	-0.53128500
C	-1.31509700	-1.18576700	-0.59707100
C	-1.74323600	-2.52875000	-1.15287900
H	-1.23251700	-2.79131200	-2.08153300
H	-1.63574400	-3.35774400	-0.44336800
C	-0.17784000	-0.71896300	-0.01997500
C	-1.46792300	1.21392400	0.90805800
C	0.82209500	-1.66039600	0.54434500
C	1.45529200	-2.67066000	-0.20794900
C	2.24399700	-3.60959500	0.46833900
H	2.74717800	-4.38038000	-0.11191500
C	2.41991300	-3.56363400	1.85052000
H	3.04010500	-4.30550100	2.34584600
C	1.80497100	-2.54872000	2.58607300
H	1.93688800	-2.49156700	3.66305000
C	1.01199200	-1.60910300	1.93558000
H	0.52841400	-0.81774000	2.50011000
C	1.41369000	-2.69831800	-1.71666600
H	0.80923700	-3.52998100	-2.10093400
H	2.42266700	-2.83411700	-2.12216200
H	1.01686500	-1.76593500	-2.12481900
C	0.77671700	1.65248900	0.05886600
C	0.38694800	2.98530400	-0.05210000
H	-0.63806100	3.26991400	0.12707700
C	1.28374900	4.02373400	-0.36395000
H	0.89788900	5.03752500	-0.41658900
C	2.61316100	3.76902400	-0.59594700
H	3.31706700	4.56519500	-0.82035400
C	3.06029900	2.43085900	-0.55638800
C	2.15097800	1.35573900	-0.25734200
C	3.83532500	-0.20604000	-0.55297400
H	4.09851400	-1.26330300	-0.55888700
C	4.81440900	0.77942700	-0.81370300
H	5.84296300	0.49519300	-1.01214600
C	4.41251000	2.09252000	-0.82365100
H	5.11445800	2.89368400	-1.04025500

2a-TS23

Charge = 0, Multiplicity = 1

O	4.31677000	0.79847600	0.94883200
O	0.18419200	-1.76713400	-1.83480000
N	-0.08084100	-0.08890400	-0.21212000
N	-2.07919600	-2.23547600	-0.52469200
C	1.92849500	-4.05999800	-0.75752200
H	0.92547900	-4.21405600	-0.34464800
H	2.53606400	-4.94121100	-0.52897000
H	1.81033400	-3.99424900	-1.84510700
C	3.86838800	-0.46702100	0.70178300
C	4.57583200	-1.65911400	0.69587700
H	5.62206700	-1.70759900	0.97835100
C	3.88690300	-2.81463400	0.26647500
H	4.42958200	-3.75627900	0.25912200
C	2.56638100	-2.81105700	-0.20743800
C	1.86688300	-1.58392100	-0.16155100
C	2.52123400	-0.46973400	0.35121300
C	2.02178600	0.86885300	0.33561900
C	3.22354900	1.73619300	0.66129400
H	3.53957600	2.38459000	-0.16437200
H	3.09568500	2.34889100	1.55689500
C	0.72688200	1.08425000	-0.01273000
C	0.58868000	-1.24951200	-0.82101300
C	0.14556500	2.41791300	-0.28795100
C	-0.68584000	2.65956200	-1.40871700
C	-1.14326500	3.96711800	-1.61884200
H	-1.77527100	4.16059900	-2.48189500
C	-0.80572700	5.01879200	-0.76875400
H	-1.18109400	6.01890900	-0.96616400
C	0.01762500	4.77631800	0.33059200
H	0.28865800	5.58101500	1.00797100
C	0.48297900	3.48608300	0.56157400
H	1.09275300	3.28908700	1.43778100
C	-1.08070800	1.58577900	-2.39282200
H	-0.24156600	0.93896400	-2.66308800
H	-1.47102300	2.04198900	-3.30818900
H	-1.86035200	0.93004000	-1.98954100
C	-1.31579100	-0.16105900	0.49007500
C	-1.56707900	0.78572600	1.48065100
H	-0.79140700	1.48038400	1.76302700
C	-2.80598900	0.88859600	2.14192700

H	-2.93401600	1.67324300	2.88198200
C	-3.82780300	0.01477700	1.86463900
H	-4.79192900	0.08886400	2.35948600
C	-3.59540500	-1.03612900	0.94616200
C	-2.33349000	-1.16600400	0.26820300
C	-3.01459600	-3.13992800	-0.72299300
H	-2.74580100	-3.97681600	-1.36687500
C	-4.30511400	-3.07391200	-0.15083500
H	-5.03959400	-3.84495000	-0.36137200
C	-4.58174900	-2.02256300	0.68858600
H	-5.54733700	-1.93374800	1.18003400

2a-TS24a

Charge = 0, Multiplicity = 1

O	-1.96103200	3.17890400	1.55249900
O	0.91963700	0.64836200	-2.54515300
N	-0.03581600	-0.38124500	-0.64441300
N	2.50531200	-1.41121800	-1.27533700
C	2.87115500	2.92463300	-1.43260600
H	3.38152900	1.96520600	-1.29103100
H	3.57274900	3.72777300	-1.18725800
H	2.62724100	2.99598800	-2.49903700
C	-0.73659500	3.25965900	0.95560600
C	0.18732500	4.29815700	0.98198200
H	0.01669100	5.20272600	1.55598900
C	1.35845700	4.13874300	0.21535500
H	2.08943300	4.94287200	0.22902400
C	1.62767000	3.01435600	-0.58704200
C	0.68481100	1.97103400	-0.56249000
C	-0.45209100	2.11755400	0.22166000
C	-1.55279300	1.19307400	0.30168100
C	-2.61442500	1.95075500	1.07782300
H	-3.47024200	2.26740700	0.47593300
H	-2.97997900	1.40484000	1.95231600
C	-1.39164700	-0.06344700	-0.18991900
C	0.61068800	0.73618300	-1.38615800
C	-2.38782300	-1.15153500	-0.25638300
C	-3.73003400	-0.92939400	-0.65454400
C	-4.62123600	-2.01377800	-0.65183500
H	-5.64809400	-1.83777200	-0.96359900
C	-4.22178100	-3.29760800	-0.29974100
H	-4.93774900	-4.11466900	-0.31142100
C	-2.88498400	-3.52849500	0.03218300

H	-2.54256500	-4.52915500	0.27984800
C	-1.98538500	-2.47147200	0.04025600
H	-0.95163000	-2.66552000	0.29277100
C	0.82308700	-0.91044400	0.37964900
C	0.43450500	-0.96112500	1.70995500
H	-0.53455300	-0.57421300	1.99688500
C	1.26667000	-1.51058300	2.70911600
H	0.90695100	-1.53026300	3.73382700
C	2.51507100	-1.99581700	2.40162700
H	3.16535000	-2.40888300	3.16770400
C	2.96211700	-1.95967900	1.05767800
C	2.11758000	-1.43084100	0.02655500
C	3.69805200	-1.87229900	-1.59158800
H	3.96329800	-1.83861100	-2.64754100
C	4.61431200	-2.39891300	-0.65066600
H	5.58358100	-2.76178400	-0.97802800
C	4.23763200	-2.44404700	0.67008700
H	4.90112800	-2.84703000	1.43104800
C	-4.24763300	0.39072200	-1.17112900
H	-4.79251500	0.95159000	-0.40078800
H	-3.44622000	1.02825800	-1.55160900
H	-4.95595200	0.21798800	-1.98823700

2a-TS24b

Charge = 0, Multiplicity = 1

O	-0.69957400	3.58430400	1.61577900
O	0.71028800	0.35550700	-2.64387500
N	-0.21338900	-0.36813100	-0.61311900
N	2.40755700	-1.24087500	-0.80977900
C	3.54675900	1.81247700	-1.69089600
H	4.23577500	1.12927200	-1.17901200
H	4.13430500	2.66232400	-2.05418100
H	3.13181200	1.28266800	-2.55121100
C	0.43408100	3.22807600	0.95638100
C	1.63462000	3.92725000	0.89120900
H	1.78888800	4.84366600	1.45077600
C	2.62566400	3.42055700	0.03751900
H	3.56666100	3.95989500	-0.03544300
C	2.45433500	2.27357000	-0.76193100
C	1.24795600	1.56988600	-0.63243600
C	0.27094000	2.04627900	0.24545900
C	-1.09462600	1.56527000	0.38039800
C	-1.75798600	2.65455800	1.22465500

H	-2.50652300	3.24970700	0.70003500
H	-2.18637100	2.26559000	2.14945800
C	-1.41892600	0.36198100	-0.18885200
C	0.70252600	0.44368600	-1.44059100
C	-2.67319800	-0.39273700	-0.44938800
C	-3.99926400	-0.00446200	-0.10553000
C	-5.05966300	-0.86617100	-0.41071800
H	-6.06443600	-0.55428000	-0.13802300
C	-4.87867700	-2.08706000	-1.05592700
H	-5.73159800	-2.72347300	-1.27382000
C	-3.59097300	-2.45770000	-1.42966300
H	-3.41025600	-3.39088200	-1.95537700
C	-2.52100100	-1.62278500	-1.13268000
H	-1.52901400	-1.91116800	-1.44927900
C	0.32762800	-1.22678500	0.36528100
C	-0.41101000	-1.67233300	1.45576100
H	-1.41735700	-1.30989600	1.61353500
C	0.11825500	-2.61048400	2.36773900
H	-0.50631900	-2.92974900	3.19741900
C	1.38865900	-3.12041800	2.22630800
H	1.79002600	-3.84537200	2.92833000
C	2.18812600	-2.67766900	1.14468700
C	1.66668300	-1.72176100	0.21681900
C	3.63555800	-1.68460700	-0.98857700
H	4.18404100	-1.27198700	-1.83260000
C	4.23810800	-2.64386400	-0.14244200
H	5.25295100	-2.97617500	-0.33632500
C	3.51461800	-3.12831100	0.92268900
H	3.94395800	-3.85650900	1.60594800
C	-4.36850400	1.30763500	0.53560100
H	-3.95639000	1.41352900	1.54227100
H	-4.03379700	2.15441600	-0.06974600
H	-5.45537900	1.38850400	0.62705300

2a-TS34'

Charge = 0, Multiplicity = 1

O	-4.26948800	0.86071200	0.90077800
O	0.13764900	-2.41547900	-1.02465400
N	0.05494400	-0.19162900	-0.36169600
N	2.57867800	-1.10301200	-1.34255400
C	-2.20195200	-4.08766800	-0.97516800
H	-1.80209700	-3.99777100	-1.99017900
H	-2.97911500	-4.85893900	-0.97278400

H	-1.37021500	-4.42849600	-0.35011100
C	-3.92428500	-0.39149000	0.49050200
C	-4.69325300	-1.54011400	0.47473300
H	-5.72111800	-1.54675500	0.82122900
C	-4.08446900	-2.71254300	-0.02185900
H	-4.67955700	-3.62133600	-0.04869700
C	-2.76235800	-2.77985400	-0.48029400
C	-1.99799500	-1.58350700	-0.43653400
C	-2.60402500	-0.43184500	0.04109300
C	-2.02184800	0.86801700	0.10276600
C	-3.19340700	1.76461800	0.49699200
H	-2.97339900	2.43738800	1.33073200
H	-3.61129900	2.35194200	-0.32755900
C	-0.68465800	1.03314400	-0.16734700
C	-0.56136900	-1.46880800	-0.70157400
C	-0.09004800	2.40602300	-0.33959400
C	1.26333900	2.85978600	-0.27114500
C	1.51091800	4.24345100	-0.31524200
H	2.54435100	4.56795400	-0.23074800
C	0.52152700	5.20227100	-0.48950300
H	0.77403100	6.25831600	-0.51424100
C	-0.78155400	4.76299500	-0.69225300
H	-1.58360800	5.45987500	-0.91770700
C	-1.05380100	3.40406800	-0.62867900
H	-2.05662400	3.10365000	-0.87638300
C	2.50857500	2.01167100	-0.24331000
H	2.47060600	1.22916100	-1.00110100
H	2.69171100	1.54567300	0.72743800
H	3.37521000	2.64060800	-0.46853400
C	1.17788100	-0.44908100	0.50859600
C	1.02769700	-0.22709600	1.86267500
H	0.09895600	0.19947800	2.22684600
C	2.05587200	-0.55682000	2.77335600
H	1.90933100	-0.36460600	3.83197100
C	3.21521500	-1.14772600	2.32515500
H	4.00253900	-1.42919100	3.01929800
C	3.40169300	-1.39003800	0.94029800
C	2.38791200	-1.01573800	0.00342400
C	3.70483300	-1.62452000	-1.77911800
H	3.82959500	-1.66734900	-2.86035700
C	4.73932600	-2.10476100	-0.93603600
H	5.63400100	-2.54062300	-1.36924900
C	4.58986600	-1.96957300	0.42149700
H	5.36827000	-2.28751900	1.11031200

2a-TS34

Charge = 0, Multiplicity = 1

O	2.83804000	2.29961700	1.60225900
O	1.41166400	-2.03246700	-2.02820800
N	0.14363100	-0.41701100	-0.95130400
N	-0.92763700	-0.55038400	1.66763600
C	4.20267100	-2.33049800	-1.37752600
H	3.57538200	-3.18014700	-1.08869200
H	5.25085700	-2.60101700	-1.21331600
H	4.04331800	-2.18584700	-2.45089400
C	3.30590100	1.20238900	0.95564300
C	4.56817800	0.64254200	1.02919100
H	5.34101900	1.06140500	1.66480300
C	4.81221800	-0.49978900	0.24008700
H	5.80041600	-0.94961500	0.28404800
C	3.85449500	-1.09349700	-0.59079400
C	2.56588700	-0.49886800	-0.62758300
C	2.32852100	0.63908300	0.13432600
C	1.13733400	1.43170200	0.15465300
C	1.49388000	2.57700800	1.10270300
H	1.55860500	3.56679900	0.65971200
H	0.82122200	2.60751400	1.96536400
C	0.01803400	0.95295700	-0.48375900
C	1.39327200	-1.04213400	-1.30773900
C	-1.28647600	1.62229500	-0.79000100
C	-1.62055100	2.98826500	-0.53339600
C	-2.93988200	3.42187700	-0.73462900
H	-3.16894500	4.45904100	-0.50379200
C	-3.93687200	2.61070700	-1.26182400
H	-4.94495400	2.99079600	-1.39957200
C	-3.57937000	1.33252300	-1.67590100
H	-4.29285200	0.68480300	-2.17714900
C	-2.28794300	0.87385300	-1.45514900
H	-2.05999700	-0.10662500	-1.82786400
C	-0.64967400	4.09154300	-0.19527600
H	-0.40317100	4.14825000	0.86820000
H	-1.09440500	5.05464700	-0.46164500
H	0.27280000	3.99677300	-0.77247500
C	-0.85546000	-1.39370500	-0.59814500
C	-1.27373000	-2.33529400	-1.52187600
H	-0.88136600	-2.29123000	-2.52741000
C	-2.21367700	-3.33113100	-1.17878800

H	-2.51549900	-4.04967500	-1.93488400
C	-2.75643000	-3.38011400	0.08351200
H	-3.49248900	-4.13369600	0.34988300
C	-2.35038000	-2.43813200	1.06049600
C	-1.37252600	-1.44000400	0.73895000
C	-1.42712300	-0.60190000	2.88494700
H	-1.03809500	0.12479200	3.59722200
C	-2.41196100	-1.53058600	3.29825900
H	-2.78522900	-1.51100100	4.31715600
C	-2.86540100	-2.44808100	2.38207100
H	-3.61382300	-3.18948300	2.64985800

2a-TS41'

Charge = 0, Multiplicity = 1

O	3.23209000	2.33850600	-1.60427900
O	1.38673600	-1.95754400	1.76353300
N	0.18672200	-0.60714700	0.29764200
N	-2.56272000	0.02255300	-0.50070600
C	4.20272000	-2.52217100	1.15545400
H	3.93241300	-2.37355900	2.20585500
H	5.25858700	-2.80557300	1.10240400
H	3.60309100	-3.36809200	0.80138000
C	3.61266600	1.12528000	-1.11406900
C	4.88963300	0.60535300	-0.97916600
H	5.76312800	1.12217900	-1.36223300
C	5.01779200	-0.61066300	-0.27485300
H	6.01388800	-1.03038700	-0.16369600
C	3.95070500	-1.27950300	0.34231500
C	2.65436600	-0.73055600	0.16751000
C	2.52502800	0.40940800	-0.61715300
C	1.34475700	1.20080400	-0.71503800
C	1.80536900	2.51925300	-1.30956800
H	1.31864500	2.76172000	-2.25703300
H	1.69966100	3.37406400	-0.63139200
C	0.18620400	0.76909900	-0.14895300
C	1.42088400	-1.16253600	0.83741800
C	-0.82542900	1.77026300	0.26995100
C	-1.27321500	1.85511400	1.61002500
C	-2.10071900	2.92616300	1.96364000
H	-2.44629100	2.99351600	2.99248200
C	-2.48454600	3.90557300	1.04675800
H	-3.12748100	4.72349100	1.35949800
C	-2.02857800	3.82312700	-0.26833900

H	-2.31535600	4.57201600	-1.00162500
C	-1.20206500	2.76698600	-0.64353300
H	-0.88440800	2.67781900	-1.67744100
C	-0.90185200	0.83640700	2.65873600
H	-1.35038100	-0.14165400	2.45345700
H	-1.24862900	1.16370300	3.64411000
H	0.18003500	0.67805300	2.72042400
C	-0.82488700	-1.58733400	-0.01733600
C	-0.47795200	-2.93724700	-0.03834200
H	0.53036000	-3.24538600	0.18834000
C	-1.40015600	-3.96174800	-0.31986500
H	-1.04702400	-4.98858500	-0.30174300
C	-2.71250000	-3.67973300	-0.61128900
H	-3.43429700	-4.46519600	-0.81558600
C	-3.11564200	-2.32829100	-0.66086300
C	-2.18077800	-1.26855700	-0.38724000
C	-3.79843600	0.33072900	-0.82446400
H	-4.02209500	1.39425400	-0.89842800
C	-4.79970900	-0.63543800	-1.07358500
H	-5.80908200	-0.32907200	-1.32938100
C	-4.44477400	-1.95995700	-0.99598600
H	-5.16670500	-2.74780200	-1.19494900

2a-TS41

Charge = 0, Multiplicity = 1

O	4.31672900	0.79858400	-0.94886700
O	0.18416600	-1.76727700	1.83468600
N	-0.08085300	-0.08894900	0.21213400
N	-2.07928100	-2.23547700	0.52471500
C	1.92866300	-4.05997000	0.75754300
H	1.81033200	-3.99414200	1.84510400
H	2.53636400	-4.94113100	0.52914500
H	0.92572300	-4.21417600	0.34453400
C	3.86839600	-0.46693100	-0.70181500
C	4.57589800	-1.65898800	-0.69586500
H	5.62214200	-1.70743200	-0.97831400
C	3.88701700	-2.81453000	-0.26644600
H	4.42974100	-3.75614900	-0.25905800
C	2.56648900	-2.81100500	0.20744700
C	1.86693000	-1.58390200	0.16152400
C	2.52123500	-0.46970200	-0.35126800
C	2.02173600	0.86886400	-0.33568700
C	3.22344900	1.73625400	-0.66140700

H	3.09554500	2.34887400	-1.55705800
H	3.53942800	2.38473900	0.16420700
C	0.72683700	1.08421700	0.01269900
C	0.58869700	-1.24956200	0.82096000
C	0.14549700	2.41786500	0.28794400
C	-0.68574900	2.65949900	1.40882900
C	-1.14318200	3.96704300	1.61900900
H	-1.77506600	4.16051600	2.48215300
C	-0.80579400	5.01871600	0.76886000
H	-1.18115900	6.01882500	0.96631400
C	0.01741100	4.77625700	-0.33060000
H	0.28833000	5.58095900	-1.00801900
C	0.48277200	3.48603300	-0.56163600
H	1.09245100	3.28904300	-1.43791200
C	-1.08039800	1.58570600	2.39301200
H	-1.85996100	0.92981500	1.98982700
H	-1.47071600	2.04190100	3.30838500
H	-0.24112800	0.93904000	2.66324900
C	-1.31578900	-0.16110700	-0.49008800
C	-1.56701800	0.78564500	-1.48070900
H	-0.79130800	1.48025500	-1.76309900
C	-2.80591900	0.88855300	-2.14199800
H	-2.93390500	1.67318000	-2.88208100
C	-3.82777800	0.01479600	-1.86468100
H	-4.79189900	0.08891700	-2.35953100
C	-3.59543400	-1.03609400	-0.94617100
C	-2.33353000	-1.16600600	-0.26819800
C	-3.01472100	-3.13988500	0.72302600
H	-2.74596400	-3.97677300	1.36692500
C	-4.30523300	-3.07382800	0.15086000
H	-5.03974500	-3.84483200	0.36140500
C	-4.58182100	-2.02248300	-0.68858100
H	-5.54740300	-1.93363800	-1.18003800

2c-Conf-1

Charge = 0, Multiplicity = 1

O	3.60390200	1.97515300	-1.59756200
O	1.17821100	-2.47154600	1.35421900
N	0.30456200	-0.57047400	0.40499100
N	-1.28727700	-1.76562100	-1.54177400
C	4.06605100	-2.92225700	1.27225300
H	3.67197200	-2.82340600	2.28902600
H	5.11099500	-3.24395600	1.33343300

H	3.48311200	-3.71798000	0.79740600
C	3.89167200	0.80781000	-0.94565900
C	5.11174900	0.19710100	-0.73858700
H	6.03981800	0.61840900	-1.11020000
C	5.10612800	-1.01843800	-0.01048600
H	6.06136900	-1.50884200	0.15741700
C	3.95940600	-1.62766400	0.50818600
C	2.71411700	-0.97493900	0.28352100
C	2.73449400	0.21080200	-0.44007100
C	1.61277400	1.01423200	-0.76041000
C	2.15394200	2.19806500	-1.53090300
H	1.78160900	2.26425600	-2.55841300
H	1.98766700	3.16249500	-1.03807700
C	0.38783200	0.62884800	-0.33290700
C	1.39378400	-1.43307000	0.73368800
C	-0.84661100	1.42020600	-0.58942400
C	-1.42045300	2.23677400	0.40714000
C	-2.55865500	2.98177500	0.07326700
H	-3.01711000	3.61822500	0.82379700
C	-3.11324800	2.93354400	-1.20530300
H	-3.99838300	3.52185100	-1.43173500
C	-2.52772700	2.13796900	-2.19003800
H	-2.94955800	2.09689300	-3.19013800
C	-1.39597100	1.38824000	-1.87861600
H	-0.93750300	0.74713000	-2.62321700
C	-0.99869700	-1.07221700	0.74088800
C	-1.45911200	-1.00716400	2.03545400
H	-0.82151700	-0.58349700	2.80302700
C	-2.74695400	-1.48556100	2.36857800
H	-3.08941000	-1.41636700	3.39642500
C	-3.55806700	-2.03058100	1.39961400
H	-4.55177600	-2.39455600	1.64626100
C	-3.10052800	-2.13758200	0.06175200
C	-1.79342800	-1.66723500	-0.28121100
C	-2.04439400	-2.31593400	-2.47026600
H	-1.61041800	-2.38707800	-3.46666900
C	-3.35541800	-2.80115200	-2.24279900
H	-3.92072700	-3.23651500	-3.06051900
C	-3.87965200	-2.70935800	-0.97574900
H	-4.87981100	-3.07087200	-0.75140800
C	-0.77667200	2.37268500	1.77880000
H	-0.14338800	1.49552400	1.93935200
C	0.14476200	3.60546100	1.80872800
H	0.91873100	3.53743400	1.03652000

H	-0.42628800	4.52522900	1.63432700
H	0.64332000	3.69320500	2.78150600
C	-1.79677400	2.42228800	2.92437600
H	-1.28003300	2.37479800	3.88999600
H	-2.37775700	3.35157000	2.91368600
H	-2.49889800	1.58397600	2.86952500

2c-Conf-2

Charge = 0, Multiplicity = 1

O	-3.83272500	2.32036000	0.50698900
O	-1.03619900	-2.59892000	-1.01654300
N	-0.32724300	-0.43739000	-0.71366600
N	1.12112200	-1.93897000	1.13019000
C	-3.81192600	-3.29976900	-0.41289400
H	-3.50515400	-3.53353000	-1.43754100
H	-4.80323800	-3.73102700	-0.23841500
H	-3.09246900	-3.80312000	0.24114000
C	-4.00446500	0.97539200	0.32671900
C	-5.14594400	0.21148100	0.46053900
H	-6.09971400	0.64210900	0.74657800
C	-5.02262000	-1.17720200	0.20709800
H	-5.91504000	-1.78876100	0.31103600
C	-3.83495000	-1.81314900	-0.16741100
C	-2.67239200	-1.00200400	-0.29768300
C	-2.80826000	0.35683800	-0.04373500
C	-1.77836800	1.32700800	-0.11158600
C	-2.42565200	2.64716900	0.24435100
H	-2.01868900	3.11163100	1.14884200
H	-2.40140400	3.38438000	-0.56536000
C	-0.52418500	0.93191900	-0.43486000
C	-1.33269100	-1.45227400	-0.69338700
C	0.61567200	1.88469700	-0.54537700
C	1.54092900	2.06928900	0.50148400
C	2.55446000	3.02065600	0.32124900
H	3.27518600	3.18398600	1.11659300
C	2.65788900	3.76857600	-0.85025800
H	3.45828100	4.49555200	-0.95799800
C	1.73030100	3.58781000	-1.87668200
H	1.79715100	4.16941700	-2.79156300
C	0.71262200	2.65091800	-1.71632500
H	-0.01734200	2.49725400	-2.50623500
C	0.99225900	-0.90241400	-1.03426200
C	1.56032000	-0.60801800	-2.25196000

H	0.99216600	-0.03559400	-2.97647300
C	2.87152800	-1.03816100	-2.56061200
H	3.29985600	-0.78395400	-3.52516800
C	3.59320200	-1.77603700	-1.65138600
H	4.59998200	-2.11316400	-1.88274300
C	3.02933200	-2.10994700	-0.39305500
C	1.70894900	-1.66767700	-0.06758400
C	1.80017100	-2.65137300	2.00619300
H	1.30268800	-2.85201100	2.95391900
C	3.10896800	-3.14626100	1.78367600
H	3.60649100	-3.72572900	2.55470000
C	3.72133600	-2.86930700	0.58516100
H	4.72698100	-3.22151700	0.37070200
C	1.41184000	1.31541000	1.81614600
C	2.75519800	0.77949900	2.33102200
H	2.59192700	0.14264000	3.20711300
H	3.26595900	0.18258800	1.56916600
H	3.42940500	1.58841500	2.63627300
C	0.73690300	2.20531900	2.87484900
H	0.60516400	1.65411000	3.81356800
H	1.34132100	3.09613400	3.08559300
H	-0.25059100	2.54137800	2.54009500
H	0.76277900	0.45148500	1.65037000

2c-Conf-3

Charge = 0, Multiplicity = 1

O	-3.60388300	1.97507800	-1.59763400
O	-1.17817400	-2.47147900	1.35434400
N	-0.30453000	-0.57043400	0.40505000
N	1.28718400	-1.76573700	-1.54170900
C	-4.06600900	-2.92221800	1.27238000
H	-3.48306400	-3.71795500	0.79756200
H	-5.11095200	-3.24392000	1.33356600
H	-3.67193500	-2.82332900	2.28915000
C	-3.89164600	0.80776200	-0.94567700
C	-5.11171800	0.19704700	-0.73859800
H	-6.03978700	0.61832600	-1.11024600
C	-5.10609200	-1.01846100	-0.01044600
H	-6.06133000	-1.50887000	0.15746500
C	-3.95937000	-1.62765200	0.50826600
C	-2.71408600	-0.97491900	0.28359200
C	-2.73446800	0.21079500	-0.44004300
C	-1.61275400	1.01422500	-0.76040200

C	-2.15392800	2.19801200	-1.53096400
H	-1.98767500	3.16247200	-1.03819000
H	-1.78157900	2.26415400	-2.55847100
C	-0.38780900	0.62886900	-0.33288000
C	-1.39375000	-1.43302600	0.73377600
C	0.84662300	1.42023500	-0.58943700
C	1.42045600	2.23687600	0.40707400
C	2.55863200	2.98189000	0.07314200
H	3.01707900	3.61839500	0.82363100
C	3.11321300	2.93360200	-1.20543100
H	3.99833000	3.52191900	-1.43190600
C	2.52770100	2.13795600	-2.19011400
H	2.94952000	2.09683700	-3.19021800
C	1.39596900	1.38821500	-1.87863500
H	0.93750400	0.74705900	-2.62319800
C	0.99872800	-1.07219600	0.74092500
C	1.45919400	-1.00710300	2.03547100
H	0.82164700	-0.58337200	2.80304700
C	2.74702700	-1.48554200	2.36857000
H	3.08952600	-1.41631400	3.39640000
C	3.55808000	-2.03064300	1.39960100
H	4.55178300	-2.39465000	1.64622800
C	3.10048400	-2.13769300	0.06176200
C	1.79339300	-1.66730200	-0.28117300
C	2.04423500	-2.31614200	-2.47020100
H	1.61021200	-2.38732800	-3.46658100
C	3.35524500	-2.80141000	-2.24276000
H	3.92049800	-3.23684800	-3.06047900
C	3.87953700	-2.70956700	-0.97573800
H	4.87968800	-3.07111700	-0.75141800
C	0.77669800	2.37285300	1.77873900
C	1.79682100	2.42254500	2.92429400
H	2.37776200	3.35185200	2.91355400
H	1.28010100	2.37507100	3.88992600
H	2.49898200	1.58426300	2.86946400
C	-0.14475600	3.60561500	1.80862300
H	-0.91875300	3.53753200	1.03644800
H	-0.64327900	3.69341000	2.78141400
H	0.42627300	4.52538200	1.63414700
H	0.14343300	1.49568800	1.93934900

2c-Conf-4

Charge = 0, Multiplicity = 1

O	3.83271800	2.32036500	0.50699600
O	1.03620500	-2.59892000	-1.01654300
N	0.32724500	-0.43739100	-0.71366800
N	-1.12111600	-1.93896500	1.13019400
C	3.81193600	-3.29976100	-0.41289900
H	3.09247600	-3.80311600	0.24112900
H	4.80324800	-3.73101700	-0.23841500
H	3.50517200	-3.53352100	-1.43754900
C	4.00446200	0.97539800	0.32672400
C	5.14594400	0.21149100	0.46054100
H	6.09971300	0.64212100	0.74657900
C	5.02262300	-1.17719200	0.20709800
H	5.91504500	-1.78874900	0.31103300
C	3.83495500	-1.81314200	-0.16741200
C	2.67239500	-1.00200000	-0.29768200
C	2.80825900	0.35684200	-0.04373000
C	1.77836500	1.32700900	-0.11158100
C	2.42564600	2.64717200	0.24435300
H	2.40139900	3.38437800	-0.56536300
H	2.01868000	3.11163900	1.14883900
C	0.52418300	0.93191800	-0.43485900
C	1.33269500	-1.45227300	-0.69338800
C	-0.61567600	1.88469200	-0.54538100
C	-1.54093400	2.06928700	0.50147900
C	-2.55446800	3.02065000	0.32123900
H	-3.27519400	3.18398100	1.11658200
C	-2.65789900	3.76856300	-0.85027200
H	-3.45829400	4.49553700	-0.95801500
C	-1.73031000	3.58779500	-1.87669500
H	-1.79716300	4.16939700	-2.79157900
C	-0.71262900	2.65090700	-1.71633300
H	0.01733600	2.49724100	-2.50624300
C	-0.99225600	-0.90241900	-1.03426300
C	-1.56031800	-0.60803100	-2.25196200
H	-0.99216400	-0.03560900	-2.97647800
C	-2.87152500	-1.03817700	-2.56061200
H	-3.29985400	-0.78397600	-3.52516900
C	-3.59319900	-1.77604800	-1.65138100
H	-4.59997900	-2.11317700	-1.88273500
C	-3.02932800	-2.10995000	-0.39304800
C	-1.70894500	-1.66767800	-0.06758000
C	-1.80016400	-2.65136400	2.00620100
H	-1.30268000	-2.85199800	2.95392700
C	-3.10896100	-3.14625300	1.78368800

H	-3.60648300	-3.72571700	2.55471500
C	-3.72133100	-2.86930500	0.58517200
H	-4.72697600	-3.22151600	0.37071600
C	-1.41184200	1.31541300	1.81614400
H	-0.76277800	0.45149000	1.65037200
C	-0.73691000	2.20532800	2.87484400
H	-1.34133000	3.09614300	3.08558400
H	-0.60517100	1.65412400	3.81356600
H	0.25058400	2.54138900	2.54009100
C	-2.75519900	0.77950000	2.33102200
H	-3.26595700	0.18258300	1.56916800
H	-2.59192600	0.14264600	3.20711600
H	-3.42940900	1.58841400	2.63626800

2c-TS12'

Charge = 0, Multiplicity = 1

O	-2.99482300	2.47777900	1.57577100
O	-1.67141400	-1.60699400	-2.34554300
N	-0.33195700	-0.30198300	-0.95226600
N	0.60898000	-0.50648900	1.73684600
C	-4.47268900	-1.99591200	-1.60154100
H	-4.33849800	-1.78257500	-2.66723300
H	-5.51716000	-2.27556200	-1.43065000
H	-3.84207100	-2.86422100	-1.38202500
C	-3.50140600	1.41118000	0.89779600
C	-4.78256700	0.89218100	0.92639100
H	-5.55884700	1.31656200	1.55420300
C	-5.04803100	-0.21716900	0.09233300
H	-6.05256100	-0.63152400	0.10204900
C	-4.10004400	-0.81196600	-0.74850200
C	-2.78834200	-0.26747800	-0.73238700
C	-2.53201400	0.82298200	0.08529800
C	-1.30774500	1.54204900	0.17234600
C	-1.65458700	2.74177900	1.04747900
H	-0.96778000	2.86729100	1.89012200
H	-1.74136100	3.69600900	0.51764000
C	-0.16808300	1.01822300	-0.38564400
C	-1.62524300	-0.76858000	-1.45938800
C	1.09593700	1.82861800	-0.47879000
C	2.45511400	1.44371500	-0.68740600
C	3.46019300	2.41575500	-0.53349000
H	4.49122000	2.09897000	-0.65459400
C	3.20779300	3.75439400	-0.27143500

H	4.02584700	4.46062700	-0.16229900
C	1.88031000	4.16817000	-0.21601900
H	1.62094900	5.21664700	-0.10019300
C	0.87331800	3.22271100	-0.33139100
H	-0.13609700	3.59505200	-0.36360800
C	0.44194700	-1.42669000	-0.49447700
C	0.73078300	-2.46828000	-1.36313300
H	0.44737400	-2.37427900	-2.40028900
C	1.39170500	-3.63384300	-0.92230000
H	1.59163100	-4.42342000	-1.64045700
C	1.79236300	-3.76585700	0.38635500
H	2.31133100	-4.65625700	0.73015600
C	1.54068400	-2.71662800	1.30267000
C	0.85216800	-1.53130000	0.87853400
C	1.01584700	-0.60587500	2.98529300
H	0.79780300	0.24222600	3.63295100
C	1.70569900	-1.72790300	3.50196100
H	2.02049600	-1.74350100	4.54045300
C	1.96152800	-2.77939300	2.65536100
H	2.49117100	-3.66379800	3.00000600
C	2.96961400	0.09276400	-1.16082100
H	2.13387700	-0.57141600	-1.30497300
C	3.63982900	0.21144700	-2.54217300
H	2.95457800	0.65404600	-3.27378700
H	4.54534800	0.82807800	-2.51359400
H	3.92506300	-0.78427800	-2.90352900
C	3.91668600	-0.56556100	-0.14343400
H	4.14714000	-1.59216200	-0.44958200
H	4.86527500	-0.02089300	-0.06632900
H	3.47140400	-0.59978100	0.85475600

2c-TS12

Charge = 0, Multiplicity = 1

O	-3.72301700	1.53754300	1.35768200
O	1.43485100	2.16121700	-1.25568000
N	0.41871100	0.33885100	-0.25883500
N	2.97692600	-0.26894400	-1.35302400
C	0.07306300	4.68924300	-1.44488100
H	1.03288200	4.70588900	-0.91869300
H	-0.28295400	5.71881200	-1.55465900
H	0.27923400	4.28273400	-2.44003800
C	-2.90692300	2.41872700	0.72064200
C	-3.08720000	3.77896700	0.54275000

H	-3.95681700	4.29521100	0.93510900
C	-2.09361300	4.46864100	-0.17915400
H	-2.22384800	5.53613500	-0.33511900
C	-0.94518100	3.86112200	-0.70504200
C	-0.78961400	2.46789200	-0.49066200
C	-1.77680200	1.78434900	0.20662100
C	-1.85124600	0.36752900	0.43454700
C	-3.24600000	0.19566600	1.03366400
H	-3.97991800	-0.19822900	0.32803100
H	-3.26384900	-0.39302500	1.95364100
C	-0.77624200	-0.41792300	0.09526200
C	0.41612300	1.68492400	-0.77816500
C	-0.65235600	-1.91545200	-0.00526300
C	-1.72072300	-2.87559000	-0.08401700
C	-1.39594800	-4.24099600	-0.06586300
H	-2.19919300	-4.96443900	-0.09748700
C	-0.09259500	-4.72420500	-0.05014700
H	0.09573100	-5.79402600	-0.03713300
C	0.94505300	-3.80534400	-0.10954400
H	1.98157900	-4.12426200	-0.16914200
C	0.65277500	-2.44898100	-0.09696200
H	1.48990900	-1.78878800	-0.18536500
C	1.59661400	0.17616600	0.57101100
C	1.47004100	0.29731000	1.93868200
H	0.48318200	0.44216000	2.36589600
C	2.60399800	0.25202300	2.78138700
H	2.47115200	0.35294000	3.85436400
C	3.86309300	0.11261600	2.24518800
H	4.74318800	0.09987100	2.88262600
C	4.02826900	-0.02891000	0.84338100
C	2.88495800	-0.02160100	-0.01666700
C	4.17422600	-0.45316200	-1.86779100
H	4.21310100	-0.66116000	-2.93632300
C	5.37798800	-0.40661000	-1.12013800
H	6.33156700	-0.54978200	-1.61847600
C	5.29871500	-0.20783400	0.23629300
H	6.18997700	-0.19492300	0.85847000
C	-3.18693600	-2.53142900	-0.32459800
H	-3.52626800	-1.90407300	0.49360700
C	-3.34985900	-1.77565300	-1.65739600
H	-2.71550600	-0.88872000	-1.72035700
H	-3.07950300	-2.43484800	-2.49047300
H	-4.39165000	-1.46391200	-1.80016500
C	-4.15980600	-3.72068800	-0.31333700

H	-5.18112600	-3.33976600	-0.42617500
H	-3.97814500	-4.41601500	-1.14048200
H	-4.12010100	-4.28199900	0.62653300

2c-TS23'

Charge = 0, Multiplicity = 1

O	-3.36343900	-2.17821900	-1.86744600
O	-1.45119500	1.86288300	1.74980100
N	-0.28561100	0.67651200	0.12126800
N	2.43070300	0.17625900	-0.86607800
C	-4.29213200	2.46236600	1.26231000
H	-3.98258800	2.24274200	2.28917600
H	-5.35196300	2.73577300	1.26708000
H	-3.71449600	3.33894900	0.94813500
C	-3.74259700	-1.00941800	-1.27806900
C	-5.01978600	-0.51944900	-1.06080800
H	-5.90060500	-1.02119200	-1.44717100
C	-5.13699200	0.64309900	-0.26852200
H	-6.13364200	1.03865100	-0.09267000
C	-4.05676600	1.28363500	0.35464400
C	-2.76068400	0.76824400	0.09352000
C	-2.64678800	-0.31292800	-0.77155000
C	-1.45991300	-1.07362900	-0.97060300
C	-1.92407900	-2.35653500	-1.63723100
H	-1.46814600	-2.52835800	-2.61485000
H	-1.78382100	-3.25267100	-1.02175700
C	-0.28295800	-0.66196200	-0.42980900
C	-1.50977400	1.16116100	0.75224100
C	0.77047000	-1.68175600	-0.17440700
C	1.26926800	-1.96237700	1.11783900
C	2.15863600	-3.03780000	1.25960900
H	2.56078000	-3.25407500	2.24529800
C	2.53479100	-3.84342200	0.18811000
H	3.22388200	-4.66924100	0.34168600
C	2.01175300	-3.58009600	-1.07955300
H	2.28848400	-4.19442300	-1.93212800
C	1.13850500	-2.51241200	-1.24819200
H	0.77144000	-2.27162500	-2.24078000
C	0.70141300	1.69902600	-0.13453700
C	0.34170600	3.03892700	0.00183900
H	-0.65725000	3.30858700	0.30468600
C	1.24040900	4.10061000	-0.20919600
H	0.87777200	5.11442800	-0.06730100

C	2.54183600	3.87026000	-0.58251200
H	3.24702400	4.68287400	-0.73107900
C	2.95485100	2.53746900	-0.79244500
C	2.04154800	1.44193300	-0.59832300
C	3.65537900	-0.07888300	-1.26839400
H	3.88514400	-1.12521700	-1.46505200
C	4.63727100	0.92166400	-1.44901800
H	5.63887900	0.65807600	-1.77370000
C	4.27295700	2.22526600	-1.21649300
H	4.97918800	3.03947000	-1.35751600
C	0.90700600	-1.15046900	2.35538800
H	0.10734900	-0.45725700	2.09852000
C	0.38047400	-2.03678000	3.49587200
H	-0.47306200	-2.64055300	3.16651200
H	1.14821200	-2.72094800	3.87533400
H	0.05101100	-1.41319600	4.33544500
C	2.10255700	-0.30206600	2.82154800
H	1.81770400	0.32908300	3.67177200
H	2.93920000	-0.93784700	3.13671100
H	2.46076200	0.34919100	2.01892900

2c-TS23

Charge = 0, Multiplicity = 1

O	0.89793200	4.26836400	-1.11625000
O	1.34331700	-0.13839400	2.16552300
N	0.04607900	-0.08619800	0.20481600
N	1.50812000	-2.50109300	0.68954400
C	4.34797700	0.47582100	1.32245800
H	4.10671300	0.47423300	2.39193300
H	5.41068500	0.71207700	1.21080300
H	4.17959600	-0.54498000	0.96147700
C	1.88233900	3.43099500	-0.67626900
C	3.23890200	3.68103900	-0.52208100
H	3.68631400	4.62212500	-0.82372500
C	4.01772600	2.67062400	0.08106500
H	5.08135400	2.85506500	0.20722200
C	3.49134500	1.46856600	0.58102400
C	2.11619900	1.23527100	0.37760000
C	1.36903200	2.19613500	-0.29565500
C	-0.05517900	2.18600500	-0.47191900
C	-0.39364500	3.59071100	-0.93699200
H	-0.90360200	3.62750100	-1.90212800
H	-0.97842400	4.16526100	-0.20924000

C	-0.74953700	1.05984700	-0.17347500
C	1.23879300	0.23282000	1.02342800
C	-2.22250300	0.91459000	-0.20897000
C	-2.95313300	0.27957700	0.82465100
C	-4.34520500	0.18550800	0.68001700
H	-4.91964700	-0.30836800	1.45781600
C	-5.01735500	0.71570000	-0.41821000
H	-6.09738000	0.62205800	-0.49048800
C	-4.29606700	1.36927400	-1.41824500
H	-4.80212600	1.78996800	-2.28243200
C	-2.91376100	1.45851900	-1.30802000
H	-2.34587100	1.92783000	-2.10572200
C	0.07516400	-1.16426800	-0.72167400
C	-0.58839400	-1.06083000	-1.93894400
H	-1.06359700	-0.13189700	-2.21446400
C	-0.67118400	-2.13913900	-2.84413000
H	-1.22219100	-1.99613000	-3.76930700
C	-0.06272000	-3.34101600	-2.57604600
H	-0.12290400	-4.17573700	-3.26853400
C	0.67880600	-3.48144200	-1.37803400
C	0.76806100	-2.39782600	-0.44161700
C	2.14287700	-3.62595700	0.94808900
H	2.72319400	-3.65141400	1.86955400
C	2.10076500	-4.75975700	0.10507500
H	2.64068300	-5.66202300	0.37473200
C	1.37057300	-4.67694600	-1.05644700
H	1.31565200	-5.51534600	-1.74616800
C	-2.30524100	-0.27701900	2.08709700
H	-1.27498400	0.07435900	2.13199000
C	-3.00564500	0.21608100	3.36418600
H	-3.06415900	1.31033000	3.38995900
H	-4.02405600	-0.17770100	3.46037200
H	-2.44290600	-0.11367000	4.24533300
C	-2.25423300	-1.81318400	2.04746600
H	-1.72746400	-2.20031100	2.92734300
H	-3.26467100	-2.24119200	2.03883000
H	-1.72812200	-2.16894500	1.15756700

2e-Conf-1

Charge = 0, Multiplicity = 1

O	3.74273700	1.44120700	-1.66063700
O	0.77144700	-2.55655500	1.43306400
N	0.14812400	-0.60403900	0.40789600

N	-1.37698800	-2.25906100	-1.21356200
C	3.57573400	-3.38645500	1.35367400
H	3.21124900	-3.21027400	2.37097100
H	4.56774500	-3.84620600	1.41401800
H	2.88387500	-4.10578900	0.90389700
C	3.88046100	0.27445000	-0.96230200
C	5.01001900	-0.48941300	-0.74771300
H	5.98054600	-0.20950700	-1.14342800
C	4.85044900	-1.67047200	0.01727800
H	5.73337200	-2.27940600	0.19301200
C	3.63716700	-2.10796800	0.55833100
C	2.48863800	-1.30166300	0.32304800
C	2.66127300	-0.14233300	-0.42332900
C	1.65092700	0.78843600	-0.77267300
C	2.33469400	1.85147100	-1.60402800
H	1.96290800	1.90712700	-2.63318200
H	2.29567500	2.84898200	-1.16006100
C	0.38524200	0.55378000	-0.35556500
C	1.12005700	-1.57871100	0.77650600
C	-0.77255200	1.42446100	-0.70013900
C	-1.05425700	2.61992100	-0.01256700
C	-2.14009700	3.41161800	-0.39590500
H	-2.34961200	4.32851700	0.14244800
C	-2.95497700	3.02311600	-1.45736500
H	-3.79851100	3.64371500	-1.74356100
C	-2.68215300	1.84112000	-2.14478500
H	-3.31105600	1.53215600	-2.97442500
C	-1.59751600	1.05133600	-1.76797600
H	-1.38135100	0.12478800	-2.28837300
C	-1.20171600	-0.93068200	0.77961100
C	-1.75566800	-0.42271300	1.93047300
H	-1.16548300	0.23564100	2.55585000
C	-3.08392600	-0.74915700	2.29284000
H	-3.50125800	-0.33424100	3.20513200
C	-3.83543100	-1.58873200	1.50395300
H	-4.85393700	-1.84853300	1.78000500
C	-3.28892700	-2.12982100	0.31145800
C	-1.95102800	-1.79741500	-0.06772400
C	-2.08876700	-3.06231200	-1.98042400
H	-1.60321200	-3.41729900	-2.88828500
C	-3.41434700	-3.46830900	-1.69102400
H	-3.93634400	-4.13469100	-2.37020300
C	-4.01247000	-2.99553300	-0.54710900
H	-5.03095100	-3.27241800	-0.28741500

C	-0.17948100	3.09980700	1.11607400
F	0.97669000	3.64893900	0.66227900
F	0.17834300	2.11121600	1.96812300
F	-0.78871700	4.05039500	1.85716800

2e-Conf-2

Charge = 0, Multiplicity = 1

O	-3.51735000	2.48901300	-0.50191500
O	-1.48069500	-2.96323300	0.18742500
N	-0.46643800	-0.99088500	-0.42065400
N	1.54652300	-0.67872000	1.50244500
C	-4.34610500	-3.00794600	0.72870100
H	-4.04224500	-3.65250200	-0.10246500
H	-5.39960200	-3.20343500	0.95451200
H	-3.74225700	-3.31662400	1.58814800
C	-3.88842000	1.21373200	-0.18199500
C	-5.13629200	0.71900200	0.13896500
H	-6.01717100	1.35118300	0.17353500
C	-5.22332600	-0.66490500	0.42710400
H	-6.20070800	-1.06481100	0.68363100
C	-4.14113400	-1.55060800	0.40425300
C	-2.86634700	-1.01501800	0.06660100
C	-2.79461100	0.34509700	-0.20750200
C	-1.62888200	1.06710600	-0.55869800
C	-2.07081700	2.50225300	-0.74795400
H	-1.62153900	3.19944200	-0.03581200
H	-1.90837800	2.88278300	-1.76234200
C	-0.45363800	0.40203500	-0.65196100
C	-1.60633500	-1.76074000	-0.02961200
C	0.82138500	1.03681900	-1.07712500
C	1.51640300	1.99203200	-0.31295200
C	2.70391300	2.55019500	-0.80487500
H	3.23296600	3.28192200	-0.20377100
C	3.21617600	2.16859900	-2.03945000
H	4.14135500	2.60703500	-2.40037000
C	2.53212100	1.22448300	-2.80637100
H	2.91523300	0.92121000	-3.77604300
C	1.35042700	0.67155800	-2.32628500
H	0.81509500	-0.06004400	-2.92117200
C	0.76515600	-1.72721700	-0.51013700
C	0.95829000	-2.61223100	-1.54735000
H	0.17008800	-2.74480100	-2.28085200
C	2.16341400	-3.33965100	-1.66299100

H	2.29000000	-4.02931700	-2.49179300
C	3.16861000	-3.17219000	-0.73713600
H	4.10143700	-3.72315200	-0.82196700
C	2.99631200	-2.27732100	0.34826100
C	1.77210600	-1.54771700	0.48079200
C	2.49865600	-0.51040400	2.39756100
H	2.28809400	0.20019800	3.19432900
C	3.74661700	-1.17985800	2.36185800
H	4.48482900	-0.98991900	3.13435500
C	3.99089000	-2.06143700	1.33634000
H	4.93353700	-2.59800600	1.26621100
C	1.06705100	2.53342300	1.02373100
F	2.11080600	2.61876100	1.88672300
F	0.10286800	1.84260200	1.64397300
F	0.59891400	3.80811400	0.87759400

2e-Conf-3

Charge = 0, Multiplicity = 1

O	-3.74259900	1.44154400	-1.66058100
O	-0.77176300	-2.55648500	1.43323400
N	-0.14822300	-0.60410700	0.40795600
N	1.37690600	-2.25880500	-1.21370500
C	-3.57601700	-3.38635000	1.35336800
H	-2.88364900	-4.10541900	0.90395700
H	-4.56792100	-3.84641800	1.41305100
H	-3.21222800	-3.21018800	2.37092800
C	-3.88044300	0.27476700	-0.96230400
C	-5.01004900	-0.48907000	-0.74784200
H	-5.98054100	-0.20909300	-1.14357300
C	-4.85057300	-1.67020100	0.01704700
H	-5.73352100	-2.27912200	0.19265500
C	-3.63734000	-2.10779900	0.55814600
C	-2.48877100	-1.30151500	0.32301700
C	-2.66131500	-0.14211200	-0.42327300
C	-1.65088000	0.78857700	-0.77256600
C	-2.33454900	1.85177300	-1.60377500
H	-2.29551400	2.84918300	-1.15955500
H	-1.96267600	1.90766800	-2.63287900
C	-0.38522300	0.55376300	-0.35546400
C	-1.12024300	-1.57862900	0.77661400
C	0.77265000	1.42431000	-0.70010400
C	1.05448200	2.61977300	-0.01258600
C	2.14033800	3.41139100	-0.39607000

H	2.34998100	4.32828100	0.14223000
C	2.95503500	3.02283300	-1.45764900
H	3.79851500	3.64342100	-1.74399600
C	2.68207400	1.84082900	-2.14500300
H	3.31083800	1.53179700	-2.97471400
C	1.59745600	1.05109900	-1.76804000
H	1.38121600	0.12451600	-2.28834600
C	1.20160400	-0.93079200	0.77970700
C	1.75550400	-0.42310300	1.93073500
H	1.16530400	0.23513600	2.55619100
C	3.08371700	-0.74968900	2.29311500
H	3.50101600	-0.33500200	3.20551600
C	3.83523300	-1.58912000	1.50407600
H	4.85370700	-1.84903500	1.78011900
C	3.28879000	-2.12991400	0.31143300
C	1.95091600	-1.79738400	-0.06775400
C	2.08868900	-3.06197300	-1.98066100
H	1.60316800	-3.41677700	-2.88860500
C	3.41424000	-3.46806300	-1.69127400
H	3.93623100	-4.13435700	-2.37053100
C	4.01233500	-2.99550400	-0.54725500
H	5.03079300	-3.27247200	-0.28757500
C	0.17985600	3.09968600	1.11619200
F	-0.17801200	2.11111700	1.96823800
F	0.78925900	4.05017900	1.85730400
F	-0.97632700	3.64895900	0.66258700

2e-Conf-4

Charge = 0, Multiplicity = 1

O	-3.51724200	2.48906500	0.50188100
O	-1.48081500	-2.96329100	-0.18719800
N	-0.46645200	-0.99094100	0.42069700
N	1.54646400	-0.67872100	-1.50245300
C	-4.34618800	-3.00787100	-0.72871000
H	-3.74224700	-3.31658500	-1.58807900
H	-5.39966700	-3.20329100	-0.95467300
H	-4.04248000	-3.65244900	0.10249200
C	-3.88835800	1.21379500	0.18197600
C	-5.13624300	0.71910100	-0.13898200
H	-6.01710800	1.35130200	-0.17355000
C	-5.22332000	-0.66480400	-0.42711300
H	-6.20071400	-1.06467400	-0.68365000
C	-4.14116300	-1.55054600	-0.40424400

C	-2.86635700	-1.01499300	-0.06658400
C	-2.79457600	0.34512600	0.20748800
C	-1.62881200	1.06710200	0.55863900
C	-2.07069800	2.50226300	0.74789200
H	-1.90824100	2.88279800	1.76227400
H	-1.62142200	3.19944000	0.03574500
C	-0.45358800	0.40198500	0.65192200
C	-1.60639000	-1.76076600	0.02971100
C	0.82140700	1.03678300	1.07715300
C	1.51640300	1.99203900	0.31300800
C	2.70390000	2.55021200	0.80496700
H	3.23295300	3.28195600	0.20388500
C	3.21615200	2.16859400	2.03953600
H	4.14131300	2.60705000	2.40047900
C	2.53210400	1.22444200	2.80642600
H	2.91519400	0.92115700	3.77610200
C	1.35043200	0.67150600	2.32631200
H	0.81509900	-0.06011200	2.92117700
C	0.76513300	-1.72730100	0.51010000
C	0.95828400	-2.61239000	1.54724900
H	0.17009000	-2.74502800	2.28074200
C	2.16341900	-3.33979300	1.66284500
H	2.29003100	-4.02949600	2.49161600
C	3.16862400	-3.17223900	0.73702200
H	4.10146100	-3.72318600	0.82184100
C	2.99629700	-2.27732700	-0.34833600
C	1.77208100	-1.54773700	-0.48082200
C	2.49857300	-0.51036300	-2.39758100
H	2.28799500	0.20028400	-3.19430600
C	3.74655300	-1.17978700	-2.36191100
H	4.48474400	-0.98981700	-3.13442000
C	3.99085400	-2.06139300	-1.33642500
H	4.93350700	-2.59795500	-1.26632500
C	1.06707200	2.53342900	-1.02369700
F	2.11088700	2.61892600	-1.88660800
F	0.10302900	1.84250900	-1.64401800
F	0.59878400	3.80808100	-0.87754800

2e-TS12'

Charge = 0, Multiplicity = 1

O	4.22160000	1.78147300	0.86242100
O	0.81287600	-2.55617600	-0.96266200
N	0.31116700	-0.35918100	-0.39418900

N	-1.85871600	-2.03055100	-1.28816500
C	3.49472700	-3.56782500	-0.90450000
H	2.77864400	-4.09648100	-0.26718800
H	4.44434800	-4.11251000	-0.88940500
H	3.08541700	-3.60703000	-1.91885900
C	4.21057300	0.47619800	0.47654800
C	5.24508300	-0.44144000	0.49529000
H	6.23637000	-0.18160300	0.85080400
C	4.95719600	-1.73814500	0.02196100
H	5.76238200	-2.46782800	0.01991100
C	3.69900300	-2.14902800	-0.44159600
C	2.65841500	-1.18433700	-0.43247900
C	2.95103400	0.09396200	0.01475500
C	2.05675200	1.20259300	0.04081900
C	2.95882700	2.37431900	0.42829600
H	3.22856000	3.03365100	-0.40239000
H	2.55999200	2.98360500	1.24420400
C	0.72022200	1.01402300	-0.22982500
C	1.23822000	-1.44724800	-0.68814200
C	-0.17057300	2.22513100	-0.37131800
C	-1.56814900	2.46337800	-0.16241400
C	-2.04266300	3.77470900	-0.01316600
H	-3.09746800	3.91538600	0.18486100
C	-1.23506100	4.89377700	-0.16960700
H	-1.64287000	5.89037900	-0.03565900
C	0.06874400	4.68924000	-0.60093900
H	0.71121500	5.52346200	-0.86682200
C	0.55737000	3.39373400	-0.70506300
H	1.54907700	3.27809700	-1.10691300
C	-0.71533700	-0.86165000	0.49575900
C	-0.61466700	-0.54667900	1.83643500
H	0.17701600	0.11987100	2.16270900
C	-1.50924100	-1.08720400	2.78430600
H	-1.40561200	-0.81438100	3.83026800
C	-2.48381900	-1.97128600	2.38516000
H	-3.16952900	-2.40882300	3.10603900
C	-2.60823900	-2.32712800	1.01845900
C	-1.72734600	-1.76365100	0.04074300
C	-2.80096200	-2.86503500	-1.66565700
H	-2.88231500	-3.04862100	-2.73668000
C	-3.69842500	-3.51195200	-0.77748400
H	-4.44620900	-4.19725300	-1.16427800
C	-3.60312200	-3.23185300	0.56202600
H	-4.27773600	-3.68400100	1.28459900

C	-2.68474900	1.45269600	-0.28938500
F	-2.98733700	0.79566500	0.85136100
F	-2.40699700	0.55939800	-1.25268300
F	-3.84756900	2.04982900	-0.66653400

2e-TS12

Charge = 0, Multiplicity = 1

O	1.31442800	-3.09468400	1.71707500
O	2.59246500	1.08692100	-2.13856600
N	0.64745100	0.56268500	-0.98958000
N	-0.08906600	1.33874100	1.64260200
C	5.06461900	-0.22299400	-1.42272500
H	4.84652000	-0.31252100	-2.49180400
H	6.08081600	-0.58840600	-1.24227300
H	5.03488800	0.84736500	-1.19409200
C	2.32138600	-2.48802200	1.04544600
C	3.67962800	-2.74544200	1.12495000
H	4.07809400	-3.50109700	1.79332700
C	4.52640600	-1.98717600	0.29437200
H	5.59455100	-2.18106000	0.34118000
C	4.07606900	-0.99426500	-0.58733300
C	2.68116300	-0.74577300	-0.62657800
C	1.84085500	-1.50298100	0.18234500
C	0.41156900	-1.47242900	0.20937900
C	0.05063700	-2.58093400	1.19217500
H	-0.52928500	-2.19796600	2.03582400
H	-0.45180200	-3.44190500	0.76604300
C	-0.23549900	-0.47199800	-0.47341200
C	2.02225200	0.33161600	-1.36283000
C	-1.68870600	-0.26336100	-0.75439300
C	-2.79742400	-1.11750900	-0.44335300
C	-4.11304000	-0.63778300	-0.51898900
H	-4.92057100	-1.30398700	-0.24099200
C	-4.41752300	0.62756400	-1.00118300
H	-5.44557100	0.97319100	-1.03491600
C	-3.37450600	1.38174900	-1.52571800
H	-3.56417100	2.32771700	-2.02433900
C	-2.06635000	0.93142200	-1.41393100
H	-1.30712200	1.54620100	-1.85811200
C	0.42368300	1.94525200	-0.64265900
C	0.61852600	2.94006300	-1.58477000
H	0.89328600	2.65900900	-2.59121400
C	0.44883900	4.30300400	-1.25851000

H	0.61214100	5.05055200	-2.02894100
C	0.06143000	4.67957300	0.00578100
H	-0.08726600	5.72547700	0.25996400
C	-0.14368500	3.69268800	1.00104400
C	0.05667800	2.30582800	0.69650300
C	-0.44029500	1.69174800	2.86168900
H	-0.53978000	0.88544800	3.58737900
C	-0.68353200	3.02791900	3.25992400
H	-0.97739800	3.24659800	4.28151600
C	-0.52945600	4.02284400	2.32554000
H	-0.69477400	5.06645300	2.58074600
C	-2.74280900	-2.60585700	-0.22109100
F	-3.86058200	-3.22059900	-0.67743300
F	-2.65464200	-2.96564900	1.08724000
F	-1.71720900	-3.18235500	-0.88853500

2e-TS23'

Charge = 0, Multiplicity = 1

O	-2.78800200	-2.82429200	-1.13823600
O	-2.15756300	2.22977600	1.58450800
N	-0.58881400	0.94878200	0.44393800
N	2.30219600	0.80420100	-0.05579600
C	-4.97193800	2.03211600	0.81280500
H	-4.75646500	2.09418100	1.88439200
H	-6.05695300	2.06286900	0.67183300
H	-4.54178300	2.93284900	0.36145700
C	-3.44953800	-1.66907800	-0.85452100
C	-4.81482200	-1.43066200	-0.85633500
H	-5.52614700	-2.17491400	-1.19803700
C	-5.25054400	-0.19027400	-0.34752600
H	-6.31837700	0.01048600	-0.34462300
C	-4.39912700	0.77674200	0.20858900
C	-3.00702600	0.50975400	0.17556400
C	-2.57875200	-0.66948500	-0.42485400
C	-1.25373500	-1.19060900	-0.35339500
C	-1.37830700	-2.63997500	-0.78098000
H	-0.79216200	-2.86627100	-1.67193100
H	-1.12746900	-3.36457200	0.00204300
C	-0.26599300	-0.43784000	0.19472700
C	-1.94960500	1.30329800	0.81685400
C	0.84185100	-1.07299800	0.95435300
C	1.71392600	-2.07007300	0.47745900
C	2.56407900	-2.74756500	1.36137400

H	3.24029800	-3.50038400	0.96824900
C	2.57421000	-2.44878200	2.71864200
H	3.23799000	-2.98388600	3.39030500
C	1.73325100	-1.44112200	3.19708500
H	1.73351600	-1.18271200	4.25220100
C	0.88035200	-0.77159400	2.32903400
H	0.21982900	0.00233500	2.70495500
C	0.23058400	2.05812700	0.01110300
C	-0.38284100	3.27244300	-0.28555800
H	-1.45156000	3.38143600	-0.18683300
C	0.33353300	4.41296200	-0.69257800
H	-0.22121900	5.32516200	-0.89128200
C	1.69861600	4.37921100	-0.83796100
H	2.26310100	5.25742500	-1.13762900
C	2.37278200	3.16054400	-0.60852100
C	1.65267400	1.98179900	-0.20434800
C	3.60244700	0.73120000	-0.23616800
H	4.04964800	-0.25317100	-0.11199500
C	4.40300200	1.84028500	-0.59087600
H	5.47443200	1.72518900	-0.71985200
C	3.77664400	3.04689700	-0.78215800
H	4.33636700	3.93092900	-1.07658500
C	1.91784200	-2.38627800	-0.97712500
F	3.23893400	-2.37914500	-1.29627000
F	1.47454700	-3.63694200	-1.29375600
F	1.31389900	-1.53346600	-1.82463600

2e-TS23

Charge = 0, Multiplicity = 1

O	-4.21620200	1.48737200	-1.13336200
O	-0.56907900	-1.65942900	1.76253800
N	-0.05211400	-0.23353100	-0.03824400
N	1.36858600	-2.78611800	0.34892600
C	-2.84091900	-3.57917200	1.02859000
H	-1.91181100	-3.98273100	0.61177000
H	-3.63072100	-4.32706400	0.90671500
H	-2.66392500	-3.43524300	2.10056300
C	-4.04097700	0.18669400	-0.75593300
C	-4.98793400	-0.81325700	-0.59328200
H	-6.03414100	-0.65970300	-0.83513800
C	-4.54017800	-2.04097300	-0.05986100
H	-5.27137000	-2.83429000	0.07126600
C	-3.22414800	-2.28163800	0.36630500

C	-2.28111300	-1.25049200	0.16192400
C	-2.71022100	-0.07878200	-0.44945600
C	-1.93094100	1.10804500	-0.60773200
C	-2.93404700	2.18502200	-0.97655700
H	-3.05882900	2.95383800	-0.20496400
H	-2.72475400	2.67625200	-1.92964100
C	-0.60236300	1.05843200	-0.33920400
C	-0.91867200	-1.15123800	0.72722800
C	0.25514900	2.26578300	-0.25323800
C	1.13353200	2.53186900	0.82172300
C	1.89306600	3.70538900	0.82846400
H	2.55972200	3.89731300	1.66049500
C	1.78840900	4.63687200	-0.20167900
H	2.38797400	5.54133800	-0.17679100
C	0.90273900	4.39995700	-1.25140000
H	0.80421000	5.11669400	-2.06139000
C	0.15286300	3.22824200	-1.27116600
H	-0.50272200	3.02759500	-2.11227300
C	1.07977300	-0.65729300	-0.78836600
C	1.48665800	0.11579500	-1.87216000
H	0.87767100	0.94463000	-2.19638100
C	2.67965500	-0.12908000	-2.58047700
H	2.94509900	0.53974000	-3.39416400
C	3.48790300	-1.18891700	-2.25386500
H	4.41834600	-1.38122100	-2.78033300
C	3.06289600	-2.08164500	-1.24100700
C	1.83870000	-1.85993500	-0.52068300
C	2.07275800	-3.87103100	0.59320300
H	1.63738100	-4.57885900	1.29781900
C	3.32224600	-4.14702300	-0.00601800
H	3.86533400	-5.05210500	0.24745900
C	3.80237200	-3.25141500	-0.93027200
H	4.74077900	-3.42792400	-1.44993100
C	1.26242800	1.61210700	2.01384200
F	1.84109100	2.24758500	3.06336300
F	2.02802800	0.52906300	1.76404400
F	0.06097800	1.17688900	2.45072600

2d-Conf-1

Charge = 0, Multiplicity = 1

O	3.61620600	2.19026400	-1.27945000
O	1.05931300	-2.52598600	1.08971100
N	0.25326700	-0.48133000	0.43164900

N	-1.36619800	-1.51979100	-1.57577700
C	3.92760500	-3.06943700	0.88201500
H	3.55820300	-3.09690300	1.91235900
H	4.95901600	-3.43704000	0.87198400
H	3.30232400	-3.76804500	0.31689300
C	3.86787400	0.93585200	-0.79613600
C	5.06533000	0.25557300	-0.70474300
H	6.00288900	0.68760900	-1.03812700
C	5.02238900	-1.04709300	-0.15007100
H	5.95935200	-1.59244800	-0.07350700
C	3.86073100	-1.67824800	0.30659700
C	2.64004300	-0.95394000	0.20360300
C	2.69728000	0.32021200	-0.34788000
C	1.60322600	1.20029100	-0.53700200
C	2.17914900	2.45842300	-1.14625300
H	1.78999100	2.68564100	-2.14438200
H	2.06225400	3.34541900	-0.51401000
C	0.37422300	0.79682300	-0.14321600
C	1.30924100	-1.42085300	0.61492500
C	-0.84324700	1.63718500	-0.27962700
C	-1.33542700	2.41904500	0.77471200
C	-2.46890600	3.21587800	0.62897400
H	-2.82517900	3.80543500	1.46650300
C	-3.12570000	3.24758000	-0.60091600
H	-4.00993100	3.86713100	-0.71715700
C	-2.64548100	2.49425700	-1.67287800
H	-3.15295300	2.52168400	-2.63219800
C	-1.51286700	1.69964500	-1.50998500
H	-1.14058900	1.09092900	-2.32589600
C	-1.06333600	-0.96539500	0.74213200
C	-1.52911500	-0.93560700	2.03530900
H	-0.88828900	-0.54591000	2.81759500
C	-2.82831400	-1.40196600	2.34240200
H	-3.17714700	-1.36252800	3.36960400
C	-3.64112200	-1.90029500	1.35029000
H	-4.64096000	-2.25945200	1.57875600
C	-3.18138600	-1.95850800	0.00964000
C	-1.86769000	-1.49094100	-0.30959400
C	-2.13137800	-2.01089300	-2.53129500
H	-1.70236100	-2.02663800	-3.53222400
C	-3.44443500	-2.49990100	-2.32580300
H	-4.01472400	-2.88725800	-3.16397300
C	-3.96649700	-2.46929300	-1.05451700
H	-4.97023100	-2.83162400	-0.84815000

Cl	-0.49990800	2.42513300	2.32344900
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2d-Conf-2

Charge = 0, Multiplicity = 1

O	-3.54976700	2.53872600	-0.06582500
O	-1.25596200	-2.85194300	-0.18491000
N	-0.33183800	-0.76448300	-0.46075000
N	1.53196700	-0.61956700	1.60556500
C	-4.12535600	-3.11513100	0.25525500
H	-3.77465500	-3.59919500	-0.66203500
H	-5.17234000	-3.39198800	0.41715700
H	-3.52397200	-3.53409800	1.06838200
C	-3.85916000	1.21396400	0.05191300
C	-5.08825100	0.61681900	0.24813000
H	-6.00141400	1.19393100	0.34747300
C	-5.11175900	-0.79724700	0.31171000
H	-6.07352400	-1.27848000	0.46843000
C	-3.98558700	-1.61654400	0.18009800
C	-2.73235500	-0.97519400	-0.02646300
C	-2.72035800	0.41348400	-0.06701300
C	-1.58578500	1.23615600	-0.27290500
C	-2.10074800	2.65843500	-0.26447900
H	-1.70587900	3.26142800	0.55842400
H	-1.93477500	3.19399600	-1.20557300
C	-0.38029200	0.64850900	-0.46948900
C	-1.43654900	-1.63727000	-0.21516200
C	0.85552500	1.39759100	-0.80024100
C	1.44778400	2.32816400	0.06900200
C	2.60473200	3.02412500	-0.28523300
H	3.03822100	3.72941900	0.41518000
C	3.19297000	2.80088300	-1.52726200
H	4.09541300	3.34104500	-1.79726600
C	2.61823100	1.89131000	-2.41680600
H	3.06361500	1.71997800	-3.39188500
C	1.46495300	1.20570700	-2.05291500
H	1.01215200	0.50396000	-2.74423200
C	0.94295400	-1.41628700	-0.57893100
C	1.24916000	-2.13807900	-1.71012900
H	0.51247600	-2.21530900	-2.50266200
C	2.50640500	-2.76827300	-1.84581500
H	2.72460100	-3.32896000	-2.74952200
C	3.44790700	-2.66577300	-0.84659700
H	4.42050900	-3.13983200	-0.94775000

C	3.15675300	-1.94161600	0.33678600
C	1.87876100	-1.31614600	0.48970900
C	2.41941500	-0.52127500	2.57442700
H	2.11250900	0.04436100	3.45252600
C	3.71472600	-1.09315400	2.52471100
H	4.39442300	-0.96686600	3.36137200
C	4.07870900	-1.80278100	1.40534700
H	5.06070900	-2.26131000	1.32235600
Cl	0.76942000	2.65527900	1.65740600

2d-Conf-3

Charge = 0, Multiplicity = 1

O	-3.61626900	2.18999700	-1.27976300
O	-1.05924700	-2.52576200	1.09020300
N	-0.25320000	-0.48127000	0.43158600
N	1.36625800	-1.52002300	-1.57568200
C	-3.92747800	-3.06946900	0.88227400
H	-3.30227600	-3.76813700	0.31713000
H	-4.95889500	-3.43706300	0.87239600
H	-3.55794000	-3.09686900	1.91257100
C	-3.86789000	0.93562900	-0.79631000
C	-5.06532900	0.25533900	-0.70478400
H	-6.00291600	0.68733600	-1.03814400
C	-5.02233900	-1.04726400	-0.14997700
H	-5.95928500	-1.59263300	-0.07331700
C	-3.86065200	-1.67833400	0.30673100
C	-2.63997900	-0.95401300	0.20360400
C	-2.69726100	0.32006200	-0.34804600
C	-1.60323800	1.20016500	-0.53726900
C	-2.17924400	2.45827500	-1.14647200
H	-2.06243100	3.34520900	-0.51410800
H	-1.79005500	2.68564500	-2.14454900
C	-0.37422300	0.79682600	-0.14341800
C	-1.30917300	-1.42078600	0.61506300
C	0.84323700	1.63722100	-0.27980400
C	1.33517800	2.41925300	0.77452600
C	2.46870300	3.21604400	0.62892400
H	2.82481800	3.80569900	1.46645200
C	3.12576200	3.24755200	-0.60082900
H	4.01002700	3.86707200	-0.71697800
C	2.64575700	2.49409700	-1.67279100
H	3.15344000	2.52140800	-2.63200300
C	1.51311100	1.69950500	-1.51003000

H	1.14097500	1.09070400	-2.32594500
C	1.06340300	-0.96525800	0.74214400
C	1.52922400	-0.93520900	2.03529900
H	0.88838900	-0.54541300	2.81753100
C	2.82843100	-1.40149100	2.34245200
H	3.17730200	-1.36181400	3.36963100
C	3.64122700	-1.89997900	1.35041500
H	4.64108900	-2.25903900	1.57892600
C	3.18146200	-1.95845100	0.00978700
C	1.86775200	-1.49097900	-0.30950000
C	2.13143000	-2.01130000	-2.53111500
H	1.70241600	-2.02720300	-3.53204400
C	3.44448800	-2.50028400	-2.32555300
H	4.01475100	-2.88780400	-3.16366600
C	3.96656500	-2.46943400	-1.05428800
H	4.97029500	-2.83173400	-0.84784400
Cl	0.49938000	2.42550000	2.32311200

2d-Conf-4

Charge = 0, Multiplicity = 1

O	3.54994200	2.53855900	-0.06591300
O	1.25542000	-2.85181100	-0.18517400
N	0.33170700	-0.76427300	-0.46125700
N	-1.53128800	-0.62076700	1.60561500
C	4.12478300	-3.11539400	0.25507500
H	3.52308200	-3.53425300	1.06802300
H	5.17167600	-3.39240300	0.41730700
H	3.77429700	-3.59942900	-0.66231200
C	3.85919700	1.21374500	0.05172600
C	5.08820500	0.61643500	0.24797800
H	6.00143800	1.19342600	0.34738100
C	5.11152600	-0.79763800	0.31151800
H	6.07321400	-1.27900100	0.46831300
C	3.98525100	-1.61678800	0.17985000
C	2.73212300	-0.97527200	-0.02679500
C	2.72032000	0.41340100	-0.06734800
C	1.58585300	1.23621600	-0.27326600
C	2.10091600	2.65844800	-0.26437800
H	1.93490200	3.19440600	-1.20522800
H	1.70613300	3.26111800	0.55882400
C	0.38031300	0.64873000	-0.46996300
C	1.43622600	-1.63716400	-0.21557200
C	-0.85550700	1.39807800	-0.80012500

C	-1.44756400	2.32802400	0.06989900
C	-2.60456700	3.02427300	-0.28358100
H	-3.03788400	3.72906900	0.41743800
C	-3.19305700	2.80192200	-1.52565700
H	-4.09556900	3.34225500	-1.79509900
C	-2.61850700	1.89299500	-2.41598200
H	-3.06410300	1.72240700	-3.39109500
C	-1.46514800	1.20713200	-2.05283700
H	-1.01250500	0.50585800	-2.74474100
C	-0.94313900	-1.41592400	-0.57963900
C	-1.24971900	-2.13694200	-1.71123800
H	-0.51321900	-2.21381500	-2.50397400
C	-2.50715200	-2.76671800	-1.84705900
H	-2.72569900	-3.32678100	-2.75106700
C	-3.44842000	-2.66461800	-0.84757100
H	-4.42117300	-3.13834000	-0.94885300
C	-3.15681000	-1.94140000	0.33626200
C	-1.87861400	-1.31637600	0.48931200
C	-2.41845000	-0.52299100	2.57479100
H	-2.11112800	0.04184300	3.45326100
C	-3.71395700	-1.09442600	2.52496600
H	-4.39341500	-0.96853300	3.36188300
C	-4.07845200	-1.80310600	1.40516900
H	-5.06061500	-2.26127200	1.32209700
Cl	-0.76877300	2.65393400	1.65840200

2d-int24

Charge = 0, Multiplicity = 1

O	-1.00200900	3.05261200	2.00031400
O	0.55529700	0.54957600	-2.65047100
N	-0.03918600	-0.54176400	-0.64697400
N	2.63807400	-0.99027000	-1.15023400
C	3.26456500	2.31995300	-1.67445000
H	4.05669800	1.66850500	-1.28478900
H	3.72377900	3.27787800	-1.93981800
H	2.87518900	1.85674000	-2.58430200
C	0.13178100	2.96855500	1.25118500
C	1.21307300	3.84541300	1.21055400
H	1.27281400	4.71022800	1.86248000
C	2.21207300	3.58347200	0.26033800
H	3.05854600	4.26355800	0.20873400
C	2.17030500	2.51103300	-0.65698800
C	1.09133500	1.62333300	-0.55752000

C	0.11262000	1.86784000	0.40753900
C	-1.14532400	1.17046700	0.54533100
C	-1.93001600	2.01806300	1.52866300
H	-2.78749600	2.53574600	1.09467800
H	-2.26695400	1.44627900	2.39850700
C	-1.30298000	-0.01558100	-0.10565400
C	0.65156300	0.50244000	-1.45144500
C	-2.47990500	-0.87994200	-0.26446900
C	-3.81067100	-0.43120100	-0.39909200
C	-4.88786800	-1.31358200	-0.49181400
H	-5.89114700	-0.91441200	-0.59216200
C	-4.66499500	-2.68663100	-0.49450900
H	-5.50560200	-3.36947900	-0.57092100
C	-3.35529100	-3.16710200	-0.43770000
H	-3.15921500	-4.23429200	-0.47564200
C	-2.29307700	-2.27981500	-0.33609600
H	-1.28286300	-2.66512300	-0.30447000
C	0.76614700	-1.20632900	0.31679400
C	0.27221900	-1.65033000	1.53568900
H	-0.74734700	-1.42640900	1.82055800
C	1.07146400	-2.40388400	2.42404100
H	0.63065500	-2.73531800	3.35993100
C	2.37846300	-2.71481800	2.12888600
H	2.99062400	-3.29514000	2.81305700
C	2.93750000	-2.25350400	0.91150300
C	2.13735400	-1.49029400	0.00497000
C	3.89325800	-1.23309500	-1.47010400
H	4.24649500	-0.81002100	-2.40838400
C	4.76280400	-1.99578400	-0.65634900
H	5.78703800	-2.16870900	-0.97083600
C	4.28237900	-2.49597900	0.53193400
H	4.92066500	-3.07541900	1.19391500
Cl	-4.20076800	1.27564300	-0.60036800

2d-TS12'

Charge = 0, Multiplicity = 1

O	4.33530500	1.35073700	0.67824300
O	0.26379400	-2.59598500	-0.56509800
N	0.10653300	-0.30752800	-0.22243600
N	-2.17829200	-1.56284700	-1.34598400
C	2.79416500	-3.93529200	-0.70868600
H	2.08506400	-4.33913000	0.02084200
H	3.66745100	-4.59455200	-0.74930400

H	2.28578400	-3.96853300	-1.67739800
C	4.12565200	0.04208800	0.36885400
C	5.03445700	-0.99853600	0.36148000
H	6.07644900	-0.85131100	0.62425000
C	4.54850700	-2.26947700	-0.01119400
H	5.25290500	-3.09658700	-0.03289600
C	3.21495900	-2.53429900	-0.34851100
C	2.30815000	-1.44219000	-0.31864900
C	2.79196300	-0.19013000	0.02682200
C	2.05299700	1.02717500	0.05131600
C	3.12717800	2.08264300	0.31694900
H	3.40804700	2.66903600	-0.56538600
H	2.88107000	2.76863400	1.13261300
C	0.68747800	1.00622700	-0.14409400
C	0.85405200	-1.53299100	-0.44448200
C	-0.07671800	2.29391900	-0.32263500
C	-1.45899100	2.63277900	-0.27129800
C	-1.89770700	3.96471200	-0.25074100
H	-2.96332400	4.14419700	-0.16457300
C	-1.02221600	5.03150700	-0.37801500
H	-1.39196700	6.05168000	-0.35713300
C	0.31978500	4.74203500	-0.60101700
H	1.03886800	5.52943200	-0.80474100
C	0.74594400	3.42387500	-0.58341700
H	1.77251900	3.25782000	-0.84717100
C	-1.06249900	-0.61111900	0.56502800
C	-1.06861600	-0.27131500	1.90006000
H	-0.22566800	0.27427900	2.31204200
C	-2.15024600	-0.63483700	2.73469100
H	-2.13336400	-0.34706700	3.78154900
C	-3.19682500	-1.37043800	2.23056100
H	-4.02389900	-1.67180100	2.86795300
C	-3.21738400	-1.73915000	0.85966300
C	-2.14994100	-1.34217600	-0.00372900
C	-3.20359900	-2.22093400	-1.84332200
H	-3.20168300	-2.37428900	-2.92195200
C	-4.28358600	-2.71695500	-1.06990000
H	-5.08874100	-3.26397700	-1.55028700
C	-4.29084800	-2.46433500	0.27978900
H	-5.10896800	-2.79773600	0.91324300
Cl	-2.81045200	1.51928200	-0.36947100

Charge = 0, Multiplicity = 1

O	-2.69024000	2.31815300	1.62256700
O	-1.56338300	-2.00216500	-2.12258100
N	-0.18493500	-0.52404100	-0.98490200
N	0.80291700	-0.82220600	1.65076300
C	-4.34862200	-2.19738900	-1.38371500
H	-4.21937100	-2.03685400	-2.45895500
H	-5.40128000	-2.42732200	-1.18932100
H	-3.74892000	-3.07846300	-1.13284500
C	-3.22698000	1.25491800	0.97608300
C	-4.51498100	0.75733900	1.06864500
H	-5.25389100	1.20796500	1.72251500
C	-4.83076400	-0.36179000	0.27333300
H	-5.83945700	-0.76161500	0.33205000
C	-3.92188800	-0.99253100	-0.58613100
C	-2.60609900	-0.46495300	-0.63957900
C	-2.29609400	0.64827800	0.13195100
C	-1.06083500	1.37140700	0.14813000
C	-1.37070200	2.56993900	1.04203900
H	-0.66387700	2.68540700	1.86591000
H	-1.46693600	3.51418800	0.51025500
C	0.02779500	0.82172800	-0.48262100
C	-1.47781400	-1.04989900	-1.35910200
C	1.38535100	1.39531000	-0.73818200
C	1.84560400	2.71456400	-0.47961900
C	3.18775000	3.08757500	-0.59087400
H	3.46149300	4.10672900	-0.34191800
C	4.14277300	2.19855700	-1.06462500
H	5.18162800	2.50201000	-1.14762400
C	3.71006800	0.94669700	-1.48997800
H	4.39989000	0.24260400	-1.94507500
C	2.38055900	0.58103000	-1.33764200
H	2.10749600	-0.38971000	-1.70454800
C	0.72331300	-1.58918600	-0.63927500
C	1.08795800	-2.53170900	-1.58435400
H	0.72498100	-2.42494900	-2.59638900
C	1.93726400	-3.60975500	-1.25210100
H	2.19996900	-4.32706100	-2.02375400
C	2.44186600	-3.74063800	0.02032700
H	3.10838500	-4.55894800	0.27869500
C	2.08694900	-2.79994200	1.01858200
C	1.20011100	-1.71776200	0.70687600
C	1.26356600	-0.94988700	2.87780400
H	0.91517300	-0.21516800	3.60259800

C	2.15937600	-1.96751600	3.28492400
H	2.50516300	-2.00871100	4.31281500
C	2.56354800	-2.89089400	2.35159000
H	3.24276200	-3.69780200	2.61430000
Cl	0.79502800	4.09779900	-0.17614900

2d-TS23'

Charge = 0, Multiplicity = 1

O	-3.09900900	-2.53038900	-1.28426900
O	-1.65638600	2.18188700	1.70551900
N	-0.31812500	0.78375100	0.41615000
N	2.49437800	0.25774800	-0.24848700
C	-4.47846300	2.47477600	0.99286700
H	-4.23700700	2.43521300	2.05996700
H	-5.54819900	2.67915500	0.88382100
H	-3.92348300	3.32637000	0.58440100
C	-3.57192800	-1.30628600	-0.92363600
C	-4.88534700	-0.86785600	-0.86745600
H	-5.70903000	-1.47857200	-1.22142300
C	-5.11698600	0.39252800	-0.27950100
H	-6.14237500	0.74854000	-0.22906700
C	-4.11635800	1.18740900	0.29954800
C	-2.78112700	0.71932000	0.20414700
C	-2.54949600	-0.47196100	-0.47484600
C	-1.31428800	-1.18441800	-0.48002300
C	-1.67005300	-2.57787800	-0.95809100
H	-1.14066100	-2.86078100	-1.86951900
H	-1.51861000	-3.36079100	-0.20577200
C	-0.20888900	-0.61528300	0.06780000
C	-1.60353300	1.29981900	0.86289300
C	0.83194700	-1.44970800	0.71235300
C	1.52599100	-2.49997700	0.09226200
C	2.36181400	-3.35495400	0.80783000
H	2.89156500	-4.14375600	0.28431300
C	2.52503300	-3.17393100	2.18061200
H	3.17640000	-3.84034200	2.73774800
C	1.85683400	-2.12900800	2.82143300
H	1.97963400	-1.97366700	3.88925500
C	1.01987300	-1.28750000	2.09678600
H	0.49373900	-0.47845400	2.59323800
C	0.64635900	1.79513700	0.04385800
C	0.22022100	3.11248200	-0.10738000
H	-0.81237600	3.37440100	0.06006200

C	1.08942900	4.16521300	-0.44825900
H	0.67567100	5.16570100	-0.53316600
C	2.42620600	3.94083300	-0.66769600
H	3.10866400	4.74883600	-0.91487000
C	2.91049300	2.61778200	-0.58470600
C	2.03053100	1.52763000	-0.25442900
C	3.76014400	0.00584400	-0.49504100
H	4.05327100	-1.04287000	-0.47092400
C	4.71111600	1.00977900	-0.78580100
H	5.74728800	0.74801700	-0.97493600
C	4.27261500	2.31000200	-0.83734200
H	4.95222000	3.12346600	-1.07785000
Cl	1.49469800	-2.67715900	-1.66164800

2d-TS23

Charge = 0, Multiplicity = 1

O	-4.32548300	1.19307800	-0.89670100
O	-0.33804900	-1.88218700	1.63008300
N	0.00134300	-0.19758000	0.02445700
N	1.83313100	-2.52527900	0.32253400
C	-2.42310900	-3.90637000	0.71684600
H	-1.48138900	-4.18943900	0.23399700
H	-3.15237100	-4.70483700	0.54740200
H	-2.21555500	-3.84871700	1.79114000
C	-4.01457200	-0.11568500	-0.66250100
C	-4.85351000	-1.21716600	-0.60358000
H	-5.91311200	-1.14640700	-0.82451800
C	-4.27684400	-2.44172500	-0.20162200
H	-4.92289300	-3.31427300	-0.15230600
C	-2.93884500	-2.59066600	0.19488500
C	-2.10546100	-1.45282100	0.09770600
C	-2.65914200	-0.27456600	-0.38817900
C	-2.00903800	0.99499000	-0.41229100
C	-3.11795200	1.99717200	-0.67269300
H	-3.31110300	2.67333600	0.16837400
H	-2.96916100	2.59459800	-1.57518300
C	-0.68123700	1.05478000	-0.13505200
C	-0.75304800	-1.28102300	0.66854100
C	0.03374900	2.32787300	0.11462400
C	0.89312500	2.54129800	1.20885500
C	1.51350800	3.77328900	1.41791600
H	2.16819600	3.89660500	2.27370800
C	1.27959900	4.83162500	0.54327900

H	1.76640700	5.78710100	0.71309100
C	0.41941000	4.65411100	-0.54116100
H	0.22997400	5.46920700	-1.23290800
C	-0.18540100	3.41917700	-0.74631100
H	-0.81896600	3.27291200	-1.61502700
C	1.25841900	-0.35410300	-0.62278400
C	1.60847100	0.58297500	-1.59267200
H	0.88185800	1.31292300	-1.91431900
C	2.88532100	0.63446900	-2.18370000
H	3.09102600	1.41900900	-2.90607700
C	3.84805900	-0.28664000	-1.85488200
H	4.84429000	-0.25047400	-2.28632000
C	3.50684000	-1.34423000	-0.97868500
C	2.19881000	-1.43011600	-0.38594800
C	2.70559500	-3.48606200	0.54072300
H	2.34603100	-4.34139000	1.11210100
C	4.03888900	-3.45804300	0.07361600
H	4.71884900	-4.27304100	0.30117000
C	4.42477200	-2.38803800	-0.69597400
H	5.42534900	-2.32908000	-1.11685200
Cl	1.18829800	1.28457700	2.39957700

2d-TS24a

Charge = 0, Multiplicity = 1

O	-1.77805500	3.08665200	1.72717300
O	0.92412500	0.67017800	-2.54246800
N	0.10173800	-0.41194600	-0.60626800
N	2.66238300	-1.30913700	-1.32688000
C	2.90421500	2.95900800	-1.49279600
H	3.43260700	2.00319800	-1.40348800
H	3.60787400	3.76529300	-1.26441900
H	2.60256300	3.05470700	-2.54247700
C	-0.58334500	3.19262300	1.07975200
C	0.32137500	4.24948200	1.07262900
H	0.16015300	5.14550100	1.66240500
C	1.45529200	4.12100200	0.24856300
H	2.17017100	4.93949000	0.23486500
C	1.70614200	3.01085400	-0.58112200
C	0.78799600	1.94894700	-0.52151100
C	-0.31072100	2.06292800	0.32237500
C	-1.39513200	1.12311400	0.43487500
C	-2.43013600	1.85037300	1.27200700
H	-3.32356000	2.14523700	0.71640700

H	-2.73549000	1.28719400	2.15866400
C	-1.23831100	-0.11653200	-0.09730800
C	0.68935600	0.72817300	-1.36515500
C	-2.21558500	-1.21962900	-0.14778900
C	-3.57338300	-1.05461800	-0.48891700
C	-4.47730900	-2.11802300	-0.48014000
H	-5.51163200	-1.93749700	-0.75134000
C	-4.03824200	-3.39846000	-0.15960200
H	-4.74279400	-4.22458500	-0.15603300
C	-2.68759300	-3.60993700	0.12277800
H	-2.32308200	-4.60792300	0.34633600
C	-1.79982200	-2.54199400	0.11908800
H	-0.75656300	-2.72305700	0.33992200
C	1.00736400	-0.92816100	0.38338800
C	0.65798300	-1.03103400	1.72158700
H	-0.31617000	-0.69027200	2.04710200
C	1.53916000	-1.57348300	2.68234300
H	1.20894000	-1.63450300	3.71531800
C	2.79637700	-2.00061500	2.32856100
H	3.48338300	-2.40781400	3.06506200
C	3.20428200	-1.90931600	0.97474600
C	2.31156500	-1.38547000	-0.01701000
C	3.86328100	-1.71188200	-1.68933600
H	4.09822500	-1.63364200	-2.75001200
C	4.82434800	-2.23058800	-0.78982500
H	5.79769900	-2.54428300	-1.15374800
C	4.48652700	-2.33016800	0.53857700
H	5.18647400	-2.72799200	1.26895600
Cl	-4.19943000	0.48613700	-1.07668600

2d-TS24b

Charge = 0, Multiplicity = 1

O	-0.85746600	3.44211700	1.57868400
O	0.85059300	0.36778900	-2.67707200
N	-0.01293300	-0.44374800	-0.65019800
N	2.66709900	-1.10194000	-0.83814000
C	3.57063000	2.03993000	-1.66887600
H	4.30614600	1.41277700	-1.14995600
H	4.09149500	2.93717800	-2.01965800
H	3.21357900	1.48318800	-2.53813600
C	0.30986100	3.18665700	0.93524300
C	1.45734600	3.97389000	0.90070000
H	1.53363400	4.89163100	1.47374800

C	2.49760100	3.55283200	0.06035300
H	3.39644200	4.16224400	0.01114900
C	2.42990600	2.40451400	-0.75519300
C	1.27966100	1.61053900	-0.65505800
C	0.25244900	2.00608500	0.20601600
C	-1.07160700	1.41874800	0.31465000
C	-1.84332400	2.45893400	1.12168100
H	-2.57881300	3.01197300	0.53562400
H	-2.32105400	2.04585800	2.01016600
C	-1.27791400	0.18681200	-0.24629900
C	0.83372400	0.44713000	-1.47409700
C	-2.45377200	-0.68216600	-0.48680300
C	-3.81819100	-0.42171400	-0.22698900
C	-4.82339900	-1.35783700	-0.46977400
H	-5.85006300	-1.09178900	-0.24393000
C	-4.51637800	-2.60293800	-1.00787700
H	-5.30672800	-3.32326000	-1.19475900
C	-3.18842200	-2.88944800	-1.31723400
H	-2.91703600	-3.84281300	-1.76017400
C	-2.19727500	-1.95189200	-1.06517200
H	-1.17575700	-2.18044800	-1.33199000
C	0.60649300	-1.20901400	0.36410800
C	-0.08339000	-1.66593600	1.48010700
H	-1.11374200	-1.37794900	1.63761400
C	0.52993300	-2.51750500	2.42473600
H	-0.05800200	-2.85069100	3.27530400
C	1.83697500	-2.92514700	2.28853100
H	2.30378700	-3.58309700	3.01562000
C	2.58780400	-2.46465100	1.17951000
C	1.97973200	-1.59753300	0.21835200
C	3.92695800	-1.44772000	-1.01208100
H	4.43163900	-1.02739100	-1.87939000
C	4.61601800	-2.31454400	-0.13271200
H	5.65371200	-2.56797000	-0.32464400
C	3.94555700	-2.81164400	0.96103900
H	4.44105400	-3.47058800	1.66930100
Cl	-4.40566700	1.12667200	0.37637800

2d-TS34'

Charge = 0, Multiplicity = 1

O	-4.33516200	1.35010400	0.67926900
O	-0.26352500	-2.59578000	-0.56620400
N	-0.10635100	-0.30740600	-0.22288600

N	2.17896500	-1.56257300	-1.34584400
C	-2.79383400	-3.93524100	-0.71008500
H	-2.28606400	-3.96804900	-1.67913900
H	-3.66703100	-4.59463600	-0.75040800
H	-2.08419100	-4.33919800	0.01884100
C	-4.12544800	0.04157600	0.36937900
C	-5.03415800	-0.99913100	0.36177800
H	-6.07611600	-0.85210600	0.62479400
C	-4.54816100	-2.26987900	-0.01148700
H	-5.25248200	-3.09705000	-0.03336000
C	-3.21465400	-2.53444600	-0.34918300
C	-2.30793700	-1.44226400	-0.31905600
C	-2.79180700	-0.19039800	0.02701300
C	-2.05295900	1.02698500	0.05177100
C	-3.12723500	2.08225300	0.31777100
H	-2.88105100	2.76824100	1.13341100
H	-3.40841200	2.66862000	-0.56448200
C	-0.68750200	1.00625300	-0.14394800
C	-0.85384100	-1.53287100	-0.44517400
C	0.07644100	2.29405800	-0.32260700
C	1.45866400	2.63305800	-0.27147000
C	1.89730900	3.96500700	-0.25131300
H	2.96293000	4.14457900	-0.16537400
C	1.02169200	5.03169700	-0.37864700
H	1.39136200	6.05190600	-0.35807100
C	-0.32034400	4.74207600	-0.60126200
H	-1.03953500	5.52938900	-0.80492700
C	-0.74640000	3.42388100	-0.58336200
H	-1.77303200	3.25768800	-0.84683100
C	1.06246200	-0.61112000	0.56490900
C	1.06808600	-0.27157300	1.90001400
H	0.22496900	0.27392100	2.31178000
C	2.14945400	-0.63512900	2.73496800
H	2.13216400	-0.34754100	3.78186900
C	3.19629800	-1.37051000	2.23107100
H	4.02319700	-1.67188500	2.86868600
C	3.21735700	-1.73898700	0.86011900
C	2.15015700	-1.34201000	-0.00357900
C	3.20449000	-2.22051100	-1.84291600
H	3.20291300	-2.37379400	-2.92155800
C	4.28429500	-2.71647600	-1.06920200
H	5.08966400	-3.26336200	-1.54938600
C	4.29109100	-2.46399200	0.28051100
H	5.10903500	-2.79737600	0.91420200

Cl	2.81010600	1.51953400	-0.36938400
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2d-TS34

Charge = 0, Multiplicity = 1

O	2.69016400	2.31799000	1.62276900
O	1.56332700	-2.00199400	-2.12278500
N	0.18487300	-0.52406300	-0.98485300
N	-0.80302200	-0.82212000	1.65088800
C	4.34865500	-2.19708400	-1.38416100
H	3.74832400	-3.07796700	-1.13418600
H	5.40105900	-2.42759000	-1.18907700
H	4.22034600	-2.03597800	-2.45944400
C	3.22693700	1.25486300	0.97612800
C	4.51499600	0.75739700	1.06849900
H	5.25393300	1.20802800	1.72233600
C	4.83079500	-0.36162800	0.27304800
H	5.83952200	-0.76138700	0.33164100
C	3.92188400	-0.99236700	-0.58638400
C	2.60605100	-0.46488500	-0.63967000
C	2.29601900	0.64822600	0.13202900
C	1.06073600	1.37131300	0.14832400
C	1.37060800	2.56980500	1.04229100
H	1.46681400	3.51407500	0.51052900
H	0.66381200	2.68523100	1.86618900
C	-0.02785700	0.82168800	-0.48252600
C	1.47775300	-1.04981900	-1.35919400
C	-1.38540200	1.39525400	-0.73816900
C	-1.84565800	2.71450600	-0.47964700
C	-3.18772300	3.08765000	-0.59147000
H	-3.46148400	4.10681000	-0.34255900
C	-4.14262300	2.19873900	-1.06566500
H	-5.18140800	2.50230600	-1.14913100
C	-3.70987300	0.94682500	-1.49081600
H	-4.39958700	0.24278600	-1.94615900
C	-2.38045400	0.58104500	-1.33797900
H	-2.10733100	-0.38972100	-1.70477800
C	-0.72330900	-1.58922800	-0.63911800
C	-1.08789500	-2.53183700	-1.58414100
H	-0.72491900	-2.42511200	-2.59617900
C	-1.93710900	-3.60993600	-1.25183100
H	-2.19975100	-4.32730700	-2.02344600
C	-2.44170300	-3.74078700	0.02060200
H	-3.10814900	-4.55914000	0.27902000

C	-2.08687000	-2.79999800	1.01879600
C	-1.20012500	-1.71775300	0.70703600
C	-1.26366000	-0.94978500	2.87793400
H	-0.91533500	-0.21499800	3.60269300
C	-2.15937600	-1.96747600	3.28510300
H	-2.50516000	-2.00865700	4.31299600
C	-2.56346100	-2.89092900	2.35180800
H	-3.24260400	-3.69788700	2.61455100
Cl	-0.79511500	4.09759000	-0.17541600

2d-TS41'

Charge = 0, Multiplicity = 1

O	-3.29004500	-2.31718900	-1.66085600
O	-1.40389600	2.01890300	1.64206400
N	-0.22367900	0.65990600	0.16443000
N	2.52408500	0.01279300	-0.63138800
C	-4.23574300	2.53673800	1.12031600
H	-3.94355000	2.39016100	2.16510200
H	-5.29449000	2.81246600	1.08826100
H	-3.64870800	3.38616100	0.75424400
C	-3.67080900	-1.10790700	-1.16025800
C	-4.94865900	-0.59890800	-0.99443500
H	-5.82727200	-1.12257900	-1.35572600
C	-5.06798600	0.61581900	-0.28731400
H	-6.06437200	1.02737400	-0.15104900
C	-3.99138100	1.29540300	0.30285200
C	-2.69582500	0.75692200	0.09761800
C	-2.57899000	-0.38240600	-0.68860300
C	-1.39448300	-1.16147500	-0.81521300
C	-1.85668700	-2.48529700	-1.39729100
H	-1.38698900	-2.72517800	-2.35405000
H	-1.73044500	-3.33731400	-0.71929600
C	-0.22738000	-0.71196100	-0.28223600
C	-1.44836500	1.20806400	0.73169000
C	0.79492200	-1.71832100	0.09560200
C	1.25964000	-1.88748700	1.41193500
C	2.09763400	-2.94446000	1.76286600
H	2.43820300	-3.03108500	2.78912900
C	2.47747200	-3.88337700	0.80574700
H	3.12783400	-4.70651900	1.08529300
C	2.00959500	-3.75518600	-0.50340100
H	2.29548900	-4.47756100	-1.26242300
C	1.17890000	-2.69276300	-0.84305200

H	0.85523300	-2.57078900	-1.87121900
C	0.80375300	1.63215000	-0.11987000
C	0.47243900	2.98588800	-0.12168200
H	-0.53490100	3.30131000	0.09806200
C	1.40984000	4.00461800	-0.37189500
H	1.06812900	5.03491600	-0.33857000
C	2.72293900	3.71301000	-0.64982700
H	3.45699300	4.49351900	-0.82756500
C	3.10980700	2.35803700	-0.72339200
C	2.15815600	1.30499000	-0.48455500
C	3.75865300	-0.30412100	-0.95153600
H	3.96827100	-1.36815100	-1.05444300
C	4.77575900	0.65383800	-1.16275400
H	5.78366000	0.34053300	-1.41575100
C	4.43735200	1.98052300	-1.05355400
H	5.17173800	2.76341400	-1.22441400
Cl	0.80062000	-0.76513300	2.68864300

2d-TS41

Charge = 0, Multiplicity = 1

O	4.32538200	1.19366000	-0.89652000
O	0.33840300	-1.88219500	1.63023400
N	-0.00124700	-0.19754200	0.02472700
N	-1.83293900	-2.52534400	0.32284600
C	2.42362600	-3.90615800	0.71664500
H	2.21628400	-3.84869300	1.79099200
H	3.15288800	-4.70456800	0.54692900
H	1.48182200	-4.18918400	0.23393700
C	4.01464200	-0.11515300	-0.66235900
C	4.85368800	-1.21656100	-0.60362900
H	5.91326300	-1.14568100	-0.82465700
C	4.27717000	-2.44122400	-0.20176000
H	4.92330900	-3.31371200	-0.15257900
C	2.93921000	-2.59034600	0.19480600
C	2.10570900	-1.45257200	0.09781100
C	2.65925600	-0.27419400	-0.38791900
C	2.00900000	0.99528500	-0.41193200
C	3.11778400	1.99760800	-0.67233200
H	2.96884800	2.59511300	-1.57474300
H	3.31093800	2.67369900	0.16879300
C	0.68118200	1.05489600	-0.13473300
C	0.75330400	-1.28095000	0.66870200
C	-0.03406400	2.32787200	0.11476200

C	-0.89380700	2.54114000	1.20873900
C	-1.51448000	3.77301600	1.41761300
H	-2.16945000	3.89621200	2.27320700
C	-1.28049800	4.83139700	0.54305200
H	-1.76752700	5.78678600	0.71272400
C	-0.41994300	4.65404700	-0.54112400
H	-0.23043900	5.46918300	-1.23280500
C	0.18515500	3.41922500	-0.74609900
H	0.81901200	3.27309200	-1.61462400
C	-1.25818400	-0.35429600	-0.62274900
C	-1.60811500	0.58260300	-1.59285100
H	-0.88149200	1.31256600	-1.91444300
C	-2.88485900	0.63392400	-2.18412600
H	-3.09048700	1.41834300	-2.90665500
C	-3.84758600	-0.28721500	-1.85536100
H	-4.84373000	-0.25120200	-2.28701600
C	-3.50646100	-1.34464500	-0.97893200
C	-2.19855600	-1.43032300	-0.38589200
C	-2.70537400	-3.48616100	0.54100000
H	-2.34587100	-4.34135700	1.11261400
C	-4.03856200	-3.45834000	0.07357800
H	-4.71849400	-4.27337300	0.30108900
C	-4.42436400	-2.38849200	-0.69627000
H	-5.42484400	-2.32970000	-1.11740300
Cl	-1.18907500	1.28439100	2.39941700

2f-(R)

Charge = 0, Multiplicity = 1

O	3.18129800	-3.29670300	-0.62072000
O	2.00230900	2.28117700	0.75747100
N	0.67719200	0.44016000	0.43980000
N	-0.44118900	2.24486700	-1.37881500
C	4.89923500	2.05524200	0.30665600
H	4.41304400	2.74955600	-0.38740000
H	5.98286100	2.14136700	0.17658900
H	4.64547200	2.39571500	1.31649100
C	3.76198000	-2.07362100	-0.41022600
C	5.08866100	-1.70843800	-0.50084100
H	5.86911000	-2.41734300	-0.75709800
C	5.39804200	-0.34784900	-0.24895300
H	6.44072200	-0.04913700	-0.31698000
C	4.45598200	0.63388400	0.07141500
C	3.09123700	0.23033900	0.15417500

C	2.80460400	-1.11139700	-0.07647900
C	1.52130400	-1.70554800	-0.07191300
C	1.72802300	-3.16088600	-0.42613900
H	1.44098600	-3.85682700	0.36739200
H	1.23549500	-3.46195800	-1.35668100
C	0.43722300	-0.92307900	0.16015600
C	1.94054800	1.08078900	0.46471200
C	-0.95247800	-1.42716900	0.11351900
C	-1.89136200	-0.91686900	-0.79234200
C	-3.19071200	-1.41845000	-0.84514000
H	-3.89101400	-1.00281700	-1.55969800
C	-3.56838700	-2.45607200	0.01850000
C	-2.63226000	-2.98604300	0.91926400
H	-2.93885800	-3.79038400	1.58097500
C	-1.34109000	-2.47631000	0.96275100
H	-0.62804400	-2.88160600	1.67459900
C	-0.43274300	1.27326700	0.82004400
C	-0.96689300	1.16440800	2.08314500
H	-0.53450700	0.45628300	2.78285400
C	-2.07305600	1.95809900	2.46708800
H	-2.48055500	1.85197300	3.46773900
C	-2.62301700	2.85699400	1.58177500
H	-3.47168800	3.47252800	1.86736500
C	-2.09028300	2.99062700	0.27317300
C	-0.97699800	2.18743300	-0.12608900
C	-0.97560200	3.09398500	-2.23789600
H	-0.53208700	3.11887500	-3.23213300
C	-2.06635700	3.94641100	-1.94071600
H	-2.44731300	4.62013400	-2.70142500
C	-2.62335000	3.89008500	-0.68524800
H	-3.46738700	4.51796300	-0.41248600
H	-1.60251200	-0.12557200	-1.47575400
O	-4.80988600	-3.01378300	0.05492700
C	-5.80070700	-2.50487800	-0.83816400
H	-6.70565900	-3.08087400	-0.63603200
H	-5.99527400	-1.44193600	-0.65187400
H	-5.50383300	-2.64637900	-1.88411900

2f-(S)

Charge = 0, Multiplicity = 1

O	3.12661000	-3.21711600	0.63617100
O	2.15919900	2.38006800	-0.81778700
N	0.76159100	0.58333500	-0.52461800

N	-0.67425400	1.40295300	1.70990100
C	5.05835000	1.99135800	-0.62609400
H	4.72724700	2.30816400	-1.62104900
H	6.15268800	2.01342100	-0.60387400
H	4.68482800	2.74130300	0.07977900
C	3.75434000	-2.02843300	0.37105500
C	5.10199700	-1.73625200	0.35115000
H	5.85997300	-2.48077800	0.57131900
C	5.46527000	-0.40559200	0.02279700
H	6.52462900	-0.16355700	0.00620300
C	4.55707500	0.61122600	-0.28584500
C	3.17075600	0.27979600	-0.26525300
C	2.82824400	-1.02402700	0.07647800
C	1.51941100	-1.55578100	0.13777800
C	1.67320400	-3.01201900	0.51584500
H	1.22928300	-3.26958000	1.48175600
H	1.29841300	-3.70709900	-0.24272700
C	0.47060900	-0.75553200	-0.17806300
C	2.05030700	1.17563800	-0.55803900
C	-0.93124500	-1.22471300	-0.19128500
C	-1.73098600	-1.15156500	-1.33853000
C	-3.04553300	-1.61663900	-1.33530400
H	-3.63532300	-1.54630600	-2.24131900
C	-3.58013800	-2.17201700	-0.16498300
C	-2.78456300	-2.26388800	0.98740700
H	-3.21315100	-2.69492100	1.88705000
C	-1.47815400	-1.79535700	0.97067700
H	-0.87735600	-1.84719500	1.87312100
C	-0.33979500	1.49687100	-0.66949700
C	-0.68533800	1.98561900	-1.90835900
H	-0.11013300	1.68259200	-2.77717400
C	-1.78770300	2.85837600	-2.05443400
H	-2.04543900	3.22711200	-3.04250800
C	-2.53446100	3.22539300	-0.95709700
H	-3.39095600	3.88587800	-1.06144600
C	-2.19254100	2.74681000	0.33355900
C	-1.06529800	1.88115600	0.49432300
C	-1.38468600	1.75202100	2.76634800
H	-1.05150300	1.35710600	3.72495300
C	-2.52408500	2.59139000	2.71723000
H	-3.05842400	2.82952700	3.63131900
C	-2.92301800	3.09025500	1.50015600
H	-3.78772800	3.74267100	1.41253700
H	-1.32420300	-0.73272800	-2.25259400

O	-4.85065600	-2.64806400	-0.04939800
C	-5.70491200	-2.56334400	-1.18995300
H	-6.66103800	-2.98652700	-0.87643500
H	-5.85058900	-1.52184300	-1.50038700
H	-5.30645700	-3.14485600	-2.02978000

2f-TS'

Charge = 0, Multiplicity = 1

O	2.30322700	-3.06330900	-1.93997000
O	2.26422000	1.02062800	2.15982800
N	0.72421500	0.56112800	0.48884400
N	-1.89585700	1.44977200	-0.52006900
C	5.07909900	0.27724400	1.71442600
H	4.93008100	1.34939700	1.54487400
H	6.15424100	0.07362500	1.69857900
H	4.70358400	0.06489400	2.72180900
C	3.13626600	-2.25271700	-1.21984700
C	4.49380000	-2.39866700	-0.98542100
H	5.07847700	-3.17803800	-1.46304800
C	5.08514100	-1.51550400	-0.05749500
H	6.15016300	-1.61696700	0.13222600
C	4.37271900	-0.55571000	0.67717300
C	2.98760500	-0.42055800	0.39975900
C	2.43461700	-1.22333400	-0.59629100
C	1.03902400	-1.37966000	-0.84614500
C	0.91981200	-2.64308000	-1.67194900
H	0.40716200	-3.46410500	-1.15594000
H	0.44330300	-2.48156000	-2.64207600
C	0.15268400	-0.58668500	-0.19012700
C	2.02409600	0.41910700	1.12029400
C	-1.20724300	-1.03491400	0.13967200
C	-1.97993100	-1.78051400	-0.75817600
C	-3.22932000	-2.29008700	-0.39523400
H	-3.80559200	-2.84724700	-1.12445700
C	-3.71800800	-2.07023400	0.89699900
C	-2.94359400	-1.33884100	1.81340000
H	-3.33027900	-1.18302200	2.81636300
C	-1.71095200	-0.83056600	1.43927400
H	-1.12360300	-0.26058800	2.15200800
C	0.38453500	1.92807100	0.15550600
C	1.37792200	2.90172300	0.22759600
H	2.38741200	2.63576000	0.50505000
C	1.13603400	4.26450900	-0.03216400

H	1.96381000	4.96145700	0.06139900
C	-0.11135000	4.70406900	-0.40265600
H	-0.31391100	5.75344100	-0.59667600
C	-1.14579500	3.75440900	-0.55651900
C	-0.91359500	2.35698600	-0.30290700
C	-3.08394800	1.84264800	-0.92772500
H	-3.82246800	1.05698900	-1.08527900
C	-3.42242400	3.19418400	-1.16489400
H	-4.42243100	3.46108200	-1.49187000
C	-2.44377200	4.14048000	-0.98304700
H	-2.63752100	5.19388700	-1.16812100
H	-1.63678800	-1.92868900	-1.77700500
O	-4.92087300	-2.52168100	1.35923200
C	-5.74426300	-3.26121100	0.46013000
H	-6.64321900	-3.52007500	1.02308000
H	-6.02229400	-2.65875500	-0.41340200
H	-5.24617600	-4.17979400	0.12655600

2f-TS

Charge = 0, Multiplicity = 1

O	-0.29808200	-4.06611300	1.24442300
O	-1.64351500	-0.19462900	-2.48038400
N	-0.23717000	0.16407400	-0.63316200
N	-2.16793100	2.21401200	-1.02969300
C	-4.45847600	-1.17776100	-1.33036800
H	-4.40493300	-0.10105000	-1.13374700
H	-5.46005600	-1.52921000	-1.06462500
H	-4.32821500	-1.31118800	-2.41163000
C	-1.42672100	-3.45049700	0.77691100
C	-2.73620900	-3.91180000	0.77837000
H	-3.01133200	-4.85366500	1.24164200
C	-3.70227100	-3.11916500	0.12385500
H	-4.73112500	-3.46886700	0.11956000
C	-3.40303700	-1.93029500	-0.56313000
C	-2.07015700	-1.47583300	-0.51207500
C	-1.13143000	-2.22425900	0.19354400
C	0.28266200	-1.98456500	0.24732300
C	0.85938900	-3.22771100	0.89364100
H	1.50804800	-3.81569500	0.23469500
H	1.39360200	-3.01709800	1.82519600
C	0.77046700	-0.80908100	-0.23038300
C	-1.40457100	-0.43207000	-1.31924300
C	2.16288300	-0.37411000	-0.33390700

C	2.48768400	0.81934100	-1.01371500
C	3.79970100	1.24943900	-1.12436600
H	4.04232900	2.16684400	-1.65230500
C	4.84270300	0.49901700	-0.55850300
C	4.54433900	-0.69053100	0.11934400
H	5.32765100	-1.29070400	0.56662700
C	3.22078300	-1.11228400	0.22626100
H	3.02706200	-2.03232400	0.76453500
C	-0.52445000	1.14123100	0.37793900
C	0.14596300	1.12877700	1.59381000
H	0.85852700	0.34528300	1.81137300
C	-0.07309400	2.11751500	2.57790800
H	0.48911100	2.05816000	3.50553100
C	-0.98558700	3.12552200	2.38083600
H	-1.16597800	3.88459000	3.13664300
C	-1.71234000	3.16915700	1.16565200
C	-1.48611000	2.18666000	0.14599600
C	-3.06523300	3.16101500	-1.22963200
H	-3.58588800	3.13988900	-2.18610000
C	-3.36493800	4.17126200	-0.28797300
H	-4.11447100	4.92259500	-0.51524800
C	-2.68268900	4.17043000	0.90538400
H	-2.87321500	4.92588300	1.66327500
H	1.69335400	1.40172700	-1.46597500
O	6.09656400	1.00135600	-0.72186600
C	7.19082500	0.26687900	-0.17268300
H	8.08646600	0.83962600	-0.42019900
H	7.10317200	0.17851500	0.91671000
H	7.26135000	-0.73251500	-0.61813200

5a-(R)

Charge = 0, Multiplicity = 1

C	-4.60986300	-0.51867600	0.22270800
C	-3.55943000	0.38111400	0.13900900
C	-2.23445200	-0.05904200	-0.06069000
C	-1.96409100	-1.44935300	-0.19882100
C	-3.05766100	-2.36680700	-0.10372900
C	-4.35018500	-1.89519500	0.10507100
H	-3.75876800	1.44231200	0.22415200
C	-1.14774700	0.89541900	-0.14726800
C	-0.59581000	-1.91407800	-0.42760800
H	-5.17967100	-2.58798200	0.17465900
C	0.11933100	0.45422900	-0.39595800

C	-6.02462000	-0.04605800	0.43396700
H	-6.66919700	-0.35281800	-0.39947900
H	-6.45202700	-0.48193100	1.34570300
H	-6.07289400	1.04352800	0.52033800
O	-2.78337800	-3.68780000	-0.22915000
C	-3.86080400	-4.62031100	-0.14889800
H	-3.40320000	-5.60263200	-0.28007200
H	-4.35627900	-4.57589600	0.82802900
H	-4.59658200	-4.45085700	-0.94371600
O	-0.22901700	-3.09167300	-0.50872700
N	0.37352600	-0.90331900	-0.56494300
C	1.73592200	-1.35268100	-0.67825700
C	2.53864500	-1.39738800	0.49634900
C	2.24897400	-1.72263000	-1.89918800
C	3.90619600	-1.79489400	0.36582000
C	3.59736600	-2.13219300	-2.01570500
H	1.61062700	-1.68683500	-2.77602100
C	2.76283100	-1.06945400	2.75928200
C	4.69850700	-1.80082400	1.54232100
C	4.41392300	-2.16079200	-0.90719000
H	3.98396400	-2.41506400	-2.98995000
C	4.13062100	-1.43540200	2.73966400
H	2.29783900	-0.78529000	3.70210600
H	5.74313700	-2.09341800	1.47781100
H	5.45427800	-2.46346500	-0.98939900
H	4.70475800	-1.42532100	3.66050100
C	-1.40640500	2.35529800	0.01227800
C	-1.77078700	2.88139000	1.26082500
C	-1.27199600	3.22960200	-1.07510300
C	-1.98500900	4.25086600	1.42025400
H	-1.87597400	2.21150900	2.10975900
C	-1.48270600	4.60004300	-0.91657200
H	-0.99241400	2.83089800	-2.04579500
C	-1.83872200	5.11496800	0.33195000
H	-2.25985800	4.64360300	2.39556600
H	-1.36951000	5.26493900	-1.76869300
H	-2.00194500	6.18203600	0.45647000
C	1.28093700	1.38091700	-0.49460600
C	1.92827600	1.59527800	-1.71875500
C	1.72296000	2.06467200	0.64522600
C	3.00486200	2.47792700	-1.79977500
H	1.58285500	1.07468400	-2.60635800
C	2.80107400	2.94557800	0.56309700
H	1.22252400	1.89816300	1.59280700

C	3.44528700	3.15329400	-0.65866500
H	3.49758300	2.63981100	-2.75447500
H	3.13792400	3.46831600	1.45401200
H	4.28530200	3.83955200	-0.72219800
N	1.98564000	-1.04681900	1.69223800

5a-(S)

Charge = 0, Multiplicity = 1

C	4.41535800	-1.33094100	0.27700200
C	3.57040900	-0.23352300	0.23621600
C	2.19276500	-0.38166500	-0.02776900
C	1.64892100	-1.67921100	-0.24298000
C	2.53386900	-2.80229100	-0.19912600
C	3.88930000	-2.61554300	0.05427600
H	3.97246500	0.75629700	0.41478500
C	1.32096800	0.77502300	-0.05400400
C	0.21849600	-1.84491700	-0.50012500
H	4.56048200	-3.46474700	0.08838900
C	-0.01615600	0.60662500	-0.26766400
C	5.88683700	-1.17080000	0.55773100
H	6.18112700	-1.74160700	1.44739300
H	6.48873100	-1.54912200	-0.27822400
H	6.15060700	-0.12170700	0.72141000
O	2.00156200	-4.03042300	-0.40880800
C	2.86582100	-5.16532300	-0.36694000
H	2.22323400	-6.02565600	-0.56297900
H	3.64203500	-5.10539800	-1.13888700
H	3.33359400	-5.27544500	0.61835300
O	-0.36515100	-2.90964700	-0.73195200
N	-0.53971600	-0.66122700	-0.49237000
C	-1.94549600	-0.81746300	-0.75820800
C	-2.81089000	-1.20215200	0.30473700
C	-2.43883600	-0.57476900	-2.01849400
C	-4.20798400	-1.32475200	0.02754400
C	-3.82342700	-0.69626700	-2.28292900
H	-1.75562100	-0.28052300	-2.80858600
C	-3.11624600	-1.75627700	2.51396000
C	-5.05598100	-1.69723300	1.10163700
C	-4.69203500	-1.06569000	-1.28131200
H	-4.19207700	-0.49556400	-3.28414300
C	-4.51296100	-1.91537000	2.34558500
H	-2.67308700	-1.91846900	3.49534800
H	-6.12315000	-1.80121400	0.92433700

H	-5.75707900	-1.16118400	-1.47448900
H	-5.12921000	-2.19971200	3.19241600
C	1.86757700	2.14349100	0.17563400
C	2.67561300	2.75820400	-0.79247400
C	1.57166700	2.84507600	1.35248400
C	3.16790300	4.04851000	-0.59280300
H	2.91021600	2.22191400	-1.70793000
C	2.06044200	4.13695800	1.55219800
H	0.94924300	2.37539500	2.10830200
C	2.85936300	4.74278200	0.57983000
H	3.78724900	4.51342500	-1.35522800
H	1.81773100	4.66935600	2.46800000
H	3.23934600	5.74902400	0.73426700
C	-0.97175300	1.74893100	-0.28213000
C	-1.87327900	1.93544100	0.77419100
C	-0.95883100	2.65862700	-1.34635800
C	-2.75418300	3.01631800	0.76133000
H	-1.87741300	1.23458100	1.60272600
C	-1.84186000	3.73883500	-1.35768100
H	-0.25634800	2.51692100	-2.16187200
C	-2.74217600	3.91905300	-0.30515600
H	-3.44767600	3.15491600	1.58615600
H	-1.82606300	4.43859500	-2.18867700
H	-3.42889800	4.76100200	-0.31391300
N	-2.28600100	-1.41429300	1.54521500

5a-TS

Charge = 0, Multiplicity = 1

C	0.08536200	4.01131200	0.68942100
C	0.96385000	2.92673700	0.62779300
C	0.57916800	1.72541300	0.01591800
C	-0.69182900	1.65643600	-0.59718400
C	-1.57351000	2.75319800	-0.55906400
C	-1.18744700	3.91950800	0.10467900
H	1.95339000	3.02456700	1.05770200
C	1.46871000	0.54874100	-0.09382400
C	-0.95023200	0.42854900	-1.36266600
H	-1.85572500	4.77095700	0.15923300
C	0.93041000	-0.66800300	-0.39028600
C	0.48941000	5.28277900	1.39125500
H	0.25653200	6.16381800	0.78196600
H	-0.05369000	5.39429400	2.33896900
H	1.56024500	5.29087900	1.61596300

O	-2.77338100	2.57509000	-1.16634700
C	-3.72199100	3.64220000	-1.11684100
H	-4.60069800	3.27695900	-1.65102300
H	-3.99401400	3.88140200	-0.08239100
H	-3.33604400	4.53879400	-1.61516400
O	-1.33869800	0.36557200	-2.50607300
N	-0.48044700	-0.75710100	-0.64512700
C	-1.26765700	-1.27547600	0.42757700
C	-2.68836700	-1.43705400	0.28575100
C	-0.67566000	-1.65183200	1.62452800
C	-3.43825000	-1.99587800	1.37164400
C	-1.42578300	-2.22523600	2.67478800
H	0.38473100	-1.50025600	1.77536200
C	-4.59611800	-1.16503200	-0.98232800
C	-4.84095900	-2.11780900	1.20040900
C	-2.78449800	-2.39967800	2.56240800
H	-0.90790300	-2.51276700	3.58537300
C	-5.42637100	-1.70149800	0.02811300
H	-5.03372300	-0.83056900	-1.92201700
H	-5.43450800	-2.53824300	2.00808000
H	-3.36969900	-2.82971700	3.37027300
H	-6.49706500	-1.77875000	-0.13234900
C	2.93814100	0.74088600	0.05285900
C	3.51103500	1.02237400	1.30262900
C	3.77478800	0.62393300	-1.06570900
C	4.89199800	1.17837600	1.42982200
H	2.87297600	1.09670400	2.17864100
C	5.15574600	0.77691300	-0.93761200
H	3.33679500	0.40441800	-2.03511900
C	5.71847600	1.05454300	0.31028800
H	5.32235600	1.38874200	2.40517800
H	5.79184600	0.67940500	-1.81321600
H	6.79388300	1.17292600	0.41037500
C	1.64274600	-1.96123300	-0.50137600
C	1.20101300	-2.89236800	-1.45778800
C	2.72637500	-2.30834400	0.32468700
C	1.83871300	-4.12340800	-1.60135200
H	0.35794800	-2.63515600	-2.09010700
C	3.35845800	-3.54149400	0.18203300
H	3.06421200	-1.62118600	1.09066600
C	2.92178200	-4.45281900	-0.78360200
H	1.48806400	-4.82556600	-2.35281300
H	4.19009700	-3.79460600	0.83392400
H	3.41778600	-5.41335200	-0.89250400

N	-3.28758800	-1.03967300	-0.86737100
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6-(4R,5S)

Charge = 0, Multiplicity = 1

C	-3.79236200	-3.74899900	-0.63727500
C	-2.51883900	-3.68447800	-0.08885300
C	-1.77941900	-2.48111500	-0.09757900
C	-2.37528100	-1.34256300	-0.68902600
C	-3.66582400	-1.41727000	-1.23846600
C	-4.37741100	-2.61169300	-1.21300500
H	-0.11828300	-3.32526300	1.00858700
H	-4.34011900	-4.68706500	-0.61529100
H	-2.07273200	-4.56714400	0.36160400
C	-0.47399000	-2.42705500	0.51647200
H	-4.11293500	-0.53159300	-1.68255100
H	-5.37723600	-2.66122100	-1.63327600
C	0.31615400	-1.32383900	0.58328500
N	-0.05344400	-0.07731900	0.05323400
P	-1.50613800	0.21946900	-0.83860400
C	-2.39668500	1.43627900	0.16486200
C	-2.64390500	1.18315500	1.52256500
C	-2.82898700	2.63483100	-0.41345400
C	-3.31575900	2.12844900	2.29522000
H	-2.30476200	0.25362200	1.97188100
C	-3.50203400	3.58011100	0.36328100
H	-2.62883500	2.82056500	-1.46383500
C	-3.74386700	3.32781300	1.71532500
H	-3.50487800	1.93395300	3.34701600
H	-3.83482100	4.51179600	-0.08528200
H	-4.26588800	4.06451800	2.31948800
O	-1.28603300	0.71722200	-2.23766200
C	0.95154200	0.93637500	-0.13136800
C	2.03631400	0.69470500	-1.03017100
C	0.84537900	2.14658900	0.52105500
C	3.02255200	1.71735300	-1.19690300
C	1.81262700	3.16090900	0.32775100
H	0.02143900	2.30995100	1.20596600
C	3.13042700	-0.70703300	-2.48881000
C	4.10690900	1.44417000	-2.06942700
C	2.88563800	2.95043800	-0.50763700
H	1.70485800	4.10189000	0.85827300
C	4.16580900	0.23175000	-2.71478100
H	3.15801300	-1.66896900	-2.99824000

H	4.87497400	2.19933900	-2.21307700
H	3.64055600	3.71835000	-0.65190300
H	4.98030600	-0.01424200	-3.38820100
C	1.60389500	-1.38561300	1.32200500
C	1.87470400	-0.49703500	2.37460700
C	2.55493500	-2.36098500	0.99118600
C	3.07615200	-0.58180600	3.07658400
H	1.13774900	0.25009900	2.64972800
C	3.75637200	-2.44476200	1.69548800
H	2.35474500	-3.03750300	0.16667100
C	4.02243900	-1.55269900	2.73674800
H	3.27155000	0.10846600	3.89243600
H	4.48780200	-3.20072900	1.42384200
H	4.96055100	-1.61348600	3.28124800
N	2.10535400	-0.49854200	-1.68363500

6-(4S,5S)

Charge = 0, Multiplicity = 1

C	3.79937500	-3.48437000	-1.29550400
C	2.43769500	-3.60406500	-1.05350900
C	1.73058900	-2.59730700	-0.36064100
C	2.45800100	-1.47695900	0.10772600
C	3.83304400	-1.35973200	-0.15192500
C	4.50462600	-2.35494600	-0.85345900
H	-0.16383200	-3.65514600	-0.41475500
H	4.32000900	-4.26952500	-1.83672800
H	1.89328100	-4.47494300	-1.40895100
C	0.30284300	-2.70823900	-0.16668000
H	4.37427900	-0.48621900	0.20213000
H	5.56811900	-2.26075100	-1.05103500
C	-0.50155800	-1.70866400	0.28242600
N	0.00444300	-0.46016500	0.68527600
P	1.65740600	-0.23753700	1.12744100
C	2.06226700	1.38004000	0.42494400
C	1.89284500	1.62426700	-0.94621100
C	2.53686300	2.39419600	1.26411900
C	2.18907200	2.88156800	-1.46853800
H	1.51317500	0.84039900	-1.59420700
C	2.83628800	3.65145100	0.73610300
H	2.66240500	2.19442100	2.32354200
C	2.66066700	3.89513200	-0.62774800
H	2.05087100	3.07281600	-2.52879800
H	3.20290000	4.43900700	1.38817500

H	2.89095400	4.87461100	-1.03745900
O	1.93447300	-0.31934600	2.60277400
C	-0.84243000	0.69343200	0.70068400
C	-1.46044300	1.12681500	-0.51326900
C	-0.99477400	1.43010400	1.85756100
C	-2.27130600	2.30470400	-0.48190200
C	-1.77617400	2.60851100	1.86988400
H	-0.51073000	1.08954400	2.76664500
C	-1.82990200	0.83710500	-2.76581600
C	-2.88584500	2.70682400	-1.69538600
C	-2.41456400	3.03368400	0.72724100
H	-1.87779700	3.16556400	2.79608000
C	-2.67096900	1.97335700	-2.83820000
H	-1.63470300	0.25482500	-3.66486000
H	-3.51433000	3.59322800	-1.70257100
H	-3.02834100	3.93006300	0.72948700
H	-3.12296200	2.25125800	-3.78472400
C	-1.96544400	-1.91400500	0.40458200
C	-2.69198400	-2.44520800	-0.67093000
C	-2.64075500	-1.59807100	1.59449300
C	-4.06561800	-2.66027400	-0.55901800
H	-2.17676000	-2.66670600	-1.60014200
C	-4.01352700	-1.81342400	1.70419700
H	-2.08559000	-1.19743100	2.43619700
C	-4.73088700	-2.34217800	0.62735200
H	-4.61751600	-3.06593000	-1.40232700
H	-4.52318500	-1.57137600	2.63264600
H	-5.80182900	-2.50366000	0.71258100
N	-1.24490900	0.42034700	-1.65816100

6-TS

Charge = 0, Multiplicity = 1

C	-0.93463100	-4.03051400	2.53587700
C	-0.65964600	-2.67008600	2.68768000
C	-0.68291400	-1.81380500	1.57868600
C	-1.03166200	-2.35254600	0.31594700
C	-1.31018900	-3.70975100	0.16919600
C	-1.25438500	-4.55518700	1.28110500
H	-0.74117800	0.06862000	2.66596600
H	-0.90180400	-4.68368100	3.40311700
H	-0.42090600	-2.26617700	3.66772100
C	-0.46390300	-0.36923600	1.71195300
H	-1.56480300	-4.10352100	-0.81042900

H	-1.46667600	-5.61426000	1.16978900
C	-0.07799400	0.44634400	0.70288400
N	0.27056700	-0.16893400	-0.58363300
P	-1.03771400	-1.20197100	-1.08173500
C	-2.48627500	-0.12219000	-0.95106200
C	-3.40790000	-0.21078300	0.10007500
C	-2.69273400	0.80791100	-1.98148000
C	-4.51339100	0.63921300	0.13078800
H	-3.26310000	-0.93465400	0.89490500
C	-3.79780300	1.65708500	-1.94583700
H	-1.98974600	0.86881200	-2.80670300
C	-4.70615700	1.57615200	-0.88743100
H	-5.22268700	0.57058700	0.95042800
H	-3.94837500	2.38090900	-2.74137100
H	-5.56573700	2.23973400	-0.85835700
O	-0.89083200	-1.82318600	-2.43859400
C	1.61718800	-0.65208500	-0.73657000
C	2.73336300	0.18527500	-0.38259400
C	1.89143600	-1.91636300	-1.24202100
C	4.06876800	-0.31453200	-0.53666600
C	3.21386000	-2.38569300	-1.40780900
H	1.08761700	-2.57278400	-1.54253500
C	3.51860300	2.20334100	0.42381500
C	5.13648100	0.54144300	-0.16120700
C	4.29347500	-1.61243700	-1.05658400
H	3.35969300	-3.38427700	-1.80951900
C	4.87028200	1.80041200	0.32226400
H	3.27254200	3.19737800	0.79585600
H	6.15691900	0.18225900	-0.26542300
H	5.31224600	-1.97139400	-1.17145400
H	5.66559800	2.47713500	0.61775500
C	-0.19705700	1.91665200	0.76253900
C	-0.35470400	2.65601200	-0.42119700
C	-0.22858300	2.60251100	1.98820900
C	-0.56020300	4.03259500	-0.38060500
H	-0.30374900	2.13908500	-1.37124400
C	-0.42295100	3.98247700	2.02693000
H	-0.07784400	2.06204900	2.91745200
C	-0.59711600	4.70542200	0.84393100
H	-0.68716600	4.58270100	-1.30919900
H	-0.43424000	4.49419000	2.98546200
H	-0.75172500	5.78024800	0.87583400
N	2.50056900	1.43697400	0.08817700

CN_163_CC_163

Charge = 0, Multiplicity = 1

O	4.26563400	-0.94793200	-0.17561300
O	-1.20650200	-2.20245400	0.99058100
N	-0.33082700	-0.26210100	-0.00599400
N	-2.82436600	-1.26600800	-0.82757400
C	0.02025900	-4.72838400	-0.02244000
H	-0.42751500	-4.77160700	0.97551400
H	0.35182900	-5.73220900	-0.30566600
H	-0.78054200	-4.41915100	-0.70237500
C	3.38554900	-1.98876100	-0.13165500
C	3.61226300	-3.34139600	-0.31562300
H	4.60518100	-3.73677200	-0.49946700
C	2.48656700	-4.19424100	-0.26672000
H	2.65129200	-5.25890400	-0.41005700
C	1.17143000	-3.75687500	-0.05664400
C	0.97545600	-2.36537700	0.09875600
C	2.08532500	-1.54051000	0.09483800
C	2.06379500	-0.12374900	0.18792500
C	3.51944200	0.28735300	0.06026200
H	3.71038000	0.96838700	-0.77650300
H	3.92173300	0.73632100	0.97076700
C	0.86606400	0.52772900	0.14584100
C	-0.28259700	-1.67589100	0.40334400
C	0.77558400	1.91616400	-0.37727600
C	1.66343300	2.95367000	-0.04549000
C	1.72290000	4.14908200	-0.76448900
H	2.40719800	4.92526900	-0.44055600
C	0.89158400	4.33727200	-1.86249700
H	0.93977300	5.26461100	-2.42482600
C	-0.01229300	3.33225500	-2.21648200
H	-0.67057500	3.46299300	-3.06993400
C	-0.05766500	2.14763600	-1.49522700
H	-0.72476300	1.35431200	-1.81013300
C	-1.55959100	0.36025200	0.43362800
C	-1.55695900	1.41269100	1.32796900
H	-0.61821200	1.77118600	1.73236400
C	-2.75553900	2.03600600	1.73822700
H	-2.70255900	2.87452500	2.42586700
C	-3.97002600	1.57445300	1.29175400
H	-4.89876100	2.04014700	1.61030300
C	-4.02091200	0.45293500	0.42717200
C	-2.81216500	-0.16782900	-0.02215800

S166

C	-3.98502600	-1.75938600	-1.19865800
H	-3.95100100	-2.63613400	-1.84463500
C	-5.23847600	-1.22406100	-0.80998800
H	-6.15839600	-1.68913600	-1.15008600
C	-5.24843300	-0.11305300	-0.00422900
H	-6.18137300	0.33816600	0.32425300
Cl	2.57057600	2.90352600	1.46997500

CN_163_CC_168

Charge = 0, Multiplicity = 1

O	4.22860200	-1.06497300	-0.14720400
O	-1.28163700	-2.17206400	0.98348000
N	-0.34349600	-0.24785200	0.01271300
N	-2.85786200	-1.17055700	-0.83919200
C	-0.12599500	-4.71864200	-0.05878400
H	-0.57700900	-4.76532500	0.93757300
H	0.17602800	-5.72704900	-0.35831200
H	-0.91570100	-4.37412000	-0.73467300
C	3.31779900	-2.07839800	-0.11797300
C	3.50559000	-3.43429800	-0.32145500
H	4.48728700	-3.85484700	-0.50961600
C	2.35608300	-4.25482200	-0.28766300
H	2.48996100	-5.32160500	-0.44651100
C	1.05386700	-3.78167800	-0.07468000
C	0.89897100	-2.38774600	0.10092000
C	2.03129200	-1.59399900	0.11343100
C	2.05108400	-0.17771800	0.22612700
C	3.52007600	0.18818600	0.10545900
H	3.73328700	0.87497800	-0.72115100
H	3.93594000	0.61063000	1.02215600
C	0.87226600	0.51132700	0.18633500
C	-0.33916100	-1.66606600	0.40767600
C	0.82307600	1.90155600	-0.34241800
C	1.78405400	2.89413000	-0.07811800
C	1.89130600	4.06208200	-0.83525300
H	2.63050200	4.80415400	-0.55503100
C	1.03773600	4.26963300	-1.91214200
H	1.12367200	5.17476800	-2.50525600
C	0.06264600	3.31244000	-2.20225100
H	-0.61504800	3.45599900	-3.03829100
C	-0.02912600	2.15443200	-1.44322500
H	-0.74793300	1.39431200	-1.72197500
C	-1.55843100	0.40054600	0.45588600

C	-1.53296200	1.44008900	1.36452800
H	-0.58669700	1.76877100	1.77693600
C	-2.71707500	2.08893100	1.77755800
H	-2.64599000	2.91595400	2.47737900
C	-3.94072400	1.66618700	1.31791800
H	-4.85864300	2.15167600	1.63823600
C	-4.01624200	0.55958100	0.43599900
C	-2.82174400	-0.08650200	-0.01553500
C	-4.02885900	-1.62633500	-1.22568200
H	-4.01406800	-2.49283100	-1.88604200
C	-5.27002400	-1.06401900	-0.83573100
H	-6.19981100	-1.49865400	-1.18899700
C	-5.25559300	0.03364500	-0.01190300
H	-6.17829900	0.50437900	0.31808400
Cl	2.71628500	2.85463100	1.42450000

CN_163_CC_173

Charge = 0, Multiplicity = 1

O	4.19745700	-1.15398100	-0.11319800
O	-1.34193400	-2.14872300	0.97049000
N	-0.35368900	-0.23538200	0.02809300
N	-2.88176000	-1.09042500	-0.85333900
C	-0.23903600	-4.70621800	-0.09760900
H	-0.69550600	-4.75818100	0.89601700
H	0.04108000	-5.71653100	-0.41166800
H	-1.01749600	-4.33296500	-0.77122500
C	3.26310300	-2.14493400	-0.10134000
C	3.42163800	-3.50193800	-0.32219500
H	4.39502400	-3.94107900	-0.51103300
C	2.25446000	-4.29694600	-0.30587800
H	2.36504800	-5.36423100	-0.47863200
C	0.96227200	-3.79674500	-0.09376800
C	0.83861000	-2.40241100	0.10002600
C	1.98721500	-1.63291700	0.13036100
C	2.03853000	-0.21811600	0.26196400
C	3.51732900	0.11197500	0.14928400
H	3.74915600	0.80070800	-0.67069300
H	3.94163400	0.51563300	1.07018900
C	0.87521500	0.50047500	0.22437800
C	-0.38407200	-1.65724200	0.40755100
C	0.85909100	1.89275800	-0.30734600
C	1.88122000	2.84131900	-0.11109300
C	2.02482100	3.98015900	-0.90502100

H	2.81061600	4.68871100	-0.66832400
C	1.14841600	4.20495500	-1.95955200
H	1.26297600	5.08647200	-2.58259500
C	0.11317900	3.29549300	-2.18497800
H	-0.58503600	3.45035800	-3.00191700
C	-0.01320400	2.16541100	-1.38954200
H	-0.77656700	1.43823800	-1.63257700
C	-1.55847900	0.42987400	0.47740700
C	-1.51666300	1.45361200	1.40288600
H	-0.56552000	1.75693400	1.82362800
C	-2.68971400	2.11932600	1.82100600
H	-2.60576300	2.93303800	2.53486800
C	-3.91914400	1.72934700	1.34807900
H	-4.82874000	2.22797300	1.67192700
C	-4.01228600	0.63996000	0.44651300
C	-2.82868000	-0.02261100	-0.00952700
C	-4.05948400	-1.51475100	-1.25497000
H	-4.05843900	-2.36905100	-1.93118400
C	-5.29121100	-0.93425300	-0.86172400
H	-6.22752900	-1.34317900	-1.22818100
C	-5.25939000	0.14773000	-0.01784900
H	-6.17428700	0.63128000	0.31532300
Cl	2.84064200	2.81754500	1.37718100

CN_163_CC_178

Charge = 0, Multiplicity = 1

O	4.17349600	-1.21787900	-0.07334100
O	-1.38871600	-2.13314000	0.95083700
N	-0.36140100	-0.22480400	0.04029000
N	-2.89807100	-1.02464900	-0.86956900
C	-0.32080800	-4.69329700	-0.14047800
H	-0.78759600	-4.74939000	0.84809000
H	-0.05465700	-5.70436100	-0.46412400
H	-1.08635600	-4.29894300	-0.81686500
C	3.22198500	-2.19124300	-0.08138000
C	3.36042700	-3.54789400	-0.31768500
H	4.32851500	-3.99982300	-0.50351200
C	2.18094700	-4.32395100	-0.32161700
H	2.27541000	-5.39068000	-0.50688500
C	0.89562600	-3.80450100	-0.11438800
C	0.79395800	-2.41105500	0.09602300
C	1.95344200	-1.65914000	0.14612400
C	2.02714000	-0.24617700	0.29622300

C	3.51339800	0.05670900	0.19385900
H	3.76130100	0.74535900	-0.62142300
H	3.94105500	0.44720400	1.11854000
C	0.87564600	0.49460900	0.26005300
C	-0.41801300	-1.65027600	0.40253100
C	0.88484000	1.88963800	-0.27240100
C	1.95646700	2.79709300	-0.14515800
C	2.12515500	3.90595300	-0.97492900
H	2.94964500	4.58303600	-0.78192200
C	1.22489700	4.14490000	-2.00574200
H	1.35907600	5.00204800	-2.65812900
C	0.14013100	3.28139500	-2.16508700
H	-0.58006800	3.44548200	-2.96088600
C	-0.00918800	2.17970400	-1.33421600
H	-0.81067700	1.48428200	-1.54106300
C	-1.55971900	0.44874600	0.49815900
C	-1.50735800	1.45379600	1.44308400
H	-0.55327900	1.73558900	1.87225200
C	-2.67262700	2.12841500	1.86893100
H	-2.58031600	2.92692300	2.59875400
C	-3.90527000	1.76583400	1.38280900
H	-4.80907100	2.27140200	1.71205900
C	-4.00989400	0.69595800	0.45930600
C	-2.83390900	0.02493500	-0.00385700
C	-4.07978100	-1.42303200	-1.28583200
H	-4.08777200	-2.26326100	-1.97940100
C	-5.30486300	-0.83227000	-0.88710700
H	-6.24513900	-1.21964700	-1.26660900
C	-5.26163100	0.23178000	-0.02120800
H	-6.17107400	0.72208500	0.31698200
Cl	2.94488700	2.79513200	1.32723700

CN_163_CC_183

Charge = 0, Multiplicity = 1

O	2.17964600	-3.23915200	1.21295800
O	-1.48217800	-0.76096200	-2.38781200
N	-0.19099700	0.23143900	-0.67961600
N	-2.72696000	1.40247500	-1.11414400
C	-2.88673800	-3.26811900	-1.34384100
H	-3.49253300	-2.40157000	-1.05639800
H	-3.45975200	-4.17594500	-1.13276100
H	-2.73456700	-3.19128100	-2.42543700
C	0.92569400	-3.38463100	0.70925000

S170

C	0.09728000	-4.49812700	0.76380500
H	0.39749400	-5.40324300	1.28023800
C	-1.14295900	-4.41309700	0.10537100
H	-1.80050200	-5.27778800	0.13717200
C	-1.56869200	-3.28351700	-0.61357700
C	-0.71383400	-2.16452700	-0.61745600
C	0.49939700	-2.23427700	0.05610400
C	1.53211100	-1.22546700	0.09031800
C	2.70502200	-1.95716500	0.74227400
H	3.51443900	-2.18879400	0.04841000
H	3.11525800	-1.43826700	1.60901600
C	1.21681500	0.03022800	-0.35067400
C	-0.88243500	-0.89702700	-1.35332400
C	1.98631000	1.29839500	-0.45204900
C	3.37285900	1.50256000	-0.27042900
C	3.95388100	2.77133200	-0.27096100
H	5.02461500	2.85193700	-0.12092800
C	3.17976400	3.90396600	-0.49449300
H	3.64136000	4.88658800	-0.49433800
C	1.82165800	3.74291200	-0.76010500
H	1.19677000	4.60146200	-0.98595600
C	1.25328000	2.47734600	-0.74557200
H	0.20642900	2.37568400	-0.98822700
C	-0.97224500	0.75453600	0.41260200
C	-0.49296000	0.74973500	1.71260700
H	0.48584600	0.33693800	1.91703300
C	-1.25152800	1.26019500	2.78785300
H	-0.82619600	1.23196000	3.78682600
C	-2.51376700	1.76272700	2.58432600
H	-3.11058300	2.14013700	3.41015100
C	-3.04528900	1.79783200	1.27204600
C	-2.27212000	1.31876400	0.16277700
C	-3.92677800	1.89869700	-1.33009800
H	-4.24372800	1.95184400	-2.37098700
C	-4.78779600	2.35889500	-0.30490000
H	-5.77078100	2.74826900	-0.55112700
C	-4.33578900	2.31456200	0.99172100
H	-4.94859700	2.67393500	1.81472500
Cl	4.53789000	0.18478100	-0.16610000

CN_163_CC_188

Charge = 0, Multiplicity = 1

O	2.12581400	-3.17757700	1.31908800
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S171

O	-1.44206700	-0.75333200	-2.42214000
N	-0.18117300	0.25620200	-0.69820200
N	-2.70146300	1.43239400	-1.16981200
C	-2.88220100	-3.24294800	-1.35662600
H	-3.48779300	-2.36750400	-1.09674300
H	-3.46458700	-4.14309300	-1.13854500
H	-2.71016600	-3.18791100	-2.43656500
C	0.88644900	-3.33648100	0.78088100
C	0.04626400	-4.44062400	0.84855900
H	0.32275200	-5.33178300	1.40124800
C	-1.17679700	-4.36381400	0.15710200
H	-1.84312800	-5.22131700	0.19903800
C	-1.57777900	-3.25105800	-0.60225900
C	-0.71276500	-2.14034500	-0.61969600
C	0.48631600	-2.20698000	0.07786600
C	1.52270700	-1.20441000	0.11167500
C	2.67610900	-1.92118200	0.80736500
H	3.49107700	-2.19120000	0.13436400
H	3.08610700	-1.37065900	1.65608700
C	1.22057900	0.04652800	-0.34845700
C	-0.86128600	-0.88011700	-1.37619600
C	2.01197800	1.29790100	-0.41104100
C	3.41259500	1.43916600	-0.29043500
C	4.03786500	2.68377800	-0.20607500
H	5.11758500	2.71883600	-0.11363100
C	3.29117200	3.85381700	-0.28386800
H	3.78511100	4.81842900	-0.21926600
C	1.91665200	3.75992100	-0.49628700
H	1.31392700	4.65522800	-0.61355100
C	1.30440800	2.51672500	-0.56446300
H	0.24358300	2.46952800	-0.75788700
C	-0.98581400	0.75721700	0.38884600
C	-0.53805300	0.72865000	1.69941100
H	0.43706500	0.31506100	1.91953400
C	-1.32421000	1.21741300	2.76491200
H	-0.92386400	1.17124500	3.77349600
C	-2.58213000	1.72173900	2.53942700
H	-3.19985200	2.08253600	3.35727600
C	-3.08114100	1.78159800	1.21526900
C	-2.27979700	1.32450600	0.11687600
C	-3.89611200	1.93175900	-1.40605700
H	-4.18711200	2.00458700	-2.45331100
C	-4.78335400	2.37192900	-0.39425300
H	-5.76010100	2.76551100	-0.65800700

C	-4.36472400	2.30295500	0.91240600
H	-4.99868200	2.64613500	1.72625100
Cl	4.52264500	0.07691900	-0.42168100

CN_163_CC_193

Charge = 0, Multiplicity = 1

O	2.12555700	-3.12049300	1.38946800
O	-1.40943600	-0.76174200	-2.43155700
N	-0.17825300	0.27201700	-0.69856500
N	-2.69785900	1.42961700	-1.21045900
C	-2.83965600	-3.26008300	-1.36651600
H	-3.45675300	-2.38829100	-1.12170900
H	-3.41665600	-4.16382200	-1.14904300
H	-2.65362900	-3.21189500	-2.44444800
C	0.89780900	-3.30076600	0.82932900
C	0.06429500	-4.40999100	0.89756700
H	0.33623500	-5.29180200	1.46725200
C	-1.14758500	-4.35029900	0.18447400
H	-1.80850300	-5.21196700	0.22673000
C	-1.54560500	-3.24976400	-0.59458100
C	-0.68836400	-2.13300800	-0.61294000
C	0.50044100	-2.18605200	0.10219200
C	1.52582900	-1.17464100	0.14236500
C	2.67443800	-1.86828900	0.86467900
H	3.50119400	-2.14280800	0.20819000
H	3.06998300	-1.29748200	1.70795500
C	1.21881200	0.07037600	-0.32686000
C	-0.83808800	-0.87738600	-1.37940700
C	2.01688100	1.31515300	-0.36686100
C	3.42437200	1.42204600	-0.31541800
C	4.07963100	2.64854900	-0.19758800
H	5.16331100	2.66021000	-0.16424200
C	3.35267100	3.83321200	-0.17128200
H	3.86849100	4.78426800	-0.08148500
C	1.96660800	3.77646700	-0.31446400
H	1.37839100	4.68826400	-0.34962000
C	1.32523500	2.55039400	-0.41678900
H	0.25424200	2.53342200	-0.54993000
C	-1.00844200	0.75634900	0.37780400
C	-0.58791100	0.71788200	1.69707200
H	0.38617800	0.31036800	1.93292200
C	-1.39976900	1.19042800	2.75042700
H	-1.02036600	1.13770000	3.76675500

C	-2.65658100	1.68751600	2.50311500
H	-3.29389800	2.03603100	3.31120500
C	-3.12867300	1.75582400	1.16951800
C	-2.30140000	1.31497900	0.08373300
C	-3.89167200	1.92094100	-1.46637800
H	-4.16269200	1.99939300	-2.51858400
C	-4.80257000	2.34629400	-0.46912800
H	-5.77687100	2.73442300	-0.74951100
C	-4.41004400	2.26982500	0.84509300
H	-5.06309600	2.60103700	1.64873500
Cl	4.48789900	0.04551000	-0.59625000

CN_163_CC_198

Charge = 0, Multiplicity = 1

O	2.15216900	-3.06564500	1.44439300
O	-1.38347300	-0.77876500	-2.42641700
N	-0.17925900	0.28341600	-0.69033600
N	-2.70473400	1.41097000	-1.24454200
C	-2.77587700	-3.29991100	-1.37449000
H	-3.41076400	-2.43827000	-1.13944700
H	-3.33954300	-4.21292900	-1.16083100
H	-2.57841300	-3.25149000	-2.45036200
C	0.93513100	-3.27135300	0.86804300
C	0.11880300	-4.39363700	0.93003900
H	0.39645600	-5.26889500	1.50702900
C	-1.08449900	-4.35574600	0.20056700
H	-1.73187900	-5.22785500	0.23787300
C	-1.49122000	-3.26482600	-0.58780000
C	-0.65196600	-2.13412700	-0.60040700
C	0.52800200	-2.16795500	0.12953700
C	1.53406000	-1.13992000	0.17929500
C	2.68434900	-1.80452300	0.92268400
H	3.52907300	-2.06318900	0.28284600
H	3.05291900	-1.21892700	1.76893100
C	1.21344300	0.09772000	-0.29622300
C	-0.81481000	-0.88192600	-1.37162700
C	2.01139600	1.34100200	-0.32240400
C	3.42060900	1.42798900	-0.34433900
C	4.09806000	2.64144600	-0.21473600
H	5.18198600	2.64064400	-0.24167700
C	3.38806400	3.83116300	-0.10131700
H	3.91994200	4.77247000	-0.00276000
C	1.99504500	3.79604000	-0.16804000

H	1.41878900	4.71541700	-0.13194900
C	1.33232800	2.58248700	-0.28348100
H	0.25486800	2.58286900	-0.35005000
C	-1.03541000	0.75434200	0.37240500
C	-0.64006600	0.71248300	1.69946900
H	0.33405700	0.31436100	1.95111100
C	-1.47640200	1.17130000	2.73946500
H	-1.11594500	1.11746400	3.76260600
C	-2.73340500	1.65665100	2.47030200
H	-3.38950400	1.99487300	3.26767200
C	-3.18131400	1.72546300	1.12842300
C	-2.32946600	1.29831900	0.05612400
C	-3.89970000	1.88841900	-1.51993000
H	-4.15373400	1.96545100	-2.57648300
C	-4.83277700	2.30119700	-0.53781400
H	-5.80641900	2.67878200	-0.83443500
C	-4.46264500	2.22585200	0.78283800
H	-5.13360000	2.54699300	1.57574800
Cl	4.44186500	0.04818400	-0.74146900

CN_163_CC_203

Charge = 0, Multiplicity = 1

O	2.19954400	-3.01098900	1.48835700
O	-1.36171100	-0.80340400	-2.41072900
N	-0.18346400	0.29158500	-0.67630900
N	-2.71892100	1.37981600	-1.27465900
C	-2.69513400	-3.35632400	-1.37917500
H	-3.35287100	-2.51052200	-1.14962100
H	-3.23860700	-4.28296000	-1.17186800
H	-2.48843500	-3.30178600	-2.45300200
C	0.99243600	-3.24510700	0.90073800
C	0.20222200	-4.38642500	0.95170800
H	0.49424600	-5.25699900	1.52869300
C	-0.99447100	-4.37415700	0.21013900
H	-1.62148000	-5.26134100	0.23881300
C	-1.41946900	-3.29129500	-0.57990300
C	-0.60696900	-2.14076200	-0.58211000
C	0.56511300	-2.15069300	0.16051600
C	1.54509300	-1.10056300	0.22142000
C	2.70143000	-1.73076100	0.98260100
H	3.56858000	-1.95628500	0.36034600
H	3.03152500	-1.13544000	1.83862300
C	1.20488300	0.12784900	-0.25997600

C	-0.79161000	-0.89198800	-1.35541200
C	1.99805100	1.37343100	-0.27878500
C	3.40427500	1.45053300	-0.37704600
C	4.09762600	2.65536900	-0.24897300
H	5.17826400	2.64978700	-0.33744000
C	3.40326500	3.84441200	-0.05828900
H	3.94665900	4.77927400	0.03893400
C	2.00821100	3.81993300	-0.04338800
H	1.44291600	4.74125200	0.05794500
C	1.33017900	2.61466100	-0.15878000
H	0.25045200	2.62290600	-0.15390600
C	-1.06544600	0.75166500	0.37051000
C	-0.69369200	0.71196700	1.70469200
H	0.28151000	0.32675300	1.97219900
C	-1.55378800	1.15839400	2.73037500
H	-1.21074100	1.10803100	3.75965800
C	-2.81218100	1.62740100	2.43928100
H	-3.48665600	1.95626500	3.22515900
C	-3.23787400	1.69038000	1.08991700
C	-2.36217500	1.27575000	0.03183100
C	-3.91654700	1.83824500	-1.56956300
H	-4.15542100	1.90885000	-2.63010300
C	-4.87101100	2.23924200	-0.60310500
H	-5.84533900	2.60179300	-0.91582100
C	-4.52082000	2.17151300	0.72327500
H	-5.20906100	2.48341800	1.50497700
Cl	4.38581800	0.07331300	-0.87134200

CN_163_CC_208

Charge = 0, Multiplicity = 1

O	2.26637500	-2.95283500	1.52374600
O	-1.34340400	-0.83546500	-2.38638500
N	-0.19041900	0.29635000	-0.65811800
N	-2.73974200	1.33561000	-1.30104100
C	-2.59654400	-3.42731800	-1.38097400
H	-3.28101400	-2.60220000	-1.15458700
H	-3.11368200	-4.37045300	-1.18073000
H	-2.38294100	-3.36322700	-2.45291300
C	1.06919300	-3.21935500	0.92847400
C	0.31353300	-4.38422100	0.96535900
H	0.62747300	-5.25058700	1.53714800
C	-0.87796700	-4.40177600	0.21508000
H	-1.47807500	-5.30764700	0.23280600

C	-1.32989200	-3.32706500	-0.57114000
C	-0.55229600	-2.15213600	-0.56004000
C	0.61244900	-2.13356900	0.19324400
C	1.55965900	-1.05659100	0.26606000
C	2.72666000	-1.64840100	1.03993700
H	3.61459400	-1.83018300	0.43247700
H	3.01440100	-1.04855200	1.90842800
C	1.19341900	0.16063100	-0.21971800
C	-0.76761400	-0.90735800	-1.33279500
C	1.97632700	1.41279900	-0.23613600
C	3.37447600	1.49009300	-0.41261600
C	4.07615100	2.69149400	-0.29650800
H	5.14991200	2.68859200	-0.44703600
C	3.39484000	3.87498900	-0.03665800
H	3.94398000	4.80743900	0.05120000
C	2.00309500	3.85029300	0.06320700
H	1.44712400	4.76878800	0.22430400
C	1.31726800	2.64822000	-0.04183800
H	0.24004100	2.65471000	0.03621500
C	-1.09822300	0.74660300	0.37132300
C	-0.74873300	0.71265400	1.71197800
H	0.22818500	0.34312100	1.99531300
C	-1.63189200	1.14693200	2.72296800
H	-1.30498300	1.10321300	3.75779300
C	-2.89252900	1.59568800	2.41031900
H	-3.58484500	1.91527400	3.18443300
C	-3.29777300	1.64800000	1.05423900
C	-2.39903200	1.24560500	0.01065500
C	-3.94121900	1.77028400	-1.61500900
H	-4.16677900	1.83010300	-2.67913600
C	-4.91625500	2.15949500	-0.66427100
H	-5.89240500	2.50283800	-0.99261000
C	-4.58372900	2.10468500	0.66712000
H	-5.28854400	2.40748000	1.43755500
Cl	4.32086500	0.11940700	-0.98758800

CN_163_CC_213

Charge = 0, Multiplicity = 1

O	2.34931500	-2.88997900	1.55072500
O	-1.32802400	-0.87460100	-2.35526300
N	-0.19920900	0.29763700	-0.63778800
N	-2.76495400	1.28001900	-1.32467600
C	-2.48479400	-3.50772300	-1.37662600

H	-3.19824900	-2.70750900	-1.15066100
H	-2.97031800	-4.46897100	-1.18335900
H	-2.26781300	-3.43135500	-2.44707400
C	1.16182700	-3.19220000	0.95191600
C	0.44715600	-4.38280400	0.97432700
H	0.78914100	-5.24419800	1.53748100
C	-0.74071800	-4.43357400	0.21926900
H	-1.30897900	-5.35989700	0.22580700
C	-1.22665800	-3.36835300	-0.55940600
C	-0.49012900	-2.16676000	-0.53472300
C	0.66821500	-2.11620700	0.22622800
C	1.57731700	-1.00954600	0.31012100
C	2.75968900	-1.56068900	1.08944700
H	3.66261800	-1.69387900	0.49092400
H	3.00832300	-0.96048600	1.96990800
C	1.17963500	0.19473800	-0.17786800
C	-0.74307200	-0.92745600	-1.30541500
C	1.94721100	1.45731600	-0.19475100
C	3.33208200	1.54355900	-0.45066400
C	4.03473700	2.74610100	-0.35280700
H	5.09788300	2.75230000	-0.56563700
C	3.36441600	3.92003400	-0.02851800
H	3.91366400	4.85367300	0.04520100
C	1.98184400	3.88578900	0.15859700
H	1.43413600	4.79758400	0.37625800
C	1.29542500	2.68234900	0.07009800
H	0.22575700	2.67926400	0.22163500
C	-1.13247200	0.73855400	0.37342600
C	-0.80383700	0.71315600	1.71983100
H	0.17520200	0.36138300	2.01850000
C	-1.70906300	1.13534000	2.71619100
H	-1.39698000	1.10068200	3.75592300
C	-2.97245900	1.56069500	2.38273700
H	-3.68191600	1.87103700	3.14501200
C	-3.35891400	1.59855800	1.02070800
C	-2.43822600	1.20830100	-0.00844900
C	-3.97104100	1.68703200	-1.65692400
H	-4.18474100	1.73293200	-2.72420100
C	-4.96558800	2.06437700	-0.72164300
H	-5.94425000	2.38527000	-1.06488700
C	-4.64877000	2.02659700	0.61404900
H	-5.36925900	2.32037000	1.37339800
Cl	4.24774900	0.18245500	-1.09444600

CN_163_CC_223

Charge = 0, Multiplicity = 1

O	2.54839300	-2.74655800	1.58429500
O	-1.29890400	-0.97015400	-2.28040000
N	-0.21949100	0.29000800	-0.59381600
N	-2.82132600	1.14000500	-1.36496900
C	-2.23383300	-3.68060100	-1.34720400
H	-3.00692200	-2.94048000	-1.11326800
H	-2.64395000	-4.67886800	-1.16708300
H	-2.02199200	-3.57383600	-2.41604600
C	1.38095400	-3.12787600	0.98872600
C	0.76095700	-4.37006300	0.98611400
H	1.17097400	-5.21593900	1.52693700
C	-0.42298300	-4.49503700	0.23213000
H	-0.91768600	-5.46258100	0.21941900
C	-0.99124700	-3.45605000	-0.52536500
C	-0.34896800	-2.20068200	-0.47767800
C	0.79910800	-2.07893800	0.28914700
C	1.61977800	-0.90994200	0.39120400
C	2.84359300	-1.37395900	1.16116700
H	3.75653100	-1.40798100	0.56241300
H	3.03250500	-0.77952400	2.06021400
C	1.14665200	0.26352900	-0.09352200
C	-0.69086100	-0.97861900	-1.24195000
C	1.87087000	1.55494600	-0.11616400
C	3.21251400	1.67917300	-0.53275500
C	3.89804100	2.89422400	-0.48065100
H	4.92774700	2.93333900	-0.81796700
C	3.24818400	4.03982700	-0.03456500
H	3.78322400	4.98384000	0.00371500
C	1.90330300	3.96532100	0.32982900
H	1.37241000	4.85487900	0.65485600
C	1.23428100	2.74868800	0.28368700
H	0.19505700	2.71026600	0.57832000
C	-1.20150500	0.71329000	0.37947100
C	-0.91049000	0.71180800	1.73521200
H	0.07286500	0.39885200	2.06264000
C	-1.85630900	1.11045900	2.70302700
H	-1.57062800	1.09972100	3.75084500
C	-3.12585500	1.48164300	2.33087800
H	-3.86694400	1.77338600	3.07007200
C	-3.47914900	1.48114700	0.95936000
C	-2.51803100	1.11492300	-0.04176100

C	-4.03759500	1.48185700	-1.73082300
H	-4.23089100	1.49200900	-2.80294700
C	-5.06807800	1.83440400	-0.82516800
H	-6.05298200	2.10165000	-1.19547600
C	-4.77811900	1.84103400	0.51693400
H	-5.52742700	2.11653400	1.25493900
Cl	4.07568500	0.34419500	-1.29334800

CN_163_CC_233

Charge = 0, Multiplicity = 1

O	2.80289600	-2.54892800	1.59716600
O	-1.26505400	-1.10384700	-2.18522100
N	-0.24394300	0.26372500	-0.54711600
N	-2.88908800	0.93752600	-1.39568600
C	-1.91253600	-3.88349200	-1.28958600
H	-2.75103200	-3.22542500	-1.03691400
H	-2.22156800	-4.91951200	-1.12087400
H	-1.72426300	-3.74071800	-2.35856100
C	1.66392100	-3.02979500	1.01608400
C	1.16553900	-4.32465300	0.99446700
H	1.66321700	-5.13972800	1.50837600
C	-0.01378500	-4.54560400	0.25379700
H	-0.41399800	-5.55560800	0.22646300
C	-0.68834000	-3.55231000	-0.47632200
C	-0.16684000	-2.24111400	-0.41212300
C	0.97064200	-2.02833500	0.34880600
C	1.67656300	-0.79076400	0.46309200
C	2.95383600	-1.14422800	1.20224400
H	3.85263600	-1.07205200	0.58399300
H	3.09974100	-0.55556800	2.11279400
C	1.10427000	0.33725700	-0.01178200
C	-0.62588300	-1.05175600	-1.16624100
C	1.75631200	1.67106800	-0.04702600
C	3.02727000	1.86505700	-0.62539300
C	3.66176600	3.10817400	-0.62471800
H	4.63794800	3.20375700	-1.08681800
C	3.02665800	4.20968200	-0.06032900
H	3.52108200	5.17640300	-0.06181700
C	1.75033400	4.06218200	0.48275900
H	1.23423400	4.91590800	0.91131800
C	1.13201600	2.81685800	0.48437200
H	0.14629400	2.71916300	0.91771100
C	-1.27436400	0.66485700	0.38645700

C	-1.01547000	0.70123500	1.74860200
H	-0.02672700	0.43645400	2.10230000
C	-1.99823100	1.07547100	2.68889700
H	-1.73453300	1.10040200	3.74222800
C	-3.27568900	1.37623300	2.28233500
H	-4.04575100	1.64829800	2.99909700
C	-3.60121000	1.31925700	0.90524700
C	-2.60351200	0.97805800	-0.06927400
C	-4.11710500	1.19441300	-1.78984600
H	-4.29425200	1.15405700	-2.86407900
C	-5.17997800	1.51944800	-0.91176600
H	-6.17273900	1.71624200	-1.30457000
C	-4.91131200	1.58979200	0.43274300
H	-5.68643100	1.84605900	1.15074400
Cl	3.85384700	0.57196200	-1.49119500

CN_168_CC_163

Charge = 0, Multiplicity = 1

O	-3.84015100	1.84872700	0.67999300
O	1.24004700	1.81287500	-1.81463800
N	0.33423100	0.10262900	-0.48248000
N	3.23944700	0.35786300	-0.87026600
C	0.93006000	4.56243200	-0.73963300
H	1.82803000	4.14190200	-0.27484700
H	0.88682900	5.63101900	-0.50751700
H	1.05949400	4.44056300	-1.81989700
C	-2.74489400	2.63706100	0.50030000
C	-2.65897200	4.01956100	0.54497100
H	-3.51045700	4.63501900	0.81372500
C	-1.42529700	4.59874800	0.18607600
H	-1.34235800	5.68195100	0.21470200
C	-0.31855700	3.86476700	-0.26491300
C	-0.43574600	2.45577400	-0.27302400
C	-1.61944900	1.88384600	0.17377300
C	-1.95656900	0.49133100	0.13750300
C	-3.44832000	0.46310900	0.43090400
H	-4.05318500	0.08202600	-0.39980000
H	-3.70073000	-0.09948200	1.32825000
C	-0.99012000	-0.40384800	-0.20124100
C	0.48022800	1.50640100	-0.92874000
C	-1.14245300	-1.81993600	-0.62169100
C	-2.14677900	-2.71805200	-0.21525300
C	-2.37197400	-3.93503600	-0.85919600

S181

H	-3.14706400	-4.59322000	-0.48271400
C	-1.58255500	-4.30502300	-1.94270300
H	-1.76120200	-5.25156600	-2.44355300
C	-0.55023100	-3.45990200	-2.35279400
H	0.08707300	-3.73608800	-3.18725800
C	-0.34853700	-2.24433600	-1.71358800
H	0.41878400	-1.56699700	-2.06785000
C	1.33424200	-0.43957700	0.40954100
C	0.90361900	-1.10659600	1.55115100
H	-0.15437700	-1.15201300	1.77272300
C	1.79216300	-1.72136900	2.45574800
H	1.38191000	-2.23896600	3.31778300
C	3.14863500	-1.64649900	2.26383000
H	3.84656600	-2.10444100	2.95931400
C	3.64792700	-0.93610400	1.14674000
C	2.75724300	-0.32569100	0.19617200
C	4.53878000	0.47269000	-1.03536600
H	4.86237700	1.03020700	-1.91401500
C	5.49811800	-0.08234300	-0.15644200
H	6.55887000	0.04922800	-0.34637200
C	5.04157500	-0.79005500	0.92789100
H	5.73104800	-1.24306400	1.63602700
Cl	-3.01172500	-2.49120300	1.30750600

CN_168_CC_168

Charge = 0, Multiplicity = 1

O	-3.61804600	2.20388300	0.73829000
O	1.34574900	1.61818000	-1.89603100
N	0.33596700	0.04440600	-0.47475000
N	3.23946200	0.05076400	-0.88229100
C	1.35264900	4.41031600	-0.85244800
H	2.21773200	3.90821100	-0.40655700
H	1.42393500	5.48103000	-0.63784700
H	1.43592300	4.26079900	-1.93385500
C	-2.45483900	2.87459200	0.51957300
C	-2.23300100	4.24288700	0.53955200
H	-3.01339800	4.94146000	0.82065800
C	-0.96029200	4.69432000	0.13837100
H	-0.77127300	5.76447600	0.14665000
C	0.05559300	3.84824700	-0.33005300
C	-0.19875800	2.45848600	-0.30952700
C	-1.41909000	2.00796700	0.17801400
C	-1.89439800	0.65341300	0.17007100

C	-3.37298400	0.78243600	0.50689800
H	-4.04120800	0.44882800	-0.29443200
H	-3.64908700	0.26625800	1.42474700
C	-1.02742800	-0.33845200	-0.17606100
C	0.59781500	1.41244900	-0.97221500
C	-1.30536500	-1.74089800	-0.58421000
C	-2.42773500	-2.52132100	-0.24493500
C	-2.74664700	-3.71022300	-0.90138700
H	-3.61310500	-4.27354900	-0.57339900
C	-1.93805300	-4.17684200	-1.93183100
H	-2.19027400	-5.10134500	-2.44207200
C	-0.79423000	-3.45523500	-2.27444800
H	-0.13953100	-3.80569000	-3.06648300
C	-0.50033800	-2.26364500	-1.62614900
H	0.35328300	-1.67755600	-1.94188400
C	1.28921000	-0.54183900	0.43692100
C	0.81327100	-1.13691200	1.59990000
H	-0.24516600	-1.09854600	1.82084100
C	1.65791400	-1.78283700	2.52490900
H	1.21412000	-2.23841100	3.40518600
C	3.01577500	-1.81500400	2.32978800
H	3.68006400	-2.29802000	3.04104900
C	3.56235800	-1.18728000	1.18550800
C	2.71519900	-0.54787700	0.21510200
C	4.54260500	0.05670500	-1.05837200
H	4.90163100	0.54925500	-1.96167200
C	5.46260100	-0.53356400	-0.16054700
H	6.52884400	-0.49269200	-0.36060300
C	4.96139900	-1.15804700	0.95492700
H	5.61954500	-1.63368200	1.67787700
Cl	-3.35770800	-2.20203400	1.22228800

CN_168_CC_173

Charge = 0, Multiplicity = 1

O	-3.29955000	2.59860400	0.80965300
O	1.43090600	1.36917800	-2.00763300
N	0.32255100	-0.03001100	-0.48119000
N	3.19343300	-0.32002100	-0.90340800
C	1.83630100	4.16395800	-0.99623900
H	2.64940300	3.56263200	-0.57582200
H	2.04838300	5.21954000	-0.80072900
H	1.85739700	3.99447300	-2.07777500
C	-2.07258500	3.11715700	0.53798500

C	-1.68431400	4.44850100	0.53589400
H	-2.36231300	5.23793600	0.84109500
C	-0.38407100	4.73989100	0.08057000
H	-0.06598400	5.77900100	0.07005900
C	0.50130500	3.77224000	-0.41698300
C	0.08040400	2.42544900	-0.36937400
C	-1.16681600	2.12669200	0.16624100
C	-1.80606000	0.83819000	0.18909400
C	-3.24456100	1.15750000	0.57869900
H	-3.98028500	0.91254200	-0.19383200
H	-3.54719700	0.68346600	1.51067500
C	-1.07364300	-0.25704700	-0.16411800
C	0.71596500	1.28037600	-1.04078900
C	-1.49892600	-1.63367100	-0.54157900
C	-2.73060700	-2.26283200	-0.26777300
C	-3.14561300	-3.42875300	-0.91140900
H	-4.09694300	-3.86816000	-0.63305700
C	-2.33138700	-4.03150400	-1.86347400
H	-2.65960400	-4.93781200	-2.36298600
C	-1.08760200	-3.46539000	-2.14030600
H	-0.42560200	-3.91989900	-2.87101100
C	-0.69782300	-2.29256900	-1.50865600
H	0.23681100	-1.82518900	-1.78840200
C	1.21729200	-0.64873200	0.46381500
C	0.69825200	-1.13854000	1.65654500
H	-0.35257400	-1.00035400	1.87382300
C	1.49225100	-1.80185100	2.61401200
H	1.01793500	-2.16945500	3.51919800
C	2.84144600	-1.96009300	2.41861400
H	3.46676700	-2.45751500	3.15481400
C	3.43141800	-1.45049200	1.23750600
C	2.63393100	-0.79760500	0.23547600
C	4.48973000	-0.44298200	-1.08906000
H	4.87961000	-0.04446700	-2.02527000
C	5.36461100	-1.05453400	-0.16084900
H	6.42763400	-1.12189800	-0.37058600
C	4.82454300	-1.56030900	0.99611600
H	5.44730300	-2.04717600	1.74255600
Cl	-3.73083100	-1.78517700	1.10726600

CN_168_CC_178

Charge = 0, Multiplicity = 1

O	2.73728300	-3.09469600	0.90946600
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S184

O	-1.46841100	-0.99708600	-2.19050000
N	-0.27333400	0.13984100	-0.51544500
N	-3.03499100	0.85205900	-0.94008900
C	-2.48377600	-3.68626900	-1.20593800
H	-3.19052200	-2.93981800	-0.82756400
H	-2.90372300	-4.68142300	-1.03105100
H	-2.40998100	-3.52020700	-2.28583100
C	1.45603500	-3.37531100	0.55671200
C	0.82397100	-4.61075500	0.53648500
H	1.32198300	-5.50710600	0.88945700
C	-0.47685900	-4.66230000	0.00215600
H	-0.98310000	-5.62359700	-0.02431600
C	-1.13406100	-3.55162100	-0.54910000
C	-0.47208800	-2.30910800	-0.47661900
C	0.78009400	-2.23790800	0.12437100
C	1.64973700	-1.08764800	0.18238900
C	2.97912300	-1.67741900	0.64856500
H	3.77983200	-1.61190900	-0.09272700
H	3.32829500	-1.24724200	1.58541200
C	1.14129700	0.12733500	-0.18202400
C	-0.84153700	-1.06135100	-1.16403900
C	1.77525200	1.44288800	-0.48906600
C	3.11086200	1.84709000	-0.27626700
C	3.65171100	3.00560800	-0.83463400
H	4.68201000	3.25811300	-0.61066600
C	2.87332700	3.83246200	-1.63595900
H	3.30181300	4.73168100	-2.06772400
C	1.54079900	3.48916300	-1.85419300
H	0.90314400	4.11449100	-2.47150200
C	1.02253800	2.32188500	-1.31132600
H	0.01015600	2.03489700	-1.55760100
C	-1.08436900	0.76947000	0.49022600
C	-0.53192600	1.07580100	1.72719200
H	0.49203100	0.79524100	1.93484700
C	-1.26440800	1.73145000	2.73847500
H	-0.77082400	1.94895600	3.68116900
C	-2.58128100	2.06935400	2.54749600
H	-3.15823900	2.56196200	3.32523400
C	-3.20075300	1.76322100	1.31194600
C	-2.46219400	1.12427200	0.25894200
C	-4.29902400	1.16133200	-1.13502800
H	-4.70450400	0.92450900	-2.11815900
C	-5.12031000	1.77236300	-0.15857200
H	-6.15895700	1.99798700	-0.37953700

C	-4.56073800	2.07496000	1.05897500
H	-5.14269900	2.55369400	1.84266600
Cl	4.16835500	1.05334900	0.89281800

CN_168_CC_183

Charge = 0, Multiplicity = 1

O	1.82750200	-3.35383700	1.29566800
O	-1.33014600	-0.63599400	-2.51717700
N	-0.14845800	0.28149400	-0.68920300
N	-2.66388900	1.46653900	-1.10801400
C	-3.15543300	-2.92206100	-1.38756600
H	-3.66902900	-1.98602500	-1.14080900
H	-3.83192500	-3.75459800	-1.17279700
H	-2.96354600	-2.89488200	-2.46551400
C	0.57372600	-3.38119400	0.77034600
C	-0.36796900	-4.40164500	0.83190200
H	-0.17471000	-5.31911800	1.37684000
C	-1.57798700	-4.20704900	0.14173900
H	-2.32244900	-4.99794700	0.17922900
C	-1.86753200	-3.05929900	-0.61696200
C	-0.90398100	-2.03620100	-0.62427700
C	0.28138400	-2.21066300	0.08195700
C	1.41512900	-1.31333300	0.11232600
C	2.49293800	-2.14672100	0.80280500
H	3.28451300	-2.48048400	0.13006400
H	2.94298200	-1.64999500	1.66320300
C	1.23816700	-0.04036100	-0.35840500
C	-0.88782200	-0.78339300	-1.40931200
C	2.12722000	1.14183500	-0.46035200
C	3.52649100	1.20127900	-0.27400000
C	4.23327600	2.40406500	-0.26445800
H	5.30675800	2.37519700	-0.11499200
C	3.57649100	3.61074500	-0.47813400
H	4.13490300	4.54172800	-0.47031500
C	2.20841700	3.59140200	-0.74260500
H	1.67430600	4.51187000	-0.95725400
C	1.51426600	2.39008400	-0.73846700
H	0.46013200	2.39349200	-0.97191400
C	-0.89229400	0.84138000	0.40326700
C	-0.38474500	0.87571300	1.69267600
H	0.58748400	0.44724700	1.89516000
C	-1.10658300	1.44992900	2.76129800
H	-0.66015100	1.44889000	3.75146500

C	-2.35695500	1.98402000	2.56491900
H	-2.92279900	2.41391000	3.38678900
C	-2.91551400	1.98235100	1.26332300
C	-2.18208300	1.43160300	0.16117400
C	-3.85225000	1.99113900	-1.32307600
H	-4.19283100	2.00037100	-2.35773800
C	-4.67172400	2.53147000	-0.30345500
H	-5.64591300	2.94379200	-0.54720100
C	-4.19353000	2.52961200	0.98491400
H	-4.77681800	2.94606500	1.80245000
Cl	4.54412100	-0.23443200	-0.18726700

CN_168_CC_188

Charge = 0, Multiplicity = 1

O	1.82289700	-3.27765100	1.38588800
O	-1.29092800	-0.64927200	-2.53687900
N	-0.14160700	0.30063200	-0.70216000
N	-2.65620900	1.46508900	-1.16030600
C	-3.11650900	-2.93750200	-1.39541400
H	-3.64070100	-2.00201300	-1.16944600
H	-3.78956900	-3.77197000	-1.17746800
H	-2.91010600	-2.92463500	-2.47091100
C	0.58111400	-3.33167000	0.83192700
C	-0.35799700	-4.35403900	0.90247900
H	-0.17357300	-5.25593800	1.47574300
C	-1.55582500	-4.18114400	0.18515600
H	-2.29809100	-4.97374400	0.22961100
C	-1.83839000	-3.05267000	-0.60520900
C	-0.87855400	-2.02631100	-0.62223500
C	0.29628200	-2.18392800	0.10401200
C	1.42181100	-1.27911000	0.13615900
C	2.49347100	-2.08583900	0.86194500
H	3.29076900	-2.44067200	0.20713800
H	2.93948100	-1.55918100	1.70786300
C	1.24163600	-0.01335300	-0.34936100
C	-0.86025000	-0.78138600	-1.42287100
C	2.13615900	1.16228700	-0.41910600
C	3.54317700	1.17938900	-0.29582500
C	4.27557100	2.36460500	-0.22294100
H	5.35424500	2.30602700	-0.13002600
C	3.63350700	3.59480500	-0.31081100
H	4.21027600	4.51288500	-0.25517300
C	2.25503800	3.62117600	-0.51822000

H	1.73342500	4.56570500	-0.63820100
C	1.53562900	2.43621400	-0.57640700
H	0.47262100	2.47723900	-0.76068500
C	-0.91388600	0.83777000	0.38394900
C	-0.43634400	0.85935600	1.68479300
H	0.53638600	0.43977200	1.90316500
C	-1.18922300	1.41011100	2.74426600
H	-0.76595900	1.40015500	3.74450200
C	-2.44093300	1.93270900	2.52606500
H	-3.03054700	2.34440700	3.34051900
C	-2.96925200	1.94373700	1.21193700
C	-2.20419900	1.41705000	0.11955600
C	-3.84517700	1.97946100	-1.39530300
H	-4.16195300	1.99989200	-2.43734100
C	-4.69440600	2.49603700	-0.38754300
H	-5.66722100	2.90109300	-0.64837400
C	-4.24660600	2.48099200	0.91152900
H	-4.85347700	2.87921500	1.72094000
Cl	4.52281800	-0.28090500	-0.40540100

CN_168_CC_193

Charge = 0, Multiplicity = 1

O	1.83767300	-3.21773300	1.45211100
O	-1.25823300	-0.66189300	-2.54123400
N	-0.13858200	0.31595100	-0.70101500
N	-2.65659700	1.45497500	-1.20043200
C	-3.06549100	-2.96819600	-1.40600900
H	-3.60479300	-2.03818100	-1.19322400
H	-3.73023600	-3.80989800	-1.19041700
H	-2.84586700	-2.96003000	-2.47890700
C	0.60586700	-3.29717300	0.87710200
C	-0.32331500	-4.32873100	0.94618100
H	-0.13947900	-5.22133400	1.53400300
C	-1.51179900	-4.17691400	0.20830500
H	-2.24620000	-4.97687200	0.25153700
C	-1.79606600	-3.06061000	-0.59904900
C	-0.84705500	-2.02408100	-0.61515700
C	0.31868000	-2.16401500	0.12815600
C	1.43081000	-1.24551000	0.16804700
C	2.50209800	-2.02607300	0.91881200
H	3.31258600	-2.38088900	0.28048000
H	2.93234000	-1.47859800	1.76070100
C	1.24131000	0.01446600	-0.32524900

C	-0.83453700	-0.78257800	-1.42348500
C	2.13769900	1.18670200	-0.37491200
C	3.54867800	1.17543400	-0.32085000
C	4.30366100	2.34469700	-0.22147100
H	5.38458800	2.26724700	-0.18645100
C	3.67679300	3.58572100	-0.21297800
H	4.26984400	4.49195200	-0.13758500
C	2.29006300	3.64289900	-0.35165500
H	1.77999000	4.60023800	-0.39579500
C	1.54879000	2.47317700	-0.43729000
H	0.47860900	2.53956400	-0.56405900
C	-0.93846800	0.83617000	0.37468200
C	-0.48867600	0.85086700	1.68543800
H	0.48434800	0.44057300	1.91991300
C	-1.26952200	1.38372400	2.73365700
H	-0.86723400	1.36964300	3.74246100
C	-2.52233900	1.89407400	2.49353100
H	-3.13350600	2.29187400	3.29896300
C	-3.02347600	1.91049600	1.16884800
C	-2.22999000	1.40222400	0.08801100
C	-3.84672900	1.95683900	-1.45513900
H	-4.14297300	1.98164700	-2.50311200
C	-4.72229000	2.45554100	-0.46079800
H	-5.69437000	2.85121800	-0.73825200
C	-4.30083300	2.43531700	0.84688600
H	-4.92867200	2.81965700	1.64696200
Cl	4.48932800	-0.29377000	-0.56622200

CN_168_CC_198

Charge = 0, Multiplicity = 1

O	1.86803700	-3.16590900	1.50591700
O	-1.23171500	-0.67736900	-2.53452400
N	-0.13866300	0.32834500	-0.69196200
N	-2.66309900	1.43688900	-1.23422300
C	-3.00271000	-3.01339100	-1.41669200
H	-3.55950000	-2.09104800	-1.21601000
H	-3.65621700	-3.86455300	-1.20387100
H	-2.77055600	-3.00789600	-2.48696700
C	0.64514800	-3.27135300	0.91457300
C	-0.26737800	-4.31817800	0.97563100
H	-0.07726000	-5.20546100	1.56947900
C	-1.44838100	-4.18865400	0.22119800
H	-2.16974200	-5.00069900	0.25816700

C	-1.74172600	-3.08036100	-0.59421100
C	-0.81011600	-2.02776200	-0.60283000
C	0.34733200	-2.14770200	0.15590900
C	1.44129000	-1.21052900	0.20646600
C	2.51620800	-1.96260200	0.97781300
H	3.34658700	-2.30112800	0.35639900
H	2.91942300	-1.39921200	1.82340900
C	1.23786000	0.04332000	-0.29281600
C	-0.81038000	-0.78759700	-1.41493400
C	2.13346500	1.21475800	-0.33029100
C	3.54466100	1.18494900	-0.34908100
C	4.31831200	2.34153500	-0.24173000
H	5.39866500	2.25265500	-0.26571800
C	3.70645700	3.58671400	-0.15148600
H	4.31296000	4.48351500	-0.07038800
C	2.31479800	3.66405400	-0.21533900
H	1.81570200	4.62792400	-0.19304300
C	1.55554700	2.50658900	-0.31023200
H	0.48072100	2.58934700	-0.37364900
C	-0.96557000	0.83550800	0.37054800
C	-0.54197200	0.84800800	1.69014100
H	0.43147500	0.44824300	1.94080800
C	-1.34875800	1.36660000	2.72562600
H	-0.96591700	1.35221200	3.74196400
C	-2.60262400	1.86345800	2.46339800
H	-3.23386300	2.25040800	3.25857900
C	-3.07861300	1.87964300	1.12948200
C	-2.25887600	1.38582900	0.06147000
C	-3.85480000	1.92411300	-1.50861600
H	-4.13283600	1.94787200	-2.56160000
C	-4.75441800	2.40887300	-0.52879700
H	-5.72625100	2.79316900	-0.82264500
C	-4.35647800	2.38968200	0.78614300
H	-5.00350300	2.76317500	1.57600500
Cl	4.44718800	-0.28599700	-0.70275500

CN_168_CC_203

Charge = 0, Multiplicity = 1

O	1.91117900	-3.11971900	1.55007700
O	-1.20933100	-0.69551000	-2.51960200
N	-0.14108100	0.33840900	-0.67713600
N	-2.67365300	1.41205400	-1.26359200
C	-2.93049900	-3.06890200	-1.42589200

S190

H	-3.50855000	-2.15803800	-1.23324300
H	-3.56844100	-3.93319700	-1.21881100
H	-2.68658900	-3.06019600	-2.49352400
C	0.69619300	-3.25141400	0.94651000
C	-0.19399500	-4.31789800	0.99513300
H	0.00827700	-5.20272700	1.58862800
C	-1.36910600	-4.21161200	0.22756200
H	-2.07304400	-5.03918100	0.25478700
C	-1.67772500	-3.10842000	-0.58928800
C	-0.76910700	-2.03544700	-0.58592600
C	0.38079000	-2.13359500	0.18659300
C	1.45275700	-1.17428100	0.24936300
C	2.53463100	-1.89667100	1.03690800
H	3.38763500	-2.20710900	0.43147800
H	2.90371600	-1.32231600	1.89128500
C	1.23198500	0.07295900	-0.25473300
C	-0.78747300	-0.79548600	-1.39930700
C	2.12471900	1.24600500	-0.28593000
C	3.53220400	1.20522600	-0.38018500
C	4.32061000	2.35251900	-0.27756600
H	5.39746600	2.25786200	-0.36159600
C	3.72386900	3.59764400	-0.11502300
H	4.34101200	4.48752700	-0.03785900
C	2.33123800	3.68685700	-0.09930800
H	1.84310500	4.65304900	-0.01645600
C	1.55780400	2.53840600	-0.19103900
H	0.48161800	2.63019600	-0.18675900
C	-0.99420500	0.83562600	0.37006300
C	-0.59559300	0.84988100	1.69760900
H	0.37839100	0.46199200	1.96468900
C	-1.42706400	1.35656400	2.71919600
H	-1.06256100	1.34514700	3.74229300
C	-2.68214300	1.83799800	2.43478800
H	-3.33253100	2.21578500	3.21887300
C	-3.13450900	1.84929400	1.09264600
C	-2.28980300	1.36765100	0.03846800
C	-3.86737100	1.88217300	-1.55773900
H	-4.12858800	1.90106300	-2.61513100
C	-4.78972900	2.35511300	-0.59328400
H	-5.76180400	2.72576500	-0.90342700
C	-4.41343300	2.34179500	0.72797600
H	-5.07862400	2.70614400	1.50694600
Cl	4.39750600	-0.26382900	-0.82332100

CN_168_CC_208

Charge = 0, Multiplicity = 1

O	1.96770400	-3.07528700	1.58653000
O	-1.19156400	-0.71726800	-2.49784100
N	-0.14567200	0.34590700	-0.65864500
N	-2.68853600	1.37956800	-1.28922900
C	-2.84802900	-3.13466900	-1.43248300
H	-3.45226900	-2.24044300	-1.24241100
H	-3.46444100	-4.01663900	-1.23488600
H	-2.59390000	-3.11502900	-2.49755300
C	0.75991800	-3.23485000	0.97415400
C	-0.10212300	-4.32465100	1.00762300
H	0.11805600	-5.20854800	1.59611600
C	-1.27284500	-4.24351900	0.22988800
H	-1.95485700	-5.08954700	0.24519300
C	-1.60304300	-3.14406600	-0.58354700
C	-0.72301300	-2.04705400	-0.56549900
C	0.42006700	-2.12102200	0.21907300
C	1.46591800	-1.13623700	0.29464200
C	2.55835200	-1.82743900	1.09394600
H	3.43357500	-2.10110900	0.50222900
H	2.88975500	-1.24667300	1.95975600
C	1.22372700	0.10358800	-0.21312000
C	-0.76543800	-0.80680400	-1.37825500
C	2.11072900	1.28116700	-0.24249000
C	3.51040900	1.23687100	-0.41380700
C	4.30851000	2.37879900	-0.32502100
H	5.37890000	2.28382400	-0.46952100
C	3.72598500	3.62046900	-0.09735800
H	4.34996900	4.50647300	-0.03107900
C	2.33679400	3.71348600	0.00077800
H	1.85911700	4.67853800	0.13932800
C	1.55410100	2.57013900	-0.07872000
H	0.48029200	2.66391300	-0.00501600
C	-1.02428200	0.83520300	0.37180600
C	-0.64932800	0.85410800	1.70643600
H	0.32531500	0.47923400	1.98963000
C	-1.50411300	1.35026700	2.71370300
H	-1.15667200	1.34427400	3.74276600
C	-2.76058700	1.81444200	2.40761600
H	-3.42913900	2.18418700	3.18018100
C	-3.19101400	1.81705300	1.05824100
C	-2.32279800	1.34609300	0.01823800

C	-3.88481900	1.83001500	-1.60253000
H	-4.13087900	1.84063600	-2.66368100
C	-4.82845100	2.29251600	-0.65363400
H	-5.80132900	2.64727000	-0.97947000
C	-4.47164300	2.28922400	0.67298400
H	-5.15381300	2.64556900	1.44089400
Cl	4.34086700	-0.22779900	-0.93193300

CN_173_CC_163

Charge = 0, Multiplicity = 1

O	3.38662200	2.50730500	-0.82230300
O	-1.35648200	1.45775700	1.97965400
N	-0.33279000	0.02006700	0.43351700
N	-3.24358400	-0.00525200	0.75199300
C	-1.73084600	4.25399100	0.86812800
H	-2.55474400	3.66309700	0.45389000
H	-1.91613000	5.31010700	0.64977300
H	-1.76292300	4.10776000	1.95297600
C	2.16796600	3.06968700	-0.59472800
C	1.82018800	4.41220300	-0.61825800
H	2.52736900	5.17765900	-0.91829200
C	0.52048400	4.74869700	-0.19108700
H	0.23433900	5.79709800	-0.20090200
C	-0.40166900	3.81663300	0.30831800
C	-0.02328600	2.45729700	0.28578900
C	1.22191300	2.11473500	-0.23088200
C	1.82655100	0.81142400	-0.20662800
C	3.28412100	1.07509800	-0.54934600
H	3.98072700	0.83329500	0.26138900
H	3.61134200	0.55973900	-1.45112900
C	1.06116000	-0.25195600	0.16554900
C	-0.68513300	1.34151000	0.98498600
C	1.47653100	-1.60094300	0.62109400
C	2.63074100	-2.30612500	0.23376200
C	3.07182300	-3.44849900	0.90186400
H	3.95727800	-3.95967200	0.54076700
C	2.35767400	-3.93608900	1.99127800
H	2.70377800	-4.82441900	2.51067400
C	1.18727300	-3.28542400	2.38499400
H	0.60845800	-3.65677700	3.22512200
C	0.76876000	-2.14057900	1.72098800
H	-0.11014500	-1.60670800	2.06130600
C	-1.23602300	-0.68700000	-0.42657200

C	-0.71021600	-1.38207700	-1.51149500
H	0.34608500	-1.30633500	-1.73172300
C	-1.50302200	-2.18266300	-2.35773200
H	-1.02019600	-2.70989100	-3.17528700
C	-2.85812700	-2.28288700	-2.16510900
H	-3.48068200	-2.89399200	-2.81259200
C	-3.45782200	-1.54961900	-1.11397700
C	-2.66567400	-0.73612600	-0.23227000
C	-4.54798500	-0.05116700	0.91543600
H	-4.95152900	0.55734200	1.72425000
C	-5.41434900	-0.83055500	0.11446000
H	-6.48390800	-0.82938600	0.30039100
C	-4.85902100	-1.57488700	-0.89745800
H	-5.47680200	-2.18647800	-1.55042600
Cl	3.45700800	-1.94027800	-1.28259900

CN_173_CC_168

Charge = 0, Multiplicity = 1

O	-3.11023200	2.79481900	0.87579100
O	1.40656000	1.26671900	-2.05898900
N	0.32100700	-0.04110700	-0.44089900
N	3.20381300	-0.30131100	-0.78778100
C	2.09680300	4.02922800	-0.97902000
H	2.87060100	3.35996800	-0.58800300
H	2.39311000	5.06208000	-0.77220400
H	2.07933600	3.87888500	-2.06373100
C	-1.85071900	3.23337500	0.60788500
C	-1.37508700	4.53681700	0.61165500
H	-1.99704000	5.36705600	0.92778000
C	-0.06345000	4.74625400	0.14376200
H	0.32194400	5.76239800	0.13744600
C	0.74927600	3.72692900	-0.37550500
C	0.24335700	2.41136400	-0.32991400
C	-1.01339500	2.18896100	0.22458800
C	-1.74186400	0.94766300	0.22846300
C	-3.15542200	1.35744700	0.61611200
H	-3.90152700	1.17895700	-0.16557900
H	-3.49728900	0.88556500	1.53587600
C	-1.08933400	-0.18846600	-0.15034300
C	0.77169000	1.23081800	-1.03527400
C	-1.61926900	-1.50592200	-0.58419700
C	-2.86481100	-2.07552100	-0.25661300
C	-3.38724200	-3.18158600	-0.92685400

H	-4.34279400	-3.58361200	-0.60908800
C	-2.66954500	-3.77452900	-1.95996600
H	-3.07997300	-4.63431000	-2.48052100
C	-1.41500100	-3.26349100	-2.29365600
H	-0.83066500	-3.71575600	-3.08911000
C	-0.91582600	-2.15093900	-1.63065300
H	0.02906400	-1.72098800	-1.93775100
C	1.17338800	-0.77104900	0.44916400
C	0.60981900	-1.38048700	1.56570100
H	-0.43880300	-1.22799700	1.78307500
C	1.35624700	-2.18935100	2.44600200
H	0.84683600	-2.64526500	3.28991900
C	2.70101900	-2.38555300	2.25362000
H	3.28735900	-3.00302700	2.92828200
C	3.33860100	-1.74898500	1.16234400
C	2.59297500	-0.93168900	0.24512200
C	4.49980200	-0.44641400	-0.96160100
H	4.93218600	0.08335300	-1.80988900
C	5.32222900	-1.23480700	-0.12391400
H	6.38680200	-1.31713600	-0.31993500
C	4.73195600	-1.88122800	0.93465300
H	5.31601400	-2.49633100	1.61478600
Cl	-3.73980700	-1.59542600	1.19974200

CN_173_CC_173

Charge = 0, Multiplicity = 1

O	-2.65919600	3.15564400	0.94256300
O	1.42025500	0.98928900	-2.19433000
N	0.28211400	-0.13231400	-0.47326200
N	3.08532500	-0.72281200	-0.84757300
C	2.58499000	3.63210400	-1.14027700
H	3.26732700	2.85404800	-0.78140000
H	3.03965600	4.60884800	-0.94921900
H	2.49823900	3.49105400	-2.22302500
C	-1.36392600	3.40700200	0.61582200
C	-0.70422700	4.62842700	0.60156500
H	-1.18558500	5.53612300	0.94861400
C	0.60137800	4.65171400	0.07627100
H	1.12888700	5.60166500	0.05477200
C	1.23486800	3.52863400	-0.47844000
C	0.54694100	2.30130500	-0.41019500
C	-0.70657900	2.25498800	0.19372600
C	-1.60745600	1.12849400	0.22993800

C	-2.92812200	1.74380100	0.67807200
H	-3.72301300	1.69072200	-0.07209200
H	-3.29773000	1.31943400	1.60993900
C	-1.13326500	-0.09270900	-0.15692500
C	0.86365500	1.05474700	-1.12854900
C	-1.82312900	-1.35302000	-0.53980500
C	-3.15388300	-1.73006400	-0.26649300
C	-3.78094400	-2.80315200	-0.89935900
H	-4.80084900	-3.04772400	-0.62445700
C	-3.09271700	-3.56258800	-1.83904900
H	-3.58604200	-4.39603800	-2.32958400
C	-1.76368700	-3.24624500	-2.11742600
H	-1.19878200	-3.82682800	-2.84028900
C	-1.15904300	-2.16272900	-1.49558200
H	-0.15139400	-1.88373400	-1.77306300
C	1.06386000	-0.86593500	0.47354600
C	0.46567500	-1.32875000	1.64035200
H	-0.56356700	-1.07003400	1.84977600
C	1.15665000	-2.12135400	2.57964000
H	0.62571700	-2.45802500	3.46531500
C	2.47665800	-2.44906300	2.39247500
H	3.01928500	-3.05320400	3.11413200
C	3.14577800	-1.97607100	1.23831700
C	2.45432800	-1.18334500	0.26067000
C	4.35702900	-1.00673000	-1.03239800
H	4.80968700	-0.61196700	-1.94138600
C	5.12888100	-1.77810800	-0.13284700
H	6.17536100	-1.97841900	-0.34081800
C	4.51434200	-2.25861400	0.99812800
H	5.06018300	-2.85621200	1.72406300
Cl	-4.06154400	-1.03351300	1.07774400

CN_173_CC_178

Charge = 0, Multiplicity = 1

O	-1.79800200	3.54043100	1.09299900
O	1.26617700	0.57175600	-2.47405400
N	0.16092500	-0.27306300	-0.57384600
N	2.74793500	-1.34160400	-0.95169400
C	3.22992100	2.81958900	-1.41942600
H	3.72191600	1.88822800	-1.11786400
H	3.92391600	3.64877200	-1.25271500
H	3.03704200	2.73524000	-2.49451100
C	-0.51877100	3.48748800	0.64004600

S196

C	0.42918200	4.50401400	0.62733200
H	0.22331100	5.47369500	1.06710100
C	1.65450700	4.23944000	-0.00962000
H	2.40342900	5.02676400	-0.03069000
C	1.94362700	3.02894400	-0.66220200
C	0.97509100	2.01416300	-0.58990300
C	-0.21522100	2.24426700	0.09699500
C	-1.36876800	1.36855000	0.16713500
C	-2.45209600	2.27874200	0.74748100
H	-3.25344000	2.51517100	0.04427100
H	-2.88523000	1.89049900	1.66772300
C	-1.21829600	0.07180600	-0.24765300
C	0.90942000	0.74315900	-1.33879800
C	-2.13793600	-1.07507900	-0.48051300
C	-3.52892400	-1.16100400	-0.25271700
C	-4.28693600	-2.27291200	-0.62096300
H	-5.34943600	-2.27090200	-0.40533400
C	-3.68959400	-3.36306200	-1.24313000
H	-4.28871600	-4.22315200	-1.52580800
C	-2.32015700	-3.32111100	-1.49380100
H	-1.82260000	-4.15008400	-1.98766200
C	-1.57937900	-2.20476300	-1.13307600
H	-0.52976900	-2.16604300	-1.38565800
C	0.86002600	-0.92450700	0.48538400
C	0.27568500	-1.09764900	1.73266500
H	-0.70638300	-0.68681100	1.92396900
C	0.93064900	-1.79093300	2.77297400
H	0.42209000	-1.89708800	3.72686800
C	2.19068700	-2.30935000	2.59789900
H	2.70281100	-2.83475900	3.39907900
C	2.83260700	-2.15605900	1.34481500
C	2.17201200	-1.47567300	0.26954900
C	3.95365400	-1.83365600	-1.14849500
H	4.36963200	-1.70172600	-2.14651900
C	4.69880300	-2.50707100	-0.15236100
H	5.69034300	-2.88813600	-0.37611400
C	4.13027900	-2.66643700	1.08898400
H	4.65847800	-3.18232700	1.88703200
Cl	-4.44972000	0.08132100	0.59190900

CN_173_CC_183

Charge = 0, Multiplicity = 1

O	-1.56430100	3.40373100	1.36358100
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S197

O	1.16643600	0.56974900	-2.60579900
N	0.10965800	-0.32003000	-0.68985100
N	2.63357700	-1.45384000	-1.09511600
C	3.31953800	2.64645900	-1.42879700
H	3.76576600	1.67116300	-1.20371100
H	4.06241600	3.42290800	-1.22368800
H	3.09885000	2.64784100	-2.50179500
C	-0.32005400	3.34536800	0.81769200
C	0.69771300	4.29113200	0.87910900
H	0.58420100	5.20978500	1.44411900
C	1.87647900	4.02022400	0.16180200
H	2.67934000	4.75180800	0.19971900
C	2.06388900	2.86938100	-0.62542800
C	1.02827700	1.92287000	-0.63049600
C	-0.12827600	2.16941800	0.10466700
C	-1.32855400	1.35950300	0.13875300
C	-2.32779100	2.25998500	0.86101200
H	-3.10215600	2.66517000	0.20759800
H	-2.80136600	1.78240600	1.71987800
C	-1.25580300	0.08372100	-0.35481200
C	0.86990600	0.69745100	-1.44882300
C	-2.22570300	-1.02824200	-0.46396700
C	-3.62468100	-0.98473100	-0.27339400
C	-4.41836600	-2.13177100	-0.27329700
H	-5.48671100	-2.02556100	-0.12185600
C	-3.85158300	-3.38163300	-0.49789700
H	-4.47703300	-4.26899900	-0.49763200
C	-2.48524400	-3.46209300	-0.76105200
H	-2.02081900	-4.41855900	-0.98036800
C	-1.70415300	-2.31546600	-0.74808500
H	-0.65131600	-2.39231300	-0.97577100
C	0.82798100	-0.90595300	0.39844300
C	0.29209500	-0.99430000	1.67426800
H	-0.68348000	-0.57318600	1.87554900
C	0.99000400	-1.61866600	2.73085400
H	0.52235500	-1.65876300	3.71039200
C	2.24090100	-2.15351900	2.53855300
H	2.78522800	-2.62454200	3.35226100
C	2.82800700	-2.09577000	1.25076100
C	2.12202200	-1.48764000	0.16203800
C	3.82470800	-1.97248200	-1.31241900
H	4.19083900	-1.92317000	-2.33705000
C	4.61476800	-2.57550300	-0.30524800
H	5.59131500	-2.98235200	-0.54861500

C	4.10820700	-2.63691700	0.97121500
H	4.67186800	-3.09861400	1.77813600
Cl	-4.52674900	0.52466300	-0.16808000

CN_173_CC_188

Charge = 0, Multiplicity = 1

O	-1.57787900	3.32443100	1.44940600
O	1.12925500	0.59035500	-2.61861800
N	0.10416100	-0.33733500	-0.70088300
N	2.63203700	-1.44211900	-1.14736800
C	3.27215700	2.67974500	-1.43434800
H	3.73093300	1.70519300	-1.23229900
H	4.00957100	3.45986700	-1.22359400
H	3.03904500	2.69836300	-2.50454300
C	-0.34327100	3.29768000	0.87715700
C	0.66788700	4.25010400	0.94614600
H	0.55799600	5.15295200	1.53677000
C	1.83721200	4.00588200	0.20365200
H	2.63483900	4.74284000	0.24747200
C	2.02390200	2.87470900	-0.61243000
C	0.99584200	1.92010400	-0.62587000
C	-0.15216100	2.14466500	0.12818100
C	-1.34126300	1.32160500	0.16437600
C	-2.34004800	2.19139300	0.91935800
H	-3.12080500	2.61187000	0.28359600
H	-2.80872700	1.68403500	1.76494400
C	-1.25979000	0.05318100	-0.34329800
C	0.84127000	0.70170400	-1.45813000
C	-2.23032500	-1.05627400	-0.42379600
C	-3.63462400	-0.97686200	-0.29707800
C	-4.44715200	-2.10943500	-0.24244700
H	-5.51923700	-1.97842700	-0.14707200
C	-3.89077100	-3.37945100	-0.34944300
H	-4.52957000	-4.25629300	-0.30808800
C	-2.51661100	-3.49865900	-0.55413600
H	-2.06156500	-4.47565000	-0.68468100
C	-1.71694300	-2.36556800	-0.59521000
H	-0.65754500	-2.47445100	-0.77412600
C	0.85267600	-0.90180000	0.38062700
C	0.34660900	-0.98246300	1.66886800
H	-0.63058400	-0.57332400	1.88659100
C	1.07669500	-1.58413600	2.71679200
H	0.63167500	-1.61932900	3.70699600

C	2.33075800	-2.10307700	2.50247800
H	2.89991600	-2.55644600	3.30920900
C	2.88817600	-2.05258500	1.20126700
C	2.14931400	-1.46786900	0.12151100
C	3.82559000	-1.94597100	-1.38467100
H	4.16834200	-1.90395600	-2.41768700
C	4.64674500	-2.52532800	-0.38832500
H	5.62349000	-2.92096800	-0.64878900
C	4.16968600	-2.57876900	0.89970900
H	4.75772600	-3.02261800	1.69921100
Cl	-4.50583800	0.55229800	-0.37224100

CN_173_CC_193

Charge = 0, Multiplicity = 1

O	-1.59851000	3.26534600	1.51491200
O	1.09371000	0.60568800	-2.62022500
N	0.10125200	-0.35164000	-0.69820000
N	2.63398100	-1.42743900	-1.18752300
C	3.21940600	2.71849800	-1.44558400
H	3.69517600	1.74944500	-1.25662400
H	3.94789600	3.50785400	-1.23826000
H	2.97245900	2.74139800	-2.51256500
C	-0.37242900	3.26551600	0.92204000
C	0.62805100	4.22940400	0.98826900
H	0.51716100	5.12330500	1.59216900
C	1.78911900	4.00807600	0.22544800
H	2.57834600	4.75415300	0.26697900
C	1.97903900	2.88867300	-0.60643400
C	0.96253900	1.92161700	-0.61761400
C	-0.17701100	2.12638100	0.15375900
C	-1.35268000	1.28718700	0.19848400
C	-2.35323600	2.13017500	0.97793100
H	-3.14847800	2.54872800	0.35910800
H	-2.80556400	1.60155600	1.82038400
C	-1.26052900	0.02411500	-0.31708100
C	0.81414500	0.70577600	-1.45689200
C	-2.23092600	-1.08369000	-0.38013700
C	-3.63757600	-0.97835200	-0.32272400
C	-4.46868100	-2.09644000	-0.24693600
H	-5.54211900	-1.94838800	-0.20876400
C	-3.92506800	-3.37626900	-0.26347800
H	-4.57714500	-4.24241400	-0.20660800
C	-2.54458200	-3.52346200	-0.39984500

H	-2.09958400	-4.51192900	-0.45932800
C	-1.72697500	-2.40429600	-0.46309800
H	-0.66215300	-2.53621500	-0.58593900
C	0.87797500	-0.90071100	0.37261000
C	0.39952800	-0.97827300	1.67153800
H	-0.57841300	-0.58007900	1.90590700
C	1.15794200	-1.56362500	2.70844800
H	0.73356600	-1.59749100	3.70771700
C	2.41386100	-2.06829200	2.47191900
H	3.00493500	-2.50903300	3.26984900
C	2.94427900	-2.01957300	1.15939000
C	2.17659400	-1.45154800	0.09080100
C	3.82912300	-1.91721300	-1.44494700
H	4.15124300	-1.87703500	-2.48466100
C	4.67717300	-2.47991800	-0.46152700
H	5.65363300	-2.86464900	-0.73887000
C	4.22630600	-2.53140600	0.83590200
H	4.83559300	-2.96256700	1.62638600
Cl	-4.47394800	0.55850200	-0.52445700

CN_173_CC_198

Charge = 0, Multiplicity = 1

O	1.62754800	-3.21751400	1.56833700
O	-1.06517900	-0.61855700	-2.61256600
N	-0.10026900	0.36491800	-0.68827100
N	-2.63816900	1.41153100	-1.22139000
C	-3.16018400	-2.76478800	-1.45895900
H	-3.65542600	-1.80367700	-1.27960300
H	-3.87726000	-3.56615700	-1.25806600
H	-2.89922200	-2.78676200	-2.52259200
C	0.40902700	-3.24268600	0.95902100
C	-0.57627100	-4.22268900	1.01562600
H	-0.45978400	-5.11244200	1.62458000
C	-1.73020700	-4.02302000	0.23573100
H	-2.50751600	-4.78187900	0.26969800
C	-1.92794900	-2.91020500	-0.60339400
C	-0.92738000	-1.92623500	-0.60537900
C	0.20380600	-2.11132400	0.18223600
C	1.36338900	-1.25312600	0.23839200
C	2.36802400	-2.06957900	1.03780900
H	3.18388900	-2.47307700	0.43602500
H	2.79435400	-1.52466100	1.88420500
C	1.25863700	0.00490800	-0.28299900

S201

C	-0.78952300	-0.71039000	-1.44779200
C	2.22879000	1.11178600	-0.33555000
C	3.63451700	0.98750300	-0.35048800
C	4.48251900	2.09288400	-0.27043100
H	5.55475000	1.93296600	-0.29028100
C	3.95332300	3.37732700	-0.20997000
H	4.61755800	4.23401800	-0.15039500
C	2.56940900	3.54498900	-0.27263200
H	2.13525700	4.54005000	-0.26974400
C	1.73555500	2.43819500	-0.34162400
H	0.66746300	2.58679500	-0.40353600
C	-0.90428000	0.90180300	0.36974400
C	-0.45267800	0.97836500	1.67839700
H	0.52558700	0.59111200	1.92949700
C	-1.23777600	1.54969200	2.70308000
H	-0.83329000	1.58395100	3.71055200
C	-2.49497700	2.04004500	2.44422800
H	-3.10680900	2.46989200	3.23240400
C	-2.99940700	1.99051600	1.12152500
C	-2.20451700	1.43695300	0.06517700
C	-3.83456900	1.88675200	-1.49883400
H	-4.13717900	1.84612100	-2.54439000
C	-4.70782500	2.43512500	-0.52933400
H	-5.68383600	2.80843200	-0.82338300
C	-4.28170300	2.48742400	0.77629800
H	-4.91089800	2.90761600	1.55703500
Cl	4.43505800	-0.55177900	-0.65293000

CN_173_CC_203

Charge = 0, Multiplicity = 1

O	1.66555600	-3.17685600	1.61334800
O	-1.03968000	-0.63267000	-2.59833300
N	-0.10133600	0.37633100	-0.67308600
N	-2.64513000	1.39109500	-1.25096100
C	-3.09488700	-2.81828500	-1.47077300
H	-3.61112200	-1.86685300	-1.29919200
H	-3.79850200	-3.63332100	-1.27738800
H	-2.82042600	-2.83651400	-2.53106000
C	0.45359000	-3.22627800	0.99130200
C	-0.51224100	-4.22611500	1.03442200
H	-0.38550100	-5.11492000	1.64271500
C	-1.66045400	-4.04790500	0.24061100
H	-2.42257300	-4.82240500	0.26401600

S202

C	-1.87071000	-2.93831800	-0.59988100
C	-0.89029300	-1.93391400	-0.58879400
C	0.23313800	-2.09856500	0.21365200
C	1.37397900	-1.21875800	0.28260100
C	2.38526600	-2.00865800	1.09800300
H	3.22469800	-2.38691500	0.51217700
H	2.77911000	-1.45183800	1.95293100
C	1.25447100	0.03411200	-0.24381600
C	-0.76625500	-0.71674500	-1.43256100
C	2.22357200	1.14135700	-0.29109200
C	3.62489200	1.00399000	-0.38065000
C	4.48723300	2.09897400	-0.30715700
H	5.55560600	1.93150900	-0.38578700
C	3.97347600	3.38455300	-0.17799400
H	4.64799800	4.23355000	-0.12379100
C	2.58969200	3.56631500	-0.16328700
H	2.16713100	4.56458400	-0.10352000
C	1.74197400	2.46963800	-0.22726300
H	0.67343400	2.62929100	-0.22504500
C	-0.93154500	0.90423500	0.37002400
C	-0.50579400	0.98297100	1.68735300
H	0.47238700	0.60677200	1.95537800
C	-1.31592500	1.54324600	2.69846500
H	-0.93035800	1.58051100	3.71322100
C	-2.57394800	2.01884700	2.41710500
H	-3.20533500	2.44018300	3.19438600
C	-3.05372500	1.96453400	1.08544600
C	-2.23337500	1.42230500	0.04260800
C	-3.84273400	1.85058900	-1.54847500
H	-4.12726600	1.80574100	-2.59893700
C	-4.73940000	2.38770000	-0.59407300
H	-5.71502300	2.74838400	-0.90471400
C	-4.33626100	2.44516600	0.71853300
H	-4.98400600	2.85677700	1.48859900
Cl	4.38915200	-0.53472100	-0.76774300

CN_173_CC_208

Charge = 0, Multiplicity = 1

O	1.71327800	-3.14026700	1.65162000
O	-1.01880800	-0.64863300	-2.57879200
N	-0.10430300	0.38549400	-0.65463600
N	-2.65525100	1.36555200	-1.27664100
C	-3.02287900	-2.87954400	-1.48051200

S203

H	-3.55782800	-1.93647100	-1.32098300
H	-3.71389300	-3.70595500	-1.28990700
H	-2.73625000	-2.89937100	-2.53757900
C	0.50701600	-3.21439800	1.01991900
C	-0.43539500	-4.23680200	1.04765100
H	-0.29417900	-5.12637700	1.65161800
C	-1.57930300	-4.08067300	0.24264400
H	-2.32320000	-4.87295300	0.25406100
C	-1.80665800	-2.97254700	-0.59534400
C	-0.85022200	-1.94503000	-0.56917900
C	0.26619600	-2.08813300	0.24641800
C	1.38547200	-1.18424400	0.32844800
C	2.40634500	-1.94736000	1.15578600
H	3.26898700	-2.29387400	0.58373500
H	2.76503600	-1.38265400	2.02130500
C	1.24817700	0.06340000	-0.20146900
C	-0.74443900	-0.72562400	-1.41282100
C	2.21473700	1.17302000	-0.24742700
C	3.60800200	1.02861700	-0.41297700
C	4.48089000	2.11632900	-0.35437400
H	5.54277800	1.94582200	-0.49209400
C	3.98249500	3.40024800	-0.16319500
H	4.66459200	4.24387500	-0.12083900
C	2.60270100	3.58958000	-0.06845200
H	2.19168600	4.58816300	0.04378500
C	1.74481200	2.49988000	-0.11895500
H	0.67892700	2.66466800	-0.05037600
C	-0.95960800	0.90678600	0.37222500
C	-0.55826100	0.99028900	1.69713100
H	0.41966600	0.62549100	1.98167600
C	-1.39158200	1.54170600	2.69406000
H	-1.02373400	1.58410000	3.71517700
C	-2.65018600	2.00197300	2.39080400
H	-3.29965500	2.41653200	3.15675700
C	-3.10706300	1.93960600	1.05147100
C	-2.26317200	1.40635500	0.02268900
C	-3.85411900	1.80815800	-1.59355200
H	-4.12223700	1.75601700	-2.64800200
C	-4.77224100	2.33638200	-0.65466200
H	-5.74766100	2.68331600	-0.98121000
C	-4.38999000	2.40261400	0.66367700
H	-5.05478800	2.80741800	1.42274200
Cl	4.33720700	-0.50749400	-0.87138700

CN_173_CC_213

Charge = 0, Multiplicity = 1

O	-1.76866300	3.10684800	1.68333900
O	0.99991700	0.66582000	-2.55559400
N	0.10849300	-0.39280600	-0.63356400
N	2.66663200	-1.33586500	-1.29923000
C	2.94703300	2.94429200	-1.48675700
H	3.51079500	2.01856800	-1.32470700
H	3.61576300	3.79196900	-1.31059900
H	2.64893700	2.94596700	-2.54076700
C	-0.56703500	3.20563200	1.04514800
C	0.34870700	4.25215000	1.05624400
H	0.18931600	5.14381300	1.65256600
C	1.48960500	4.11820500	0.24257700
H	2.21264100	4.92964200	0.24079800
C	1.73789200	3.01032500	-0.58963800
C	0.80852900	1.95811300	-0.54711200
C	-0.30155200	2.07928400	0.27996300
C	-1.39745900	1.15017700	0.37469600
C	-2.43103800	1.88818400	1.20784500
H	-3.31278000	2.19989100	0.64429500
H	-2.75787700	1.32013800	2.08390100
C	-1.24045900	-0.09233300	-0.15692600
C	0.72348700	0.73609400	-1.38969400
C	-2.20317700	-1.20616100	-0.20435400
C	-3.58455000	-1.06022100	-0.44690900
C	-4.46410800	-2.14361100	-0.40884200
H	-5.51672400	-1.97389700	-0.60591400
C	-3.98111800	-3.42356600	-0.15990400
H	-4.66779300	-4.26415700	-0.13365500
C	-2.60956100	-3.61466300	0.01678000
H	-2.21038900	-4.61126700	0.17855100
C	-1.74529000	-2.52896900	-0.01467300
H	-0.68548300	-2.69398900	0.12047400
C	0.98780000	-0.90880300	0.37618200
C	0.61029000	-0.99813100	1.70790900
H	-0.36674900	-0.64405500	2.00896600
C	1.46556600	-1.54214700	2.69018800
H	1.11480800	-1.59063400	3.71703700
C	2.72419900	-1.98712000	2.36533200
H	3.39081700	-2.39603700	3.11950100
C	3.15911200	-1.91469500	1.01917800
C	2.29296700	-1.38895500	0.00496400

S205

C	3.86668300	-1.76055500	-1.63515300
H	4.11936600	-1.69895500	-2.69291700
C	4.80493600	-2.28150000	-0.71220800
H	5.78013000	-2.61382500	-1.05427600
C	4.44233800	-2.35906400	0.61098000
H	5.12317600	-2.75826700	1.35871200
Cl	-4.28039100	0.47192300	-0.96642800

CN_173_CC_223

Charge = 0, Multiplicity = 1

O	-1.90293500	3.03939300	1.73270900
O	0.97142400	0.71070000	-2.50102700
N	0.12022600	-0.39919600	-0.58966800
N	2.69517400	-1.26001000	-1.33746100
C	2.78658700	3.08556900	-1.48044400
H	3.40525300	2.19613000	-1.31564800
H	3.40764000	3.97259100	-1.32450900
H	2.47392600	3.05583800	-2.52973000
C	-0.70773600	3.19085100	1.09059700
C	0.14774600	4.28664300	1.07312400
H	-0.05706600	5.18111900	1.65109700
C	1.28765400	4.19997800	0.25067700
H	1.96361900	5.05066700	0.22605900
C	1.58841700	3.09432700	-0.56650800
C	0.71965800	1.99152700	-0.49581600
C	-0.38194800	2.06610000	0.34661000
C	-1.42537800	1.08368900	0.46194500
C	-2.49454300	1.77188300	1.29085000
H	-3.40042300	2.01298000	0.72929500
H	-2.77299400	1.20401800	2.18359100
C	-1.22078700	-0.14799800	-0.06862600
C	0.68497500	0.76573200	-1.33668200
C	-2.17072500	-1.27600200	-0.12338700
C	-3.51604700	-1.14183900	-0.52143100
C	-4.39781500	-2.22403900	-0.53105700
H	-5.42294500	-2.06656500	-0.84718600
C	-3.94721900	-3.48952500	-0.17073300
H	-4.63457500	-4.32996200	-0.18170200
C	-2.60615700	-3.66868100	0.17284400
H	-2.23276600	-4.65506500	0.43056400
C	-1.73984800	-2.58325100	0.18633000
H	-0.70289900	-2.73657300	0.45343400
C	1.04361600	-0.90938000	0.38432000

C	0.70907200	-1.01617700	1.72661800
H	-0.26509900	-0.68202100	2.05892300
C	1.60249300	-1.55168500	2.67918600
H	1.28214600	-1.61730600	3.71499500
C	2.86037900	-1.96585300	2.31392600
H	3.55681100	-2.36846700	3.04417800
C	3.25688200	-1.86492900	0.95776000
C	2.35202800	-1.34770700	-0.02704200
C	3.89791000	-1.64564100	-1.70827700
H	4.12462300	-1.55684000	-2.77001700
C	4.87072900	-2.15846600	-0.81714400
H	5.84611600	-2.45848500	-1.18739900
C	4.54120900	-2.26856100	0.51223400
H	5.24972300	-2.66150000	1.23722900
Cl	-4.14845400	0.37728000	-1.14917400

CN_173_CC_233

Charge = 0, Multiplicity = 1

O	-2.06667900	2.96248400	1.76871500
O	0.95280500	0.77076400	-2.43743800
N	0.13572800	-0.39397000	-0.54461600
N	2.73153900	-1.15908100	-1.36581400
C	2.60945000	3.24254100	-1.45227400
H	3.27911800	2.39084700	-1.28810500
H	3.17960900	4.16453800	-1.30486900
H	2.29183400	3.18935300	-2.49913200
C	-0.87665400	3.17389200	1.13163200
C	-0.09075700	4.31949800	1.09184100
H	-0.35141900	5.21233700	1.64952300
C	1.05295300	4.28643800	0.26960500
H	1.67473300	5.17684200	0.22723700
C	1.41898700	3.18824500	-0.53004100
C	0.61950800	2.03420600	-0.43754900
C	-0.47789500	2.05677500	0.41188700
C	-1.46026200	1.01756400	0.54167600
C	-2.57686100	1.65216200	1.34875600
H	-3.48970400	1.82390200	0.77131000
H	-2.82763500	1.08772500	2.25155500
C	-1.19689100	-0.20081200	0.01624700
C	0.64825900	0.80750700	-1.27678400
C	-2.12487100	-1.35127900	-0.05132400
C	-3.41596300	-1.24846500	-0.60567800
C	-4.28505200	-2.33888400	-0.66561200

S207

H	-5.26925100	-2.20784600	-1.10127700
C	-3.87096000	-3.58060400	-0.19413200
H	-4.54748800	-4.42844700	-0.24406000
C	-2.58119000	-3.72756500	0.31810600
H	-2.23810000	-4.69536500	0.67094600
C	-1.72724600	-2.63265400	0.37921700
H	-0.72835700	-2.75955700	0.77572900
C	1.09884400	-0.90196600	0.39256400
C	0.80140900	-1.03315100	1.74171400
H	-0.16868800	-0.71691100	2.10285200
C	1.72619900	-1.56692600	2.66493000
H	1.43147900	-1.65521500	3.70666800
C	2.98274800	-1.94968500	2.26338700
H	3.70380600	-2.35149700	2.96980300
C	3.34763200	-1.81017900	0.90178800
C	2.41103000	-1.29397700	-0.05396900
C	3.93758600	-1.50131900	-1.76652000
H	4.14452800	-1.37491700	-2.82852400
C	4.93812600	-2.01383700	-0.90651500
H	5.91463500	-2.27763100	-1.30064900
C	4.63393200	-2.16857100	0.42430900
H	5.36473600	-2.56109000	1.12706700
Cl	-3.98682800	0.24909200	-1.33569700

CN_178_CC_163

Charge = 0, Multiplicity = 1

O	3.70880600	2.10323200	-0.86651600
O	-1.14274000	1.43706700	1.81661700
N	-0.33877500	0.11049200	0.05793700
N	-3.17272800	0.78419900	0.25777600
C	-1.14434700	4.38699100	0.94498100
H	-2.03260300	3.95476700	0.47181400
H	-1.18178500	5.47482200	0.83286300
H	-1.21116800	4.14046300	2.01010800
C	2.57006900	2.80986900	-0.62392400
C	2.41409000	4.18567500	-0.52632300
H	3.22763100	4.86750900	-0.74827800
C	1.16867700	4.66181500	-0.07243800
H	1.03160100	5.73671600	0.01133100
C	0.11977100	3.82688600	0.34513300
C	0.30203700	2.43808900	0.19572000
C	1.49117900	1.96944000	-0.36169800
C	1.92264600	0.59952600	-0.39686300

C	3.41414500	0.68554400	-0.66521200
H	4.04015100	0.32371900	0.15872800
H	3.70916100	0.16560400	-1.57681800
C	1.01459000	-0.37055300	-0.08240700
C	-0.51595800	1.36245400	0.78661000
C	1.28400100	-1.69782400	0.51867600
C	2.38532400	-2.52596400	0.24357300
C	2.71081800	-3.62651500	1.03703500
H	3.55990600	-4.24189700	0.76111100
C	1.93079900	-3.93623600	2.14606600
H	2.18544100	-4.79184200	2.76382900
C	0.81391200	-3.15000200	2.43735000
H	0.18949500	-3.37995800	3.29518600
C	0.50747100	-2.05188200	1.64599300
H	-0.32761000	-1.41365500	1.91035800
C	-1.38151200	-0.66906100	-0.49462700
C	-1.04941600	-1.76048300	-1.29513600
H	-0.01460600	-1.94324500	-1.54913400
C	-2.01640800	-2.65292500	-1.79466700
H	-1.68235700	-3.49571600	-2.39264700
C	-3.35221200	-2.46965000	-1.53159300
H	-4.10447300	-3.16320700	-1.89616100
C	-3.75405600	-1.32179900	-0.80928300
C	-2.78597500	-0.38095900	-0.31781900
C	-4.45322600	1.02800400	0.43541300
H	-4.70137200	1.98294400	0.89726400
C	-5.48203300	0.13509200	0.05621000
H	-6.52176300	0.38443000	0.24373600
C	-5.12249100	-1.02923600	-0.57732800
H	-5.87271500	-1.73559200	-0.92406000
Cl	3.28280500	-2.36052200	-1.26710000

CN_178_CC_168

Charge = 0, Multiplicity = 1

O	3.52920700	2.32701800	-0.93310900
O	-1.18681400	1.35586300	1.90082300
N	-0.34002700	0.06736600	0.13462300
N	-3.21331900	0.53539900	0.38124300
C	-1.41521800	4.28868000	1.00371300
H	-2.28395400	3.78383500	0.56776900
H	-1.53576200	5.36849800	0.87404800
H	-1.43034800	4.05933000	2.07468600
C	2.35268400	2.95321800	-0.65708800

S209

C	2.10299300	4.31614200	-0.57222300
H	2.85932700	5.04928100	-0.83006100
C	0.84203900	4.71120200	-0.08580800
H	0.63229700	5.77498300	-0.01107700
C	-0.13261800	3.81057500	0.37291300
C	0.14322800	2.43627800	0.23501500
C	1.34588900	2.04179200	-0.34987300
C	1.86926700	0.70249700	-0.39353000
C	3.34216500	0.89408200	-0.71412200
H	4.02018600	0.58517200	0.08928400
H	3.64268400	0.39126100	-1.63304600
C	1.03619900	-0.32674800	-0.05597400
C	-0.58287700	1.31393600	0.85642800
C	1.38436700	-1.65097100	0.51497600
C	2.56247400	-2.38243400	0.27978100
C	2.94492900	-3.46664800	1.06986600
H	3.85311300	-4.00382100	0.82012700
C	2.14888600	-3.86283500	2.13907200
H	2.44893300	-4.70544600	2.75428900
C	0.95860200	-3.17842800	2.39069800
H	0.31854200	-3.47436300	3.21617600
C	0.59698400	-2.09342400	1.60455300
H	-0.29421900	-1.52904800	1.84989100
C	-1.33302300	-0.71861200	-0.49789200
C	-0.92893700	-1.72021500	-1.37888300
H	0.11794200	-1.82002000	-1.63043300
C	-1.83597700	-2.62288000	-1.96530000
H	-1.44628900	-3.39179200	-2.62594700
C	-3.18325800	-2.53849800	-1.71133200
H	-3.88960200	-3.23929600	-2.14698300
C	-3.65926800	-1.48481000	-0.89649400
C	-2.75333100	-0.53806800	-0.30708600
C	-4.50732800	0.68360000	0.56692000
H	-4.81488300	1.56790500	1.12391600
C	-5.47803700	-0.22364300	0.08335500
H	-6.53234300	-0.05557400	0.27981100
C	-5.04444300	-1.29663900	-0.65640500
H	-5.74837100	-2.00886300	-1.07975800
Cl	3.50345300	-2.13631500	-1.19394900

CN_178_CC_173

Charge = 0, Multiplicity = 1

O	2.00450300	3.50097500	-1.04783100
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S210

O	-1.27389800	0.68247700	2.37050800
N	-0.20962200	-0.23555000	0.48806900
N	-2.91507600	-1.03861900	0.83135700
C	-3.13043900	3.01343300	1.28803300
H	-3.66794300	2.11656400	0.96111200
H	-3.77271800	3.88407100	1.12518500
H	-2.96108100	2.89988100	2.36450100
C	0.70080000	3.50662500	-0.66355000
C	-0.18042900	4.58080000	-0.63767700
H	0.10249500	5.55357500	-1.02462600
C	-1.44024500	4.37078000	-0.04823000
H	-2.13804700	5.20343400	-0.01698400
C	-1.82061500	3.16148400	0.55722000
C	-0.91761300	2.08821700	0.47174800
C	0.29643000	2.26185200	-0.19230200
C	1.39978000	1.32621200	-0.24911100
C	2.55689300	2.17873500	-0.75884100
H	3.36726900	2.30966600	-0.03583400
H	2.97524300	1.80664900	-1.69253600
C	1.17937800	0.04089200	0.16407500
C	-0.92326800	0.81996400	1.22797400
C	2.07951600	-1.08182000	0.52719100
C	3.45287000	-1.22459800	0.24104200
C	4.24927600	-2.20318600	0.83485300
H	5.29483300	-2.26602000	0.55473100
C	3.69911400	-3.09876000	1.74565200
H	4.32461500	-3.85802000	2.20490200
C	2.33890500	-3.01156400	2.03823600
H	1.88095600	-3.70067800	2.74116100
C	1.56188100	-2.02080900	1.45433000
H	0.52333800	-1.91850100	1.73899000
C	-0.89534300	-1.01533400	-0.48078700
C	-0.24856300	-1.42567600	-1.64109200
H	0.75928000	-1.08699300	-1.84044600
C	-0.86978800	-2.27207400	-2.58304200
H	-0.30854600	-2.56405900	-3.46599000
C	-2.15880200	-2.71236100	-2.40390700
H	-2.64242600	-3.36097100	-3.12875300
C	-2.87192400	-2.30086100	-1.25206400
C	-2.25244700	-1.45103500	-0.27724300
C	-4.15829300	-1.42919000	1.02178600
H	-4.64252900	-1.06844500	1.92832400
C	-4.85963800	-2.27024300	0.12709400
H	-5.88390000	-2.56062400	0.33914900

C	-4.21024200	-2.69907700	-1.00610700
H	-4.70652500	-3.34317500	-1.72780800
Cl	4.23885700	-0.31701200	-1.05142200

CN_178_CC_178

Charge = 0, Multiplicity = 1

O	-1.38872000	3.55635400	1.25918500
O	1.07850100	0.48598300	-2.60744900
N	0.09227700	-0.32987300	-0.62905300
N	2.64439500	-1.39964600	-0.98074700
C	3.44879900	2.42429300	-1.47556700
H	3.88207800	1.46519700	-1.16953900
H	4.20868200	3.20210200	-1.35575500
H	3.20516700	2.33249900	-2.53951900
C	-0.14253400	3.39500900	0.74254200
C	0.91787200	4.29502100	0.75852100
H	0.84215800	5.24839100	1.26977400
C	2.08325400	3.93503500	0.06022800
H	2.91848800	4.63049100	0.06158000
C	2.21271900	2.74193500	-0.67374000
C	1.13671300	1.84434100	-0.63019800
C	-0.00436900	2.16918100	0.10365200
C	-1.25110400	1.42638800	0.16363800
C	-2.20265900	2.41650100	0.83554300
H	-2.97102500	2.80875800	0.16674200
H	-2.67617100	2.01512400	1.73076200
C	-1.25446700	0.13766200	-0.30530500
C	0.88352800	0.62176700	-1.42948000
C	-2.27796900	-0.91968300	-0.49021600
C	-3.66768800	-0.86115700	-0.24502000
C	-4.51254900	-1.95358300	-0.44147000
H	-5.56944100	-1.83731700	-0.22948500
C	-4.01015400	-3.16189500	-0.91158700
H	-4.67668200	-4.00559000	-1.06159800
C	-2.65076100	-3.25408300	-1.20171700
H	-2.23031100	-4.17520000	-1.59337200
C	-1.82012400	-2.16107800	-1.00112800
H	-0.77451100	-2.23669900	-1.26147300
C	0.75911700	-0.97801800	0.44548100
C	0.16091000	-1.15274900	1.68547300
H	-0.82035200	-0.73774400	1.87138800
C	0.80356700	-1.86067600	2.72428900
H	0.28796700	-1.96792500	3.67431400

C	2.05781200	-2.39620800	2.55454600
H	2.55620900	-2.93435900	3.35581400
C	2.71009900	-2.24408700	1.30642300
C	2.06409500	-1.54419700	0.23688300
C	3.84466000	-1.90461200	-1.18181600
H	4.26681800	-1.76237900	-2.17559200
C	4.57435600	-2.60353800	-0.19187000
H	5.56054100	-2.99690100	-0.41775600
C	4.00083700	-2.76975700	1.04690000
H	4.52091100	-3.30242300	1.83920500
Cl	-4.49348400	0.59829600	0.29289300

CN_178_CC_183

Charge = 0, Multiplicity = 1

O	-1.36206000	3.41749100	1.42573700
O	1.02907300	0.53246600	-2.65751900
N	0.07504100	-0.35231000	-0.68802200
N	2.62244400	-1.40105900	-1.07673600
C	3.42447700	2.43263300	-1.46337400
H	3.85938100	1.46038000	-1.20446800
H	4.18698500	3.20316100	-1.31640100
H	3.17058100	2.38860800	-2.52792900
C	-0.13135900	3.29745700	0.85919900
C	0.93801200	4.18549800	0.91572700
H	0.88462100	5.10053400	1.49527200
C	2.08682700	3.86204600	0.17288400
H	2.92910300	4.54814600	0.20648400
C	2.19699900	2.71506000	-0.63558300
C	1.11289900	1.82693300	-0.63487700
C	-0.01633100	2.12373000	0.12670200
C	-1.26202100	1.38245100	0.16787600
C	-2.19697400	2.32722300	0.91772600
H	-2.95592100	2.78616800	0.28190900
H	-2.68539200	1.86347300	1.77599500
C	-1.27051100	0.11172800	-0.34580300
C	0.84860500	0.63013900	-1.47411400
C	-2.29957500	-0.94125000	-0.46664400
C	-3.69314300	-0.82041500	-0.27109700
C	-4.55078200	-1.92015700	-0.28775400
H	-5.61124000	-1.75611800	-0.13246500
C	-4.05566200	-3.19655800	-0.53261800
H	-4.73060500	-4.04678100	-0.54560200
C	-2.69573400	-3.35144900	-0.79656800

S213

H	-2.28672300	-4.32998500	-1.02850000
C	-1.85060100	-2.25152800	-0.76726100
H	-0.80247700	-2.38312300	-0.99247900
C	0.77412600	-0.96276700	0.39238900
C	0.21144500	-1.11406300	1.65111400
H	-0.77265900	-0.71276600	1.85129900
C	0.89383900	-1.78204100	2.69129900
H	0.40575700	-1.87192600	3.65750400
C	2.15244100	-2.30043900	2.50201700
H	2.68163700	-2.80704700	3.30413100
C	2.76783600	-2.17441100	1.23235900
C	2.08070600	-1.51621900	0.16206400
C	3.82451000	-1.89360600	-1.29668600
H	4.21563000	-1.77638700	-2.30629800
C	4.59413500	-2.54992000	-0.30751200
H	5.57979300	-2.93445300	-0.55025200
C	4.05912800	-2.68775500	0.95172500
H	4.61004800	-3.18841600	1.74405000
Cl	-4.50334100	0.73744400	-0.13434200

CN_178_CC_188

Charge = 0, Multiplicity = 1

O	-1.38106000	3.33848900	1.51051300
O	0.99018300	0.55712100	-2.66720700
N	0.06988400	-0.36861500	-0.69802900
N	2.62251600	-1.38545800	-1.12956000
C	3.37658900	2.47258800	-1.46821700
H	3.82355100	1.49938700	-1.23454800
H	4.13333900	3.24715300	-1.31298300
H	3.11188200	2.44856400	-2.53078200
C	-0.15836800	3.25126600	0.91870000
C	0.90357900	4.14785600	0.98170000
H	0.85200900	5.04726200	1.58537800
C	2.04426500	3.85274800	0.21439100
H	2.88075100	4.54562800	0.25312600
C	2.15547500	2.72530800	-0.62162600
C	1.07963200	1.82727900	-0.62824600
C	-0.04189800	2.10000000	0.15230600
C	-1.27638400	1.34367600	0.19585300
C	-2.21266700	2.25649700	0.97863800
H	-2.97988700	2.72746100	0.36198100
H	-2.69452900	1.76277100	1.82503700
C	-1.27519000	0.08032800	-0.33274900

S214

C	0.81941100	0.63752600	-1.48141100
C	-2.30358200	-0.97160900	-0.42766000
C	-3.70089600	-0.81649100	-0.29601300
C	-4.57464700	-1.90329900	-0.26355500
H	-5.63787400	-1.71558300	-0.16379700
C	-4.08880000	-3.19968700	-0.39640800
H	-4.77509000	-4.04055000	-0.37255000
C	-2.72278300	-3.39122200	-0.60181300
H	-2.32244200	-4.38954000	-0.74915500
C	-1.86177900	-2.30347400	-0.62138900
H	-0.80863600	-2.46531600	-0.79844900
C	0.79959400	-0.95949100	0.37525500
C	0.26638800	-1.10649000	1.64705700
H	-0.71960200	-0.71857400	1.86386000
C	0.98078400	-1.75333500	2.67904900
H	0.51487200	-1.84084000	3.65634700
C	2.24303600	-2.25404400	2.46774900
H	2.79712300	-2.74412300	3.26331200
C	2.82915300	-2.13189300	1.18393700
C	2.10923100	-1.49553700	0.12193300
C	3.82722500	-1.86168500	-1.36963100
H	4.19514600	-1.74929700	-2.38847900
C	4.62802200	-2.49548100	-0.39040600
H	5.61421200	-2.86726300	-0.65025700
C	4.12207200	-2.62841100	0.88121800
H	4.69730000	-3.11223100	1.66670100
Cl	-4.48274500	0.76124600	-0.33059000

CN_178_CC_193

Charge = 0, Multiplicity = 1

O	-1.40293200	3.28145700	1.57444000
O	0.95424800	0.57191600	-2.66646800
N	0.06635900	-0.38344500	-0.69479200
N	2.62340200	-1.37107300	-1.17017000
C	3.32519700	2.51311200	-1.48043800
H	3.78801300	1.54379000	-1.26184800
H	4.07351200	3.29614300	-1.32683700
H	3.04777400	2.49575500	-2.53986700
C	-0.18773800	3.22085800	0.96243800
C	0.86403400	4.12970100	1.02157100
H	0.81126600	5.02074800	1.63742000
C	1.99707600	3.85749400	0.23428800
H	2.82557200	4.56007000	0.26996300

S215

C	2.11145900	2.74110000	-0.61641200
C	1.04660000	1.82992100	-0.61970000
C	-0.06672000	2.08245800	0.17825700
C	-1.28865000	1.30927900	0.23091300
C	-2.22730500	2.19563500	1.03791900
H	-3.01000400	2.66410200	0.43915500
H	-2.69208400	1.68076100	1.88218600
C	-1.27696700	0.05062300	-0.30530100
C	0.79203800	0.64208100	-1.47907900
C	-2.30500200	-1.00018000	-0.38440200
C	-3.70351900	-0.81921000	-0.32156500
C	-4.59399400	-1.89199900	-0.27173500
H	-5.65785700	-1.68716800	-0.22821200
C	-4.12025900	-3.19870500	-0.31904100
H	-4.81846700	-4.02926300	-0.28269600
C	-2.74940700	-3.41793400	-0.45704600
H	-2.35888900	-4.42772600	-0.53737100
C	-1.87224000	-2.34367600	-0.49504400
H	-0.81504200	-2.52825900	-0.61791200
C	0.82479500	-0.95936200	0.36831100
C	0.31974800	-1.10397400	1.65181300
H	-0.66684200	-0.72741600	1.88557800
C	1.06293400	-1.73429600	2.67357300
H	0.61804800	-1.82090300	3.66069600
C	2.32715200	-2.21987100	2.43991700
H	2.90365900	-2.69710800	3.22732600
C	2.88562100	-2.09899600	1.14372000
C	2.13626600	-1.47962900	0.09196900
C	3.82955100	-1.83257000	-1.43045400
H	4.17607400	-1.72210100	-2.45699700
C	4.65796100	-2.44922100	-0.46318600
H	5.64375200	-2.80957200	-0.74010800
C	4.17891300	-2.58046200	0.81889600
H	4.77578400	-3.05132400	1.59606200
Cl	-4.45225800	0.76712000	-0.47509800

CN_178_CC_198

Charge = 0, Multiplicity = 1

O	-1.43019300	3.23485500	1.62941800
O	0.92020900	0.58571900	-2.65840800
N	0.06495600	-0.39691400	-0.68423900
N	2.62625200	-1.35452000	-1.20507500
C	3.26868200	2.56027400	-1.49442400

H	3.74661100	1.59472800	-1.29233800
H	4.00885800	3.35121300	-1.34193800
H	2.97798500	2.55059700	-2.55040800
C	-0.22166200	3.19887300	1.00089800
C	0.81639500	4.12394200	1.05046500
H	0.75895000	5.01099100	1.67164600
C	1.94248400	3.87329900	0.24580400
H	2.76020300	4.58872600	0.27400200
C	2.06333800	2.76335300	-0.61266100
C	1.01307400	1.83513000	-0.60667100
C	-0.09182600	2.06773200	0.20807400
C	-1.29925200	1.27540000	0.27215100
C	-2.24201200	2.13611500	1.09924700
H	-3.04574000	2.59088700	0.51789400
H	-2.68169000	1.60409000	1.94706000
C	-1.27606500	0.02125300	-0.27044300
C	0.76611000	0.64727600	-1.46968700
C	-2.30447700	-1.02815000	-0.34033600
C	-3.70112200	-0.82687500	-0.34940800
C	-4.60746100	-1.88654800	-0.29683000
H	-5.66955100	-1.66874500	-0.31054000
C	-4.14810500	-3.19882800	-0.26967200
H	-4.85771800	-4.01961500	-0.23183000
C	-2.77506400	-3.43985800	-0.33526300
H	-2.39566300	-4.45685700	-0.35570800
C	-1.88263900	-2.37839000	-0.37744900
H	-0.82327200	-2.58056400	-0.44135200
C	0.85095700	-0.96158400	0.36596400
C	0.37337700	-1.10697300	1.65993100
H	-0.61313500	-0.74143800	1.91122500
C	1.14341600	-1.72477300	2.66930700
H	0.71881700	-1.81299000	3.66518200
C	2.40857400	-2.19595500	2.41255100
H	3.00606300	-2.66347100	3.19009700
C	2.94040100	-2.07258400	1.10541300
C	2.16364300	-1.46600500	0.06604500
C	3.83311000	-1.80148000	-1.48618100
H	4.15948100	-1.68913100	-2.51911800
C	4.68695200	-2.40535800	-0.53298000
H	5.67188600	-2.75412900	-0.82724600
C	4.23335300	-2.53905400	0.75799100
H	4.85025500	-3.00019400	1.52528200
Cl	-4.41506000	0.76293800	-0.60034200

CN_178_CC_203

Charge = 0, Multiplicity = 1

O	-1.46311200	3.19764200	1.67618800
O	0.88930800	0.59864400	-2.64416400
N	0.06516200	-0.40877100	-0.66819000
N	2.63046700	-1.33555800	-1.23475300
C	3.20726100	2.61285900	-1.50923100
H	3.70042500	1.65180200	-1.32324100
H	3.93884300	3.41209200	-1.35851000
H	2.90295700	2.60976400	-2.56145400
C	-0.26056100	3.18430300	1.03430000
C	0.76018800	4.12910000	1.06963800
H	0.69420500	5.01590900	1.69031900
C	1.88017000	3.89886800	0.25015800
H	2.68439200	4.62977500	0.26719800
C	2.01093900	2.79124200	-0.61001900
C	0.97891800	1.84268400	-0.58993800
C	-0.11769900	2.05546900	0.24070600
C	-1.30877600	1.24215700	0.31811200
C	-2.25725600	2.07837700	1.16172100
H	-3.08552800	2.51009500	0.59720400
H	-2.66479000	1.53362100	2.01801800
C	-1.27305900	-0.00760600	-0.22994100
C	0.74184900	0.65307900	-1.45440900
C	-2.30151400	-1.05638900	-0.29612400
C	-3.69307000	-0.84009800	-0.37917800
C	-4.61315600	-1.88853300	-0.33562600
H	-5.67101700	-1.66167500	-0.40723600
C	-4.16934600	-3.20318700	-0.24340600
H	-4.88886800	-4.01563400	-0.21292600
C	-2.79739800	-3.46024200	-0.23303400
H	-2.42985100	-4.48126700	-0.19994200
C	-1.89164200	-2.40967900	-0.26778300
H	-0.83257600	-2.62450700	-0.26972700
C	0.87723100	-0.96545900	0.36715300
C	0.42587100	-1.11446700	1.67026100
H	-0.56000000	-0.75954300	1.93904100
C	1.22074300	-1.72296000	2.66584800
H	0.81541500	-1.81508100	3.66937200
C	2.48616400	-2.18004900	2.38604900
H	3.10302700	-2.64051500	3.15260300
C	2.99279400	-2.05083200	1.06949400
C	2.19072800	-1.45362700	0.04386000

S218

C	3.83764200	-1.76771100	-1.53655900
H	4.14515500	-1.65047100	-2.57473800
C	4.71481500	-2.36218400	-0.59870700
H	5.69863600	-2.69905200	-0.91008500
C	4.28501500	-2.50194400	0.69967000
H	4.92036700	-2.95600400	1.45605300
Cl	-4.37122700	0.75068700	-0.70974300

CN_178_CC_208

Charge = 0, Multiplicity = 1

O	-1.50278300	3.16584400	1.71629000
O	0.86236000	0.61116400	-2.62561600
N	0.06683200	-0.41932600	-0.64895600
N	2.63609800	-1.31408800	-1.26068500
C	3.14208800	2.66936600	-1.52191300
H	3.65309400	1.71543600	-1.34794500
H	3.86238500	3.47962300	-1.37575700
H	2.82460700	2.66721100	-2.57026100
C	-0.30520800	3.17453500	1.06400700
C	0.69521600	4.14125800	1.08299500
H	0.61741400	5.03008700	1.69940900
C	1.81029700	3.93087700	0.25120200
H	2.59866500	4.67903900	0.25553300
C	1.95445600	2.82324000	-0.60683700
C	0.94345100	1.85231000	-0.57060900
C	-0.14524700	2.04523800	0.27456400
C	-1.31820300	1.20927900	0.36561000
C	-2.27473700	2.02217200	1.22133600
H	-3.12684500	2.42535500	0.67085300
H	-2.64854800	1.46888000	2.08782700
C	-1.26821400	-0.03634800	-0.18635000
C	0.71913800	0.65990200	-1.43521800
C	-2.29644400	-1.08542100	-0.25225900
C	-3.67936000	-0.85867100	-0.41047000
C	-4.61067400	-1.89796900	-0.38336300
H	-5.66172600	-1.66530200	-0.51301500
C	-4.18341300	-3.21264200	-0.23218600
H	-4.91094100	-4.01834500	-0.21478300
C	-2.81620900	-3.48085500	-0.14365400
H	-2.46139900	-4.50360000	-0.06115900
C	-1.89959800	-2.43915000	-0.16337300
H	-0.84368300	-2.66220100	-0.10186900
C	0.90364800	-0.97012600	0.37028900

C	0.47759500	-1.12441400	1.68147700
H	-0.50712100	-0.77973500	1.96763200
C	1.29579900	-1.72546600	2.66254100
H	0.90891500	-1.82288700	3.67282800
C	2.56101300	-2.16833900	2.36013300
H	3.19610000	-2.62309100	3.11513400
C	3.04364600	-2.03095700	1.03538500
C	2.21779200	-1.44136100	0.02419100
C	3.84345100	-1.73067700	-1.58265100
H	4.13324200	-1.60645400	-2.62512300
C	4.74246100	-2.31747100	-0.66074200
H	5.72515000	-2.64168200	-0.98870900
C	4.33505300	-2.46584800	0.64380900
H	4.98769200	-2.91412900	1.38883700
Cl	-4.32181800	0.73146300	-0.80851900

CN_183_CC_163

Charge = 0, Multiplicity = 1

O	3.22761300	2.74244400	-0.89077200
O	-1.28052300	1.00332900	1.83836800
N	-0.34253800	-0.01619200	-0.05564200
N	-3.15368200	0.40725900	0.04741100
C	-1.94240400	3.96406100	1.06162400
H	-2.74626000	3.48721500	0.48912500
H	-2.14064300	5.03883800	1.11222400
H	-1.98973000	3.54560300	2.07214100
C	1.97719700	3.20524700	-0.61263000
C	1.56394500	4.52039700	-0.44637500
H	2.22940300	5.35430600	-0.64071700
C	0.26043000	4.72829200	0.04357300
H	-0.07771600	5.75202800	0.18078000
C	-0.60082500	3.68914000	0.43300700
C	-0.16121100	2.37049000	0.21413100
C	1.08331400	2.16248000	-0.38265700
C	1.77404500	0.90463300	-0.47050500
C	3.21722300	1.28877400	-0.73592000
H	3.90797100	1.03064700	0.07550100
H	3.60151000	0.86431300	-1.66396800
C	1.07841000	-0.23614700	-0.18003200
C	-0.72910200	1.12624900	0.76922500
C	1.62398700	-1.46544900	0.43829700
C	2.87498600	-2.04364300	0.16357800
C	3.43647900	-3.03053200	0.97477300

S220

H	4.39469400	-3.45664800	0.69903800
C	2.75308300	-3.47158600	2.10289900
H	3.19107400	-4.23831100	2.73442500
C	1.49876700	-2.93213700	2.39786200
H	0.94988100	-3.26612000	3.27298100
C	0.95462700	-1.94529100	1.58812200
H	0.00837000	-1.49031200	1.85728700
C	-1.25827400	-1.00327200	-0.46682100
C	-0.82349600	-2.17123300	-1.08620300
H	0.22753400	-2.31755600	-1.28942200
C	-1.71698000	-3.19517100	-1.45771900
H	-1.31142200	-4.09150200	-1.91778000
C	-3.06834200	-3.07892000	-1.23505800
H	-3.75751500	-3.87679500	-1.49615400
C	-3.57081400	-1.87300800	-0.69138000
C	-2.68203200	-0.80263600	-0.34558800
C	-4.45021600	0.58201700	0.18739500
H	-4.77272700	1.57561500	0.49583600
C	-5.40638800	-0.43296000	-0.04958100
H	-6.46290200	-0.23501800	0.10141300
C	-4.95905400	-1.64995700	-0.50372400
H	-5.65423000	-2.45213400	-0.73853100
Cl	3.70208200	-1.71687300	-1.36053500

CN_183_CC_168

Charge = 0, Multiplicity = 1

O	3.20884600	2.73220900	-0.94852500
O	-1.25320000	0.98716000	1.86531300
N	-0.34324300	-0.02267200	-0.04687000
N	-3.15842100	0.40067100	0.09661000
C	-1.91757200	3.95137500	1.11478200
H	-2.73192400	3.46477700	0.56594400
H	-2.11991900	5.02564600	1.15967500
H	-1.93951100	3.54282600	2.13026000
C	1.96496700	3.19283300	-0.64218300
C	1.55461900	4.50821200	-0.46892300
H	2.21542700	5.34176500	-0.67992400
C	0.26254400	4.71655500	0.04916600
H	-0.07311100	5.74026800	0.19248900
C	-0.58949200	3.67703400	0.45783600
C	-0.15381500	2.35886300	0.23051000
C	1.07802000	2.14894000	-0.39194200
C	1.76748100	0.89007800	-0.49607000

S221

C	3.20517600	1.27939700	-0.78817800
H	3.91036300	1.02814600	0.01247900
H	3.57544800	0.85359900	-1.72102600
C	1.07481200	-0.25219100	-0.19782000
C	-0.71519400	1.11428000	0.79015600
C	1.61504700	-1.48640900	0.41934700
C	2.89354100	-2.03159500	0.20437400
C	3.44558600	-3.00388900	1.03875000
H	4.42552900	-3.40373300	0.80302800
C	2.72751000	-3.46545600	2.13656900
H	3.15880000	-4.22019100	2.78683300
C	1.44754600	-2.96074200	2.37451300
H	0.86943800	-3.30858400	3.22507500
C	0.91363800	-1.98705100	1.54225300
H	-0.05059700	-1.55422600	1.77948100
C	-1.26744900	-0.98790600	-0.48867400
C	-0.83785500	-2.13409600	-1.15158300
H	0.21219200	-2.27273100	-1.36614200
C	-1.73414700	-3.14393200	-1.55295700
H	-1.33232300	-4.02349600	-2.04739400
C	-3.08401500	-3.03494600	-1.31748700
H	-3.77561000	-3.82236700	-1.60275600
C	-3.58165600	-1.84958700	-0.72642500
C	-2.69001000	-0.79256600	-0.34748400
C	-4.45379900	0.56968100	0.25363800
H	-4.77352800	1.55018900	0.60402900
C	-5.41201700	-0.43514100	-0.01593100
H	-6.46734300	-0.24326300	0.15046300
C	-4.96837000	-1.63371400	-0.51996200
H	-5.66549700	-2.42632800	-0.78011000
Cl	3.77400400	-1.70125900	-1.29014900

CN_183_CC_173

Charge = 0, Multiplicity = 1

O	1.66625900	3.59936600	-1.12224600
O	-1.13018100	0.55717500	2.44829800
N	-0.15955400	-0.29049000	0.48587100
N	-2.83588700	-1.08316000	0.79875600
C	-3.33816000	2.67418600	1.36065900
H	-3.86312200	1.79805700	0.96311400
H	-4.01191800	3.53471800	1.31241900
H	-3.11773000	2.45766600	2.41136100
C	0.37859600	3.48963700	-0.70125900

S222

C	-0.59633200	4.47993900	-0.66362000
H	-0.41363600	5.46839200	-1.07058500
C	-1.81375500	4.16593900	-0.03439700
H	-2.58320100	4.93236800	0.00778800
C	-2.06539700	2.93566200	0.59724900
C	-1.07288200	1.94816300	0.49864400
C	0.10382700	2.22067400	-0.20250900
C	1.29158300	1.39096900	-0.27563200
C	2.35012400	2.34280200	-0.82197300
H	3.15534400	2.56634000	-0.11630200
H	2.78710900	1.99498200	-1.75665900
C	1.20218100	0.09416600	0.15416600
C	-0.91947100	0.69523000	1.27183100
C	2.19842700	-0.94178800	0.51582300
C	3.57708800	-0.96665100	0.22067500
C	4.45536600	-1.88015900	0.80217000
H	5.50111700	-1.85303900	0.51705100
C	3.98698700	-2.82496300	1.70925800
H	4.67622600	-3.53320800	2.15865900
C	2.62653000	-2.85197400	2.01223300
H	2.23237900	-3.58094800	2.71360800
C	1.76599900	-1.92596200	1.43928400
H	0.72403500	-1.91136300	1.72943500
C	-0.80329600	-1.09933800	-0.47667900
C	-0.13204800	-1.54133900	-1.61122600
H	0.87719300	-1.20328700	-1.80482500
C	-0.73456400	-2.42550700	-2.53079200
H	-0.15838000	-2.74293600	-3.39521300
C	-2.02164500	-2.87576400	-2.35522300
H	-2.48590700	-3.55536600	-3.06399700
C	-2.75670400	-2.43221600	-1.22922600
C	-2.15811700	-1.53996200	-0.28205700
C	-4.07884600	-1.47385000	0.99327400
H	-4.57755200	-1.07535900	1.87555900
C	-4.75959900	-2.36091600	0.12754800
H	-5.78348900	-2.65193500	0.34027800
C	-4.09430700	-2.83126000	-0.98042200
H	-4.57870800	-3.50862500	-1.67933200
Cl	4.27942300	0.02543900	-1.05705500

CN_183_CC_178

Charge = 0, Multiplicity = 1

O	1.21504400	3.55658400	-1.31997400
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S223

O	-0.97362000	0.44944300	2.63906100
N	-0.06009500	-0.36072000	0.62646100
N	-2.63745800	-1.33479100	0.95367400
C	-3.52349600	2.24655900	1.50768400
H	-4.01892200	1.35607700	1.10286100
H	-4.24892500	3.06524900	1.52598900
H	-3.23457600	2.00739700	2.53601900
C	-0.01402600	3.34580800	-0.78033200
C	-1.11225800	4.19981700	-0.78679300
H	-1.08627400	5.14982400	-1.30910700
C	-2.24674500	3.79935800	-0.06154400
H	-3.11051400	4.45903800	-0.05331600
C	-2.31151200	2.61052100	0.68908000
C	-1.20025900	1.75894500	0.63609900
C	-0.08703900	2.12357600	-0.12418700
C	1.19353500	1.43898000	-0.19398500
C	2.08773500	2.46326200	-0.89167200
H	2.84438400	2.90134000	-0.23810900
H	2.56944600	2.07131800	-1.78684900
C	1.26589000	0.15852500	0.29255800
C	-0.86550900	0.56006900	1.44697200
C	2.33878000	-0.84385900	0.48997900
C	3.72310400	-0.72100900	0.23850700
C	4.62085400	-1.76736700	0.44975700
H	5.67031000	-1.60319000	0.23253000
C	4.17903700	-2.99104200	0.94090500
H	4.88642300	-3.79852100	1.10260900
C	2.82621700	-3.14565000	1.23567000
H	2.45243700	-4.08039300	1.64208200
C	1.94250400	-2.09814100	1.01983500
H	0.90150800	-2.22027900	1.28139400
C	-0.70935000	-1.03511100	-0.43636800
C	-0.08645000	-1.27592700	-1.65332400
H	0.90590300	-0.88687500	-1.83668900
C	-0.71938000	-2.02312200	-2.67055400
H	-0.18515700	-2.18352200	-3.60266600
C	-1.98483000	-2.53406900	-2.50424500
H	-2.47244100	-3.10407500	-3.28985300
C	-2.66334600	-2.30951600	-1.28129900
C	-2.02980500	-1.56476800	-0.23613000
C	-3.85232900	-1.80340800	1.15559700
H	-4.29669500	-1.59036600	2.12659500
C	-4.56871700	-2.54885200	0.19033800
H	-5.56715100	-2.91143200	0.41371600

C	-3.96942500	-2.79646800	-1.02284000
H	-4.48207600	-3.36369300	-1.79572200
Cl	4.47204300	0.76881200	-0.32725700

CN_183_CC_183

Charge = 0, Multiplicity = 1

O	1.20023500	3.41334900	-1.48244600
O	-0.92795700	0.50402300	2.68528400
N	-0.04352600	-0.38178700	0.68663300
N	-2.61979000	-1.33139300	1.05177400
C	-3.49738200	2.26490800	1.49111600
H	-4.00476100	1.36595000	1.12100000
H	-4.21604800	3.08976500	1.48871500
H	-3.20038600	2.05795600	2.52399200
C	-0.01551600	3.24735100	-0.89562700
C	-1.12047800	4.09173000	-0.94275200
H	-1.11298900	5.00241400	-1.53147000
C	-2.24093500	3.73174400	-0.17515200
H	-3.10991500	4.38418500	-0.19911900
C	-2.29095700	2.59042300	0.64837900
C	-1.17365400	1.74593900	0.63841300
C	-0.07008700	2.07871100	-0.14823500
C	1.20791800	1.39282300	-0.19843000
C	2.08935400	2.36792200	-0.97286800
H	2.83570400	2.86828900	-0.35365800
H	2.58619900	1.91412400	-1.83168800
C	1.28213700	0.13147600	0.33348400
C	-0.83124500	0.57401800	1.48981900
C	2.35816800	-0.86974500	0.46903700
C	3.74411600	-0.68805800	0.26696700
C	4.65192400	-1.74617700	0.30463100
H	5.70337600	-1.53649100	0.14312800
C	4.21688400	-3.03887300	0.57691600
H	4.93074300	-3.85626100	0.60634900
C	2.86553300	-3.25197300	0.84481300
H	2.50263400	-4.24393200	1.09569900
C	1.97017800	-2.19338300	0.79455200
H	0.92853400	-2.36825100	1.02095700
C	-0.72656600	-1.01832800	-0.38341300
C	-0.13909700	-1.23606400	-1.62129800
H	0.85566300	-0.86057500	-1.81893500
C	-0.81094100	-1.94328500	-2.64245900
H	-0.30376800	-2.08664500	-3.59226400

C	-2.08072900	-2.43622800	-2.45713400
H	-2.59880200	-2.97477800	-3.24547600
C	-2.72306100	-2.23651400	-1.21047000
C	-2.04913500	-1.53361200	-0.16159800
C	-3.83663300	-1.78631600	1.27188800
H	-4.25105000	-1.59688600	2.26086500
C	-4.59208300	-2.48921400	0.30423400
H	-5.59028800	-2.84183200	0.54397000
C	-4.02997600	-2.70975900	-0.93166100
H	-4.57263300	-3.24488800	-1.70694000
Cl	4.47860800	0.90259100	0.08967000

CN_183_CC_188

Charge = 0, Multiplicity = 1

O	1.22111100	3.33447000	-1.56681300
O	-0.88691000	0.53080100	2.69311300
N	-0.03818600	-0.39811100	0.69603200
N	-2.61963300	-1.31422900	1.10542200
C	-3.45007500	2.30773200	1.49638500
H	-3.96959500	1.40557500	1.15174500
H	-4.16116600	3.13901900	1.48280500
H	-3.14447000	2.12110200	2.53063800
C	0.01243400	3.20171400	-0.95508000
C	-1.08521400	4.05535400	-1.00816500
H	-1.07914100	4.95036700	-1.62046100
C	-2.19810300	3.72450400	-0.21632200
H	-3.06134800	4.38432900	-0.24508000
C	-2.24953000	2.60278800	0.63425800
C	-1.14036500	1.74769100	0.63101600
C	-0.04410800	2.05543100	-0.17469700
C	1.22325200	1.35368100	-0.22761000
C	2.10661800	2.29622800	-1.03550600
H	2.86236400	2.80744200	-0.43703700
H	2.59603600	1.81223700	-1.88325600
C	1.28770900	0.09955700	0.31952300
C	-0.80148700	0.58289300	1.49628400
C	2.36248300	-0.90158900	0.43101800
C	3.75094500	-0.68577700	0.29256300
C	4.67336000	-1.73202600	0.28471700
H	5.72681600	-1.49852000	0.17819700
C	4.24717400	-3.04573100	0.44904100
H	4.97121400	-3.85465200	0.44462600
C	2.89106200	-3.29503200	0.65862300

H	2.53677500	-4.30717700	0.82795300
C	1.98136500	-2.24758000	0.65379000
H	0.93585900	-2.45216400	0.83258700
C	-0.75252100	-1.01514900	-0.36730400
C	-0.19513300	-1.22956300	-1.61941700
H	0.80118200	-0.86776600	-1.83420500
C	-0.89904100	-1.91622400	-2.63299100
H	-0.41431200	-2.05795900	-3.59467800
C	-2.17221400	-2.39104700	-2.42528900
H	-2.71539100	-2.91337100	-3.20764300
C	-2.78476200	-2.19413000	-1.16326300
C	-2.07790800	-1.51246900	-0.12197400
C	-3.83857600	-1.75261800	1.34621500
H	-4.22924000	-1.56728700	2.34559300
C	-4.62527400	-2.43368400	0.38777700
H	-5.62362400	-2.77327200	0.64508000
C	-4.09276900	-2.65019000	-0.86178600
H	-4.65976100	-3.16891100	-1.63077700
Cl	4.45782300	0.92686100	0.28014800

CN_183_CC_193

Charge = 0, Multiplicity = 1

O	-1.24314200	3.27602300	1.63316900
O	0.84794300	0.54874300	-2.69088100
N	0.03464100	-0.41307800	-0.69277100
N	2.62012700	-1.29820600	-1.14775000
C	3.39925100	2.35126400	-1.50851800
H	3.92976100	1.44700700	-1.18689900
H	4.10382700	3.18790700	-1.48738700
H	3.08344500	2.18144100	-2.54264200
C	-0.04126900	3.17061800	1.00128800
C	1.04637800	4.03729100	1.05033200
H	1.03905700	4.92374900	1.67493700
C	2.15181100	3.73041500	0.23818200
H	3.00719600	4.40051900	0.26391400
C	2.20630100	2.62017200	-0.62751300
C	1.10795000	1.75113300	-0.62077000
C	0.01998300	2.03731700	0.20302600
C	-1.23551900	1.31811000	0.26463600
C	-2.12145200	2.23308200	1.09800600
H	-2.89404700	2.74149700	0.51905100
H	-2.59292200	1.72654900	1.94368700
C	-1.29004700	0.06907200	-0.29190600

S227

C	0.77340600	0.58901100	-1.49315100
C	-2.36472300	-0.93072200	-0.38902700
C	-3.75340400	-0.68786600	-0.31881500
C	-4.69143800	-1.72021100	-0.29410900
H	-5.74489900	-1.46863800	-0.24319900
C	-4.27735900	-3.04548600	-0.37438000
H	-5.01254400	-3.84415000	-0.35784300
C	-2.91769300	-3.32352800	-0.51793700
H	-2.57346300	-4.34790000	-0.62190200
C	-1.99289600	-2.28948900	-0.53096100
H	-0.94443600	-2.51747400	-0.65706100
C	0.77813300	-1.01587900	0.36030800
C	0.24946300	-1.22943100	1.62491900
H	-0.74713700	-0.87928600	1.85733000
C	0.98230200	-1.90059200	2.62826700
H	0.51893800	-2.04258900	3.60038600
C	2.25722400	-2.35974400	2.39752900
H	2.82302100	-2.87004800	3.17175300
C	2.84162600	-2.16240200	1.12226900
C	2.10513200	-1.49663900	0.09117300
C	3.84008100	-1.72133100	-1.40950600
H	4.20886200	-1.53642400	-2.41725500
C	4.65463600	-2.38620700	-0.46294300
H	5.65230800	-2.71374600	-0.73790000
C	4.14958600	-2.60269400	0.79789100
H	4.73837100	-3.10921400	1.55859600
Cl	-4.42834700	0.93471000	-0.42482200

CN_183_CC_198

Charge = 0, Multiplicity = 1

O	-1.26861800	3.23000000	1.68945600
O	0.81063900	0.56430400	-2.68149900
N	0.03278600	-0.42667000	-0.68211400
N	2.62142600	-1.28101600	-1.18367400
C	3.34524500	2.39838000	-1.52172100
H	3.88632500	1.49279600	-1.22227600
H	4.04353700	3.24008300	-1.49448300
H	3.01853900	2.24387700	-2.55492900
C	-0.07284100	3.14870800	1.04123800
C	1.00192600	4.03184700	1.08066800
H	0.99027800	4.91448700	1.71059300
C	2.10057700	3.74647700	0.25125000
H	2.94590600	4.42945500	0.26963300

C	2.16072900	2.64251500	-0.62232700
C	1.07611300	1.75633700	-0.60636700
C	-0.00341500	2.02212800	0.23454100
C	-1.24564700	1.28382600	0.30746000
C	-2.13528800	2.17309900	1.16196700
H	-2.93052700	2.66794500	0.60210300
H	-2.58026700	1.64828000	2.01157800
C	-1.28997000	0.03937000	-0.25672100
C	0.74702000	0.59477800	-1.48308200
C	-2.36528700	-0.95850300	-0.34585700
C	-3.75123900	-0.69341900	-0.34684700
C	-4.70460300	-1.71192900	-0.32060300
H	-5.75574900	-1.44598400	-0.32620100
C	-4.30520600	-3.04401900	-0.32879200
H	-5.05140000	-3.83241600	-0.31169000
C	-2.94447700	-3.34568000	-0.40136300
H	-2.61189100	-4.37810000	-0.44779600
C	-2.00484300	-2.32509600	-0.41733200
H	-0.95514100	-2.57198800	-0.48633500
C	0.80362600	-1.01956400	0.35790600
C	0.30233800	-1.23605800	1.63319400
H	-0.69399700	-0.89734400	1.88340600
C	1.06189500	-1.89602400	2.62394800
H	0.61885700	-2.04122900	3.60502700
C	2.33771100	-2.34001500	2.36980600
H	2.92440600	-2.84163100	3.13409900
C	2.89539600	-2.13818900	1.08330900
C	2.13155100	-1.48390500	0.06473100
C	3.84176400	-1.68892400	-1.46669200
H	4.18993100	-1.50092400	-2.48119100
C	4.68188500	-2.34192700	-0.53425000
H	5.67845500	-2.65725900	-0.82691900
C	4.20268400	-2.56266000	0.73583100
H	4.81155200	-3.06031300	1.48651500
Cl	-4.39119600	0.93413600	-0.54809700

CN_183_CC_203

Charge = 0, Multiplicity = 1

O	-1.29694500	3.19434500	1.73700700
O	0.77503600	0.57615600	-2.66701400
N	0.03190600	-0.43955300	-0.66576100
N	2.62271200	-1.26374200	-1.21409900
C	3.28779700	2.44706100	-1.53734600

H	3.84041900	1.54220000	-1.25751900
H	3.97889500	3.29456700	-1.50737300
H	2.94935600	2.30374500	-2.56845500
C	-0.10679600	3.13425400	1.07510300
C	0.95260200	4.03631700	1.10021100
H	0.93412700	4.91901500	1.72989600
C	2.04482200	3.77008600	0.25570100
H	2.87815800	4.46784300	0.26304100
C	2.11261500	2.66810400	-0.61993600
C	1.04419400	1.76253600	-0.58989900
C	-0.02648500	2.00931800	0.26740300
C	-1.25436600	1.25091300	0.35385400
C	-2.14861400	2.11746000	1.22498500
H	-2.96829400	2.59153500	0.68234000
H	-2.56246700	1.57941300	2.08252600
C	-1.28811900	0.01022700	-0.21561300
C	0.72164100	0.59950400	-1.46811400
C	-2.36461000	-0.98577000	-0.30163200
C	-3.74465700	-0.70303100	-0.37573200
C	-4.71180100	-1.70897900	-0.35982000
H	-5.75823000	-1.43194900	-0.42230000
C	-4.32873200	-3.04475900	-0.30572400
H	-5.08486200	-3.82379700	-0.29713100
C	-2.97003000	-3.36510500	-0.30399600
H	-2.65010000	-4.40255800	-0.29952900
C	-2.01704000	-2.35672700	-0.31109900
H	-0.96838600	-2.61831500	-0.32036900
C	0.82888300	-1.02472400	0.35961100
C	0.35453900	-1.24511500	1.64464100
H	-0.64064100	-0.91668200	1.91292400
C	1.13928600	-1.89602600	2.62160500
H	0.71616700	-2.04525000	3.61084200
C	2.41499400	-2.32589300	2.34390800
H	3.02138700	-2.82052900	3.09730400
C	2.94661500	-2.11808400	1.04734600
C	2.15701200	-1.47304200	0.04249100
C	3.84276800	-1.65680600	-1.51834400
H	4.17110700	-1.46402200	-2.53855300
C	4.70681100	-2.30025300	-0.60120200
H	5.70179800	-2.60357100	-0.91144100
C	4.25253200	-2.52712100	0.67686500
H	4.88025300	-3.01765400	1.41662900
Cl	-4.34828900	0.92700000	-0.65325600

CN_183_CC_208

Charge = 0, Multiplicity = 1

O	-1.33075800	3.16464500	1.77922300
O	0.74125600	0.58811300	-2.64811600
N	0.03274700	-0.45088900	-0.64551000
N	2.62530900	-1.24333600	-1.24025700
C	3.22605200	2.50110100	-1.55236500
H	3.78881000	1.59612300	-1.29423200
H	3.91089100	3.35348000	-1.51785800
H	2.87560500	2.37135800	-2.58136400
C	-0.14538400	3.12498400	1.10624300
C	0.89564800	4.04846600	1.11466200
H	0.86720100	4.93363400	1.74050100
C	1.98231600	3.80094000	0.25703100
H	2.80133000	4.51546500	0.25142800
C	2.06086100	2.69840500	-0.61701400
C	1.01170300	1.77092300	-0.57030100
C	-0.05035700	1.99854700	0.30242300
C	-1.26229600	1.21842100	0.40294300
C	-2.16321000	2.06353700	1.28676800
H	-3.00738700	2.51128200	0.75890700
H	-2.54367900	1.51615800	2.15413600
C	-1.28426400	-0.01870400	-0.17086200
C	0.69757000	0.60521900	-1.44886200
C	-2.36185000	-1.01336100	-0.25779100
C	-3.73263400	-0.71719300	-0.40634900
C	-4.71123700	-1.71236800	-0.40850000
H	-5.75049200	-1.42728800	-0.52822900
C	-4.34553300	-3.04957900	-0.29822200
H	-5.10989900	-3.82059500	-0.30398500
C	-2.99231600	-3.38413300	-0.21988600
H	-2.68584200	-4.42440500	-0.16874700
C	-2.02820100	-2.38617300	-0.21036200
H	-0.98317200	-2.65849600	-0.15846100
C	0.85431400	-1.03097000	0.36352100
C	0.40596400	-1.25774200	1.65693300
H	-0.58733400	-0.93888300	1.94354700
C	1.21416000	-1.90270300	2.61859500
H	0.81016600	-2.05797400	3.61487900
C	2.48900700	-2.31889200	2.31735300
H	3.11365900	-2.80901400	3.05868700
C	2.99580400	-2.10188200	1.01235500
C	2.18227800	-1.46286500	0.02275600

S231

C	3.84470500	-1.62118700	-1.56558400
H	4.15437600	-1.42059800	-2.59012700
C	4.73072300	-2.25849500	-0.66527000
H	5.72384800	-2.54945600	-0.99284600
C	4.29993800	-2.49509000	0.61909700
H	4.94511000	-2.98103200	1.34678000
Cl	-4.29977300	0.91367800	-0.74808100

CN_183_CC_213

Charge = 0, Multiplicity = 1

O	1.36985300	3.13869800	-1.81644600
O	-0.71091000	0.60026800	2.62649700
N	-0.03468100	-0.46068600	0.62368900
N	-2.62884300	-1.22068100	1.26328600
C	-3.16238800	2.55763400	1.56404100
H	-3.73314000	1.65147800	1.32903400
H	-3.84239100	3.41354500	1.52249000
H	-2.80069900	2.44406000	2.59118700
C	0.18817700	3.11905800	-1.13508100
C	-0.83273200	4.06466900	-1.12695400
H	-0.79196800	4.95331500	-1.74716400
C	-1.91512100	3.83533200	-0.25850000
H	-2.71842300	4.56726200	-0.24003900
C	-2.00695400	2.73116900	0.61209000
C	-0.97875200	1.78101600	0.54864000
C	0.07546000	1.98979500	-0.33766300
C	1.27032300	1.18714300	-0.45146800
C	2.18053900	2.01294700	-1.34286700
H	3.04540100	2.43297300	-0.82500900
H	2.53108800	1.46015100	-2.21951100
C	1.27899100	-0.04697700	0.12487900
C	-0.67508000	0.61207000	1.42703500
C	2.35743400	-1.04117700	0.21482100
C	3.71547800	-0.73552500	0.43855000
C	4.70301400	-1.72168100	0.46321300
H	5.73254400	-1.43128200	0.64037400
C	4.35573200	-3.05843600	0.29991200
H	5.12643100	-3.82281600	0.32335700
C	3.01178200	-3.40312800	0.14318500
H	2.71967900	-4.44439400	0.04742600
C	2.03893900	-2.41376400	0.11264500
H	1.00035400	-2.69332000	-0.00117200
C	-0.87952000	-1.03725500	-0.36832200

S232

C	-0.45615600	-1.27152000	-1.66897500
H	0.53461000	-0.96132400	-1.97369100
C	-1.28608100	-1.91241000	-2.61475400
H	-0.90038100	-2.07462400	-3.61717100
C	-2.55941900	-2.31554000	-2.29052700
H	-3.20099100	-2.80264500	-3.01929400
C	-3.04260800	-2.08760900	-0.97843300
C	-2.20693100	-1.45263700	-0.00470000
C	-3.84721700	-1.58335500	1.60894900
H	-4.13944500	-1.37312000	2.63669000
C	-4.75339100	-2.21666100	0.72604400
H	-5.74444900	-2.49520200	1.07026900
C	-4.34462800	-2.46498800	-0.56324300
H	-5.00586600	-2.94787300	-1.27843500
Cl	4.24632000	0.89486100	0.83625400

CN_183_CC_223

Charge = 0, Multiplicity = 1

O	1.45695300	3.09702600	-1.87728200
O	-0.65451000	0.62608000	2.57859200
N	-0.03960300	-0.47472700	0.57711800
N	-2.63538600	-1.16991700	1.30132100
C	-3.03892900	2.66644500	1.57342000
H	-3.63099400	1.76634700	1.37054700
H	-3.70312100	3.53443000	1.52702000
H	-2.65841700	2.56824700	2.59552900
C	0.27948000	3.11422200	-1.18657900
C	-0.69916100	4.10257200	-1.14783400
H	-0.62906300	4.99960500	-1.75318900
C	-1.77679300	3.90629600	-0.26463600
H	-2.54720200	4.67182700	-0.22237500
C	-1.89984800	2.79712600	0.59531400
C	-0.91501700	1.80362300	0.50106400
C	0.12625700	1.97748400	-0.40686100
C	1.28625600	1.13102600	-0.54404500
C	2.22176600	1.92651800	-1.43499000
H	3.11380200	2.29371700	-0.92123300
H	2.53016200	1.37299800	-2.32687300
C	1.26593900	-0.09902200	0.03214600
C	-0.63339200	0.62829000	1.37890600
C	2.34584400	-1.09422300	0.13145600
C	3.66749200	-0.78067500	0.50668700
C	4.66563400	-1.75348500	0.58257200

S233

H	5.66771800	-1.45984600	0.87451300
C	4.35920800	-3.08425100	0.31798800
H	5.13701500	-3.83915200	0.38166500
C	3.04597100	-3.43804200	0.00231700
H	2.78600000	-4.47644800	-0.17910700
C	2.06269000	-2.46082800	-0.07709900
H	1.04593800	-2.74649700	-0.31360800
C	-0.92654800	-1.04843100	-0.37948200
C	-0.55013500	-1.29937900	-1.69174100
H	0.43317100	-1.00188400	-2.03190500
C	-1.41813200	-1.93784200	-2.60454400
H	-1.06663100	-2.11544000	-3.61690200
C	-2.68626200	-2.31831600	-2.23614900
H	-3.35749800	-2.80393500	-2.93871700
C	-3.12596200	-2.06484000	-0.91344800
C	-2.25143400	-1.43206100	0.02726600
C	-3.85058200	-1.50330100	1.68533300
H	-4.11149000	-1.26913400	2.71634200
C	-4.79157100	-2.13494600	0.83845500
H	-5.77782400	-2.38923900	1.21386700
C	-4.42262900	-2.41171000	-0.45695700
H	-5.11190200	-2.89313300	-1.14619400
Cl	4.12616800	0.84480600	1.00233600

CN_183_CC_233

Charge = 0, Multiplicity = 1

O	-1.55519700	3.06033300	1.92809600
O	0.60992200	0.65821700	-2.52622800
N	0.04605500	-0.48017300	-0.53085500
N	2.64271400	-1.11133600	-1.33001400
C	2.92205500	2.77520600	-1.56089300
H	3.53872000	1.88722100	-1.37955500
H	3.56528400	3.65875500	-1.51286100
H	2.52846500	2.68118100	-2.57856500
C	-0.37822400	3.11396800	1.23629600
C	0.55747100	4.14159400	1.17492200
H	0.45377700	5.04523300	1.76547300
C	1.63534500	3.97739200	0.28454200
H	2.37213800	4.77418600	0.22436100
C	1.79478000	2.86513800	-0.56475400
C	0.85354900	1.83151800	-0.44740600
C	-0.17946900	1.97209300	0.47455800
C	-1.30402300	1.08344800	0.62793600

C	-2.27378600	1.85413800	1.50226700
H	-3.17565800	2.17674900	0.97384200
H	-2.56542300	1.30556300	2.40249400
C	-1.25070000	-0.14338000	0.05562100
C	0.59796600	0.65131700	-1.32657000
C	-2.33089500	-1.14226700	-0.05637400
C	-3.60025000	-0.83472200	-0.58423200
C	-4.60162800	-1.79868000	-0.70993700
H	-5.56427400	-1.51166100	-1.11804500
C	-4.34567500	-3.11506500	-0.33903000
H	-5.12502800	-3.86416000	-0.44141900
C	-3.08134900	-3.46372900	0.13885000
H	-2.86178200	-4.49190200	0.40990900
C	-2.09440300	-2.49384900	0.26558700
H	-1.11268100	-2.77564600	0.62505700
C	0.96840700	-1.05700900	0.38986300
C	0.63371500	-1.32705500	1.70982800
H	-0.33930900	-1.03582000	2.08372000
C	1.53155600	-1.97189800	2.58879100
H	1.21013800	-2.16672900	3.60798200
C	2.79175500	-2.33580700	2.17928200
H	3.48617600	-2.82726400	2.85473600
C	3.19424700	-2.05188600	0.85088000
C	2.28928900	-1.41166800	-0.05565900
C	3.85348100	-1.41814500	-1.74830400
H	4.08916300	-1.15315100	-2.77795100
C	4.82066900	-2.05907500	-0.93880300
H	5.80138200	-2.29133000	-1.34200200
C	4.48435500	-2.37140500	0.35733000
H	5.19513900	-2.85919100	1.01972600
Cl	-3.98146100	0.77759400	-1.17842900

CN_188_CC_163

Charge = 0, Multiplicity = 1

O	2.93587500	3.00523800	-0.92590700
O	-1.34967700	0.82636800	1.87228100
N	-0.33137400	-0.08772600	-0.02977500
N	-3.13129000	0.20587600	-0.02435000
C	-2.29021100	3.72409300	1.12708900
H	-3.06593400	3.25733000	0.50855200
H	-2.54788400	4.77799600	1.26802200
H	-2.31556900	3.21611200	2.09584200
C	1.65382300	3.34568100	-0.61675600

S235

C	1.12332800	4.61498200	-0.43043300
H	1.70392200	5.50885000	-0.63021600
C	-0.18341700	4.69591100	0.08707000
H	-0.61325200	5.68232600	0.24014600
C	-0.93594900	3.57795800	0.48319700
C	-0.37909800	2.30709500	0.24693700
C	0.86725900	2.22151500	-0.37602000
C	1.67252500	1.03627900	-0.48977700
C	3.06615900	1.55645800	-0.78433000
H	3.79666300	1.35842300	0.00909200
H	3.46715400	1.17625600	-1.72453300
C	1.09893100	-0.16836100	-0.19023200
C	-0.82015800	1.01147800	0.79988800
C	1.78405100	-1.33101300	0.41730900
C	3.07936800	-1.78100300	0.10947500
C	3.76215600	-2.69656400	0.91144700
H	4.75052000	-3.02568300	0.61045400
C	3.16089700	-3.19221500	2.06339600
H	3.69339800	-3.90314700	2.68752600
C	1.86715600	-2.78011100	2.39225300
H	1.38157300	-3.15831200	3.28658800
C	1.20138900	-1.86312900	1.59147900
H	0.22147700	-1.50401800	1.88457100
C	-1.17105800	-1.15124500	-0.41019700
C	-0.66963000	-2.32999300	-0.95163000
H	0.39217600	-2.44830700	-1.10946100
C	-1.51268400	-3.40486500	-1.29997700
H	-1.05825900	-4.30694800	-1.69912800
C	-2.87425900	-3.33183000	-1.12738600
H	-3.52261900	-4.16901500	-1.36921000
C	-3.44133600	-2.12208700	-0.66031400
C	-2.60475500	-1.00350200	-0.34290200
C	-4.43707300	0.33790700	0.06920600
H	-4.80562200	1.33202800	0.31832500
C	-5.34707100	-0.72353600	-0.14505400
H	-6.41422600	-0.55879900	-0.03473500
C	-4.84194200	-1.94356900	-0.52485000
H	-5.49996200	-2.78208700	-0.73871600
Cl	3.82441700	-1.38652400	-1.44050400

CN_188_CC_168

Charge = 0, Multiplicity = 1

O	2.92665800	2.98414500	-0.98113500
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S236

O	-1.31481900	0.81168600	1.89689000
N	-0.33178900	-0.09451200	-0.02698200
N	-3.13380100	0.21563400	0.02006200
C	-2.25356100	3.71711900	1.17781100
H	-3.04195000	3.24882200	0.57675000
H	-2.50722400	4.77178600	1.32027000
H	-2.25991600	3.21261400	2.14869900
C	1.65257400	3.32637100	-0.64507800
C	1.12889800	4.59755300	-0.45072800
H	1.70757700	5.48921100	-0.66536400
C	-0.16607400	4.68315200	0.09373600
H	-0.59035900	5.67086000	0.25377800
C	-0.91280000	3.56734300	0.50704400
C	-0.36386700	2.29528200	0.26129400
C	0.86975600	2.20371900	-0.38638100
C	1.67020900	1.01520000	-0.51651100
C	3.05926000	1.53638500	-0.83489100
H	3.80137500	1.34398800	-0.05132000
H	3.44684300	1.15282300	-1.77908600
C	1.09609200	-0.18937500	-0.21120800
C	-0.80159200	1.00030900	0.81752100
C	1.77268100	-1.35864300	0.39708500
C	3.09306600	-1.77562400	0.15003500
C	3.76261900	-2.67784600	0.97720700
H	4.77063200	-2.98093600	0.71686800
C	3.12553500	-3.19481700	2.10004000
H	3.64832700	-3.89467100	2.74452900
C	1.80869600	-2.81715300	2.37091000
H	1.29280900	-3.21003800	3.24164000
C	1.15677600	-1.91206500	1.54543800
H	0.16086600	-1.57443200	1.80586000
C	-1.18507200	-1.13602800	-0.43463500
C	-0.69516400	-2.29997600	-1.01789900
H	0.36492200	-2.41757800	-1.18906100
C	-1.54702900	-3.35896700	-1.39162500
H	-1.10144100	-4.25016300	-1.82385700
C	-2.90661900	-3.28460700	-1.20349200
H	-3.56177200	-4.11021900	-1.46585800
C	-3.46245900	-2.08804600	-0.69134900
C	-2.61695700	-0.98435200	-0.34586000
C	-4.43781900	0.35061600	0.13260500
H	-4.79847000	1.33713900	0.42047700
C	-5.35540700	-0.69848300	-0.10836400
H	-6.42049100	-0.53260200	0.01899200

C	-4.86061100	-1.90727500	-0.53490300
H	-5.52524300	-2.73483600	-0.76996600
Cl	3.89359700	-1.37617800	-1.37222300

CN_188_CC_173

Charge = 0, Multiplicity = 1

O	2.88156500	2.99204600	-1.04370800
O	-1.27584300	0.78241800	1.93436800
N	-0.32768500	-0.10642000	-0.01499800
N	-3.13267300	0.19616100	0.07811700
C	-2.25286700	3.68520500	1.23342500
H	-3.05061200	3.21286300	0.64801800
H	-2.51035900	4.73791600	1.38323500
H	-2.23547300	3.17891000	2.20320900
C	1.61358900	3.32208400	-0.67641400
C	1.08183500	4.58955200	-0.47758800
H	1.64636700	5.48506300	-0.71285000
C	-0.19987100	4.66636800	0.09747600
H	-0.62999300	5.65081500	0.26196600
C	-0.92571700	3.54537600	0.53406800
C	-0.37009100	2.27794800	0.28230000
C	0.84991100	2.19278400	-0.39209900
C	1.65884400	1.00975500	-0.53753600
C	3.03574400	1.54784000	-0.88472600
H	3.79225200	1.37622600	-0.11075400
H	3.41404400	1.16051700	-1.83088700
C	1.09810600	-0.20078200	-0.22496700
C	-0.78761900	0.97944000	0.84545600
C	1.77783200	-1.37400000	0.37693400
C	3.12254000	-1.74685300	0.19081800
C	3.78277000	-2.63794300	1.03667000
H	4.81052000	-2.90500700	0.81738400
C	3.11427300	-3.19093100	2.12338200
H	3.63039500	-3.88146400	2.78308300
C	1.77510900	-2.85976500	2.33565800
H	1.23182900	-3.27909000	3.17689000
C	1.13331600	-1.96372400	1.49235800
H	0.12018600	-1.65788600	1.72034300
C	-1.18644600	-1.12716400	-0.45859100
C	-0.69938100	-2.26617100	-1.09227900
H	0.35985000	-2.37322200	-1.27671300
C	-1.55230100	-3.31130400	-1.50015100
H	-1.10899500	-4.18329300	-1.97212700

C	-2.91050000	-3.24796200	-1.29709900
H	-3.56631600	-4.06362500	-1.58736100
C	-3.46379000	-2.07524800	-0.73020600
C	-2.61734500	-0.98467100	-0.34679800
C	-4.43566100	0.32267800	0.21116600
H	-4.79506500	1.29418400	0.54754200
C	-5.35338500	-0.71704800	-0.06697700
H	-6.41744500	-0.55978700	0.07862300
C	-4.86057100	-1.90472300	-0.55138200
H	-5.52602700	-2.72286500	-0.81532800
Cl	3.97891900	-1.32227000	-1.29522100

CN_188_CC_178

Charge = 0, Multiplicity = 1

O	1.09110300	3.55645600	-1.36566100
O	-0.91366500	0.41277100	2.64519000
N	-0.03688800	-0.38607200	0.61463800
N	-2.64749200	-1.25341400	0.90543300
C	-3.56050300	2.13598200	1.54932000
H	-4.13107700	1.33003900	1.07200100
H	-4.23240700	2.98667300	1.69817600
H	-3.23774400	1.76466800	2.52625200
C	-0.12274600	3.31180300	-0.80657200
C	-1.24183900	4.13852700	-0.79369000
H	-1.24880600	5.08828100	-1.31704900
C	-2.34978600	3.71243000	-0.04407100
H	-3.22887500	4.35117500	-0.01790200
C	-2.36949300	2.52441800	0.71155700
C	-1.24009700	1.69924000	0.63795600
C	-0.15187000	2.08945800	-0.14716700
C	1.14839700	1.44373300	-0.23272600
C	2.00179200	2.49162600	-0.94581200
H	2.75377700	2.95461600	-0.30417700
H	2.48218100	2.11018700	-1.84610700
C	1.26995600	0.17161200	0.26489900
C	-0.85594800	0.51240600	1.44800500
C	2.38012900	-0.78367700	0.48778000
C	3.75892600	-0.61714400	0.23125000
C	4.69782200	-1.61481000	0.49310800
H	5.74012500	-1.41905900	0.26775400
C	4.30465500	-2.83134200	1.04017500
H	5.04390000	-3.60056500	1.24108900
C	2.95751300	-3.02903100	1.33514500

H	2.62006100	-3.95969000	1.78082800
C	2.03290500	-2.02925900	1.07000700
H	0.99641200	-2.18166400	1.33372700
C	-0.66968000	-1.09618300	-0.42959700
C	-0.01970400	-1.41489300	-1.61469600
H	0.98538100	-1.05699700	-1.79220400
C	-0.64196600	-2.20610500	-2.60475800
H	-0.08664200	-2.42901800	-3.51136600
C	-1.92099300	-2.68577300	-2.44522100
H	-2.39745300	-3.29186000	-3.21029000
C	-2.62879500	-2.37569900	-1.25825800
C	-2.00845900	-1.58088900	-0.24333400
C	-3.87881400	-1.67889600	1.10238300
H	-4.34744300	-1.38622300	2.04048500
C	-4.58161000	-2.47463700	0.16795700
H	-5.59437600	-2.80004700	0.38373700
C	-3.95309100	-2.81554600	-1.00754100
H	-4.45737400	-3.42068700	-1.75677400
Cl	4.44537200	0.86462600	-0.42714700

CN_188_CC_183

Charge = 0, Multiplicity = 1

O	1.06628800	3.39694100	-1.54266900
O	-0.86304800	0.47618000	2.69825600
N	-0.01661800	-0.40887600	0.68496400
N	-2.62507500	-1.25430400	1.01574000
C	-3.53813700	2.15015400	1.53386200
H	-4.12185400	1.33261500	1.09341100
H	-4.20120100	3.01170900	1.65830800
H	-3.20737600	1.81301200	2.52029900
C	-0.13289600	3.19929200	-0.93220700
C	-1.26192400	4.01241800	-0.96478600
H	-1.29152800	4.91732500	-1.56164900
C	-2.35360600	3.63027200	-0.16866000
H	-3.24028200	4.25896600	-0.17833300
C	-2.35408800	2.49645600	0.66805400
C	-1.21576400	1.68180800	0.64211000
C	-0.13848800	2.03778700	-0.17208500
C	1.16178100	1.39503700	-0.23414500
C	1.99781200	2.38918200	-1.03385900
H	2.73535200	2.92292500	-0.43236500
H	2.49724000	1.94056800	-1.89391800
C	1.28937000	0.14631500	0.31650000

S240

C	-0.81923400	0.52767700	1.49825600
C	2.40383800	-0.80823500	0.47192700
C	3.78154000	-0.57847600	0.26218000
C	4.73006100	-1.59877200	0.32903600
H	5.77233700	-1.35285800	0.15935500
C	4.34630700	-2.89917800	0.63908500
H	5.09178200	-3.68664500	0.69136200
C	3.00410900	-3.15773500	0.91298300
H	2.68018900	-4.15589100	1.19117600
C	2.06806000	-2.13689100	0.83340800
H	1.03345600	-2.34575600	1.06354100
C	-0.68510000	-1.07452400	-0.37199900
C	-0.07300500	-1.36219900	-1.58392100
H	0.93323500	-1.01559100	-1.77609700
C	-0.73498900	-2.10806900	-2.58382500
H	-0.20840900	-2.30787400	-3.51266900
C	-2.01717700	-2.57166800	-2.40535500
H	-2.52495400	-3.14197100	-3.17780600
C	-2.68663600	-2.29408900	-1.18831600
C	-2.02489500	-1.54694200	-0.16344800
C	-3.85725800	-1.66798500	1.23120400
H	-4.29440800	-1.40458300	2.19290200
C	-4.59990600	-2.41609700	0.28807100
H	-5.61150600	-2.73338500	0.52073100
C	-4.01048300	-2.72255700	-0.91672500
H	-4.54539100	-3.29136800	-1.67314500
Cl	4.45255900	1.03283600	0.03065900

CN_188_CC_188

Charge = 0, Multiplicity = 1

O	1.08707300	3.31482800	-1.62934400
O	-0.81942900	0.50742200	2.70570200
N	-0.01071700	-0.42522000	0.69582000
N	-2.62401500	-1.23534200	1.07241900
C	-3.49265500	2.19352900	1.53595200
H	-4.09067800	1.37462300	1.11772000
H	-4.14430600	3.06512000	1.65041500
H	-3.15547500	1.87171200	2.52532000
C	-0.10559400	3.15119000	-0.99430200
C	-1.22789500	3.97347300	-1.03397200
H	-1.25904200	4.86178000	-1.65519700
C	-2.31226000	3.62164400	-0.21377500
H	-3.19362300	4.25766500	-0.22921300

S241

C	-2.31391300	2.50866700	0.65114700
C	-1.18311500	1.68360200	0.63331900
C	-0.11291900	2.01326200	-0.20011700
C	1.17756500	1.35482300	-0.26364700
C	2.01558700	2.31522300	-1.09791600
H	2.76188000	2.86093900	-0.51853800
H	2.50843100	1.83545000	-1.94606400
C	1.29590800	0.11402100	0.30396400
C	-0.78877500	0.53826600	1.50497700
C	2.40913600	-0.84082800	0.43565200
C	3.78814500	-0.57539200	0.28843600
C	4.75023500	-1.58512900	0.30785100
H	5.79372600	-1.31415300	0.19231700
C	4.37556600	-2.90929200	0.50958300
H	5.13051600	-3.68926500	0.52652300
C	3.03010700	-3.20525500	0.72714500
H	2.71526400	-4.22542000	0.92405500
C	2.08066200	-2.19428900	0.69463200
H	1.04336400	-2.43369600	0.87850900
C	-0.71117200	-1.07123600	-0.35513700
C	-0.12997900	-1.35564500	-1.58268500
H	0.87719600	-1.02226600	-1.79276200
C	-0.82418600	-2.08138100	-2.57559700
H	-0.32067300	-2.27971900	-3.51744500
C	-2.10928800	-2.52685100	-2.37400600
H	-2.64231700	-3.08140400	-3.14091100
C	-2.74831600	-2.25142000	-1.14017800
C	-2.05338900	-1.52517700	-0.12220200
C	-3.85790800	-1.63176800	1.30917100
H	-4.27091100	-1.37128300	2.28228500
C	-4.63202500	-2.35855400	0.37458800
H	-5.64345400	-2.66226500	0.62540400
C	-4.07279900	-2.66209500	-0.84518000
H	-4.63220700	-3.21479700	-1.59579900
Cl	4.43199600	1.06191600	0.22462500

CN_188_CC_193

Charge = 0, Multiplicity = 1

O	1.10928500	3.25369100	-1.69803900
O	-0.77703700	0.52921100	2.70247200
N	-0.00683100	-0.44065200	0.69312600
N	-2.62358900	-1.21733800	1.11734800
C	-3.44266900	2.23866900	1.54533900

H	-4.05243300	1.41739600	1.14931900
H	-4.08537400	3.11797800	1.65088000
H	-3.09713100	1.93218700	2.53673600
C	-0.07703900	3.11819400	-1.04314100
C	-1.18949600	3.95400000	-1.07953800
H	-1.21934500	4.83325900	-1.71356500
C	-2.26657700	3.62734400	-0.23914000
H	-3.14016400	4.27405200	-0.25223800
C	-2.27129400	2.52660600	0.64167600
C	-1.15119800	1.68708600	0.62123600
C	-0.08913500	1.99381600	-0.23042600
C	1.19006100	1.31750100	-0.30192100
C	2.03051500	2.24841600	-1.16372000
H	2.79597200	2.79074000	-0.60665400
H	2.50329100	1.74387500	-2.00990300
C	1.29907000	0.08241100	0.27697800
C	-0.75997000	0.54568000	1.50152900
C	2.41234200	-0.87088400	0.39519800
C	3.79051600	-0.57624000	0.31535500
C	4.76780900	-1.57180700	0.31698200
H	5.81063700	-1.28107700	0.25656300
C	4.40572100	-2.90947900	0.43460700
H	5.17146200	-3.67905800	0.43871500
C	3.05792100	-3.23629700	0.58745800
H	2.75386300	-4.27013400	0.71928800
C	2.09377300	-2.23893900	0.57377400
H	1.05449400	-2.50315000	0.70597000
C	-0.73709500	-1.07267300	-0.34755900
C	-0.18541400	-1.35778200	-1.58842900
H	0.82184600	-1.03671900	-1.81688300
C	-0.90915600	-2.06863700	-2.57095300
H	-0.42759300	-2.26854600	-3.52387900
C	-2.19594900	-2.49734300	-2.34548700
H	-2.75215100	-3.04021400	-3.10426200
C	-2.80604400	-2.21978600	-1.09752900
C	-2.08075800	-1.50894500	-0.08983000
C	-3.85820000	-1.59737300	1.37605300
H	-4.24846300	-1.33598000	2.35828000
C	-4.66094500	-2.30824600	0.45338900
H	-5.67150100	-2.59882900	0.72261300
C	-4.13017900	-2.61338900	-0.77857700
H	-4.71199700	-3.15414500	-1.52081600
Cl	4.40175800	1.07350900	0.37182900

CN_188_CC_198

Charge = 0, Multiplicity = 1

O	1.13329100	3.20688000	-1.75565300
O	-0.73589800	0.54602600	2.69206500
N	-0.00451200	-0.45503600	0.68211400
N	-2.62334400	-1.19922000	1.15450300
C	-3.38930200	2.28546400	1.55804100
H	-4.01030100	1.46283900	1.18284400
H	-4.02348600	3.17164700	1.65713700
H	-3.03427400	1.99188600	2.55005900
C	-0.04696900	3.09547900	-1.08418100
C	-1.14683700	3.94823200	-1.11059500
H	-1.17272500	4.82383600	-1.74983300
C	-2.21683000	3.64335300	-0.25275500
H	-3.08055000	4.30327800	-0.25830800
C	-2.22653900	2.54882200	0.63595600
C	-1.11985400	1.69184000	0.60615800
C	-0.06664300	1.97755300	-0.26310300
C	1.20000000	1.28185600	-0.34619500
C	2.04334600	2.18603500	-1.23099700
H	2.83406400	2.71418200	-0.69590000
H	2.48659500	1.66148400	-2.08173800
C	1.29973000	0.05152900	0.24128800
C	-0.73248500	0.55149900	1.49114300
C	2.41393700	-0.89926600	0.35274600
C	3.78852400	-0.58021900	0.34324200
C	4.78080600	-1.56118300	0.34423700
H	5.82077700	-1.25440600	0.33953800
C	4.43384600	-2.90710700	0.39183600
H	5.21034800	-3.66584800	0.39605900
C	3.08598400	-3.25964700	0.47528200
H	2.79412900	-4.30255200	0.55168100
C	2.10732100	-2.27644600	0.46368900
H	1.06765700	-2.56110000	0.54083000
C	-0.76258000	-1.07715500	-0.34550100
C	-0.23920600	-1.36600500	-1.59777400
H	0.76740500	-1.05655500	-1.84487000
C	-0.99030400	-2.06594100	-2.56749400
H	-0.52979800	-2.26974500	-3.52995600
C	-2.27778400	-2.47881100	-2.31784600
H	-2.85539600	-3.01314300	-3.06662600
C	-2.86021900	-2.19580600	-1.05791500
C	-2.10684400	-1.49630600	-0.06289500

S244

C	-3.85795800	-1.56312600	1.43530400
H	-4.22658300	-1.29798000	2.42487000
C	-4.68696500	-2.26234500	0.52701600
H	-5.69604600	-2.54010500	0.81469100
C	-4.18321800	-2.57271000	-0.71489800
H	-4.78570700	-3.10473400	-1.44688800
Cl	4.36423500	1.07623700	0.49329800

CN_188_CC_203

Charge = 0, Multiplicity = 1

O	1.16042200	3.17092200	-1.80368900
O	-0.69632600	0.55937700	2.67665400
N	-0.00337400	-0.46884400	0.66596700
N	-2.62317000	-1.18140000	1.18601300
C	-3.33347800	2.33329500	1.57203900
H	-3.96471300	1.50952200	1.21703500
H	-3.95990600	3.22553700	1.66556200
H	-2.96845500	2.05176300	2.56401100
C	-0.01461000	3.08049600	-1.11886100
C	-1.09952000	3.95253700	-1.13118200
H	-1.11885100	4.82852700	-1.77012200
C	-2.16311000	3.66669200	-0.25857800
H	-3.01516300	4.34160600	-0.25337100
C	-2.18001300	2.57388800	0.63225700
C	-1.08905800	1.69730100	0.58884900
C	-0.04485700	1.96367100	-0.29684700
C	1.20811700	1.24752200	-0.39343500
C	2.05561200	2.12841900	-1.29582300
H	2.87286600	2.63489300	-0.77954200
H	2.46561000	1.58921600	-2.15455800
C	1.29849000	0.02107500	0.20010800
C	-0.70624500	0.55603000	1.47590800
C	2.41431400	-0.92694100	0.30917000
C	3.78225000	-0.58774000	0.37172800
C	4.78817300	-1.55495100	0.38375400
H	5.82298400	-1.23523800	0.43489700
C	4.45807200	-2.90586700	0.37124600
H	5.24442600	-3.65431400	0.38458800
C	3.11306400	-3.27962600	0.38212300
H	2.83445000	-4.32857800	0.40976100
C	2.12118600	-2.30979500	0.36087800
H	1.08319300	-2.61101600	0.38034700
C	-0.78775200	-1.08339000	-0.34715900

C	-0.29177000	-1.37739300	-1.60941500
H	0.71349600	-1.07881700	-1.87513700
C	-1.06857800	-2.06851200	-2.56512400
H	-0.62847600	-2.27730600	-3.53602800
C	-2.35590700	-2.46621900	-2.29148600
H	-2.95359800	-2.99363600	-3.02933800
C	-2.91165800	-2.17610100	-1.02113200
C	-2.13196300	-1.48568400	-0.04006500
C	-3.85709800	-1.52973500	1.48866900
H	-4.20505900	-1.25914800	2.48423900
C	-4.71068200	-2.21928400	0.59585200
H	-5.71788100	-2.48430800	0.90158300
C	-4.23288000	-2.53665300	-0.65447200
H	-4.85473400	-3.06155000	-1.37532700
Cl	4.32130900	1.07258600	0.59587100

CN_188_CC_208

Charge = 0, Multiplicity = 1

O	1.19079700	3.14209300	-1.84642700
O	-0.65851900	0.57135300	2.65723600
N	-0.00337400	-0.48096000	0.64559800
N	-2.62341700	-1.16136900	1.21269400
C	-3.27477800	2.38392700	1.58586500
H	-3.91485500	1.55822300	1.25191700
H	-3.89461000	3.28136200	1.67297300
H	-2.89928200	2.11564400	2.57771600
C	0.02037900	3.07100000	-1.15050500
C	-1.04734500	3.96403800	-1.14642700
H	-1.05771900	4.84282800	-1.78172700
C	-2.10513300	3.69600900	-0.26083200
H	-2.94378400	4.38727800	-0.24304100
C	-2.13128600	2.60234600	0.62868500
C	-1.05828000	1.70445600	0.56912600
C	-0.02309000	1.95207200	-0.33208400
C	1.21533900	1.21472700	-0.44279600
C	2.06844300	2.07525800	-1.35816300
H	2.91057800	2.55669600	-0.85748500
H	2.44485900	1.52613800	-2.22625800
C	1.29549600	-0.00852900	0.15512500
C	-0.68132700	0.56107900	1.45687200
C	2.41315100	-0.95414200	0.26540600
C	3.77122700	-0.59888300	0.40149100
C	4.78860500	-1.55385800	0.43230600

H	5.81589900	-1.22405000	0.53980300
C	4.47637000	-2.90745300	0.36569300
H	5.27093600	-3.64678600	0.39398700
C	3.13745200	-3.29817000	0.30168600
H	2.87277400	-4.35096300	0.28482000
C	2.13445300	-2.34014200	0.26310900
H	1.10048500	-2.65426500	0.22375200
C	-0.81244000	-1.09052000	-0.35120200
C	-0.34308800	-1.39154900	-1.62213500
H	0.65983900	-1.10240700	-1.90697600
C	-1.14368700	-2.07705400	-2.56213400
H	-0.72331700	-2.29223400	-3.54036700
C	-2.42981300	-2.46092800	-2.26435000
H	-3.04602000	-2.98410700	-2.98988400
C	-2.95993600	-2.16109300	-0.98530000
C	-2.15595800	-1.47633800	-0.01994000
C	-3.85608500	-1.49429600	1.53702700
H	-4.18455100	-1.21545600	2.53694300
C	-4.73202400	-2.17804400	0.66156000
H	-5.73687000	-2.43057600	0.98510500
C	-4.27871900	-2.50563300	-0.59519500
H	-4.91832900	-3.02620400	-1.30354300
Cl	4.27327800	1.06340700	0.68767200

CN_193_CC_163

Charge = 0, Multiplicity = 1

O	2.74864600	3.13343700	-0.96891200
O	-1.40886200	0.72654000	1.89350500
N	-0.32126800	-0.13490300	0.01073800
N	-3.11045800	0.09777600	-0.08721300
C	-2.46237800	3.57783200	1.19862300
H	-3.23092000	3.10588600	0.57501300
H	-2.75364300	4.61735300	1.37641100
H	-2.45698100	3.03758300	2.14963500
C	1.45860700	3.40525900	-0.62687500
C	0.86805100	4.64467700	-0.42346700
H	1.39693200	5.56791100	-0.63305800
C	-0.42880900	4.65588800	0.12392500
H	-0.90565100	5.61815900	0.29084300
C	-1.11408900	3.49948100	0.53109100
C	-0.49746500	2.25880400	0.27941300
C	0.73775300	2.24074600	-0.37047700
C	1.60147400	1.10096000	-0.50769800

C	2.95761200	1.69340400	-0.83767100
H	3.71886000	1.53048000	-0.06537300
H	3.35165500	1.33700900	-1.79017300
C	1.10457500	-0.13306000	-0.19214200
C	-0.87098800	0.94149500	0.82969000
C	1.87739800	-1.24438500	0.40595000
C	3.18776000	-1.61912100	0.06241100
C	3.95038800	-2.47820100	0.85504000
H	4.94707000	-2.75151200	0.52683900
C	3.41761200	-2.99033300	2.03320500
H	4.01237000	-3.65711200	2.64978900
C	2.11194800	-2.65266800	2.39831100
H	1.67915800	-3.04527300	3.31331000
C	1.36611200	-1.79130100	1.60655200
H	0.37445300	-1.48932900	1.92404600
C	-1.11732000	-1.24021600	-0.34913500
C	-0.57839000	-2.43159800	-0.82025100
H	0.48963700	-2.54211300	-0.93178500
C	-1.39283400	-3.53350400	-1.15482100
H	-0.91042700	-4.44382900	-1.49858300
C	-2.76042800	-3.47633900	-1.03467300
H	-3.38650300	-4.33359500	-1.26468800
C	-3.36300200	-2.25854200	-0.63754500
C	-2.55514800	-1.11495500	-0.33784700
C	-4.42062900	0.21169700	-0.04499400
H	-4.81326100	1.20859800	0.15008500
C	-5.30642700	-0.87223800	-0.24732600
H	-6.37911400	-0.72045700	-0.18112300
C	-4.77000900	-2.09831300	-0.55854300
H	-5.40729200	-2.95570900	-0.75992000
Cl	3.85701300	-1.20451700	-1.51630400

CN_193_CC_168

Charge = 0, Multiplicity = 1

O	2.74801400	3.10391100	-1.02368000
O	-1.37161100	0.71513500	1.91549800
N	-0.32208800	-0.14180000	0.00969200
N	-3.11434800	0.11931100	-0.04655300
C	-2.41446800	3.57770700	1.24854600
H	-3.19722200	3.10807300	0.64112800
H	-2.69724500	4.61890600	1.43012500
H	-2.39287100	3.03913300	2.20027600
C	1.46718700	3.38136400	-0.65511900

S248

C	0.88730000	4.62452700	-0.44254100
H	1.41689500	5.54414800	-0.66574400
C	-0.39742800	4.64420700	0.13144900
H	-0.86568100	5.60928300	0.30627800
C	-1.08016500	3.49180300	0.55440500
C	-0.47539400	2.24797000	0.29202200
C	0.74683700	2.22038400	-0.38231700
C	1.60237000	1.07478000	-0.53621600
C	2.95523900	1.66434800	-0.88808800
H	3.72593400	1.50523100	-0.12477400
H	3.33639800	1.30332200	-1.84379600
C	1.10172300	-0.15799600	-0.21559600
C	-0.84952300	0.93209700	0.84450400
C	1.86357500	-1.27728600	0.38566600
C	3.19825300	-1.62002000	0.10317300
C	3.94551100	-2.46581600	0.92352000
H	4.96113500	-2.71399100	0.63602500
C	3.37557000	-2.99807200	2.07493700
H	3.95886600	-3.65370500	2.71397500
C	2.04746300	-2.69394700	2.38170100
H	1.58326100	-3.10058600	3.27491900
C	1.31752900	-1.84441500	1.56265900
H	0.31068500	-1.56263900	1.84708500
C	-1.13569700	-1.22490200	-0.37510900
C	-0.61189400	-2.40641100	-0.88731300
H	0.45429600	-2.52083100	-1.01406000
C	-1.43887500	-3.49153300	-1.24428800
H	-0.96806800	-4.39509800	-1.62046400
C	-2.80463800	-3.42714700	-1.10644200
H	-3.44036800	-4.27215600	-1.35452000
C	-3.39243800	-2.21720400	-0.66580000
C	-2.57194300	-1.08921300	-0.34148300
C	-4.42295900	0.24189800	0.01566500
H	-4.80515300	1.23513900	0.24680900
C	-5.31976600	-0.82844500	-0.20933200
H	-6.39033000	-0.67056700	-0.12533200
C	-4.79706000	-2.04844000	-0.56467800
H	-5.44368800	-2.89423900	-0.78447600
Cl	3.92465500	-1.20210600	-1.45079500

CN_193_CC_173

Charge = 0, Multiplicity = 1

O	2.71488200	3.09897100	-1.08200500
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S249

O	-1.33060200	0.69044300	1.94811900
N	-0.31833400	-0.15302300	0.01641400
N	-3.11408600	0.11589300	0.00567100
C	-2.39911300	3.55395200	1.29943700
H	-3.19313500	3.08819000	0.70371800
H	-2.67854000	4.59391400	1.49289200
H	-2.35931700	3.00938000	2.24709200
C	1.44192200	3.36941500	-0.68456300
C	0.85948000	4.61074100	-0.46657400
H	1.37879800	5.53165100	-0.70785100
C	-0.41170200	4.62695700	0.13581800
H	-0.88153300	5.59032400	0.31576000
C	-1.07845800	3.47263800	0.57915600
C	-0.47244900	2.23141700	0.30987300
C	0.73603700	2.20524900	-0.38947000
C	1.59496500	1.06228500	-0.55869800
C	2.93744700	1.66302800	-0.93548900
H	3.71888600	1.52109500	-0.18029800
H	3.31014600	1.29693900	-1.89234100
C	1.10294200	-0.17398900	-0.23247900
C	-0.83202500	0.91388400	0.86774800
C	1.86391700	-1.29845700	0.36492500
C	3.22155900	-1.59870400	0.14389100
C	3.95678700	-2.43288000	0.98589700
H	4.99085600	-2.64662400	0.73954300
C	3.35412000	-2.99873600	2.10409000
H	3.92854000	-3.64459500	2.76084000
C	2.00506200	-2.73957300	2.35174000
H	1.51241700	-3.17101200	3.21767200
C	1.28786500	-1.89953300	1.51164500
H	0.26529100	-1.64763900	1.76327800
C	-1.14191100	-1.21507000	-0.40079300
C	-0.62544800	-2.37797200	-0.96184500
H	0.43952100	-2.48741300	-1.10445100
C	-1.45776500	-3.44849200	-1.34830500
H	-0.99267400	-4.33811100	-1.76291400
C	-2.82198500	-3.38801400	-1.19253500
H	-3.46164300	-4.22264900	-1.46440900
C	-3.40286400	-2.19497100	-0.69998200
C	-2.57714400	-1.08046300	-0.34315300
C	-4.42166800	0.23720200	0.08954600
H	-4.79947200	1.22078300	0.36488600
C	-5.32245900	-0.82281100	-0.16619800
H	-6.39170900	-0.66748000	-0.06287500

C	-4.80587900	-2.02863400	-0.57504800
H	-5.45649800	-2.86461100	-0.81930100
Cl	4.00443300	-1.15931500	-1.37803300

CN_193_CC_178

Charge = 0, Multiplicity = 1

O	2.61497600	3.14103900	-1.14913700
O	-1.27817600	0.64133100	2.00398100
N	-0.30494400	-0.17314300	0.03947300
N	-3.10541500	0.06089600	0.08418500
C	-2.45033000	3.48259800	1.35295600
H	-3.25299500	3.03387300	0.75526600
H	-2.73060100	4.51471500	1.58370700
H	-2.39193400	2.90851300	2.28176600
C	1.34755500	3.37942900	-0.71729400
C	0.73564000	4.60719400	-0.50065800
H	1.22228000	5.53842800	-0.76890400
C	-0.51895900	4.59654100	0.13430400
H	-1.01106400	5.54871200	0.31437600
C	-1.14225000	3.42944900	0.60749300
C	-0.50830600	2.20288900	0.33856400
C	0.68476100	2.19971100	-0.38791800
C	1.57071900	1.07683300	-0.57020000
C	2.88688000	1.71588000	-0.98063200
H	3.68274300	1.61711100	-0.23458400
H	3.25765000	1.34562700	-1.93635100
C	1.11308500	-0.17184000	-0.23608800
C	-0.82148400	0.87847800	0.90896100
C	1.89243800	-1.29513500	0.34550800
C	3.27219200	-1.53372000	0.18609400
C	4.00252400	-2.36145200	1.03795800
H	5.05496800	-2.52363500	0.83382300
C	3.37537300	-2.98707900	2.10980400
H	3.94659600	-3.62727600	2.77480300
C	2.00672000	-2.79282900	2.29734500
H	1.49147000	-3.26980100	3.12539700
C	1.29514000	-1.95643300	1.44859500
H	0.25545100	-1.75203000	1.66709000
C	-1.12396700	-1.21561300	-0.42732200
C	-0.59959800	-2.34087900	-1.05525300
H	0.46535400	-2.42721100	-1.21509900
C	-1.42323400	-3.40004300	-1.48774500
H	-0.95246700	-4.26023700	-1.95480600

C	-2.78648400	-3.36602400	-1.31360400
H	-3.41881900	-4.19307300	-1.62306500
C	-3.37581900	-2.20960300	-0.74933100
C	-2.55933900	-1.10568500	-0.34149000
C	-4.41298900	0.16057000	0.19395500
H	-4.79820000	1.12101800	0.53307600
C	-5.30405300	-0.89443900	-0.11161600
H	-6.37357300	-0.75932400	0.01481900
C	-4.77881800	-2.06813200	-0.59630900
H	-5.42298000	-2.89688000	-0.87925200
Cl	4.11116700	-1.03386800	-1.28781700

CN_193_CC_183

Charge = 0, Multiplicity = 1

O	0.95291800	3.36899200	-1.60966400
O	-0.83034700	0.44698200	2.70479200
N	0.00611000	-0.43477400	0.68722300
N	-2.63740400	-1.17858100	0.97002200
C	-3.55093900	2.08527900	1.59478900
H	-4.20391600	1.33901500	1.12585000
H	-4.15593200	2.97052800	1.81470600
H	-3.19327900	1.65949700	2.53576400
C	-0.22841900	3.15335900	-0.97135200
C	-1.37206200	3.94652900	-0.98507900
H	-1.43221800	4.84414000	-1.59058900
C	-2.43400000	3.55589400	-0.15500400
H	-3.33080000	4.17021200	-0.14618600
C	-2.39283800	2.43189700	0.69481600
C	-1.24366400	1.63374700	0.64679300
C	-0.19406200	2.00098000	-0.19827500
C	1.12062500	1.39041900	-0.27418600
C	1.91795900	2.39313200	-1.10205900
H	2.65068200	2.95497800	-0.52092100
H	2.41480100	1.94364600	-1.96316800
C	1.29184400	0.15757400	0.29788800
C	-0.81236200	0.49052600	1.50330100
C	2.43911800	-0.75378200	0.47612100
C	3.80836800	-0.48542600	0.25621600
C	4.79068800	-1.47060900	0.35560000
H	5.82384600	-1.19557700	0.17520000
C	4.45164500	-2.77205700	0.70992100
H	5.22345500	-3.53155800	0.78755900
C	3.11886700	-3.06660700	0.99312800

H	2.82853100	-4.06542800	1.30409800
C	2.14910000	-2.08104100	0.88064000
H	1.12183300	-2.31698700	1.11741600
C	-0.64987000	-1.13094100	-0.35545100
C	-0.01298200	-1.48828100	-1.53629100
H	1.00465600	-1.17126100	-1.71891900
C	-0.66406800	-2.27076200	-2.51492700
H	-0.11743800	-2.52648300	-3.41814400
C	-1.95873400	-2.70384700	-2.34797800
H	-2.45609000	-3.30495900	-3.10358800
C	-2.65544600	-2.34910200	-1.16707500
C	-2.00672000	-1.55922600	-0.16661300
C	-3.88355300	-1.55366000	1.17443900
H	-4.34321800	-1.22059700	2.10324800
C	-4.61274700	-2.34495900	0.25658500
H	-5.63699600	-2.62828900	0.47724800
C	-3.99567300	-2.73379500	-0.91009900
H	-4.52145600	-3.33482500	-1.64773600
Cl	4.42597500	1.13695300	-0.03698000

CN_193_CC_188

Charge = 0, Multiplicity = 1

O	0.97181300	3.28056800	-1.70163800
O	-0.78358800	0.48376700	2.71244300
N	0.01278900	-0.45141600	0.69996000
N	-2.63517700	-1.15781200	1.03073000
C	-3.50516300	2.13120300	1.59497600
H	-4.17162600	1.38196900	1.15034800
H	-4.09783500	3.02802400	1.80117200
H	-3.14193800	1.72284900	2.54152700
C	-0.20280200	3.10058000	-1.03827500
C	-1.34003600	3.90299700	-1.06026700
H	-1.40236300	4.78247800	-1.69161200
C	-2.39400200	3.54503500	-0.20524200
H	-3.28558400	4.16697300	-0.20308000
C	-2.35323500	2.44399700	0.67486100
C	-1.21148100	1.63504000	0.63614300
C	-0.16940100	1.97382800	-0.22907500
C	1.13630900	1.34802600	-0.30497400
C	1.93476400	2.31436500	-1.17039300
H	2.67659500	2.88953900	-0.61461200
H	2.42453300	1.83143400	-2.01856100
C	1.29942500	0.12479200	0.28730900

C	-0.78103600	0.50279800	1.51059500
C	2.44564000	-0.78680600	0.44206100
C	3.81489000	-0.48006700	0.28317900
C	4.81049000	-1.45587900	0.33147500
H	5.84397900	-1.15356100	0.20438900
C	4.48145200	-2.78494000	0.57574500
H	5.26247100	-3.53795700	0.61528800
C	3.14699900	-3.11923600	0.80523600
H	2.86689300	-4.14282900	1.03424100
C	2.16404000	-2.14235000	0.74312000
H	1.13527200	-2.41060200	0.93522500
C	-0.67574400	-1.12801600	-0.33702000
C	-0.07036900	-1.48320100	-1.53469400
H	0.94807700	-1.18008200	-1.73581200
C	-0.75418200	-2.24575000	-2.50682500
H	-0.23108000	-2.50092900	-3.42400800
C	-2.05176200	-2.65964700	-2.31618200
H	-2.57484400	-3.24500300	-3.06679300
C	-2.71740700	-2.30584000	-1.11714000
C	-2.03487100	-1.53685900	-0.12291000
C	-3.88293400	-1.51433000	1.25708700
H	-4.31779700	-1.18309100	2.19843600
C	-4.64427400	-2.28419800	0.34703300
H	-5.66829500	-2.55282400	0.58635400
C	-4.05813400	-2.67138300	-0.83599000
H	-4.60895700	-3.25623800	-1.56833800
Cl	4.40413900	1.17440100	0.16444500

CN_193_CC_193

Charge = 0, Multiplicity = 1

O	0.99399600	3.21632700	-1.77201700
O	-0.73767700	0.50911300	2.70860900
N	0.01697400	-0.46750600	0.69766300
N	-2.63407100	-1.13743100	1.07782200
C	-3.45438800	2.17822800	1.60234400
H	-4.13400700	1.42836300	1.17922200
H	-4.03502400	3.08482200	1.79980500
H	-3.08406900	1.78260600	2.55158700
C	-0.17439500	3.06531500	-1.08911600
C	-1.30167200	3.88188000	-1.10842200
H	-1.36265800	4.75185600	-1.75292800
C	-2.34814500	3.55035100	-0.23338700
H	-3.23183500	4.18344400	-0.22941900

C	-2.31032900	2.46227500	0.66325400
C	-1.17954100	1.63823100	0.62263100
C	-0.14573800	1.95263900	-0.26098400
C	1.14902200	1.30854000	-0.34426300
C	1.94961300	2.24356400	-1.23867400
H	2.71230300	2.81477800	-0.70762600
H	2.41757700	1.73404300	-2.08459500
C	1.30329800	0.09168500	0.26079700
C	-0.75126500	0.51112400	1.50705300
C	2.44956600	-0.81818800	0.40282200
C	3.81705000	-0.47999200	0.31012700
C	4.82744900	-1.44152400	0.34041900
H	5.85967100	-1.11768000	0.26753200
C	4.51144000	-2.78624500	0.50186000
H	5.30294700	-3.52883000	0.52843500
C	3.17572000	-3.15350500	0.66851200
H	2.90703200	-4.19231100	0.83389200
C	2.17842900	-2.19024600	0.62537900
H	1.14856500	-2.48468700	0.76766300
C	-0.70210300	-1.12992800	-0.32917200
C	-0.12712700	-1.48702400	-1.54108900
H	0.89123400	-1.19690500	-1.76140000
C	-0.84123800	-2.23502800	-2.50272400
H	-0.34079100	-2.49280600	-3.43174300
C	-2.14044900	-2.63111700	-2.28731900
H	-2.68727500	-3.20502200	-3.02981500
C	-2.77630800	-2.27371900	-1.07321400
C	-2.06256100	-1.51992600	-0.08929700
C	-3.88246400	-1.47601600	1.32695400
H	-4.29379800	-1.14239900	2.27801000
C	-4.67322700	-2.23024400	0.42891600
H	-5.69625600	-2.48458100	0.68734100
C	-4.11649900	-2.62071600	-0.76712900
H	-4.69043100	-3.19377200	-1.49101100
Cl	4.37300700	1.18986000	0.31154300

CN_193_CC_198

Charge = 0, Multiplicity = 1

O	1.01882900	3.16852000	-1.82949000
O	-0.69325800	0.52803300	2.69693100
N	0.01934400	-0.48322700	0.68657200
N	-2.63323900	-1.11760600	1.11637000
C	-3.39916800	2.22663700	1.61415600

H	-4.09002600	1.47567700	1.21166200
H	-3.96965400	3.14118200	1.80410800
H	-3.02044800	1.84275700	2.56498600
C	-0.14369800	3.04181700	-1.13063100
C	-1.25744400	3.87704100	-1.13906400
H	-1.31364000	4.74419400	-1.78779600
C	-2.29659900	3.56799700	-0.24693200
H	-3.16965000	4.21556700	-0.23478500
C	-2.26426600	2.48541300	0.65683500
C	-1.14788900	1.64242200	0.60618700
C	-0.12338000	1.93452400	-0.29541600
C	1.15886200	1.27003500	-0.39032900
C	1.96204200	2.17658600	-1.30921900
H	2.75396400	2.73054800	-0.80319500
H	2.39575400	1.64504900	-2.16065000
C	1.30455100	0.05858400	0.22469000
C	-0.72264900	0.51701000	1.49587700
C	2.45165600	-0.84852900	0.36124700
C	3.81487300	-0.48389100	0.33770000
C	4.83970100	-1.43034800	0.36835500
H	5.86867300	-1.08893700	0.35011600
C	4.53884300	-2.78488700	0.46229100
H	5.34070100	-3.51627400	0.48976800
C	3.20384100	-3.17979700	0.56142800
H	2.94754200	-4.22877600	0.67383400
C	2.19260500	-2.23108300	0.51939800
H	1.16298800	-2.54723000	0.60896900
C	-0.72858300	-1.13491400	-0.32764300
C	-0.18325700	-1.49592100	-1.55201000
H	0.83400800	-1.21747500	-1.79217100
C	-0.92578200	-2.23274800	-2.50072500
H	-0.44747300	-2.49470500	-3.44017600
C	-2.22544800	-2.61228900	-2.25998300
H	-2.79447800	-3.17754900	-2.99236700
C	-2.83238000	-2.24876800	-1.03291100
C	-2.08942700	-1.50660100	-0.06182300
C	-3.88141500	-1.43877400	1.38847800
H	-4.27015800	-1.10023100	2.34728700
C	-4.69953700	-2.18103600	0.50503700
H	-5.72090200	-2.42144100	0.78267600
C	-4.17113400	-2.57780500	-0.70171000
H	-4.76660800	-3.14189700	-1.41515800
Cl	4.33544600	1.19464100	0.43018100

CN_193_CC_203

Charge = 0, Multiplicity = 1

O	1.04653600	3.13115000	-1.87936300
O	-0.65172800	0.54511700	2.68039200
N	0.02031800	-0.49660400	0.67066200
N	-2.63276000	-1.09619000	1.14864900
C	-3.34353500	2.27623100	1.62347000
H	-4.04552000	1.52596900	1.23931700
H	-3.90360600	3.19825900	1.80798300
H	-2.95694700	1.90140200	2.57482200
C	-0.11093600	3.02612700	-1.16762100
C	-1.20935500	3.88150400	-1.16302700
H	-1.25852800	4.74895100	-1.81193800
C	-2.24231100	3.59238700	-0.25680800
H	-3.10343700	4.25547200	-0.23497600
C	-2.21760500	2.51177600	0.64969600
C	-1.11727700	1.64860100	0.58689700
C	-0.10167400	1.91998700	-0.33089200
C	1.16696200	1.23401900	-0.43868800
C	1.97372300	2.11443200	-1.37788800
H	2.79613100	2.64459000	-0.89500600
H	2.36857100	1.56534200	-2.23761800
C	1.30357800	0.02709400	0.18408800
C	-0.69628300	0.52326100	1.48014600
C	2.45209400	-0.87707400	0.31900200
C	3.80809400	-0.49018100	0.36667200
C	4.84597600	-1.42222100	0.40794400
H	5.86952400	-1.06634800	0.44507400
C	4.56174600	-2.78315900	0.44217800
H	5.37299600	-3.50375900	0.47836300
C	3.23013100	-3.20144100	0.47016700
H	2.98711300	-4.25761100	0.53458300
C	2.20624900	-2.26671200	0.41902400
H	1.17868800	-2.60105600	0.45241700
C	-0.75381000	-1.14181300	-0.32829700
C	-0.23596700	-1.51066200	-1.56232700
H	0.77963500	-1.24335400	-1.82201600
C	-1.00413000	-2.24071600	-2.49577900
H	-0.54634200	-2.50975900	-3.44342300
C	-2.30344100	-2.60455400	-2.23031300
H	-2.89243200	-3.16453600	-2.95087400
C	-2.88363100	-2.23090600	-0.99333600
C	-2.11444600	-1.49569800	-0.03748800

S257

C	-3.88008700	-1.40042100	1.44316500
H	-4.24799300	-1.05364900	2.40725300
C	-4.72265200	-2.13525200	0.57662700
H	-5.74196500	-2.36194500	0.87274300
C	-4.22035400	-2.54235300	-0.63778500
H	-4.83518800	-3.10101200	-1.33898000
Cl	4.29185700	1.19346600	0.53446500

CN_193_CC_208

Charge = 0, Multiplicity = 1

O	1.07701000	3.10225000	-1.92126100
O	-0.61103700	0.55824000	2.66044000
N	0.02049900	-0.50951700	0.65064900
N	-2.63202600	-1.07467000	1.17589500
C	-3.28617200	2.32499100	1.63359700
H	-3.99872100	1.57615100	1.26649500
H	-3.83613500	3.25381600	1.81412100
H	-2.89154300	1.95745500	2.58458400
C	-0.07623200	3.01624100	-1.19921900
C	-1.15764400	3.89280700	-1.17919000
H	-1.19773600	4.76336500	-1.82455200
C	-2.18505100	3.62115500	-0.26101100
H	-3.03292800	4.30061000	-0.22749900
C	-2.16961300	2.53934700	0.64428100
C	-1.08695000	1.65502800	0.56667900
C	-0.08027500	1.90752200	-0.36600800
C	1.17415700	1.19982500	-0.48756200
C	1.98628700	2.05965500	-1.43988600
H	2.83455400	2.56385900	-0.97349200
H	2.34581800	1.49994800	-2.30852800
C	1.30107700	-0.00418300	0.13948600
C	-0.67070200	0.52809200	1.46116600
C	2.45150500	-0.90548000	0.27569600
C	3.79722300	-0.50017500	0.39586300
C	4.84622900	-1.41883300	0.45634100
H	5.86203600	-1.05107400	0.54887600
C	4.57990700	-2.78373200	0.43812100
H	5.39914700	-3.49432400	0.48958400
C	3.25480500	-3.22140400	0.39282500
H	3.02575600	-4.28243700	0.41447100
C	2.22009800	-2.29954700	0.32404500
H	1.19688400	-2.64893100	0.30106800
C	-0.77869200	-1.14933600	-0.33212000

C	-0.28811000	-1.52576000	-1.57508000
H	0.72488900	-1.26808200	-1.85452600
C	-1.08044800	-2.25058800	-2.49232200
H	-0.64286000	-2.52676600	-3.44743100
C	-2.37838400	-2.60002100	-2.20210300
H	-2.98623800	-3.15596600	-2.91001200
C	-2.93236400	-2.21563100	-0.95637200
C	-2.13838300	-1.48592100	-0.01671300
C	-3.87786100	-1.36242700	1.49245700
H	-4.22563100	-1.00634300	2.46062900
C	-4.74336200	-2.09148600	0.64382800
H	-5.76015000	-2.30477200	0.95804600
C	-4.26637400	-2.51000500	-0.57688000
H	-4.89945300	-3.06440400	-1.26510100
Cl	4.24395200	1.18661600	0.62320700

CN_193_CC_213

Charge = 0, Multiplicity = 1

O	1.10954200	3.07807400	-1.95860200
O	-0.57196500	0.56928600	2.63809500
N	0.02023000	-0.52158000	0.62822000
N	-2.63067700	-1.05276000	1.19978200
C	-3.22825900	2.37280600	1.64236100
H	-3.94885200	1.62311000	1.29321400
H	-3.77068600	3.30714900	1.81680800
H	-2.82521600	2.01508400	2.59368000
C	-0.04027800	3.00956300	-1.22830300
C	-1.10371100	3.90727100	-1.19238500
H	-1.13338000	4.78219300	-1.83239600
C	-2.12628400	3.65154100	-0.26389700
H	-2.96013700	4.34743100	-0.21828500
C	-2.12129400	2.56717200	0.63830200
C	-1.05715400	1.66167800	0.54519300
C	-0.05921100	1.89659900	-0.40104000
C	1.18086700	1.16755300	-0.53590600
C	2.00062700	2.01170900	-1.49464600
H	2.86828000	2.49144400	-1.03715600
H	2.33262100	1.44713400	-2.37115800
C	1.29751700	-0.03470000	0.09290700
C	-0.64615700	0.53248300	1.43996400
C	2.45038900	-0.93311000	0.23231300
C	3.78248700	-0.51271100	0.42584400
C	4.84067200	-1.41901800	0.51005400

H	5.84626200	-1.04152400	0.65819400
C	4.59372700	-2.78608100	0.44279700
H	5.41945900	-3.48752700	0.51304700
C	3.27866800	-3.23989000	0.32248700
H	3.06466500	-4.30412300	0.30367300
C	2.23502100	-2.32976700	0.23141500
H	1.21865100	-2.69156500	0.15112200
C	-0.80272600	-1.15737900	-0.33733700
C	-0.33906300	-1.54184200	-1.58832200
H	0.67060100	-1.29286600	-1.88754700
C	-1.15450700	-2.26220100	-2.48869300
H	-0.73687700	-2.54561000	-3.45060600
C	-2.45032900	-2.59792500	-2.17399600
H	-3.07611800	-3.15049600	-2.86879100
C	-2.97853400	-2.20223600	-0.92060500
C	-2.16092100	-1.47693600	0.00208400
C	-3.87448200	-1.32418800	1.53798800
H	-4.20263900	-0.95796700	2.50923100
C	-4.76160800	-2.04888800	0.70816100
H	-5.77544400	-2.24900200	1.04009800
C	-4.30926000	-2.47977200	-0.51759000
H	-4.95963800	-3.03085000	-1.19221500
Cl	4.19198800	1.17583000	0.70424900

CN_193_CC_223

Charge = 0, Multiplicity = 1

O	1.18245300	3.03945600	-2.02312900
O	-0.50011300	0.59330000	2.58806400
N	0.01811400	-0.54012800	0.58098500
N	-2.62745300	-1.00457500	1.23871500
C	-3.11774500	2.46609500	1.64564600
H	-3.85258300	1.71618200	1.32827300
H	-3.64602400	3.41049400	1.80840900
H	-2.70068200	2.12550800	2.59747100
C	0.03599500	3.00306300	-1.28329900
C	-0.99064200	3.94087800	-1.21977700
H	-0.99567400	4.82533100	-1.84724600
C	-2.00751000	3.71390600	-0.27681700
H	-2.81270500	4.44110300	-0.21000300
C	-2.02736400	2.62343100	0.61733300
C	-1.00089100	1.67767300	0.49699000
C	-0.01716600	1.88041200	-0.47072300
C	1.19374800	1.11002200	-0.62804800

S260

C	2.03607700	1.93137800	-1.58533400
H	2.92886500	2.36642000	-1.12923200
H	2.33186300	1.36635300	-2.47434100
C	1.28764200	-0.09085800	-0.00018000
C	-0.60161100	0.54398400	1.39260600
C	2.44599300	-0.98429400	0.14871400
C	3.74044500	-0.54348800	0.49078100
C	4.81122200	-1.42855100	0.62664900
H	5.78867000	-1.03811200	0.88701300
C	4.60802200	-2.79485600	0.46272600
H	5.44238500	-3.48072800	0.57370700
C	3.32445000	-3.27136300	0.18880500
H	3.14444300	-4.33744200	0.08951500
C	2.26840300	-2.38104200	0.04845100
H	1.27388100	-2.76069100	-0.14816600
C	-0.84740400	-1.17278500	-0.34841900
C	-0.43434900	-1.57492500	-1.61174800
H	0.56576400	-1.33767100	-1.95063800
C	-1.28994900	-2.29376300	-2.47551600
H	-0.90974300	-2.59323100	-3.44804800
C	-2.57874400	-2.60698900	-2.11284500
H	-3.23565800	-3.15880200	-2.77891000
C	-3.05949200	-2.18463900	-0.84898600
C	-2.20083000	-1.46059200	0.03668700
C	-3.86574600	-1.24538600	1.61790900
H	-4.15876600	-0.85353500	2.59039900
C	-4.78985200	-1.96936200	0.82885400
H	-5.79684100	-2.14439200	1.19415200
C	-4.38215100	-2.43073600	-0.40143800
H	-5.06244600	-2.98106300	-1.04652300
Cl	4.07403600	1.14364000	0.86309800

CN_193_CC_233

Charge = 0, Multiplicity = 1

O	1.25640100	3.00701900	-2.08211500
O	-0.43582000	0.61877200	2.53393100
N	0.01562500	-0.55263500	0.53279900
N	-2.62159000	-0.95503500	1.26807900
C	-3.01576200	2.55208000	1.63488600
H	-3.76348700	1.80391300	1.34485300
H	-3.53052500	3.50550800	1.78756200
H	-2.58691700	2.22515300	2.58650500
C	0.11073300	2.99969300	-1.33820900

S261

C	-0.88046500	3.97283400	-1.25249900
H	-0.85975700	4.86554600	-1.86785000
C	-1.89435400	3.77158600	-0.29966100
H	-2.67185000	4.52659800	-0.21563800
C	-1.94006200	2.67615600	0.58685500
C	-0.94957800	1.69484100	0.44426700
C	0.02224200	1.86882300	-0.54019500
C	1.20549900	1.06103000	-0.71455400
C	2.07599900	1.86776600	-1.65746900
H	2.97831500	2.26816800	-1.18626800
H	2.35945200	1.30892600	-2.55402300
C	1.27618800	-0.13956400	-0.09028100
C	-0.56194100	0.55800700	1.34146500
C	2.44203700	-1.02660100	0.07267200
C	3.68336800	-0.57592500	0.56426100
C	4.76199000	-1.44154700	0.75180700
H	5.69937000	-1.04525900	1.12582100
C	4.61463500	-2.79955300	0.48727600
H	5.45409500	-3.47144400	0.63852800
C	3.38033000	-3.28814000	0.05538900
H	3.24430800	-4.34952700	-0.12839500
C	2.31602400	-2.41552900	-0.13400400
H	1.35632800	-2.80569600	-0.44953700
C	-0.88570100	-1.18758200	-0.35948300
C	-0.51888300	-1.60897400	-1.63093200
H	0.46884800	-1.37770300	-2.00832100
C	-1.40743900	-2.33331900	-2.45607600
H	-1.06138700	-2.64993500	-3.43593300
C	-2.68661100	-2.62925800	-2.04785300
H	-3.36894100	-3.18595100	-2.68359900
C	-3.12497400	-2.17730500	-0.77876900
C	-2.23247100	-1.44722700	0.06769100
C	-3.85277800	-1.16840600	1.68495100
H	-4.11528400	-0.74720800	2.65389700
C	-4.80661100	-1.89940600	0.93895300
H	-5.80572700	-2.05181400	1.33475300
C	-4.43802300	-2.39532200	-0.29023000
H	-5.14274900	-2.95056600	-0.90412200
Cl	3.93309700	1.10257100	1.02938500

CN_198_CC_163

Charge = 0, Multiplicity = 1

O	2.63935500	3.18218300	-1.01995700
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S262

O	-1.46950400	0.67574400	1.89998400
N	-0.31681900	-0.16648600	0.05247900
N	-3.09505200	0.05164000	-0.15657700
C	-2.51878700	3.50253300	1.29023100
H	-3.27734800	2.94137400	0.73325600
H	-2.86418000	4.53440000	1.40479800
H	-2.45166500	3.03477800	2.27700200
C	1.35283600	3.42289200	-0.64267800
C	0.73911100	4.64731600	-0.42058600
H	1.24014300	5.58328200	-0.64182900
C	-0.54304400	4.62649500	0.16054800
H	-1.03776000	5.57689800	0.34267100
C	-1.19074700	3.45360700	0.58094800
C	-0.55242700	2.22748400	0.30911200
C	0.66630600	2.24098800	-0.37017400
C	1.55317700	1.12367700	-0.53091200
C	2.88528000	1.74761400	-0.89762600
H	3.67102600	1.60043300	-0.14683600
H	3.26099400	1.40117800	-1.86125800
C	1.10029400	-0.12147100	-0.19441200
C	-0.90060700	0.90229400	0.85368800
C	1.93046000	-1.19404900	0.39734100
C	3.24176400	-1.52826200	0.01724100
C	4.06215000	-2.33976300	0.80242700
H	5.05669300	-2.58441300	0.44630600
C	3.58890000	-2.84238300	2.00974500
H	4.22861200	-3.47182200	2.62053200
C	2.28424000	-2.54464800	2.41195100
H	1.89753600	-2.93144400	3.34978400
C	1.48053800	-1.73033500	1.62719200
H	0.48784400	-1.45957200	1.96926600
C	-1.09354200	-1.29595200	-0.28435000
C	-0.53938200	-2.50685100	-0.67949700
H	0.53129900	-2.62502900	-0.74237500
C	-1.34237200	-3.62264900	-0.99780900
H	-0.84833400	-4.54726000	-1.28166900
C	-2.71294800	-3.56020500	-0.93314700
H	-3.33122000	-4.42666500	-1.14954200
C	-3.32872600	-2.32640600	-0.61232000
C	-2.53134500	-1.17074500	-0.33257900
C	-4.40583800	0.16553700	-0.17211600
H	-4.80570200	1.16973200	-0.03877000
C	-5.28452800	-0.92654200	-0.36064100
H	-6.35875200	-0.77231200	-0.34356100

C	-4.73757400	-2.16480100	-0.59516700
H	-5.36697800	-3.03116400	-0.78239500
Cl	3.83958500	-1.12730300	-1.59325800

CN_198_CC_168

Charge = 0, Multiplicity = 1

O	2.64046600	3.15110200	-1.07336900
O	-1.43204400	0.66414500	1.92018400
N	-0.31762800	-0.17408100	0.04815800
N	-3.09983100	0.07886200	-0.11993100
C	-2.46668100	3.50360500	1.34010300
H	-3.23994000	2.94863200	0.79738300
H	-2.80234900	4.53771400	1.46298000
H	-2.38343400	3.03380900	2.32465900
C	1.36376600	3.39810500	-0.67016400
C	0.76193000	4.62682600	-0.43787200
H	1.26435200	5.55900100	-0.67159400
C	-0.50754300	4.61516900	0.16955600
H	-0.99262700	5.56878000	0.36058500
C	-1.15347600	3.44635400	0.60437800
C	-0.52848400	2.21658200	0.32060100
C	0.67696100	2.21999700	-0.38282000
C	1.55476000	1.09624500	-0.56056500
C	2.88361600	1.71664400	-0.94780200
H	3.67808900	1.57234600	-0.20607700
H	3.24662800	1.36582300	-1.91445500
C	1.09768800	-0.14773700	-0.21979300
C	-0.87855100	0.89261800	0.86625100
C	1.91629600	-1.22869400	0.37694300
C	3.25287800	-1.52995700	0.05820300
C	4.05663200	-2.32815700	0.87298900
H	5.07074600	-2.54712000	0.55775300
C	3.54417100	-2.85159300	2.05504700
H	4.17146800	-3.46986200	2.68961800
C	2.21613500	-2.58832100	2.39851700
H	1.79627500	-2.98985000	3.31567800
C	1.42957100	-1.78584700	1.58463200
H	0.42119700	-1.53563100	1.89290500
C	-1.11313200	-1.28242700	-0.31171000
C	-0.57513900	-2.48708800	-0.74727400
H	0.49395900	-2.61197500	-0.82675200
C	-1.39221000	-3.58642000	-1.08549400
H	-0.91056600	-4.50727400	-1.40110900

C	-2.76137400	-3.51343300	-1.00145600
H	-3.39042000	-4.36794400	-1.23367300
C	-3.36141600	-2.28356500	-0.63875700
C	-2.54989600	-1.14309000	-0.33729200
C	-4.40961400	0.20490000	-0.11511800
H	-4.79844100	1.20841100	0.05171900
C	-5.30068100	-0.87358700	-0.32283000
H	-6.37312200	-0.71027600	-0.28756400
C	-4.76836200	-2.10967100	-0.59888100
H	-5.40823700	-2.96468400	-0.80211400
Cl	3.91083400	-1.12529900	-1.52931800

CN_198_CC_173

Charge = 0, Multiplicity = 1

O	2.61399300	3.13848500	-1.13171000
O	-1.39120100	0.64126400	1.94929600
N	-0.31450700	-0.18528700	0.05045800
N	-3.10143300	0.08634800	-0.07280900
C	-2.43968700	3.48545200	1.39082600
H	-3.22611600	2.94064200	0.85667500
H	-2.76752500	4.51985800	1.53101700
H	-2.34015300	3.00446500	2.36833500
C	1.34671900	3.38185900	-0.69975300
C	0.74635600	4.61022300	-0.46032500
H	1.24088300	5.54229900	-0.71066000
C	-0.50855200	4.59832700	0.17553100
H	-0.99204100	5.55138800	0.37321400
C	-1.14140600	3.42922400	0.62906300
C	-0.51939300	2.20050600	0.33656400
C	0.67149100	2.20246700	-0.39185800
C	1.54927300	1.07925600	-0.58545200
C	2.86880400	1.70721700	-0.99584700
H	3.67227600	1.57813000	-0.26158900
H	3.22357000	1.35069000	-1.96320500
C	1.09815700	-0.16698900	-0.23979300
C	-0.85913500	0.87550900	0.88604600
C	1.91380900	-1.25339300	0.35608300
C	3.27358600	-1.51297900	0.09906300
C	4.06352800	-2.29815100	0.93877100
H	5.09603600	-2.48376000	0.66460400
C	3.51658400	-2.85247500	2.09086000
H	4.13363000	-3.45978200	2.74570700
C	2.16747900	-2.63321300	2.37505900

H	1.71776700	-3.05758600	3.26744800
C	1.39531400	-1.84169300	1.53671400
H	0.37156900	-1.61994400	1.81188500
C	-1.12278500	-1.27322300	-0.33849400
C	-0.59460200	-2.46470400	-0.82107600
H	0.47340600	-2.58913300	-0.91777400
C	-1.41963900	-3.54937700	-1.18521500
H	-0.94547400	-4.46072100	-1.53765500
C	-2.78757300	-3.47479900	-1.08162400
H	-3.42260600	-4.31886400	-1.33472200
C	-3.37834100	-2.25607000	-0.66976800
C	-2.55895700	-1.12895800	-0.33978100
C	-4.41059800	0.21647000	-0.04621900
H	-4.79352700	1.21460900	0.16134900
C	-5.30809700	-0.85124600	-0.28011100
H	-6.37940000	-0.68582000	-0.22538000
C	-4.78398100	-2.07876200	-0.60578300
H	-5.42970200	-2.92400000	-0.83031200
Cl	3.98979500	-1.09122000	-1.46023900

CN_198_CC_178

Charge = 0, Multiplicity = 1

O	2.53828300	3.15924400	-1.19575100
O	-1.34244800	0.59966800	1.99530700
N	-0.30357400	-0.20255200	0.06525900
N	-3.09727200	0.05728300	-0.00580900
C	-2.46204200	3.43340400	1.43992700
H	-3.26224600	2.91947200	0.89504900
H	-2.77768800	4.46438600	1.62575900
H	-2.35261200	2.91209000	2.39506200
C	1.27932900	3.38103400	-0.73108300
C	0.66093400	4.60039800	-0.48997900
H	1.13090300	5.53869100	-0.76330900
C	-0.57691500	4.57156200	0.17679900
H	-1.07380400	5.51717000	0.37705900
C	-1.17660000	3.39482300	0.65566400
C	-0.53787100	2.17577900	0.36078800
C	0.63705500	2.19173800	-0.39350900
C	1.53185700	1.08200500	-0.60104500
C	2.83009800	1.73711000	-1.04054300
H	3.64445500	1.64325300	-0.31378200
H	3.18240900	1.37426300	-2.00616400
C	1.10537200	-0.17243300	-0.24937000

C	-0.84420100	0.84591300	0.91910300
C	1.93171600	-1.25978000	0.33593600
C	3.31260200	-1.46372700	0.14140400
C	4.09284200	-2.24040600	0.99711800
H	5.14275400	-2.37997600	0.76510200
C	3.51754200	-2.84578100	2.10895300
H	4.12756800	-3.44577700	2.77695200
C	2.14973400	-2.68537100	2.33248200
H	1.67444600	-3.14863000	3.19164900
C	1.38793700	-1.89964500	1.47899200
H	0.34857400	-1.71953300	1.72068000
C	-1.11386800	-1.27106700	-0.36618900
C	-0.58360700	-2.43543600	-0.91035900
H	0.48433800	-2.54578300	-1.02608900
C	-1.40568300	-3.50824600	-1.31311400
H	-0.93001400	-4.39866500	-1.71377800
C	-2.77290200	-3.44912200	-1.18862100
H	-3.40527100	-4.28524500	-1.47273200
C	-3.36642400	-2.25580300	-0.71187500
C	-2.55050400	-1.13913600	-0.33965700
C	-4.40677900	0.17615800	0.04675500
H	-4.79334600	1.15955100	0.31013700
C	-5.29989400	-0.88571000	-0.22696500
H	-6.37142800	-0.73143700	-0.14900000
C	-4.77215600	-2.09194800	-0.61969900
H	-5.41545200	-2.92996600	-0.87601000
Cl	4.08707100	-0.99506800	-1.37768500

CN_198_CC_183

Charge = 0, Multiplicity = 1

O	0.85052800	3.33319100	-1.68131100
O	-0.81980400	0.41329500	2.71013600
N	0.02625200	-0.45936400	0.69386200
N	-2.65509100	-1.10859600	0.91574300
C	-3.54251500	2.05508400	1.67164400
H	-4.26586900	1.38260400	1.19444900
H	-4.07911500	2.95986500	1.97519500
H	-3.16459900	1.55375600	2.56555700
C	-0.31104700	3.10972200	-1.01049700
C	-1.46235100	3.89173600	-1.00036400
H	-1.54923900	4.78139200	-1.61429900
C	-2.49240000	3.50247700	-0.13155000
H	-3.39375000	4.10949500	-0.10009400

S267

C	-2.41390700	2.38946500	0.73060400
C	-1.26120600	1.59812000	0.65515300
C	-0.24190400	1.96754600	-0.22466100
C	1.08165700	1.38086700	-0.31790600
C	1.84379700	2.38482500	-1.17691800
H	2.57522700	2.97108700	-0.61915600
H	2.33338200	1.93013000	-2.03941900
C	1.29065400	0.16639500	0.27748200
C	-0.80767400	0.45979100	1.50819400
C	2.46720700	-0.70315200	0.47997200
C	3.82782000	-0.40291200	0.24661700
C	4.83964200	-1.35349200	0.38218100
H	5.86355300	-1.05455700	0.18766500
C	4.54144400	-2.64962100	0.78847000
H	5.33628200	-3.38146600	0.89424100
C	3.21841700	-2.97327700	1.08488300
H	2.95844700	-3.96758500	1.43476200
C	2.21923700	-2.02270200	0.93565600
H	1.19966600	-2.28064200	1.18254300
C	-0.61941000	-1.18816400	-0.33231100
C	0.04345500	-1.61540700	-1.47588700
H	1.07271000	-1.32938200	-1.64315800
C	-0.59472900	-2.43198200	-2.43438200
H	-0.02662500	-2.74309800	-3.30644100
C	-1.90222900	-2.83249700	-2.28578100
H	-2.38879800	-3.46252900	-3.02461400
C	-2.62678000	-2.40202900	-1.14806700
C	-1.99271600	-1.57190700	-0.17079600
C	-3.91406500	-1.44849000	1.10118500
H	-4.39649900	-1.05313600	1.99295400
C	-4.62868600	-2.27897200	0.20696000
H	-5.66495300	-2.53020500	0.40950000
C	-3.98282700	-2.74457000	-0.91498700
H	-4.49738100	-3.37544000	-1.63539700
Cl	4.39825600	1.22190800	-0.11891100

CN_198_CC_188

Charge = 0, Multiplicity = 1

O	0.86899500	3.23581400	-1.77808900
O	-0.76822200	0.45726300	2.71905400
N	0.03397800	-0.47772200	0.70948800
N	-2.65105700	-1.08556400	0.98258600
C	-3.49560800	2.10434400	1.66821000

H	-4.23469600	1.43179700	1.21579700
H	-4.01533500	3.02358400	1.95744600
H	-3.11365100	1.61830500	2.56880600
C	-0.28591900	3.05015300	-1.08261500
C	-1.43097200	3.84168800	-1.08304400
H	-1.52044600	4.71131000	-1.72468600
C	-2.45259700	3.48810500	-0.18899300
H	-3.34873400	4.10318500	-0.16594700
C	-2.37411000	2.40070900	0.70608000
C	-1.22901200	1.59781300	0.64215600
C	-0.21742900	1.93608400	-0.25820300
C	1.09756500	1.33436300	-0.34927500
C	1.85988700	2.29705300	-1.25035200
H	2.60361800	2.89584000	-0.72328600
H	2.33939100	1.80453300	-2.09902300
C	1.29953800	0.13198000	0.27035200
C	-0.77491700	0.47338500	1.51676700
C	2.47531100	-0.73757800	0.44855400
C	3.83443100	-0.39532600	0.27437200
C	4.85956200	-1.33828000	0.35226100
H	5.88283700	-1.00892700	0.21057400
C	4.57264400	-2.66749000	0.64365900
H	5.37665000	-3.39428000	0.70636100
C	3.24962700	-3.03427000	0.88912700
H	3.00140000	-4.05742700	1.15406200
C	2.23721600	-2.09059300	0.79657900
H	1.21735200	-2.38332200	1.00020900
C	-0.64589700	-1.18450300	-0.31253100
C	-0.01672300	-1.60881900	-1.47571200
H	1.01294600	-1.33691900	-1.66326000
C	-0.68959700	-2.40429300	-2.42842000
H	-0.14674900	-2.71453500	-3.31671600
C	-1.99981400	-2.78483000	-2.25422900
H	-2.51351700	-3.39814600	-2.98876500
C	-2.69126200	-2.35558400	-1.09553000
C	-2.02127900	-1.54769300	-0.12372400
C	-3.91148200	-1.40539300	1.19196400
H	-4.36733200	-1.01114400	2.09813600
C	-4.66020000	-2.21338100	0.30496600
H	-5.69601600	-2.44884000	0.52774900
C	-4.04751100	-2.67762600	-0.83599000
H	-4.58883300	-3.29138100	-1.55155200
Cl	4.37504500	1.27027300	0.09548700

CN_198_CC_193

Charge = 0, Multiplicity = 1

O	0.89100100	3.16703900	-1.85172000
O	-0.71951600	0.48705400	2.71468800
N	0.03839900	-0.49437500	0.70793600
N	-2.64935300	-1.06221200	1.03230700
C	-3.44237000	2.15500800	1.67311300
H	-4.19442600	1.48215600	1.24308700
H	-3.94819400	3.08537500	1.95117000
H	-3.05446300	1.68183600	2.57804700
C	-0.25730600	3.01187200	-1.13669900
C	-1.39173400	3.81878700	-1.13487300
H	-1.47966200	4.67833600	-1.79015600
C	-2.40521000	3.49372900	-0.22064100
H	-3.29284500	4.12095900	-0.19618800
C	-2.32970000	2.42021500	0.69180100
C	-1.19640800	1.60099500	0.62659100
C	-0.19370100	1.91264200	-0.29275900
C	1.11035900	1.29184200	-0.39050300
C	1.87391000	2.21932600	-1.32406100
H	2.64247300	2.81233700	-0.82705900
H	2.32609600	1.69668800	-2.17077100
C	1.30404200	0.09739800	0.24467100
C	-0.74418400	0.48301100	1.51286400
C	2.47962600	-0.77038500	0.41105500
C	3.83611300	-0.39416100	0.30166100
C	4.87563700	-1.32296300	0.35969100
H	5.89710700	-0.97017800	0.27130300
C	4.60209100	-2.67044000	0.56816300
H	5.41625400	-3.38697700	0.61642600
C	3.27885100	-3.07246000	0.75322700
H	3.04265200	-4.11270800	0.95514400
C	2.25244700	-2.14219800	0.68133100
H	1.23232200	-2.46269500	0.83725500
C	-0.67274000	-1.18686200	-0.30390600
C	-0.07497600	-1.61400500	-1.48236900
H	0.95430200	-1.35523700	-1.69031100
C	-0.77901000	-2.39542200	-2.42422800
H	-0.25965100	-2.70917800	-3.32523700
C	-2.09069900	-2.75749000	-2.22394600
H	-2.62872800	-3.35983700	-2.95010300
C	-2.75146100	-2.32313800	-1.04926000
C	-2.04936400	-1.52993100	-0.08816600

S270

C	-3.91036600	-1.36257200	1.26545900
H	-4.34199300	-0.96387000	2.18153100
C	-4.68937700	-2.15552100	0.39099500
H	-5.72413800	-2.37541800	0.63369500
C	-4.10705900	-2.62516300	-0.76357200
H	-4.67223500	-3.22756700	-1.47028000
Cl	4.34267400	1.29039200	0.24665600

CN_198_CC_198

Charge = 0, Multiplicity = 1

O	0.91709500	3.11652200	-1.91060100
O	-0.67319200	0.50970800	2.70221600
N	0.04067800	-0.51054300	0.69729300
N	-2.64835000	-1.03928700	1.07249600
C	-3.38535700	2.20630200	1.68100200
H	-4.14709000	1.53098900	1.27238400
H	-3.88100200	3.14531900	1.94787300
H	-2.99022300	1.74648500	2.58978200
C	-0.22539400	2.98680400	-1.18029100
C	-1.34540800	3.81368300	-1.16843200
H	-1.42786300	4.67037000	-1.82815900
C	-2.35151000	3.51248100	-0.23775500
H	-3.22778600	4.15514900	-0.20595900
C	-2.28221400	2.44473300	0.68223200
C	-1.16428400	1.60539000	0.60810100
C	-0.17102200	1.89298700	-0.32901000
C	1.12026200	1.25054200	-0.43769000
C	1.88606700	2.14631200	-1.39776700
H	2.68738000	2.71935200	-0.92972600
H	2.29881400	1.59887000	-2.24976700
C	1.30554500	0.06243800	0.20915200
C	-0.71528100	0.49012700	1.50125100
C	2.48183200	-0.80232500	0.37069500
C	3.83337900	-0.39729700	0.32911400
C	4.88692200	-1.31051000	0.38713000
H	5.90477200	-0.93841200	0.35246200
C	4.62863400	-2.66956100	0.52924400
H	5.45283500	-3.37451200	0.57810700
C	3.30679300	-3.10150200	0.64883500
H	3.08328700	-4.15323600	0.79915600
C	2.26686300	-2.18623000	0.57839000
H	1.24750300	-2.52991500	0.68359300
C	-0.69972500	-1.19288000	-0.30128800

C	-0.13205700	-1.62634200	-1.49223800
H	0.89628100	-1.38060300	-1.72040500
C	-0.86522500	-2.39706600	-2.42064600
H	-0.36839800	-2.71683200	-3.33218600
C	-2.17760000	-2.74087500	-2.19447700
H	-2.73841600	-3.33483100	-2.91023600
C	-2.80889000	-2.29807700	-1.00674200
C	-2.07682600	-1.51594100	-0.05905100
C	-3.90927400	-1.32019400	1.32909400
H	-4.31772000	-0.91438100	2.25267800
C	-4.71646000	-2.10155200	0.46982200
H	-5.74966900	-2.30580500	0.73202800
C	-4.16315100	-2.58002000	-0.69533800
H	-4.75057300	-3.17378500	-1.39113200
Cl	4.30415400	1.29801100	0.36576600

CN_198_CC_203

Charge = 0, Multiplicity = 1

O	0.94766700	3.07822000	-1.96011100
O	-0.62950500	0.52911700	2.68432500
N	0.04097000	-0.52492000	0.68109200
N	-2.64839100	-1.01462800	1.10484600
C	-3.32643000	2.25921500	1.68790700
H	-4.09792100	1.58396900	1.29787100
H	-3.81135200	3.20599800	1.94668200
H	-2.92470600	1.80897200	2.59868300
C	-0.18997500	2.97098200	-1.21775500
C	-1.29276000	3.82050400	-1.19237200
H	-1.36642800	4.67855700	-1.85136400
C	-2.29273100	3.54027500	-0.24838700
H	-3.15562100	4.20022900	-0.20662600
C	-2.23260400	2.47349600	0.67354400
C	-1.13258500	1.61186300	0.58709100
C	-0.14851500	1.87698100	-0.36619000
C	1.12859600	1.21110900	-0.48751400
C	1.89793300	2.07858000	-1.46900900
H	2.73326200	2.62359000	-1.02714700
H	2.26580500	1.51191200	-2.32954700
C	1.30455500	0.02804500	0.16820900
C	-0.68832400	0.49695400	1.48447700
C	2.48182500	-0.83378400	0.32934500
C	3.82576000	-0.40420300	0.35769200
C	4.89187200	-1.30211600	0.42752100

H	5.90409800	-0.91391600	0.44706400
C	4.65003300	-2.66898100	0.51276000
H	5.48328400	-3.36250300	0.57120600
C	3.33202300	-3.12643300	0.56336600
H	3.12174200	-4.18635700	0.66851700
C	2.27986800	-2.22587600	0.48267300
H	1.26299200	-2.58949800	0.53481600
C	-0.72630200	-1.20056000	-0.30194600
C	-0.18701400	-1.64314100	-1.50274600
H	0.83945200	-1.40903400	-1.75142700
C	-0.94650700	-2.40788900	-2.41487200
H	-0.47083900	-2.73609200	-3.33466900
C	-2.25845500	-2.73501100	-2.16302500
H	-2.83974800	-3.32428000	-2.86620800
C	-2.86230100	-2.27999900	-0.96559900
C	-2.10318100	-1.50426900	-0.03412100
C	-3.90856800	-1.27651000	1.38416300
H	-4.29558700	-0.86029500	2.31236100
C	-4.74101100	-2.05097700	0.54289500
H	-5.77221700	-2.23982500	0.82387200
C	-4.21456200	-2.54235500	-0.62931100
H	-4.82202200	-3.13108600	-1.31205200
Cl	4.25933000	1.29778800	0.46646500

CN_198_CC_208

Charge = 0, Multiplicity = 1

O	0.97872200	3.04827500	-2.00186200
O	-0.58669300	0.54289600	2.66379800
N	0.04115900	-0.53888200	0.66091900
N	-2.64696900	-0.99105700	1.13250600
C	-3.26774000	2.30770000	1.69552200
H	-4.04697000	1.63124300	1.32338200
H	-3.74431900	3.26075300	1.94638400
H	-2.85876500	1.86725900	2.60798300
C	-0.15465200	2.96040100	-1.24961500
C	-1.23974800	3.83181500	-1.20934000
H	-1.30389700	4.69332800	-1.86481000
C	-2.23402700	3.56924900	-0.25400300
H	-3.08312300	4.24606000	-0.20109400
C	-2.18355800	2.50094700	0.66671600
C	-1.10179400	1.61768900	0.56624700
C	-0.12693100	1.86340400	-0.40142400
C	1.13595200	1.17498600	-0.53611400

S273

C	1.91052600	2.02175700	-1.53034100
H	2.77144000	2.54052000	-1.10534100
H	2.24231500	1.44447600	-2.39871800
C	1.30236100	-0.00551500	0.12361900
C	-0.66213300	0.50141200	1.46531100
C	2.48150900	-0.86416700	0.28636600
C	3.81482900	-0.41385100	0.38613300
C	4.89168300	-1.29726900	0.47588600
H	5.89602600	-0.89538400	0.54979600
C	4.66758000	-2.66939800	0.51074200
H	5.50851900	-3.35207300	0.58501300
C	3.35632400	-3.14865500	0.48979600
H	3.15987600	-4.21447600	0.55434300
C	2.29376800	-2.26198000	0.39081000
H	1.28140600	-2.64256900	0.38922100
C	-0.75170600	-1.20877900	-0.30564200
C	-0.24055500	-1.65996100	-1.51563300
H	0.78334800	-1.43650900	-1.78458800
C	-1.02529100	-2.41893900	-2.41112000
H	-0.57061800	-2.75503200	-3.33865900
C	-2.33594500	-2.73030200	-2.13390300
H	-2.93682100	-3.31512600	-2.82421300
C	-2.91261300	-2.26355500	-0.92756800
C	-2.12760700	-1.49375900	-0.01279100
C	-3.90562000	-1.23466900	1.43431200
H	-4.27158400	-0.80792200	2.36628200
C	-4.76207700	-2.00290000	0.61162100
H	-5.79070700	-2.17691200	0.91103100
C	-4.26208100	-2.50705600	-0.56672900
H	-4.88870500	-3.09115800	-1.23599200
Cl	4.21143000	1.29247600	0.55161000

CN_203_CC_163

Charge = 0, Multiplicity = 1

O	2.52514800	3.22900800	-1.06884000
O	-1.52343000	0.62295100	1.91178100
N	-0.30956100	-0.19664800	0.09843100
N	-3.07071800	0.00408000	-0.22078800
C	-2.57305700	3.42425000	1.38391800
H	-3.30809500	2.76752900	0.90744100
H	-2.98319600	4.43782800	1.42780700
H	-2.44332300	3.04840100	2.40379200
C	1.24381400	3.43788900	-0.65612800

C	0.60574500	4.64642800	-0.41766300
H	1.07672300	5.59461300	-0.65252400
C	-0.65999100	4.59361900	0.19678500
H	-1.17335700	5.53147300	0.39196000
C	-1.26759700	3.40508600	0.63249600
C	-0.60631000	2.19493800	0.34286100
C	0.59428100	2.23925500	-0.36572300
C	1.50370600	1.14510600	-0.55003700
C	2.80905400	1.80102900	-0.95499300
H	3.61946900	1.67214600	-0.22732000
H	3.16491800	1.46353700	-1.92939600
C	1.09609200	-0.10988000	-0.19308400
C	-0.92703000	0.86244400	0.88261500
C	1.98072400	-1.14445700	0.38705800
C	3.28997000	-1.43986000	-0.03058300
C	4.16489900	-2.20462300	0.74270700
H	5.15502100	-2.42191100	0.35768500
C	3.75126600	-2.69659100	1.97598700
H	4.43351600	-3.28943300	2.57726700
C	2.45096400	-2.43626000	2.41688800
H	2.11031600	-2.81566100	3.37537700
C	1.59268200	-1.66828600	1.64346000
H	0.60154700	-1.42714100	2.01170800
C	-1.06745300	-1.34844100	-0.21673000
C	-0.50076600	-2.57532500	-0.53339600
H	0.57065700	-2.69932800	-0.54215600
C	-1.29304500	-3.70295400	-0.83976200
H	-0.79002500	-4.63943500	-1.06224700
C	-2.66446000	-3.63592200	-0.83700500
H	-3.27550900	-4.50980900	-1.04405300
C	-3.29046400	-2.38959200	-0.59234200
C	-2.50252200	-1.22457800	-0.32678700
C	-4.37939900	0.11757700	-0.29771000
H	-4.78245700	1.12654400	-0.22234400
C	-5.25200300	-0.98039500	-0.48025000
H	-6.32556700	-0.82473100	-0.51527400
C	-4.69843800	-2.22740200	-0.64088900
H	-5.32113200	-3.10055300	-0.81875100
Cl	3.81851200	-1.05177000	-1.66800900

CN_203_CC_168

Charge = 0, Multiplicity = 1

O	2.52948800	3.19388600	-1.12187700
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S275

O	-1.48575900	0.61343700	1.93116400
N	-0.31089200	-0.20529300	0.09249500
N	-3.07740300	0.03677600	-0.18587700
C	-2.51475200	3.42843500	1.43358000
H	-3.26316500	2.77441000	0.97475700
H	-2.91784700	4.44459500	1.48274700
H	-2.36608400	3.05525300	2.45188900
C	1.25870400	3.41091700	-0.68375100
C	0.63449800	4.62481100	-0.43467300
H	1.10802000	5.56870400	-0.68137700
C	-0.61817600	4.58293800	0.20575000
H	-1.12036400	5.52485600	0.41019100
C	-1.22537700	3.39915600	0.65523000
C	-0.57959500	2.18421600	0.35305700
C	0.60739400	2.21679700	-0.37935000
C	1.50615700	1.11494900	-0.58045200
C	2.80887300	1.76567800	-1.00457100
H	3.62670900	1.63875000	-0.28521800
H	3.15289600	1.42301000	-1.98117900
C	1.09311100	-0.13863600	-0.21943600
C	-0.90423000	0.85337000	0.89383800
C	1.96611200	-1.18159700	0.36738400
C	3.30142100	-1.44283100	0.00994300
C	4.16000900	-2.19316300	0.81426600
H	5.17012300	-2.38402100	0.46931500
C	3.70668100	-2.70599600	2.02479900
H	4.37669900	-3.28670500	2.65111500
C	2.38214700	-2.48178100	2.40778900
H	2.00796500	-2.87643400	3.34744000
C	1.54063500	-1.72666300	1.60373000
H	0.53340200	-1.50675800	1.93841900
C	-1.08935200	-1.33619200	-0.24448600
C	-0.53998600	-2.56014800	-0.60181800
H	0.53026600	-2.69375300	-0.62886000
C	-1.34809900	-3.67102000	-0.92646900
H	-0.85828900	-4.60641600	-1.18075600
C	-2.71871600	-3.58994300	-0.90280600
H	-3.34181700	-4.45165600	-1.12438100
C	-3.32789200	-2.34412600	-0.61689800
C	-2.52405300	-1.19456300	-0.33138600
C	-4.38570700	0.16600500	-0.24233300
H	-4.77687000	1.17678300	-0.13539400
C	-5.27236100	-0.91764600	-0.44183600
H	-6.34454300	-0.74986700	-0.45854600

C	-4.73452900	-2.16578300	-0.64230000
H	-5.36901000	-3.02728500	-0.83471500
Cl	3.88956600	-1.05209000	-1.60805200

CN_203_CC_173

Charge = 0, Multiplicity = 1

O	2.51031000	3.17334600	-1.18095100
O	-1.44588500	0.59433900	1.95686500
N	-0.30875100	-0.21631400	0.09129400
N	-3.08127600	0.05447200	-0.14362500
C	-2.47320400	3.41670400	1.48786000
H	-3.23113800	2.76002900	1.04910800
H	-2.87574400	4.43283500	1.54185900
H	-2.30119600	3.04826400	2.50425900
C	1.25050500	3.39047300	-0.71405200
C	0.63182000	4.60574800	-0.45638600
H	1.09972900	5.54814900	-0.71897700
C	-0.60511600	4.56721200	0.21302400
H	-1.10242300	5.50996200	0.42539200
C	-1.20195000	3.38480700	0.68043700
C	-0.56370800	2.16922500	0.36744800
C	0.60765000	2.19707100	-0.39043200
C	1.50276600	1.09326300	-0.60772900
C	2.79737400	1.74769000	-1.05390200
H	3.62296800	1.63364700	-0.34180600
H	3.13293700	1.39834500	-2.03081800
C	1.09273700	-0.16126900	-0.24180100
C	-0.88286300	0.83817500	0.91063000
C	1.96053000	-1.21028600	0.34687400
C	3.31940900	-1.43100900	0.05111700
C	4.16237400	-2.16788300	0.88302300
H	5.19100500	-2.32659800	0.57900000
C	3.67247900	-2.70977300	2.06631000
H	4.33081700	-3.27915900	2.71497100
C	2.32644300	-2.52860400	2.38989900
H	1.92072800	-2.94507700	3.30677200
C	1.50105300	-1.78484300	1.55867300
H	0.47846300	-1.59218000	1.85975700
C	-1.10284100	-1.32692400	-0.27220800
C	-0.56561200	-2.54247300	-0.67534700
H	0.50378300	-2.67996500	-0.72129200
C	-1.38442200	-3.63819000	-1.02274600
H	-0.90381500	-4.56796200	-1.31275300

C	-2.75426700	-3.55031200	-0.97772500
H	-3.38543500	-4.40118800	-1.21750800
C	-3.35188900	-2.31061900	-0.64507700
C	-2.53744400	-1.17481100	-0.33463900
C	-4.38942600	0.19293900	-0.17867700
H	-4.77305100	1.20204400	-0.03508000
C	-5.28510400	-0.87893200	-0.40012500
H	-6.35637100	-0.70460800	-0.39759500
C	-4.75760000	-2.12332000	-0.64624000
H	-5.39988700	-2.97468700	-0.85700500
Cl	3.96736700	-1.02675200	-1.54226600

CN_203_CC_178

Charge = 0, Multiplicity = 1

O	2.45957300	3.17095100	-1.24912100
O	-1.40164800	0.56376000	1.99201300
N	-0.30153500	-0.23051700	0.09706100
N	-3.08185800	0.05263300	-0.09022700
C	-2.45193300	3.38506100	1.55062900
H	-3.21196900	2.71278300	1.14049200
H	-2.86642900	4.39643800	1.60343800
H	-2.24797600	3.03190700	2.56664500
C	1.21178700	3.37793400	-0.74832700
C	0.58768500	4.58948500	-0.48442000
H	1.03883700	5.53380200	-0.76854800
C	-0.62960300	4.54490900	0.21867100
H	-1.13027000	5.48442200	0.43739200
C	-1.20239600	3.35991900	0.70985800
C	-0.56136100	2.14882600	0.38792100
C	0.59141200	2.18054600	-0.39818000
C	1.49248400	1.08233400	-0.63105500
C	2.77096400	1.75223100	-1.10468300
H	3.60542700	1.66559800	-0.39990700
H	3.10141800	1.39399100	-2.07985400
C	1.09655500	-0.17598900	-0.25839200
C	-0.86258300	0.81544200	0.93559600
C	1.96670900	-1.22847200	0.32648400
C	3.34609000	-1.40140200	0.09398900
C	4.17424600	-2.12855400	0.94804500
H	5.21964800	-2.24812900	0.68636800
C	3.65131400	-2.71179300	2.09707400
H	4.29853200	-3.27287200	2.76387900
C	2.28707900	-2.58151000	2.35944400

H	1.85232700	-3.02954600	3.24767300
C	1.47705700	-1.84481700	1.50662000
H	0.43995500	-1.68679100	1.77354400
C	-1.10546200	-1.32079700	-0.30064700
C	-0.57372500	-2.51973000	-0.75889600
H	0.49537000	-2.65314000	-0.82561100
C	-1.39681800	-3.60186800	-1.13614700
H	-0.92019700	-4.51927300	-1.46900600
C	-2.76611200	-3.51704800	-1.06816100
H	-3.40044100	-4.35844000	-1.33177800
C	-3.35901400	-2.29164000	-0.67937100
C	-2.54057700	-1.16784300	-0.33621600
C	-4.39043900	0.19171400	-0.10213300
H	-4.77221400	1.19417900	0.08582900
C	-5.28878700	-0.87132100	-0.35299200
H	-6.35994400	-0.69788700	-0.32937400
C	-4.76458800	-2.10500400	-0.65406500
H	-5.40972900	-2.94784900	-0.88898400
Cl	4.05459500	-0.96443300	-1.46629700

CN_203_CC_183

Charge = 0, Multiplicity = 1

O	2.35940100	3.19472900	-1.32808300
O	-1.34929200	0.51831800	2.04297500
N	-0.28637700	-0.24957100	0.11506900
N	-3.07813000	0.01799100	-0.01776900
C	-2.46640300	3.32408400	1.62146900
H	-3.22201400	2.63044300	1.24004800
H	-2.90255200	4.32612300	1.67755600
H	-2.22447800	2.98578200	2.63423500
C	1.12518000	3.37648800	-0.78711700
C	0.47831700	4.57601900	-0.52094400
H	0.89566000	5.52670100	-0.83403400
C	-0.71400700	4.51172600	0.22125000
H	-1.23100000	5.44151100	0.44353700
C	-1.24215700	3.31921800	0.74412800
C	-0.58177400	2.12063400	0.41701000
C	0.54864400	2.16906800	-0.40028000
C	1.47053100	1.08847700	-0.64734900
C	2.71941500	1.79021500	-1.15700100
H	3.56426900	1.75144800	-0.46161400
H	3.04890700	1.42151300	-2.12835600
C	1.10675800	-0.17750000	-0.26470500

C	-0.84449800	0.78249100	0.97358400
C	1.99137900	-1.22904200	0.30691200
C	3.38758300	-1.34324300	0.13920300
C	4.20352000	-2.06829000	1.00601700
H	5.26348200	-2.13784700	0.78875100
C	3.65393700	-2.71306800	2.10871500
H	4.29216000	-3.27172800	2.78610700
C	2.27543400	-2.64523300	2.30760400
H	1.81622600	-3.14079100	3.15744000
C	1.47815800	-1.90767800	1.44323100
H	0.42752700	-1.79602600	1.67465500
C	-1.09107500	-1.31893600	-0.33006900
C	-0.55383700	-2.48722000	-0.85802600
H	0.51588200	-2.60340500	-0.94746200
C	-1.37076600	-3.55787600	-1.27745500
H	-0.88966300	-4.45140600	-1.66448400
C	-2.73994900	-3.49254500	-1.18483200
H	-3.36928900	-4.32637000	-1.48216700
C	-3.33939700	-2.29568600	-0.72445200
C	-2.52778500	-1.18155500	-0.33521000
C	-4.38818700	0.14291000	-0.00295900
H	-4.77769600	1.12959100	0.24333400
C	-5.27878600	-0.91567800	-0.29626800
H	-6.35124000	-0.75583500	-0.24812100
C	-4.74627200	-2.12607600	-0.66882700
H	-5.38613800	-2.96266500	-0.93804600
Cl	4.15746200	-0.84121000	-1.37314000

CN_203_CC_188

Charge = 0, Multiplicity = 1

O	0.76942600	3.18310600	-1.86016600
O	-0.76777100	0.42583300	2.72702200
N	0.05393800	-0.50127400	0.72283400
N	-2.67103900	-1.01796600	0.92734200
C	-3.46666400	2.10259900	1.75464800
H	-4.28047400	1.51899400	1.30706600
H	-3.89768900	3.03922000	2.12415200
H	-3.07561700	1.53904600	2.60387000
C	-0.36217700	3.00056400	-1.12680300
C	-1.50965100	3.78812000	-1.10083800
H	-1.62501100	4.64670900	-1.75310600
C	-2.49519000	3.44707900	-0.16340100
H	-3.39175000	4.06033300	-0.11638700

S280

C	-2.38013800	2.37485500	0.74632900
C	-1.23714800	1.57131800	0.65322600
C	-0.26027900	1.90080600	-0.28680100
C	1.05962400	1.31632600	-0.39785700
C	1.78537100	2.26715800	-1.34083400
H	2.53693600	2.88639000	-0.85064800
H	2.24534000	1.75902000	-2.19132400
C	1.29695900	0.13754200	0.25126600
C	-0.76824800	0.44949200	1.52441500
C	2.49976600	-0.69008300	0.45372500
C	3.84845000	-0.31698400	0.26024200
C	4.90020600	-1.22726800	0.36827200
H	5.91294600	-0.87471500	0.20795000
C	4.65318500	-2.55165500	0.71281500
H	5.47795900	-3.25230500	0.79891400
C	3.34232200	-2.94548400	0.98028100
H	3.12418200	-3.96389400	1.28675200
C	2.30325800	-2.03512200	0.85610900
H	1.29293300	-2.34843300	1.07617200
C	-0.61980700	-1.24194000	-0.28025700
C	0.03395400	-1.73576500	-1.40263200
H	1.07423100	-1.49450700	-1.57171100
C	-0.62546700	-2.56383600	-2.33594400
H	-0.06181200	-2.92887700	-3.18978500
C	-1.94794300	-2.91022500	-2.18424800
H	-2.45166800	-3.55103700	-2.90199900
C	-2.66571800	-2.40571400	-1.07347800
C	-2.01033500	-1.55965000	-0.12361300
C	-3.94372500	-1.30256800	1.11087000
H	-4.42197000	-0.84926400	1.97656200
C	-4.67839100	-2.14599100	0.24551600
H	-5.72583500	-2.34858000	0.44490600
C	-4.03708200	-2.68508300	-0.84526700
H	-4.56640300	-3.32682700	-1.54505500
Cl	4.34408100	1.35417400	0.01606700

CN_203_CC_193

Charge = 0, Multiplicity = 1

O	0.79463000	3.10867600	-1.93620500
O	-0.71571000	0.46193700	2.72215600
N	0.05815500	-0.51966800	0.72245000
N	-2.66920900	-0.99084700	0.98084700
C	-3.40906100	2.15956600	1.75517100

H	-4.23344700	1.57299200	1.33146500
H	-3.82684700	3.10871200	2.10742900
H	-3.01303000	1.61231100	2.61277300
C	-0.33036600	2.95903600	-1.18424300
C	-1.46519700	3.76492700	-1.15633400
H	-1.57745200	4.61356400	-1.82202700
C	-2.44240300	3.45531900	-0.19921300
H	-3.32884900	4.08301300	-0.15114800
C	-2.33201700	2.39725200	0.72810500
C	-1.20296800	1.57453000	0.63437100
C	-0.23537500	1.87413100	-0.32486500
C	1.07268900	1.26839000	-0.44151400
C	1.79917200	2.17707600	-1.42177500
H	2.58378600	2.78419100	-0.96986700
H	2.22117700	1.63297400	-2.27090700
C	1.30188400	0.09998700	0.22692400
C	-0.73645700	0.46059500	1.51982800
C	2.50416800	-0.72569100	0.41835600
C	3.84931700	-0.31571700	0.28790600
C	4.91515600	-1.21219800	0.37344800
H	5.92560500	-0.83397400	0.26569700
C	4.68183300	-2.55809600	0.63400200
H	5.51651700	-3.24879800	0.70358700
C	3.37170000	-2.98992500	0.84347300
H	3.16621000	-4.02784900	1.08673500
C	2.31894800	-2.09252100	0.74257900
H	1.30903600	-2.43534100	0.91690400
C	-0.64839100	-1.24467700	-0.27075300
C	-0.02783100	-1.74261700	-1.40985800
H	1.01207400	-1.51579800	-1.60086500
C	-0.72044700	-2.55615400	-2.33198300
H	-0.18169900	-2.92593900	-3.19974400
C	-2.04461600	-2.88216200	-2.15253200
H	-2.57412700	-3.51158900	-2.86175400
C	-2.72994400	-2.37099300	-1.02433500
C	-2.04029600	-1.54013600	-0.08553600
C	-3.94256500	-1.25382000	1.18995900
H	-4.39482000	-0.79467700	2.06653000
C	-4.70956600	-2.08181500	0.33778500
H	-5.75590700	-2.26718200	0.55856900
C	-4.10071400	-2.62804300	-0.76797700
H	-4.65565200	-3.25809100	-1.45848400
Cl	4.31020800	1.37898300	0.17344100

CN_203_CC_198

Charge = 0, Multiplicity = 1

O	0.82408300	3.05561300	-1.99541600
O	-0.66679400	0.48842700	2.70868700
N	0.05982800	-0.53723400	0.71196700
N	-2.66841000	-0.96433200	1.02240800
C	-3.34753500	2.21586000	1.75977100
H	-4.18047500	1.62618400	1.35760800
H	-3.75472700	3.17478000	2.09744800
H	-2.94538900	1.68281200	2.62355800
C	-0.29516900	2.93283300	-1.22917000
C	-1.41315400	3.76174900	-1.19093800
H	-1.51790500	4.60849500	-1.86025500
C	-2.38287500	3.47774700	-0.21822900
H	-3.25610200	4.12308100	-0.16268700
C	-2.28059900	2.42462100	0.71603000
C	-1.16937900	1.57906800	0.61343800
C	-0.21172300	1.85219400	-0.36356300
C	1.08264600	1.22247800	-0.49065400
C	1.81084600	2.09508900	-1.49991000
H	2.63377700	2.67584100	-1.08244500
H	2.18413200	1.52315800	-2.35442000
C	1.30331100	0.06184300	0.19166600
C	-0.70685100	0.46843200	1.50720400
C	2.50591500	-0.76071800	0.37951800
C	3.84551200	-0.31931800	0.31531800
C	4.92503500	-1.19955600	0.40114000
H	5.93157200	-0.80012100	0.34614500
C	4.70701700	-2.55893500	0.59696800
H	5.55148900	-3.23759200	0.66725300
C	3.39883000	-3.02319500	0.74282100
H	3.20632600	-4.07404600	0.93610900
C	2.33288200	-2.14126300	0.64343400
H	1.32414400	-2.50883400	0.76919400
C	-0.67680400	-1.25153200	-0.26772100
C	-0.08739300	-1.75762500	-1.41966800
H	0.95155200	-1.54505000	-1.63217700
C	-0.81065900	-2.56034900	-2.32774500
H	-0.29539300	-2.93766100	-3.20646500
C	-2.13570100	-2.86631000	-2.12145600
H	-2.68892000	-3.48728300	-2.81995600
C	-2.79046100	-2.34469000	-0.97988400
C	-2.06935000	-1.52489700	-0.05524600

S283

C	-3.94175900	-1.20569100	1.25596900
H	-4.36970200	-0.73755300	2.14000700
C	-4.73841300	-2.02204400	0.41982600
H	-5.78324200	-2.18993200	0.66083300
C	-4.15999300	-2.57933800	-0.69671300
H	-4.73842600	-3.20073200	-1.37568200
Cl	4.26964600	1.38849300	0.29152400

CN_203_CC_203

Charge = 0, Multiplicity = 1

O	0.85518300	3.01537600	-2.04406100
O	-0.62071000	0.50768000	2.69110500
N	0.06035300	-0.55332700	0.69582200
N	-2.66782800	-0.93801100	1.05570500
C	-3.28603300	2.26852400	1.76498500
H	-4.12645400	1.67671300	1.38192300
H	-3.68392400	3.23533300	2.09080400
H	-2.87765500	1.74710400	2.63305700
C	-0.25893100	2.91563500	-1.26619700
C	-1.35888700	3.76770000	-1.21524100
H	-1.45460000	4.61599400	-1.88395400
C	-2.32195500	3.50504700	-0.22973600
H	-3.18102400	4.16823400	-0.16475900
C	-2.22911200	2.45277100	0.70656900
C	-1.13659700	1.58442900	0.59249200
C	-0.18866600	1.83466700	-0.39996000
C	1.09134400	1.18073700	-0.53933800
C	1.82278400	2.02550400	-1.56842500
H	2.67725000	2.57850000	-1.17650100
H	2.15209200	1.43543300	-2.42913300
C	1.30271300	0.02458400	0.15083400
C	-0.67898700	0.47427200	1.49084500
C	2.50622900	-0.79495200	0.33812900
C	3.83775100	-0.32632500	0.34224300
C	4.92967100	-1.18994900	0.44108700
H	5.93028400	-0.77226600	0.43883400
C	4.72832200	-2.55860400	0.58317800
H	5.58168100	-3.22487300	0.66411200
C	3.42438100	-3.05100600	0.66216400
H	3.24525600	-4.11110100	0.81328600
C	2.34639900	-2.18497400	0.55123500
H	1.34063600	-2.57452000	0.62738600
C	-0.70419900	-1.25965500	-0.26836900

C	-0.14426600	-1.77535900	-1.43073900
H	0.89338500	-1.57664200	-1.66295400
C	-0.89521900	-2.57052900	-2.32289600
H	-0.40191900	-2.95687600	-3.21025700
C	-2.22023500	-2.85758300	-2.09080300
H	-2.79503700	-3.47255900	-2.77707000
C	-2.84632300	-2.32348600	-0.93886800
C	-2.09661000	-1.51182100	-0.03002900
C	-3.94050100	-1.15855700	1.31235900
H	-4.34571000	-0.68001600	2.20156300
C	-4.76393100	-1.96635200	0.49398500
H	-5.80672900	-2.11754500	0.75409300
C	-4.21390700	-2.53662900	-0.63034800
H	-4.81367800	-3.15164600	-1.29648800
Cl	4.22419300	1.38983100	0.38612300

CN_203_CC_208

Charge = 0, Multiplicity = 1

O	0.89111300	2.98525300	-2.08395900
O	-0.57691800	0.52313300	2.66956900
N	0.05960200	-0.56839000	0.67545400
N	-2.66713300	-0.91093600	1.08287100
C	-3.22359900	2.32081700	1.76931500
H	-4.07196800	1.72953500	1.40331700
H	-3.61111400	3.29469100	2.08623800
H	-2.80979300	1.80769600	2.63986800
C	-0.21941500	2.90568200	-1.29778900
C	-1.29958000	3.78174000	-1.23249500
H	-1.38358200	4.63453900	-1.89704600
C	-2.25743100	3.53750300	-0.23695500
H	-3.10102800	4.21913500	-0.16125600
C	-2.17651700	2.48265000	0.69758600
C	-1.10446300	1.59072700	0.57009000
C	-0.16556900	1.82041600	-0.43580000
C	1.09928800	1.14184600	-0.58765200
C	1.83743300	1.96578700	-1.62765200
H	2.71740700	2.48957300	-1.25117300
H	2.12968900	1.36605400	-2.49526000
C	1.30017600	-0.01207900	0.10638000
C	-0.65270500	0.47907600	1.47075900
C	2.50482000	-0.82917600	0.29559900
C	3.82580000	-0.33828400	0.37010500
C	4.92736500	-1.18704500	0.49000000

S285

H	5.92034700	-0.75455700	0.54123900
C	4.74234500	-2.56218800	0.58409000
H	5.60254900	-3.21735000	0.68178600
C	3.44489600	-3.07798600	0.59300900
H	3.27855100	-4.14493200	0.70569600
C	2.35764400	-2.22607100	0.46280300
H	1.35603500	-2.63357300	0.48714800
C	-0.73131000	-1.26800800	-0.27228800
C	-0.20060500	-1.79296000	-1.44426500
H	0.83387700	-1.60449900	-1.69890200
C	-0.97781600	-2.58248400	-2.31891900
H	-0.50641100	-2.97725900	-3.21444000
C	-2.30134700	-2.85314100	-2.06027000
H	-2.89639500	-3.46386500	-2.73293500
C	-2.89933100	-2.30588400	-0.89952700
C	-2.12273200	-1.49993100	-0.00842500
C	-3.93829700	-1.11147300	1.36244500
H	-4.32168800	-0.62068900	2.25467500
C	-4.78662500	-1.91342300	0.56399700
H	-5.82677800	-2.04843200	0.84292600
C	-4.26404300	-2.49849100	-0.56584800
H	-4.88378100	-3.10909800	-1.21761000
Cl	4.17664400	1.38326500	0.46722500

CN_203_CC_213

Charge = 0, Multiplicity = 1

O	0.92689100	2.96067700	-2.11951600
O	-0.53404400	0.53615100	2.64621900
N	0.05885500	-0.58184700	0.65294000
N	-2.66502300	-0.88401800	1.10642300
C	-3.16374000	2.36831100	1.77122900
H	-4.02054500	1.78051700	1.41948600
H	-3.53973700	3.34836800	2.08272600
H	-2.74562400	1.85954500	2.64237500
C	-0.18084700	2.89885700	-1.32685100
C	-1.24171000	3.79700900	-1.24787800
H	-1.31380000	4.65482600	-1.90735700
C	-2.19507600	3.56864300	-0.24398600
H	-3.02358900	4.26732000	-0.15794200
C	-2.12596900	2.51054600	0.68774600
C	-1.07371700	1.59692700	0.54725000
C	-0.14350300	1.80849000	-0.47048800
C	1.10666300	1.10687000	-0.63424200

C	1.85365200	1.91666100	-1.67817100
H	2.75112700	2.41569100	-1.30805000
H	2.12007900	1.31352800	-2.55176300
C	1.29693600	-0.04653600	0.06050300
C	-0.62724900	0.48332600	1.44910000
C	2.50323600	-0.86136400	0.25252400
C	3.81072500	-0.35188400	0.39893200
C	4.91980300	-1.18702900	0.54341400
H	5.90292800	-0.74204700	0.64890700
C	4.75209200	-2.56684700	0.59124700
H	5.61752300	-3.21188300	0.70845700
C	3.46423600	-3.10264300	0.52749000
H	3.31109700	-4.17487400	0.60251300
C	2.36976200	-2.26350400	0.37430600
H	1.37448400	-2.68678400	0.34448800
C	-0.75679600	-1.27591500	-0.27752800
C	-0.25469900	-1.80990800	-1.45810000
H	0.77563400	-1.62994200	-1.73523500
C	-1.05641000	-2.59542500	-2.31415000
H	-0.60637500	-2.99856400	-3.21692200
C	-2.37743600	-2.85137100	-2.02908900
H	-2.99131800	-3.45914500	-2.68733500
C	-2.94812600	-2.29066800	-0.86099000
C	-2.14641200	-1.48880500	0.01127700
C	-3.93388500	-1.06560400	1.40848000
H	-4.29630600	-0.56195100	2.30232100
C	-4.80528800	-1.86353600	0.63112200
H	-5.84221800	-1.98323600	0.92844300
C	-4.30917700	-2.46394600	-0.50262500
H	-4.94749900	-3.07146200	-1.13915900
Cl	4.12659800	1.37309300	0.54304400

CN_203_CC_223

Charge = 0, Multiplicity = 1

O	1.00058800	2.91814700	-2.18470200
O	-0.45414600	0.56024700	2.59541800
N	0.05678100	-0.60506400	0.60612400
N	-2.65855100	-0.83033900	1.14583100
C	-3.04925200	2.45712200	1.76580900
H	-3.91895100	1.87262800	1.44124800
H	-3.40737300	3.44781200	2.06403800
H	-2.62225300	1.95977500	2.63946000
C	-0.10361800	2.88882800	-1.38342600

S287

C	-1.12616100	3.82776500	-1.28033400
H	-1.17280400	4.69548800	-1.92907000
C	-2.07280300	3.62810100	-0.26336200
H	-2.87129700	4.35847000	-0.15889200
C	-2.02877500	2.56348600	0.66206100
C	-1.01562100	1.60959000	0.49831700
C	-0.10105500	1.78829300	-0.53932300
C	1.12009500	1.04332800	-0.72344700
C	1.89096300	1.83430000	-1.76291000
H	2.80953400	2.29245600	-1.38874200
H	2.12745100	1.23320300	-2.64625600
C	1.28803400	-0.11122000	-0.03123600
C	-0.57988500	0.49229400	1.40223500
C	2.49977500	-0.92004600	0.16933900
C	3.76993900	-0.38128700	0.46131700
C	4.88991100	-1.19092500	0.65794800
H	5.84543800	-0.72581800	0.87307400
C	4.76353700	-2.57542000	0.61332400
H	5.63619900	-3.20170200	0.77179500
C	3.50615400	-3.14392100	0.40045000
H	3.38452300	-4.22280900	0.39945200
C	2.40108400	-2.32843900	0.19794700
H	1.42653500	-2.77856300	0.05803100
C	-0.80401400	-1.29123900	-0.28829000
C	-0.35686600	-1.84312300	-1.48278900
H	0.66314600	-1.67683000	-1.80383600
C	-1.20267500	-2.62427800	-2.29972100
H	-0.79347800	-3.04406300	-3.21428800
C	-2.51635500	-2.85422600	-1.96333300
H	-3.16419000	-3.45904000	-2.59103300
C	-3.03519500	-2.26583800	-0.78459800
C	-2.18820500	-1.46836500	0.04790900
C	-3.92105700	-0.97668000	1.49069700
H	-4.24421500	-0.44614100	2.38406800
C	-4.83349100	-1.77083100	0.75784600
H	-5.86268200	-1.86203000	1.09012700
C	-4.38715100	-2.40314500	-0.37929300
H	-5.05878800	-3.00751900	-0.98372600
Cl	4.01295200	1.34591700	0.69331300

CN_203_CC_233

Charge = 0, Multiplicity = 1

O	1.07879400	2.87739900	-2.24741200
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S288

O	-0.38513800	0.58904800	2.53931300
N	0.05342100	-0.62228400	0.56017600
N	-2.65081600	-0.77530200	1.17574100
C	-2.94540300	2.54155700	1.74050400
H	-3.82586900	1.96050900	1.43974500
H	-3.28760300	3.54192700	2.02440300
H	-2.51194600	2.05555800	2.61757900
C	-0.02584700	2.87870800	-1.44434600
C	-1.01109400	3.85444700	-1.32458600
H	-1.02961100	4.73010500	-1.96402100
C	-1.95538100	3.68225700	-0.29974400
H	-2.72476100	4.44133700	-0.18241100
C	-1.93895500	2.61352200	0.62129400
C	-0.96357700	1.62305300	0.44124100
C	-0.06097800	1.77023200	-0.61130200
C	1.13237400	0.98530300	-0.80815600
C	1.93506200	1.76347600	-1.83170300
H	2.86183300	2.18962500	-1.43744500
H	2.16405300	1.16893700	-2.72105900
C	1.27667800	-0.16994300	-0.11799000
C	-0.53934200	0.50502100	1.35067200
C	2.49690700	-0.96930600	0.09576500
C	3.71401400	-0.40885600	0.53428600
C	4.84300300	-1.19193800	0.77966100
H	5.75852400	-0.71171400	1.10646600
C	4.77330300	-2.57390000	0.63485500
H	5.65189700	-3.18087500	0.83143200
C	3.56449800	-3.16784800	0.26807800
H	3.48691900	-4.24750500	0.18350600
C	2.44994000	-2.37681900	0.01956600
H	1.50969500	-2.84944600	-0.23559100
C	-0.84537200	-1.30804900	-0.29523300
C	-0.44781400	-1.88263100	-1.49657500
H	0.55977400	-1.72677400	-1.85946500
C	-1.33036800	-2.66653800	-2.27103700
H	-0.95785600	-3.10653100	-3.19179100
C	-2.63484200	-2.87305900	-1.88703500
H	-3.31098900	-3.48044500	-2.48149100
C	-3.10754700	-2.25190300	-0.70563100
C	-2.22267100	-1.45157700	0.08360400
C	-3.90575100	-0.88823600	1.55881200
H	-4.19458200	-0.32669100	2.44497300
C	-4.85197600	-1.68540000	0.87372800
H	-5.87281400	-1.74910300	1.23678100

C	-4.44934400	-2.35479100	-0.25854900
H	-5.14870900	-2.96134200	-0.82836400
Cl	3.87102800	1.31313300	0.86053200

CN_208_CC_163

Charge = 0, Multiplicity = 1

O	2.40199100	3.27915300	-1.10659200
O	-1.57214400	0.56739100	1.93155100
N	-0.29846000	-0.22569000	0.15328000
N	-3.03883200	-0.05288000	-0.27349100
C	-2.64702600	3.34014700	1.45543100
H	-3.36011800	2.63234100	1.02153600
H	-3.10167900	4.33553200	1.47132100
H	-2.48044400	3.01043500	2.48611800
C	1.12573500	3.45335200	-0.66279800
C	0.45893200	4.64379000	-0.41395700
H	0.89699600	5.60421600	-0.66241300
C	-0.79183600	4.55686100	0.22711300
H	-1.32775200	5.48040000	0.42986700
C	-1.35690400	3.35315900	0.67763000
C	-0.66647600	2.16104600	0.37908900
C	0.51750900	2.23767800	-0.35330900
C	1.45173700	1.16957700	-0.55829700
C	2.72722100	1.85973300	-0.99975900
H	3.56048100	1.75310800	-0.29449900
H	3.06529500	1.53045200	-1.98334900
C	1.09243700	-0.09498900	-0.18392800
C	-0.95368800	0.82183800	0.91805400
C	2.03108200	-1.09143500	0.37767400
C	3.33565700	-1.34547700	-0.08020400
C	4.26449100	-2.06394600	0.67446900
H	5.24804500	-2.25190400	0.25843600
C	3.91251000	-2.54831000	1.92968700
H	4.63668700	-3.10492600	2.51636700
C	2.61952300	-2.32758900	2.41198000
H	2.32671600	-2.70165200	3.38821800
C	1.70736300	-1.60528000	1.65648800
H	0.72035900	-1.39484400	2.05384400
C	-1.03475900	-1.39839000	-0.14747400
C	-0.45404400	-2.63434300	-0.39040500
H	0.61619500	-2.75749100	-0.34355700
C	-1.23162600	-3.77417900	-0.69216300
H	-0.71894800	-4.71727700	-0.85720700

S290

C	-2.60144600	-3.70954500	-0.75413800
H	-3.20191500	-4.59150200	-0.95812200
C	-3.23942400	-2.45732200	-0.57918600
C	-2.46472000	-1.28262300	-0.31949600
C	-4.34318100	0.05453500	-0.40964400
H	-4.75027000	1.06434200	-0.38216500
C	-5.20572600	-1.05084800	-0.59585500
H	-6.27699000	-0.89917000	-0.68164900
C	-4.64426100	-2.30090700	-0.69277900
H	-5.25772600	-3.18105200	-0.86820700
Cl	3.79252200	-0.96662200	-1.74106400

CN_208_CC_168

Charge = 0, Multiplicity = 1

O	2.40612200	3.24369100	-1.15904000
O	-1.53310800	0.55835700	1.95157700
N	-0.29941000	-0.23559000	0.14648100
N	-3.04699200	-0.01793500	-0.23898700
C	-2.58763000	3.34477900	1.50475800
H	-3.31432000	2.64103300	1.08730800
H	-3.03488200	4.34335500	1.52826000
H	-2.40187100	3.01592400	2.53246200
C	1.14067400	3.42621700	-0.69023100
C	0.48778100	4.62233800	-0.43061900
H	0.92823800	5.57861100	-0.69057000
C	-0.74959200	4.54650400	0.23621300
H	-1.27430200	5.47433000	0.44845600
C	-1.31401500	3.34737100	0.70015800
C	-0.63920600	2.15018700	0.38880800
C	0.53094300	2.21490200	-0.36730800
C	1.45434800	1.13885300	-0.58911700
C	2.72687600	1.82396600	-1.04931800
H	3.56722800	1.71900900	-0.35259500
H	3.05314700	1.48948400	-2.03491100
C	1.08987100	-0.12450400	-0.21079500
C	-0.93017600	0.81242300	0.92883500
C	2.01723500	-1.12937100	0.35851300
C	3.34886600	-1.34781000	-0.03959700
C	4.26112900	-2.05167800	0.74745000
H	5.26534100	-2.21213500	0.37119100
C	3.86837200	-2.55815900	1.98161100
H	4.58018200	-3.10252500	2.59430200
C	2.55010000	-2.37533800	2.40618100

H	2.22274500	-2.76602700	3.36478300
C	1.65482400	-1.66598800	1.61869600
H	0.65094900	-1.47799100	1.98223000
C	-1.05701300	-1.38798600	-0.17613200
C	-0.49332800	-2.62319900	-0.46114500
H	0.57651900	-2.75783300	-0.43402500
C	-1.28755500	-3.74628700	-0.78091900
H	-0.78783400	-4.69004600	-0.97869900
C	-2.65750400	-3.66551300	-0.82037600
H	-3.27061100	-4.53526500	-1.03858900
C	-3.27887600	-2.41157400	-0.60336100
C	-2.48759100	-1.25229700	-0.32416500
C	-4.35181100	0.10727600	-0.35425000
H	-4.74708700	1.12042400	-0.29565600
C	-5.22916200	-0.98350700	-0.55651000
H	-6.29970100	-0.81794100	-0.62364300
C	-4.68327500	-2.23677800	-0.69312300
H	-5.30904500	-3.10525700	-0.88265900
Cl	3.86648700	-0.96516600	-1.68329100

CN_208_CC_173

Charge = 0, Multiplicity = 1

O	2.38881100	3.22030400	-1.21708000
O	-1.49282000	0.53996800	1.97605100
N	-0.29716000	-0.24752900	0.14307200
N	-3.05215000	0.00463800	-0.19925800
C	-2.54168900	3.33460800	1.55900300
H	-3.27660500	2.62720300	1.16297900
H	-2.98939600	4.33287800	1.58658400
H	-2.33205500	3.01279600	2.58441000
C	1.13509800	3.40402000	-0.71995600
C	0.48910000	4.60210900	-0.45078300
H	0.92462100	5.55649000	-0.72555700
C	-0.73210600	4.53074300	0.24465900
H	-1.25085900	5.45989900	0.46554100
C	-1.28690800	3.33347700	0.72539500
C	-0.62099600	2.13502300	0.40229500
C	0.53302700	2.19398800	-0.37916100
C	1.45169900	1.11526900	-0.61737900
C	2.71610200	1.80302400	-1.09869500
H	3.56349400	1.70977100	-0.40938900
H	3.03392300	1.46184800	-2.08451000
C	1.08959000	-0.14880300	-0.23462000

S292

C	-0.90779600	0.79723300	0.94403200
C	2.01136000	-1.15971100	0.33812800
C	3.36723100	-1.33672800	0.00136800
C	4.26345500	-2.02641500	0.81789700
H	5.28658200	-2.15418800	0.48234500
C	3.83311900	-2.56200900	2.02696900
H	4.53292900	-3.09442700	2.66348200
C	2.49263700	-2.42344200	2.39224700
H	2.13288400	-2.83637300	3.32968800
C	1.61380900	-1.72613300	1.57567800
H	0.59424600	-1.56584000	1.90539600
C	-1.07186000	-1.38015100	-0.20479900
C	-0.52100400	-2.61010600	-0.53590800
H	0.54859200	-2.75142000	-0.52935900
C	-1.32752400	-3.71780800	-0.87678200
H	-0.83750100	-4.65844800	-1.11046500
C	-2.69749200	-3.62691700	-0.89308100
H	-3.31990100	-4.48565300	-1.12787900
C	-3.30654500	-2.37587500	-0.62990800
C	-2.50308700	-1.23053900	-0.32782100
C	-4.35747800	0.14235600	-0.29285600
H	-4.74444200	1.15610900	-0.19974700
C	-5.24542100	-0.93601600	-0.51435200
H	-6.31553000	-0.76112300	-0.56184700
C	-4.71072500	-2.18858400	-0.69476300
H	-5.34548800	-3.04670900	-0.90083900
Cl	3.94577500	-0.94120100	-1.62059700

CN_208_CC_178

Charge = 0, Multiplicity = 1

O	2.34325200	3.21148400	-1.28308700
O	-1.44815800	0.51045900	2.00823300
N	-0.29037000	-0.26256000	0.14479900
N	-3.05400200	0.01110200	-0.15035500
C	-2.51269800	3.30631100	1.62035900
H	-3.25050200	2.58829900	1.24998200
H	-2.96901300	4.30057500	1.65125700
H	-2.27336700	2.99587800	2.64284700
C	1.10265500	3.38770500	-0.75313200
C	0.45415500	4.58306100	-0.47617600
H	0.87481500	5.53830700	-0.77039800
C	-0.74698800	4.50805900	0.25200500
H	-1.26674000	5.43482600	0.48044400

S293

C	-1.28014400	3.30952800	0.75432500
C	-0.61441800	2.11446000	0.42079000
C	0.52058200	2.17524100	-0.38826000
C	1.44254000	1.10057400	-0.64247800
C	2.69170700	1.80067200	-1.14844300
H	3.54584800	1.73264300	-0.46527200
H	3.00566800	1.45083600	-2.13214400
C	1.09267500	-0.16650200	-0.25418300
C	-0.88610600	0.77486400	0.96577700
C	2.01599000	-1.18038600	0.31703200
C	3.39276200	-1.30940700	0.04346600
C	4.27344600	-1.98778200	0.88506600
H	5.31342800	-2.07663300	0.59148500
C	3.80921500	-2.56282300	2.06306700
H	4.49734000	-3.08557700	2.71996700
C	2.45016700	-2.47521900	2.36735600
H	2.06061000	-2.91843100	3.27869000
C	1.58736400	-1.78670900	1.52620000
H	0.55342800	-1.66037200	1.82181600
C	-1.07725100	-1.37539000	-0.23437700
C	-0.53380900	-2.59348100	-0.61931800
H	0.53593600	-2.73498400	-0.63525500
C	-1.34732600	-3.68712400	-0.98669300
H	-0.86280700	-4.61928400	-1.26216500
C	-2.71741800	-3.59412900	-0.97802800
H	-3.34498500	-4.44300900	-1.23388900
C	-3.31976200	-2.35248700	-0.66099700
C	-2.50958200	-1.21963100	-0.33006500
C	-4.36024600	0.15449900	-0.22039900
H	-4.74360100	1.16499700	-0.08634300
C	-5.25353400	-0.91396500	-0.46677200
H	-6.32382200	-0.73566600	-0.49278700
C	-4.72430400	-2.16038300	-0.69864900
H	-5.36398200	-3.00950900	-0.92572800
Cl	4.03315000	-0.88444500	-1.54938900

CN_208_CC_183

Charge = 0, Multiplicity = 1

O	2.25466800	3.22428100	-1.35907500
O	-1.39652700	0.46679700	2.05265300
N	-0.27631800	-0.28123700	0.15538000
N	-3.05143000	-0.00781600	-0.08706700
C	-2.50999400	3.25194600	1.69222000

S294

H	-3.23981100	2.50945200	1.35647300
H	-2.98993300	4.23507300	1.72148100
H	-2.23213700	2.96525100	2.71202400
C	1.02933500	3.37999900	-0.79008100
C	0.36377500	4.56524400	-0.50806200
H	0.75432800	5.52485700	-0.82840600
C	-0.81160200	4.47488400	0.25833100
H	-1.34335300	5.39339100	0.49246300
C	-1.30462300	3.27102600	0.78906800
C	-0.62534900	2.08670300	0.44731400
C	0.48643600	2.16021200	-0.39252800
C	1.42400400	1.10014100	-0.66236200
C	2.64565200	1.82695700	-1.20129500
H	3.50819800	1.80171500	-0.52698200
H	2.95803500	1.46669100	-2.18148400
C	1.10166300	-0.17275100	-0.26604000
C	-0.86517700	0.74309600	0.99797800
C	2.03567900	-1.18593100	0.29594700
C	3.42944200	-1.25809900	0.08794200
C	4.29570100	-1.93202000	0.94700300
H	5.35014200	-1.97288700	0.69788700
C	3.80247900	-2.56405700	2.08330100
H	4.47981000	-3.08256600	2.75459600
C	2.42908200	-2.53706500	2.32355200
H	2.01326100	-3.02451700	3.20000800
C	1.58113300	-1.84990800	1.46586800
H	0.53414200	-1.76759800	1.72582200
C	-1.06764200	-1.37418400	-0.26526600
C	-0.52263600	-2.56958400	-0.71600200
H	0.54804100	-2.70076900	-0.75677500
C	-1.33454500	-3.65127300	-1.11906700
H	-0.84848500	-4.56606900	-1.44541300
C	-2.70514600	-3.56931900	-1.08336600
H	-3.33119900	-4.41020100	-1.36764300
C	-3.31005000	-2.34788300	-0.70032200
C	-2.50205600	-1.22515600	-0.33044700
C	-4.35950400	0.12982800	-0.13105400
H	-4.74707500	1.13055100	0.05411300
C	-5.24955500	-0.93265200	-0.41215400
H	-6.32121400	-0.76080300	-0.41426900
C	-4.71614900	-2.16373800	-0.70774800
H	-5.35402200	-3.00607100	-0.96341300
Cl	4.13225100	-0.77524900	-1.46315700

CN_208_CC_188

Charge = 0, Multiplicity = 1

O	0.66763500	3.13609900	-1.93486600
O	-0.77957100	0.38022300	2.73460900
N	0.07267600	-0.52012900	0.73333700
N	-2.69287200	-0.95538400	0.85743600
C	-3.42187600	2.11390700	1.85758000
H	-3.03730100	1.46118500	2.64255100
H	-4.31326600	1.64450500	1.42370500
H	-3.74050300	3.05709600	2.31528200
C	-0.43640700	2.95977100	-1.15956800
C	-1.58234600	3.74772900	-1.10014500
H	-1.72378400	4.59687700	-1.75959000
C	-2.52781900	3.42080400	-0.11821000
H	-3.42195600	4.03492000	-0.04285200
C	-2.37559100	2.36139800	0.80117000
C	-1.23852000	1.55373800	0.67279400
C	-0.30087900	1.87186200	-0.30900400
C	1.02048900	1.29934500	-0.44869400
C	1.70828400	2.24026800	-1.43007700
H	2.46665600	2.87707800	-0.97497800
H	2.14792500	1.72000000	-2.28392500
C	1.29173300	0.14243000	0.22398900
C	-0.76086400	0.42682300	1.53233500
C	2.51964900	-0.64312900	0.45252900
C	3.85813800	-0.24520400	0.23695600
C	4.93435000	-1.12008900	0.38943400
H	5.93661400	-0.74905700	0.20662700
C	4.72501700	-2.43049700	0.80446600
H	5.56893600	-3.10265100	0.92517300
C	3.42564900	-2.84499200	1.09512500
H	3.23506100	-3.85125700	1.45536800
C	2.36234900	-1.97084400	0.92549700
H	1.36131000	-2.29960100	1.16453800
C	-0.59539800	-1.30182800	-0.24409800
C	0.08477300	-1.86892200	-1.31616800
H	1.13488200	-1.65792700	-1.46170800
C	-0.55773400	-2.73242300	-2.22778500
H	0.02853200	-3.15434800	-3.03912500
C	-1.89182400	-3.04398900	-2.10605300
H	-2.38401200	-3.71353800	-2.80532800
C	-2.63735200	-2.46169800	-1.05393600
C	-1.99950500	-1.57566100	-0.12740400

S296

C	-3.97787500	-1.20313000	1.00375300
H	-4.48074400	-0.68998900	1.82020000
C	-4.69618600	-2.08170400	0.16008200
H	-5.75531600	-2.24996200	0.32694600
C	-4.02324100	-2.69804400	-0.86830000
H	-4.53757100	-3.36911200	-1.55155300
Cl	4.31231300	1.42048700	-0.10425300

CN_208_CC_193

Charge = 0, Multiplicity = 1

O	0.69674300	3.04944700	-2.01826700
O	-0.72275400	0.42781200	2.73127100
N	0.07708900	-0.54100700	0.73743500
N	-2.69080600	-0.92370500	0.91858400
C	-3.35900100	2.17978100	1.85033500
H	-2.97141500	1.54513800	2.64860800
H	-4.25987400	1.70695900	1.44033800
H	-3.66302500	3.13846100	2.28511100
C	-0.40072100	2.91051400	-1.22500300
C	-1.53149900	3.72047200	-1.16564300
H	-1.66803900	4.55858500	-1.84006600
C	-2.46831200	3.43018000	-0.16390500
H	-3.35042100	4.06152900	-0.08922100
C	-2.32272700	2.38692100	0.77555000
C	-1.20215300	1.55659100	0.64914500
C	-0.27447300	1.83924300	-0.35270800
C	1.03400100	1.24290400	-0.49504500
C	1.72116800	2.12987400	-1.52254500
H	2.52363800	2.74703900	-1.11930200
H	2.10776100	1.56341400	-2.37418300
C	1.29742300	0.10118200	0.20421800
C	-0.72743600	0.44088400	1.52838400
C	2.52442700	-0.68197300	0.42118700
C	3.85796000	-0.24253200	0.26555700
C	4.94821100	-1.10536100	0.38484700
H	5.94729000	-0.70509700	0.25332100
C	4.75371200	-2.44351100	0.70879200
H	5.60741000	-3.10730100	0.80460000
C	3.45700200	-2.89999300	0.94725800
H	3.28090400	-3.93033300	1.24066100
C	2.37984700	-2.03705200	0.81101200
H	1.38050900	-2.39824700	1.00800300
C	-0.62612900	-1.30409300	-0.23132000

C	0.01824100	-1.87525600	-1.32293100
H	1.06782000	-1.67947200	-1.49315600
C	-0.66029900	-2.72299500	-2.22340400
H	-0.10102800	-3.14995800	-3.05100600
C	-1.99625000	-3.01253800	-2.07132700
H	-2.51621300	-3.66974100	-2.76216900
C	-2.70689200	-2.42277200	-0.99926800
C	-2.03182800	-1.55322300	-0.08381700
C	-3.97665200	-1.14754100	1.09298200
H	-4.45127500	-0.62752600	1.92196000
C	-4.73008400	-2.00954800	0.26287500
H	-5.78812000	-2.15876400	0.45314000
C	-4.09234800	-2.63426400	-0.78283400
H	-4.63471100	-3.29263600	-1.45669500
Cl	4.27539900	1.45632300	0.07409000

CN_208_CC_198

Charge = 0, Multiplicity = 1

O	0.73129500	2.99046900	-2.07982000
O	-0.67211600	0.45988500	2.71791000
N	0.07785500	-0.56038100	0.72865900
N	-2.69108900	-0.89265000	0.96285400
C	-3.29135600	2.24394800	1.84984000
H	-2.89861700	1.62608900	2.65879800
H	-4.19890400	1.76573900	1.46129100
H	-3.58556900	3.21451800	2.26426700
C	-0.36037300	2.88149300	-1.27313200
C	-1.47109800	3.71826800	-1.20431000
H	-1.59763000	4.55488100	-1.88253700
C	-2.40029200	3.45694000	-0.18751500
H	-3.26666500	4.10887900	-0.10605600
C	-2.26560300	2.41849400	0.75934200
C	-1.16605100	1.56179800	0.62527500
C	-0.24873400	1.81421200	-0.39423600
C	1.04437400	1.19049000	-0.54588100
C	1.73200300	2.03334200	-1.60763800
H	2.58069600	2.61547700	-1.24881500
H	2.05561100	1.43311100	-2.46339900
C	1.29866300	0.05883900	0.17074500
C	-0.69734800	0.45032600	1.51547800
C	2.52557900	-0.72089800	0.38460300
C	3.85269100	-0.24640700	0.29269000
C	4.95661500	-1.09223500	0.40974200

H	5.95128700	-0.66810200	0.32952200
C	4.77802900	-2.44670600	0.66884000
H	5.64149900	-3.09796200	0.76330900
C	3.48420700	-2.93900300	0.84706600
H	3.32196000	-3.98435900	1.09125100
C	2.39376200	-2.09217000	0.71465100
H	1.39636000	-2.48042400	0.86660400
C	-0.65687100	-1.31167700	-0.22627900
C	-0.04478700	-1.89331100	-1.33080300
H	1.00446500	-1.71444200	-1.52188600
C	-0.75557700	-2.72991200	-2.21678500
H	-0.22068400	-3.16658500	-3.05536900
C	-2.09296800	-2.99646200	-2.03739300
H	-2.63789500	-3.64494700	-2.71714300
C	-2.77183300	-2.39382100	-0.95186100
C	-2.06353100	-1.53576400	-0.05100300
C	-3.97718900	-1.09244800	1.16248400
H	-4.42616700	-0.56196300	1.99914500
C	-4.76207300	-1.94220200	0.34893400
H	-5.81873500	-2.07187900	0.56002500
C	-4.15637500	-2.58004800	-0.70788000
H	-4.72375500	-3.22934400	-1.36983900
Cl	4.23169200	1.46936500	0.19621600

CN_208_CC_203

Charge = 0, Multiplicity = 1

O	0.76961200	2.94899300	-2.12656500
O	-0.62477300	0.48190100	2.69941900
N	0.07712900	-0.57842200	0.71251900
N	-2.69161400	-0.86201900	0.99662600
C	-3.22391700	2.30288100	1.85101300
H	-2.82541800	1.69956200	2.66821300
H	-4.13662800	1.81943900	1.48142600
H	-3.51072200	3.28269900	2.24820400
C	-0.31780700	2.86459800	-1.31032600
C	-1.40709200	3.72804900	-1.22909800
H	-1.52129100	4.56774600	-1.90570500
C	-2.33015600	3.48969500	-0.20091800
H	-3.17968400	4.16222300	-0.11018400
C	-2.20832900	2.45065700	0.74718000
C	-1.13098200	1.56775000	0.60198500
C	-0.22337700	1.79519100	-0.43205700
C	1.05384800	1.14426300	-0.59465900

C	1.74611400	1.95733800	-1.67513000
H	2.62769200	2.50593800	-1.34247900
H	2.02120700	1.33929300	-2.53563100
C	1.29752400	0.01737800	0.13047100
C	-0.66923900	0.45660400	1.49794200
C	2.52456100	-0.76014800	0.34430900
C	3.84361300	-0.25680000	0.31939600
C	4.95873900	-1.08595800	0.44990900
H	5.94772500	-0.64233300	0.42162500
C	4.79537700	-2.45140000	0.65670700
H	5.66684800	-3.09025100	0.76198600
C	3.50559200	-2.97352600	0.76951900
H	3.35563500	-4.02939800	0.97295300
C	2.40435200	-2.14239300	0.62569700
H	1.40968300	-2.55354200	0.73002300
C	-0.68697700	-1.31993300	-0.22713600
C	-0.10614100	-1.91194400	-1.34297200
H	0.94132300	-1.74714100	-1.55639600
C	-0.84665900	-2.74010700	-2.21250500
H	-0.33517900	-3.18649500	-3.06053400
C	-2.18405000	-2.98622900	-2.00586000
H	-2.75191900	-3.62822700	-2.67286600
C	-2.83251800	-2.36978100	-0.90944500
C	-2.09364100	-1.52042900	-0.02522400
C	-3.97703500	-1.03910900	1.22056400
H	-4.40181100	-0.49684000	2.06234100
C	-4.79053500	-1.87988300	0.42595500
H	-5.84509000	-1.99121000	0.65710000
C	-4.21512100	-2.53231800	-0.63888800
H	-4.80538000	-3.17482800	-1.28732200
Cl	4.18640200	1.46897800	0.28834400

CN_208_CC_208

Charge = 0, Multiplicity = 1

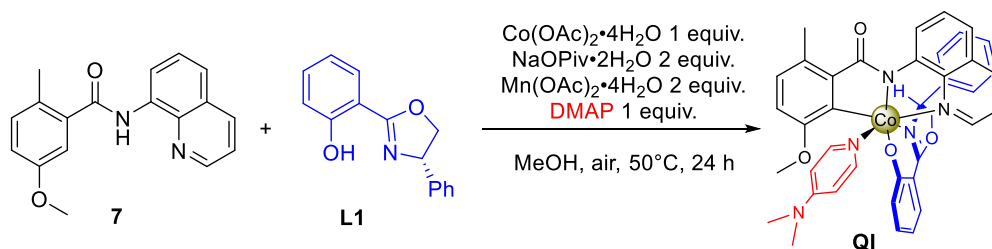
O	0.80864800	2.91869200	-2.16423900
O	-0.57914900	0.49782100	2.67807100
N	0.07608500	-0.59510000	0.69227300
N	-2.69064600	-0.83261400	1.02437200
C	-3.15885100	2.35505300	1.85209300
H	-2.75614200	1.76035600	2.67368300
H	-4.07754300	1.87122700	1.49811100
H	-3.43624500	3.34194300	2.23802400
C	-0.27554500	2.85466100	-1.34097200

S300

C	-1.34347400	3.74303500	-1.24634800
H	-1.44450400	4.58795900	-1.91853400
C	-2.26140600	3.52309600	-0.20927000
H	-3.09415800	4.21485700	-0.10835900
C	-2.15293000	2.48067000	0.73676400
C	-1.09756600	1.57341400	0.57915600
C	-0.19917200	1.78015300	-0.46719800
C	1.06230100	1.10349200	-0.64135300
C	1.76220300	1.89702600	-1.73035200
H	2.66700600	2.41572400	-1.41085800
H	2.00173300	1.27144300	-2.59620300
C	1.29504600	-0.02199300	0.08662300
C	-0.64232900	0.46066400	1.47786600
C	2.52264900	-0.79796700	0.30179400
C	3.83141300	-0.27075300	0.34630100
C	4.95501300	-1.08478100	0.49853700
H	5.93671500	-0.62505400	0.52304300
C	4.80640900	-2.45818400	0.65898800
H	5.68383300	-3.08570400	0.78173600
C	3.52268600	-3.00548200	0.70269000
H	3.38417700	-4.06936900	0.86914800
C	2.41340800	-2.18856400	0.53899100
H	1.42247100	-2.61879100	0.59322900
C	-0.71541100	-1.32803400	-0.23130700
C	-0.16496600	-1.92953300	-1.35748600
H	0.87948900	-1.77621700	-1.59382200
C	-0.93334700	-2.75018200	-2.20990600
H	-0.44481300	-3.20518000	-3.06684900
C	-2.26953600	-2.97807100	-1.97620000
H	-2.85875600	-3.61446000	-2.62991900
C	-2.88853600	-2.34843300	-0.87021300
C	-2.12112100	-1.50645800	-0.00356800
C	-3.97447900	-0.98838000	1.27204500
H	-4.37599000	-0.43406900	2.11741800
C	-4.81448400	-1.82178400	0.49746000
H	-5.86626600	-1.91589700	0.74807800
C	-4.26824600	-2.48882400	-0.57372400
H	-4.87982300	-3.12565100	-1.20784700
Cl	4.14037400	1.46151400	0.36554600

9. Synthesis of Quasi-Intermediate

Synthesis and characterization of quasi-intermediate (QI)



5-methoxy-2-methyl-*N*-(quinolin-8-yl)benzamide **7** (58.4 mmol, 0.2 mmol), DMAP (24.4 mg, 0.2 mmol), **L1** (47.8 mg, 0.2 mmol), cobalt(II) acetate tetrahydrate (49.8 mg, 0.2 mmol), NaOPiv·*x*H₂O (64 mg, 0.4 mmol), manganese(II) acetate tetrahydrate (49.0 mg, 0.4 mmol) and methanol (2 mL) was added to a 10 mL sealed tube. Then the tube was sealed and heated on an aluminum heat transfer block for 17 h. Then the mixture was filtered through a pad of celite and the filtrate was evaporated. Purification by flash chromatography (20:30:50 EA:DCM:PE) gave **QI** as a dark greenish-brown amorphous solid (56.6 mg, 40%).

The product was then dissolved in chloroform. A slow evaporation of the solvent at room temperature gave dark brown crystals for XRD. The crystal contains solvent of crystallization, whose chemical formula is C₄₀H₃₆CoN₅O₄·5/2CHCl₃.

¹H NMR (400 MHz, Chloroform-*d*) δ 9.13 (d, *J* = 7.9 Hz, 1H), 9.04 (dd, *J* = 4.7, 1.4 Hz, 1H), 7.85 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.59 – 7.51 (m, 3H), 7.38 (dd, *J* = 8.2, 4.7 Hz, 1H), 7.33 – 7.22 (m, 3H), 7.13 (d, *J* = 8.5 Hz, 1H), 6.94 (dd, *J* = 21.3, 8.0 Hz, 2H), 6.57 (dd, *J* = 21.3, 7.7 Hz, 2H), 6.45 (dt, *J* = 14.5, 7.4 Hz, 3H), 6.23 (d, *J* = 7.4 Hz, 2H), 5.95 (d, *J* = 6.8 Hz, 2H), 4.25 (dd, *J* = 9.2, 3.3 Hz, 1H), 3.97 (t, *J* = 8.8 Hz, 1H), 3.75 (dd, *J* = 8.3, 3.3 Hz, 1H), 3.26 (s, 3H), 2.78 (s, 3H), 2.70 (s, 6H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 178.48, 171.74, 165.98, 163.15, 153.63, 150.04, 147.39, 146.96, 146.51, 145.13, 139.62, 136.19, 133.31, 131.70, 129.04, 128.75, 128.38, 127.94, 126.93, 126.37, 124.46, 122.56, 121.38, 121.18, 117.42, 112.15, 111.97, 109.56, 106.52, 74.36, 66.21, 55.62, 38.76, 19.83.

HRMS (ESI) *m/z*: [M+H]⁺ Calculated for C₄₀H₃₇CoN₅O₄⁺ 710.2172; found: 710.2175.

[α]_D²⁰ = +969° (*c* = 0.261, THF)

10.X-ray Crystallographic Data of 2a, 2d, 2m and QI

Single crystals of **2a** were obtained by evaporation from its acetone solution.

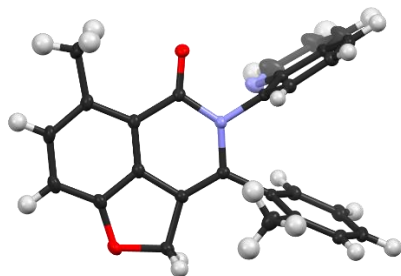


Figure S19. X-Ray crystallographic data of **2a**. The ellipsoids drawn at 30% probability level.

CCDC 2132392

Table S16. Crystal data and structure refinement for **2a**

Identification code	cu_201214_WBJ_1140_2_0m
Empirical formula	C ₂₇ H ₂₀ N ₂ O ₂
Formula weight	404.45
Temperature/K	170.0
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	11.1485(12)
b/Å	11.6290(11)
c/Å	16.013(3)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	2076.0(4)
Z	4
ρ _{calc} /cm ³	1.294
μ/mm ⁻¹	0.654
F(000)	848.0
Crystal size/mm ³	0.48 × 0.38 × 0.32
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	9.398 to 136.768
Index ranges	-13 ≤ h ≤ 13, -13 ≤ k ≤ 14, -19 ≤ l ≤ 19
Reflections collected	22740
Independent reflections	3797 [R _{int} = 0.0238, R _{sigma} = 0.0167]
Data/restraints/parameters	3797/0/282

Goodness-of-fit on F^2	1.093
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0316$, $wR_2 = 0.0786$
Final R indexes [all data]	$R_1 = 0.0316$, $wR_2 = 0.0786$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.16/-0.26
Flack parameter	0.04(3)

Single crystals of **2d** were obtained by evaporation from its acetone solution.

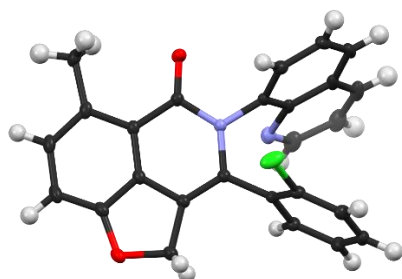


Figure S20. X-Ray crystallographic data of **2d**. The ellipsoids drawn at 30% probability level.

CCDC 2132395

For the single crystals of **2d**, each asymmetric unit has two molecules whose dihedral angles of the C-C and C-N axes are different. But their absolute configurations of both axes are identical. Only one is shown here and in the article for clarity.

Table S17. Crystal data and structure refinement for **2d**

Identification code	mo_210406_WBJ_2006_2_0m
Empirical formula	C ₂₆ H ₁₇ ClN ₂ O ₂
Formula weight	424.86
Temperature/K	170.0
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	10.593(2)
b/Å	11.753(2)
c/Å	32.743(6)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	4076.8(13)
Z	8
ρ _{calc} /cm ³	1.384
μ/mm ⁻¹	0.214
F(000)	1760.0
Crystal size/mm ³	0.49 × 0.42 × 0.38
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.266 to 54.26
Index ranges	-13 ≤ h ≤ 13, -15 ≤ k ≤ 15, -41 ≤ l ≤ 41
Reflections collected	83005
Independent reflections	9024 [R _{int} = 0.0536, R _{sigma} = 0.0249]

Data/restraints/parameters 9024/0/561
Goodness-of-fit on F^2 1.032
Final R indexes [$I \geq 2\sigma(I)$] $R_1 = 0.0302$, $wR_2 = 0.0749$
Final R indexes [all data] $R_1 = 0.0363$, $wR_2 = 0.0789$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$ 0.14/-0.26
Flack parameter 0.017(15)

Single crystals of **2m** were obtained by evaporation from its acetone/chloroform solution.

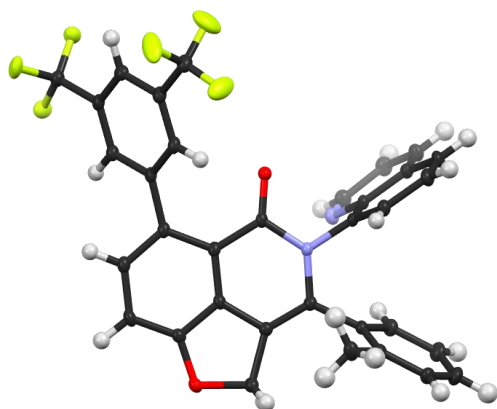


Figure S21. X-Ray crystallographic data of **2m**. The ellipsoids drawn at 30% probability level.

CCDC 2132394

Table S18. Crystal data and structure refinement for **2m**

Identification code	cu_210420_wbj_2015_2_0m
Empirical formula	C _{36.49} H _{24.72} Cl _{0.77} F ₆ N ₂ O _{2.74}
Formula weight	676.32
Temperature/K	170.0
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	8.032(4)
b/Å	15.966(9)
c/Å	23.757(13)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	3047(3)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.475
μ/mm^{-1}	1.611
F(000)	1387.0
Crystal size/mm ³	0.604 × 0.158 × 0.116
Radiation	CuK α (λ = 1.54178)
2 θ range for data collection/°	6.67 to 137.11
Index ranges	-9 ≤ h ≤ 9, -18 ≤ k ≤ 19, -28 ≤ l ≤ 28
Reflections collected	26718
Independent reflections	5614 [R _{int} = 0.0670, R _{sigma} = 0.0452]
Data/restraints/parameters	5614/59/473

Goodness-of-fit on F^2	1.107
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0411$, $wR_2 = 0.0957$
Final R indexes [all data]	$R_1 = 0.0441$, $wR_2 = 0.0969$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.25/-0.23
Flack parameter	0.100(19)

Single crystals of **QI** were obtained by slow evaporation from its chloroform solution.

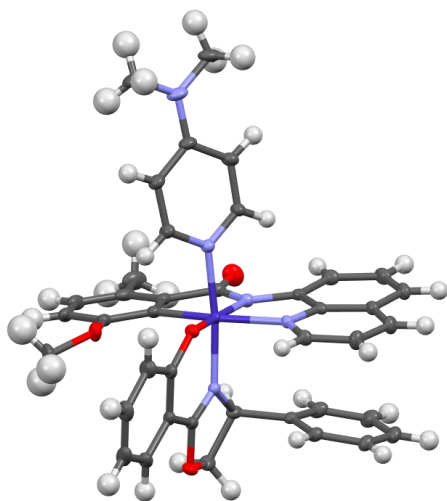


Figure S22. X-Ray crystallographic data of **QI**. The ellipsoids drawn at 30% probability level.

CCDC 2132393

Table S19 Crystal data and structure refinement for **QI**

Identification code	mo_210329_WBJ_2004_2_0m
Empirical formula	C ₈₅ H ₇₇ Cl ₁₅ Co ₂ N ₁₀ O ₈
Formula weight	2016.17
Temperature/K	170.0
Crystal system	monoclinic
Space group	C2
a/Å	21.1851(11)
b/Å	13.4394(6)
c/Å	16.0551(9)
α/°	90
β/°	99.028(2)
γ/°	90
Volume/Å ³	4514.5(4)
Z	2
ρ _{calc} /cm ³	1.483
μ/mm ⁻¹	0.871
F(000)	2060.0
Crystal size/mm ³	0.29 × 0.23 × 0.18
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.598 to 54.24
Index ranges	-26 ≤ h ≤ 27, -17 ≤ k ≤ 17, -20 ≤ l ≤ 20
Reflections collected	49493

Independent reflections	9959 [$R_{\text{int}} = 0.0466$, $R_{\text{sigma}} = 0.0380$]
Data/restraints/parameters	9959/7/563
Goodness-of-fit on F^2	1.050
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0481$, $wR_2 = 0.1289$
Final R indexes [all data]	$R_1 = 0.0566$, $wR_2 = 0.1358$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	1.26/-0.55
Flack parameter	0.018(5)

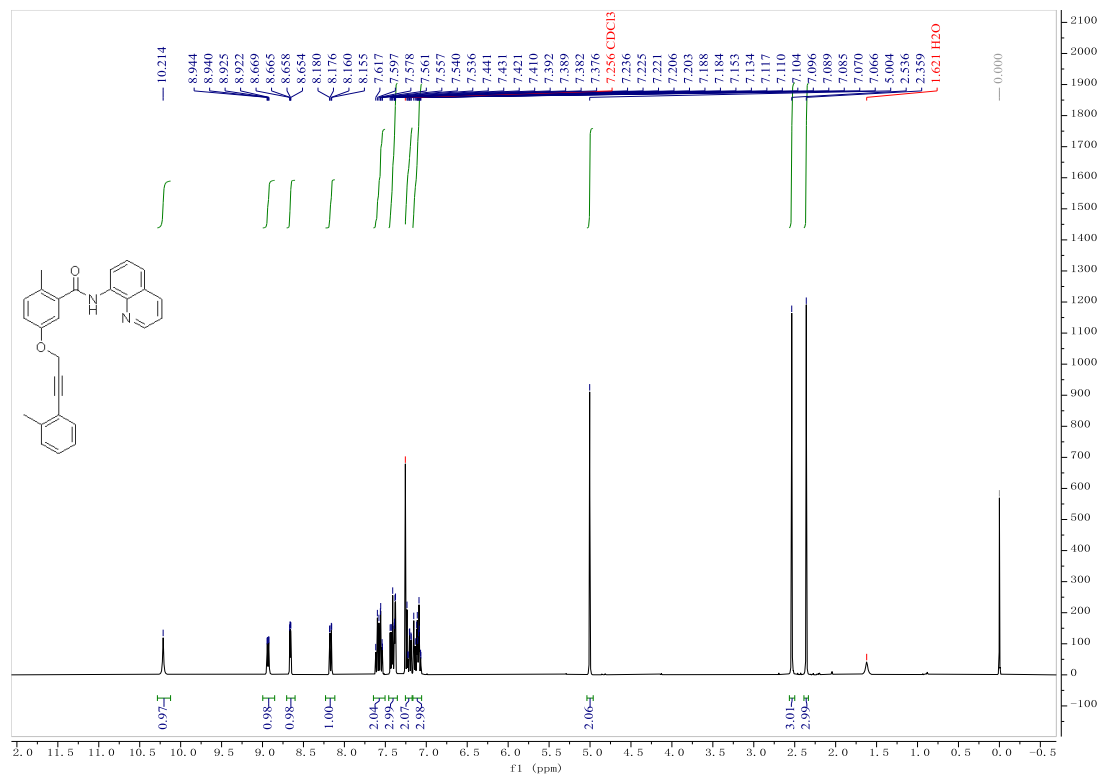
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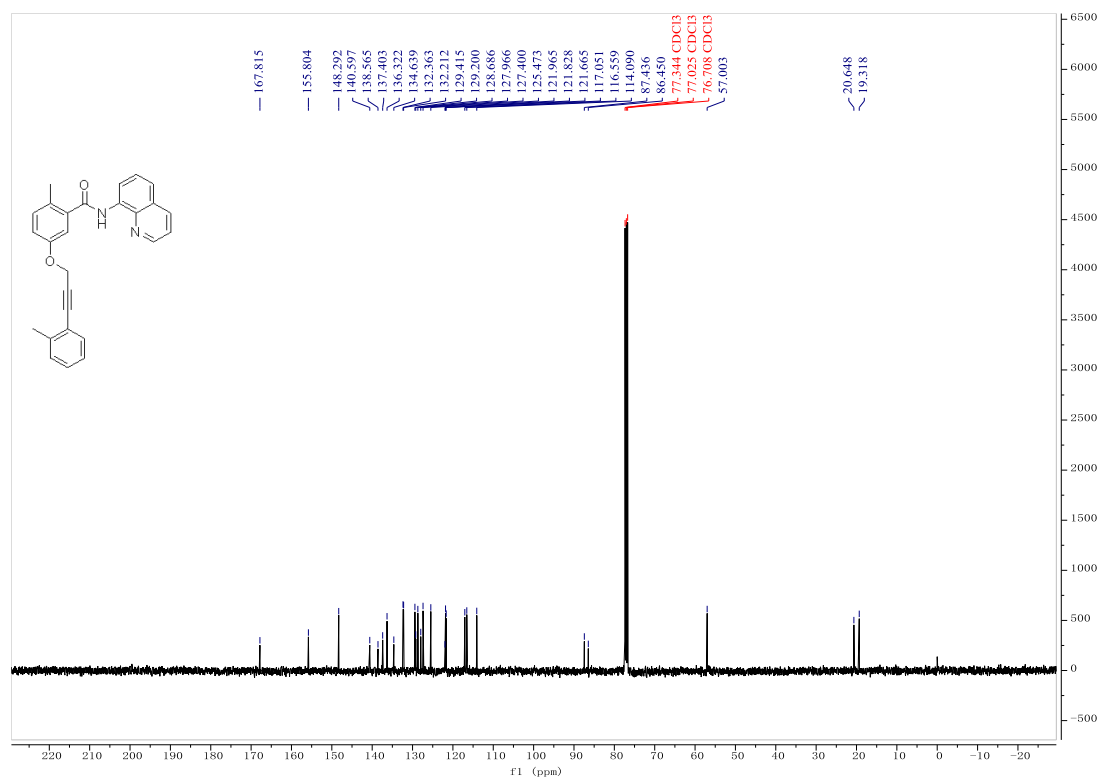
12. NMR Spectra

1a

¹H NMR (400 MHz, Chloroform-*d*)

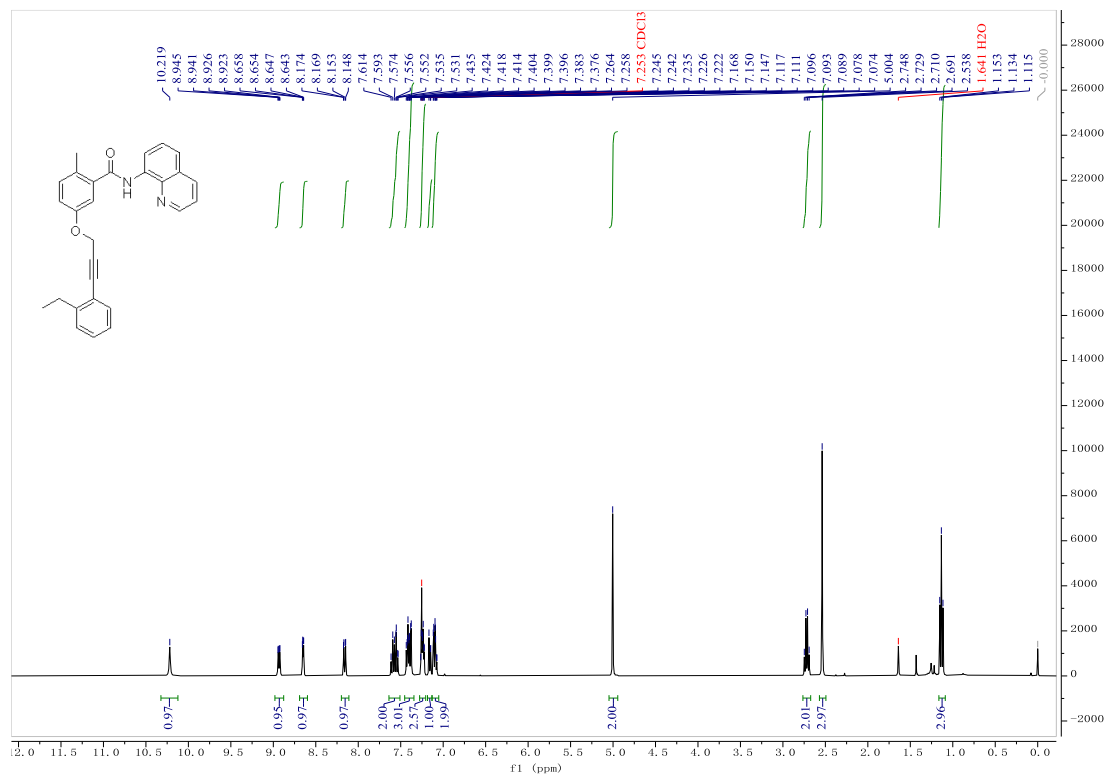


¹³C NMR (101 MHz, Chloroform-*d*)

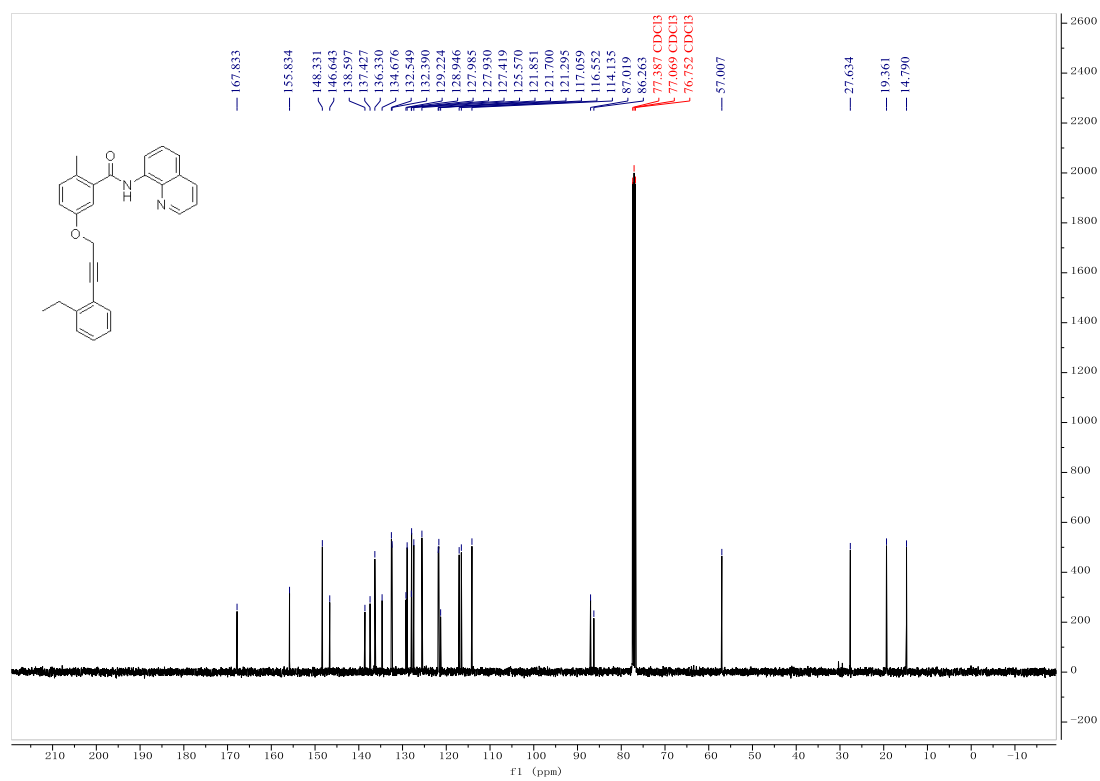


1b

¹H NMR (400 MHz, Chloroform-*d*)

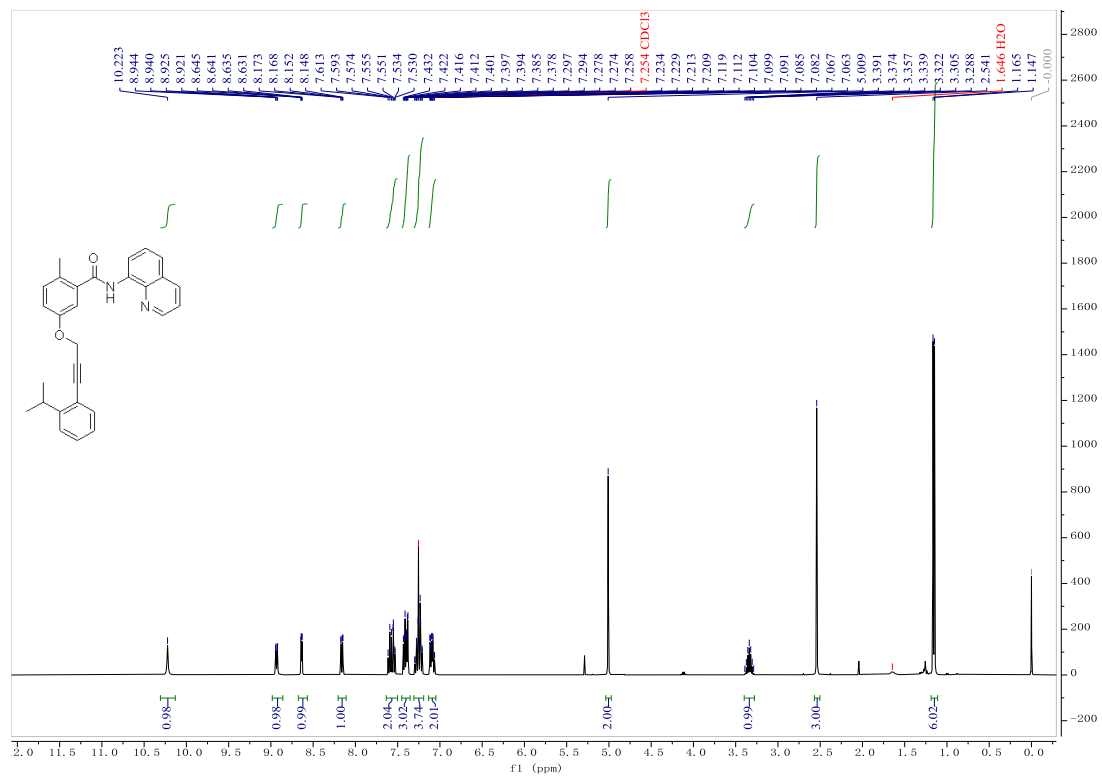


¹³C NMR (101 MHz, Chloroform-*d*)

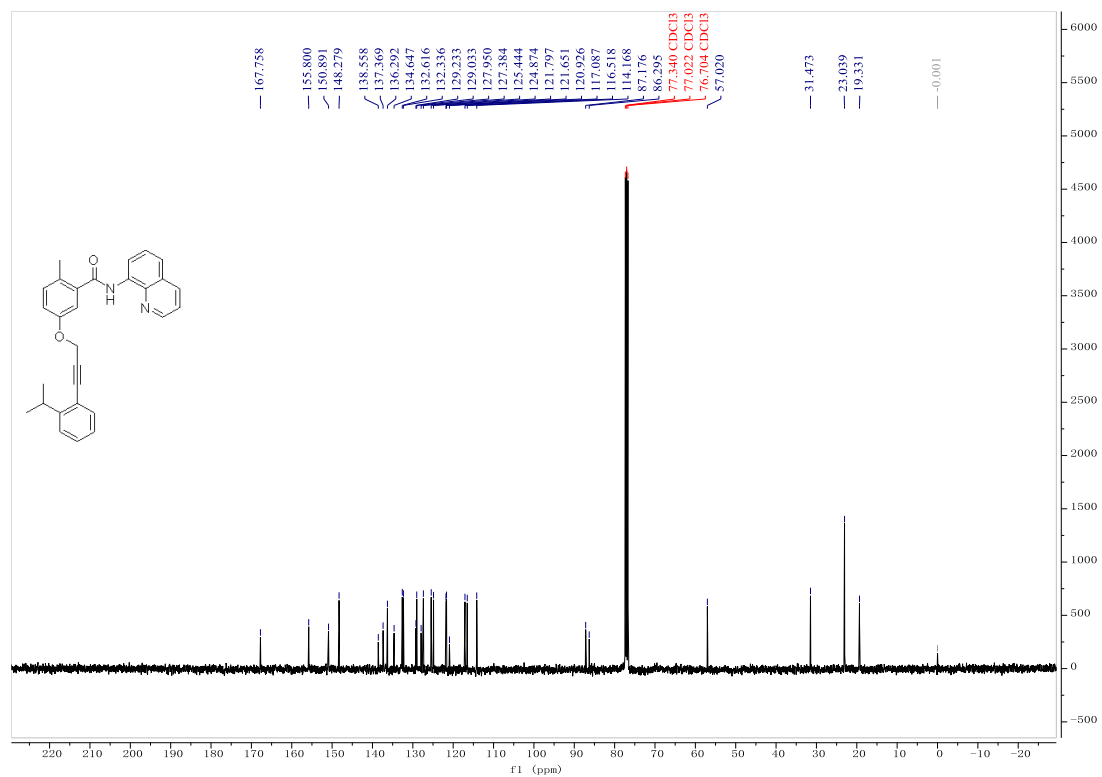


1c

¹H NMR (400 MHz, Chloroform-*d*)

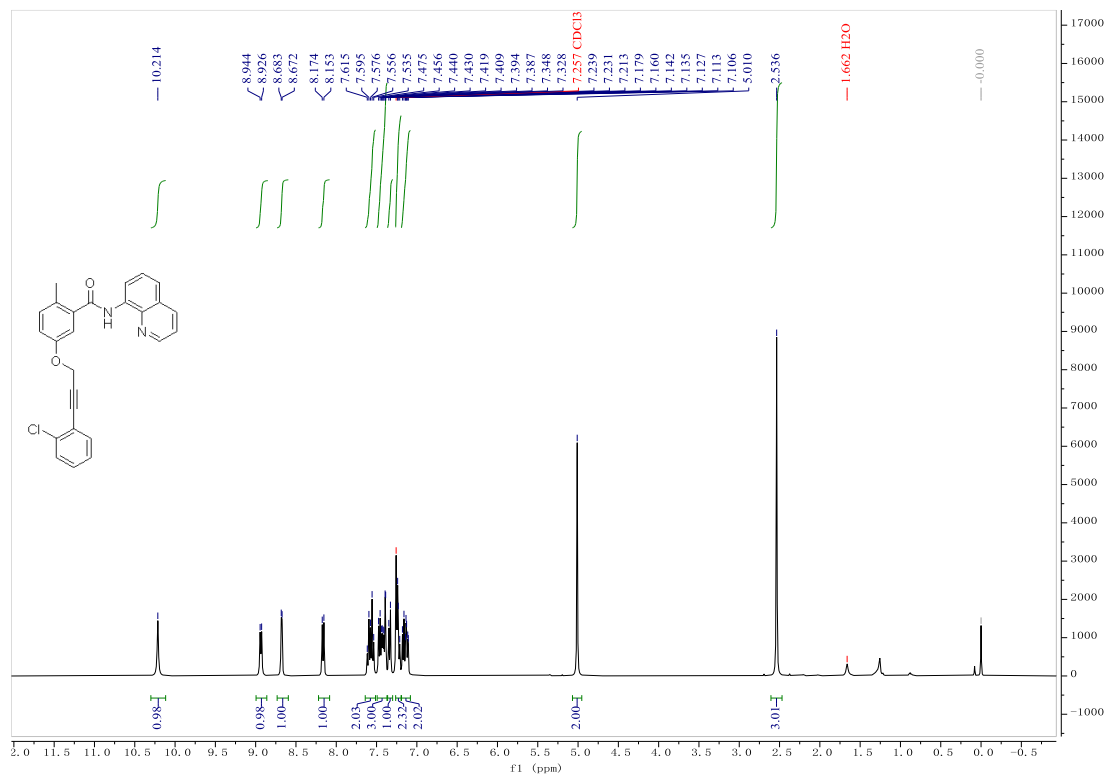


¹³C NMR (101 MHz, Chloroform-*d*)

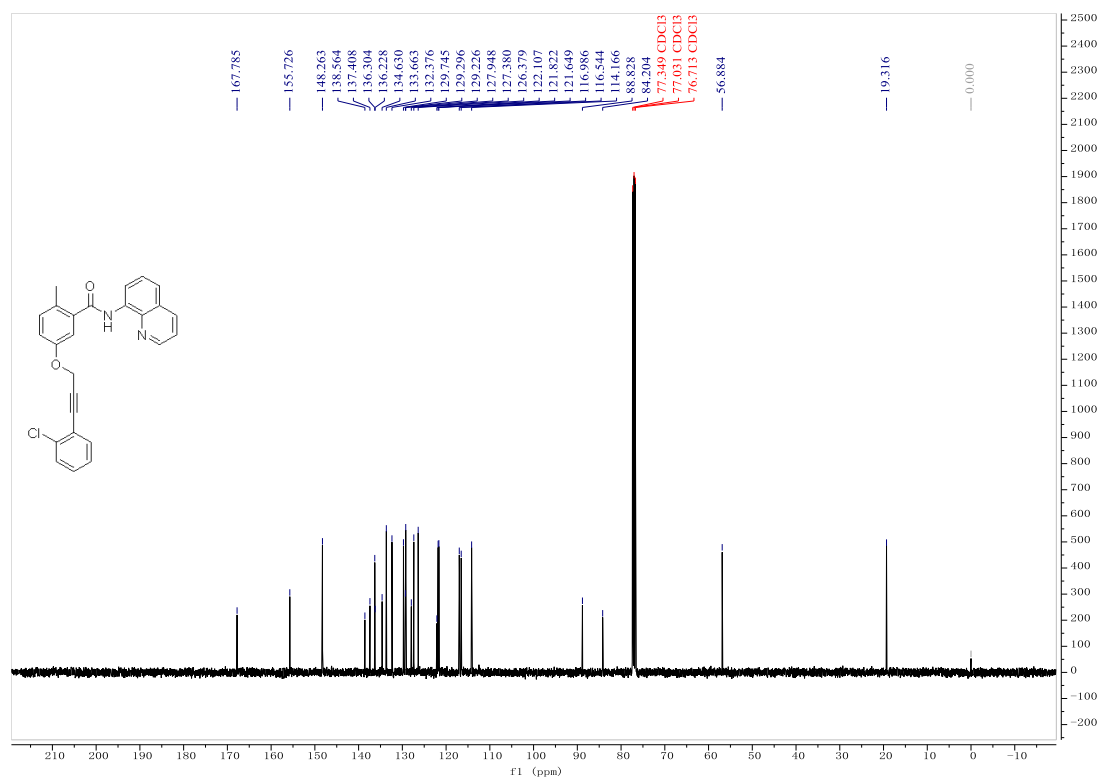


1d

¹H NMR (400 MHz, Chloroform-*d*)

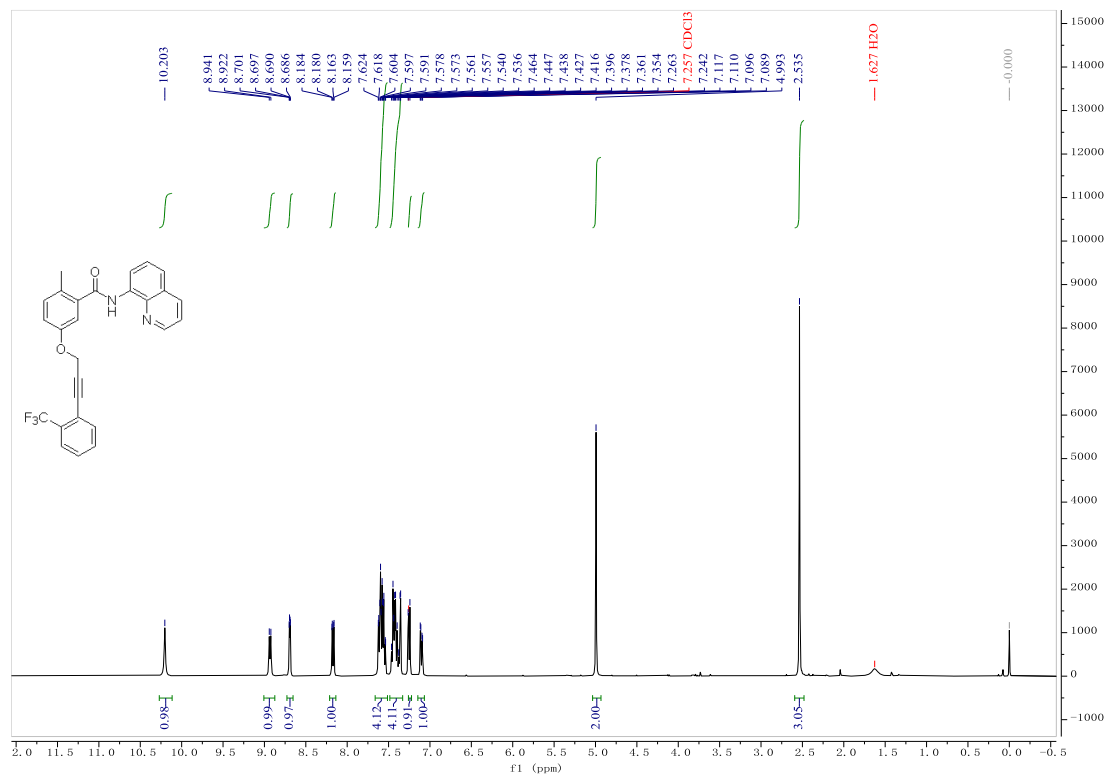


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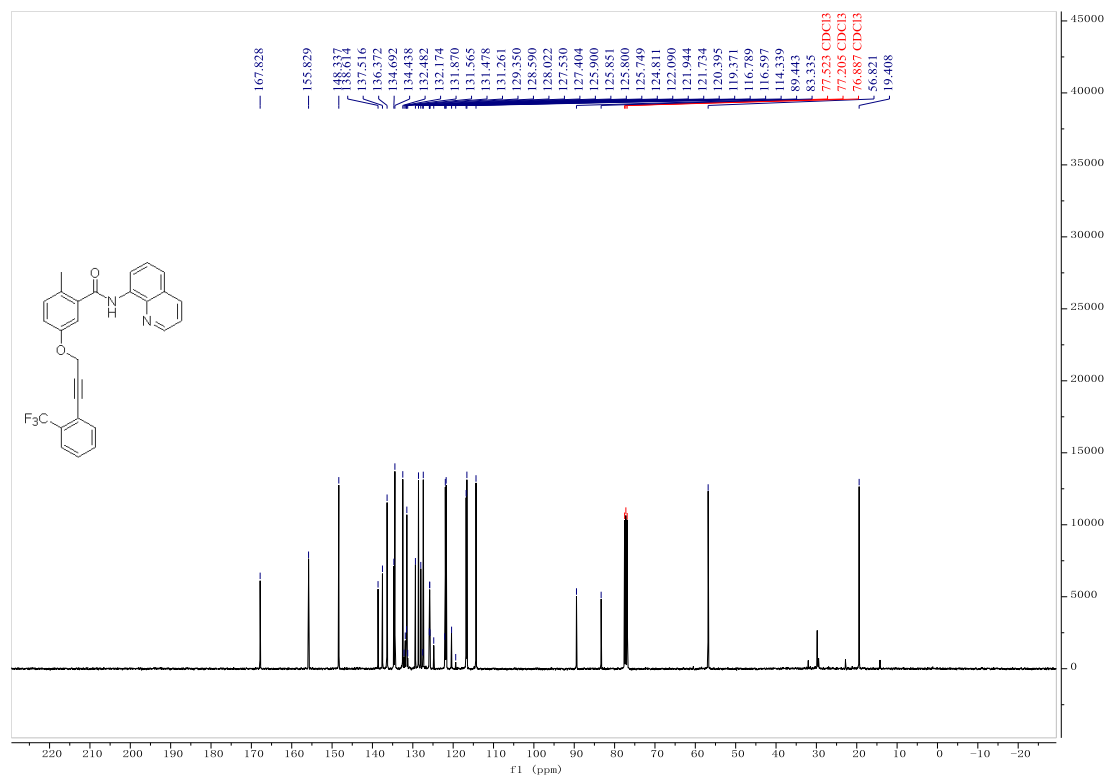


1e

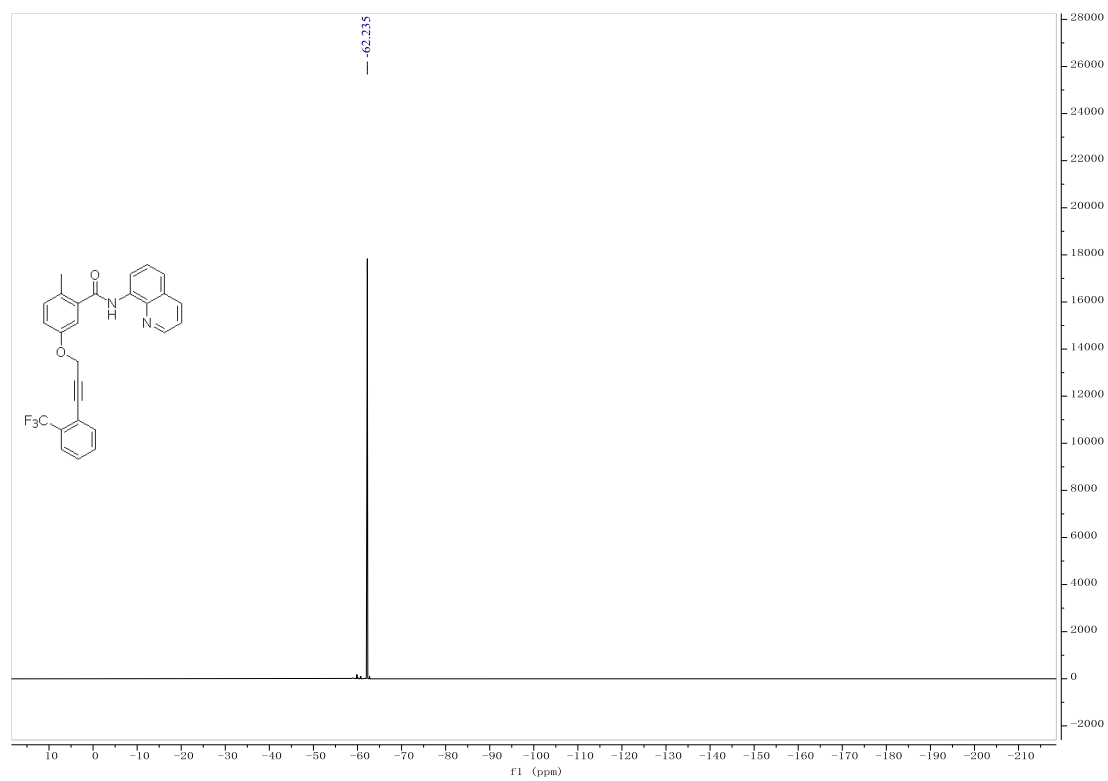
¹H NMR (400 MHz, Chloroform-*d*)



¹³C NMR (101 MHz, Chloroform-*d*)

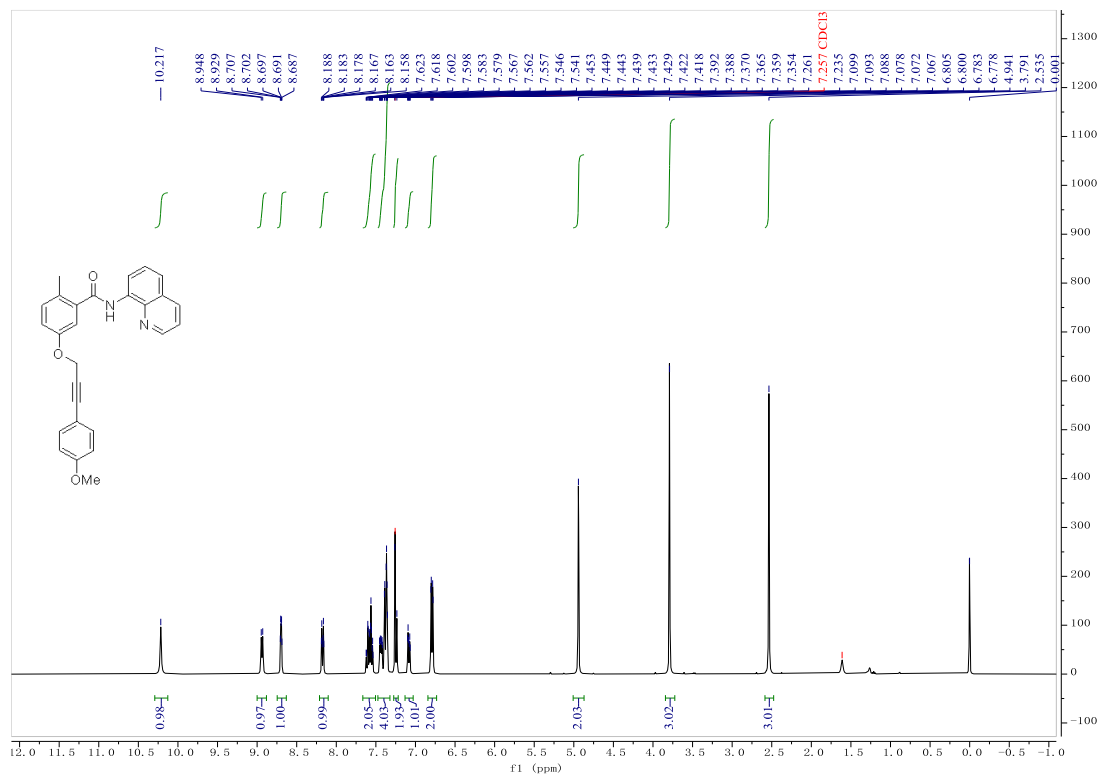


¹⁹F NMR (376 MHz, Chloroform-*d*)

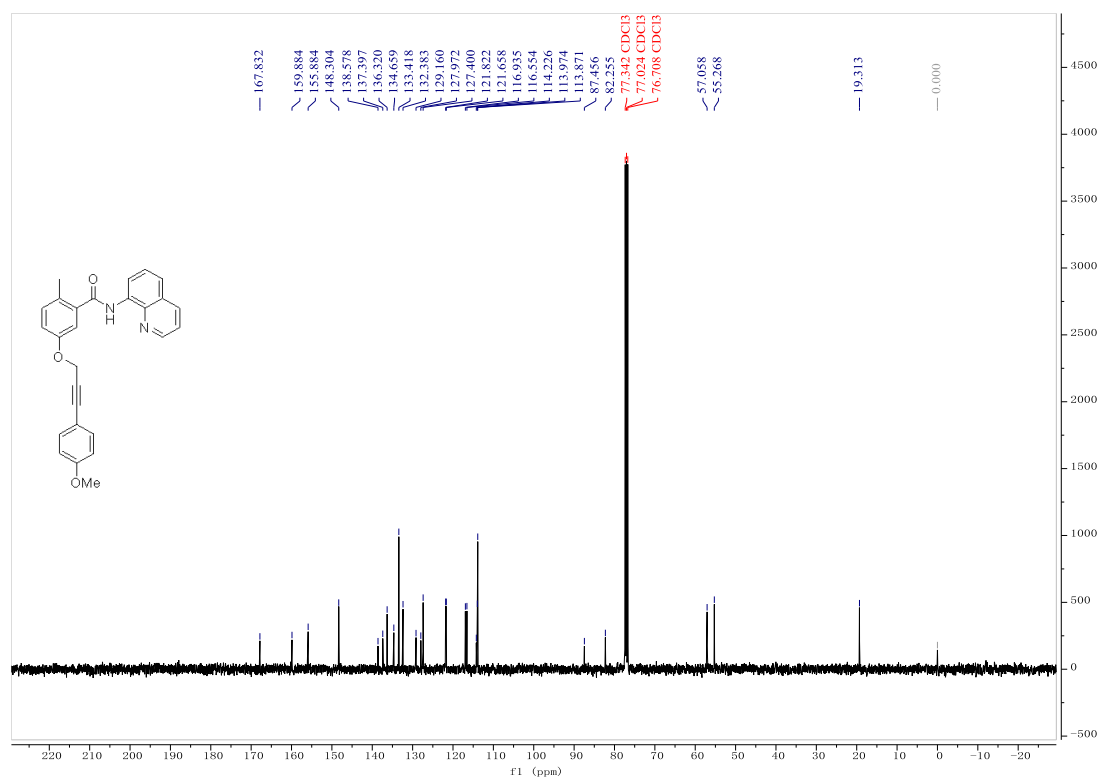


1f

¹H NMR (400 MHz, Chloroform-*d*)

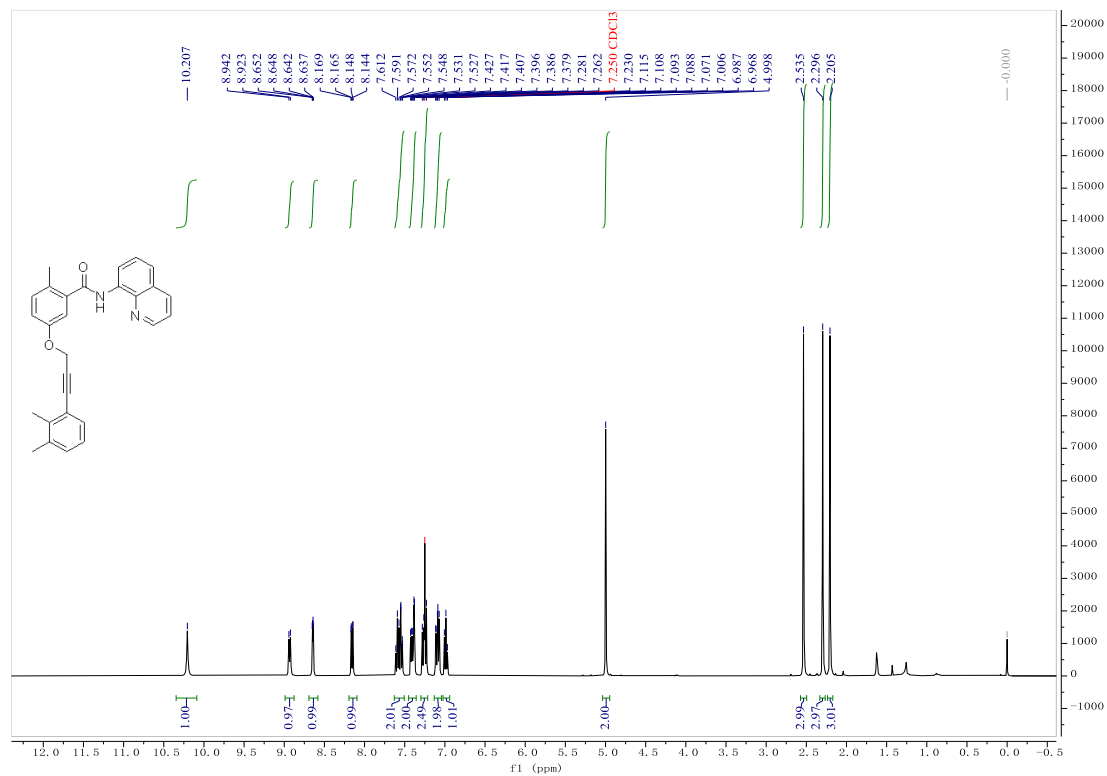


¹³C NMR (101 MHz, Chloroform-*d*)

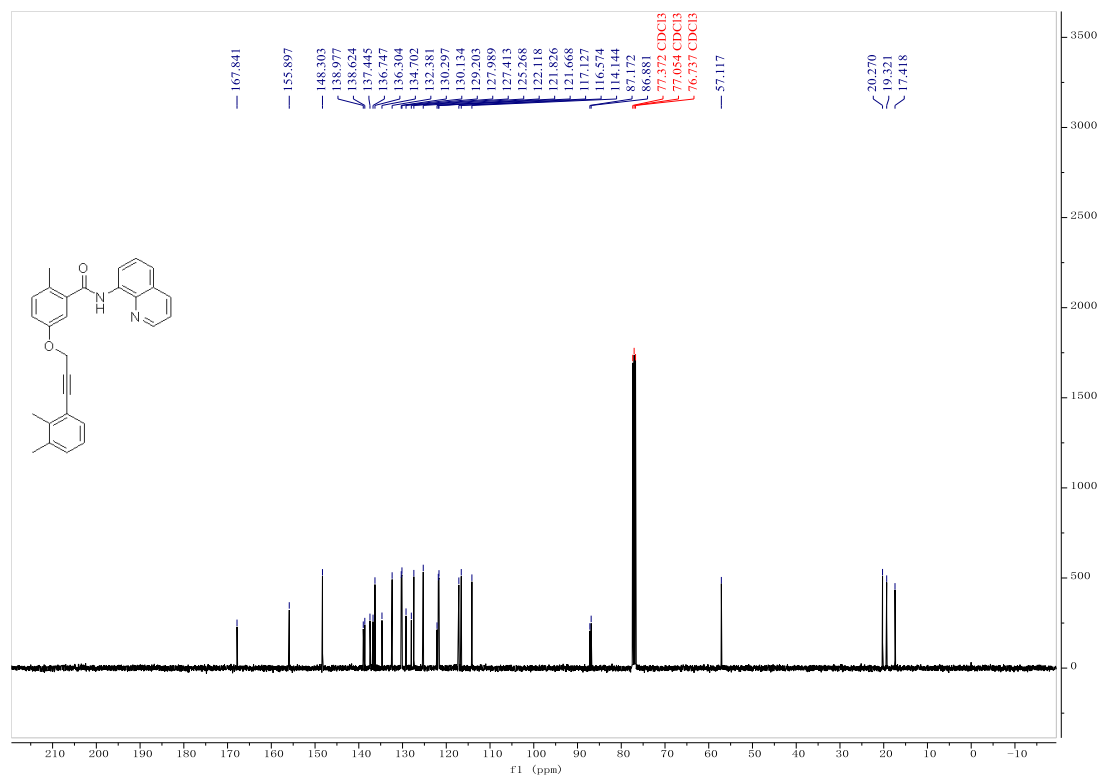


1g

¹H NMR (400 MHz, Chloroform-*d*)

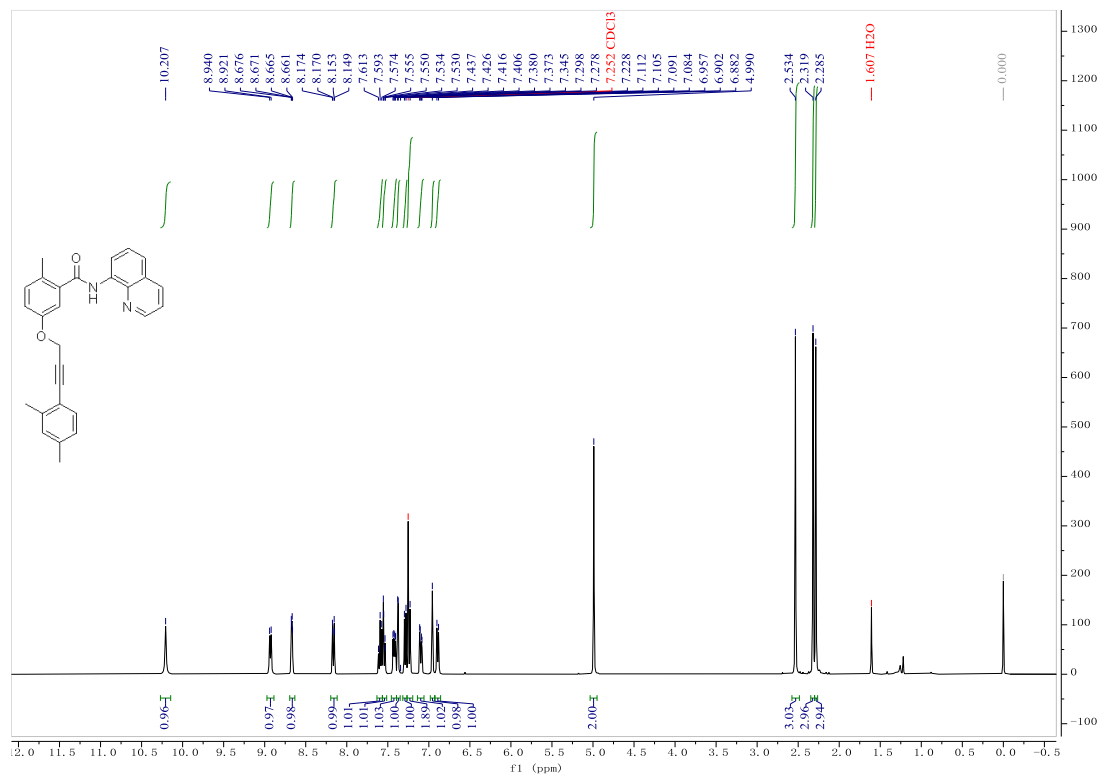


¹³C NMR (101 MHz, Chloroform-*d*)

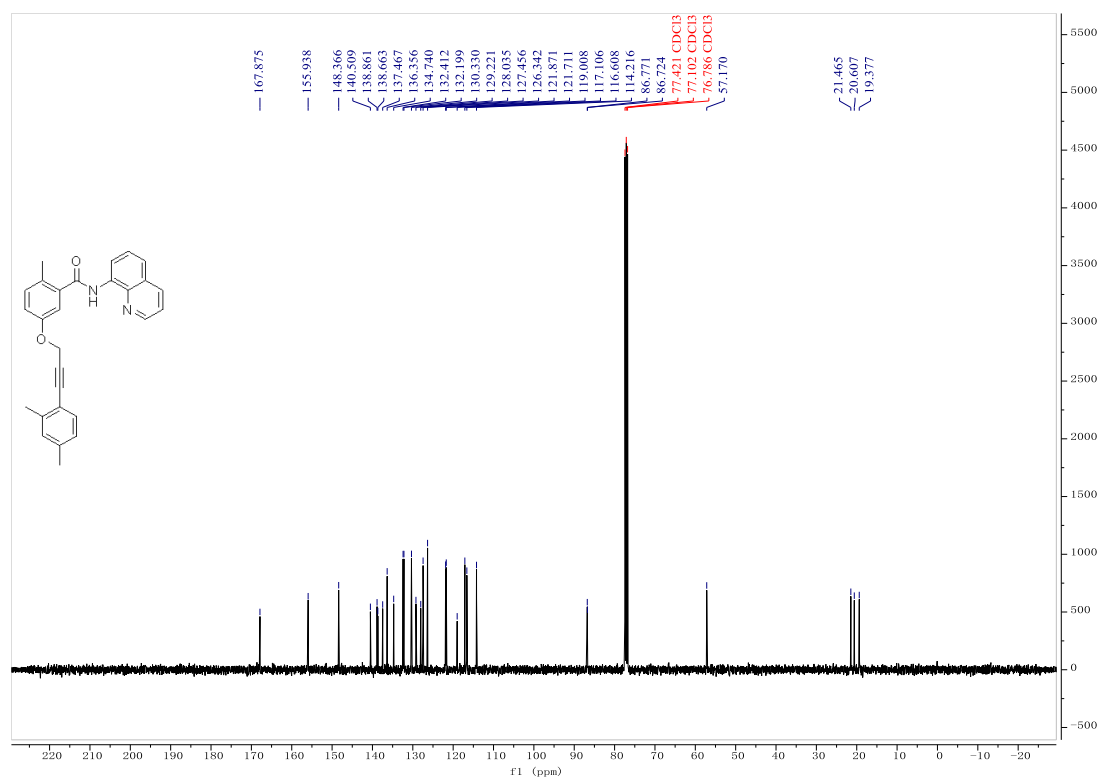


1h

¹H NMR (400 MHz, Chloroform-*d*)

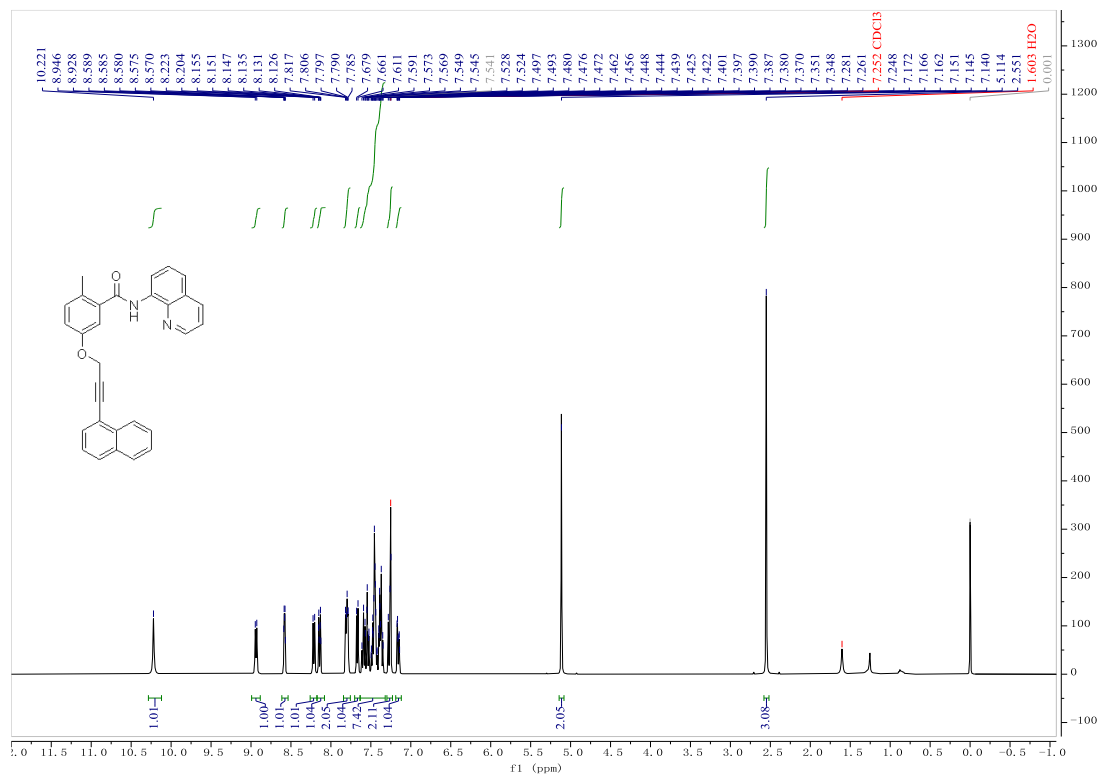


¹³C NMR (101 MHz, Chloroform-*d*)

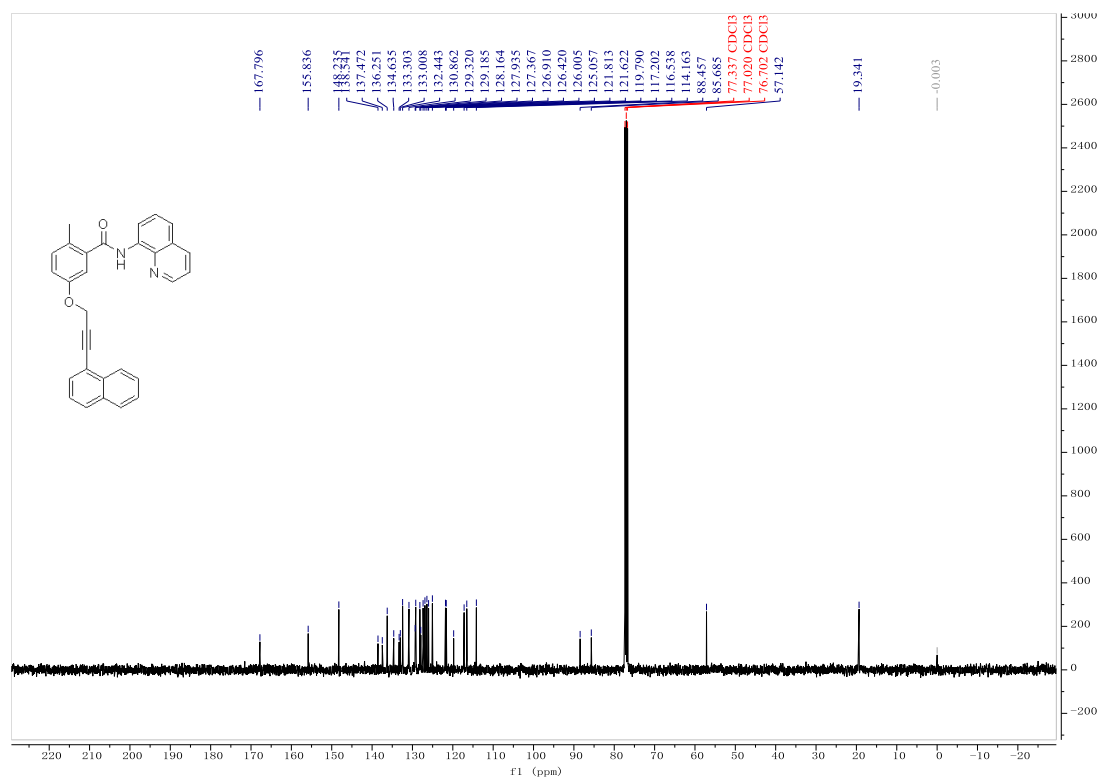


1i

¹H NMR (400 MHz, Chloroform-*d*)

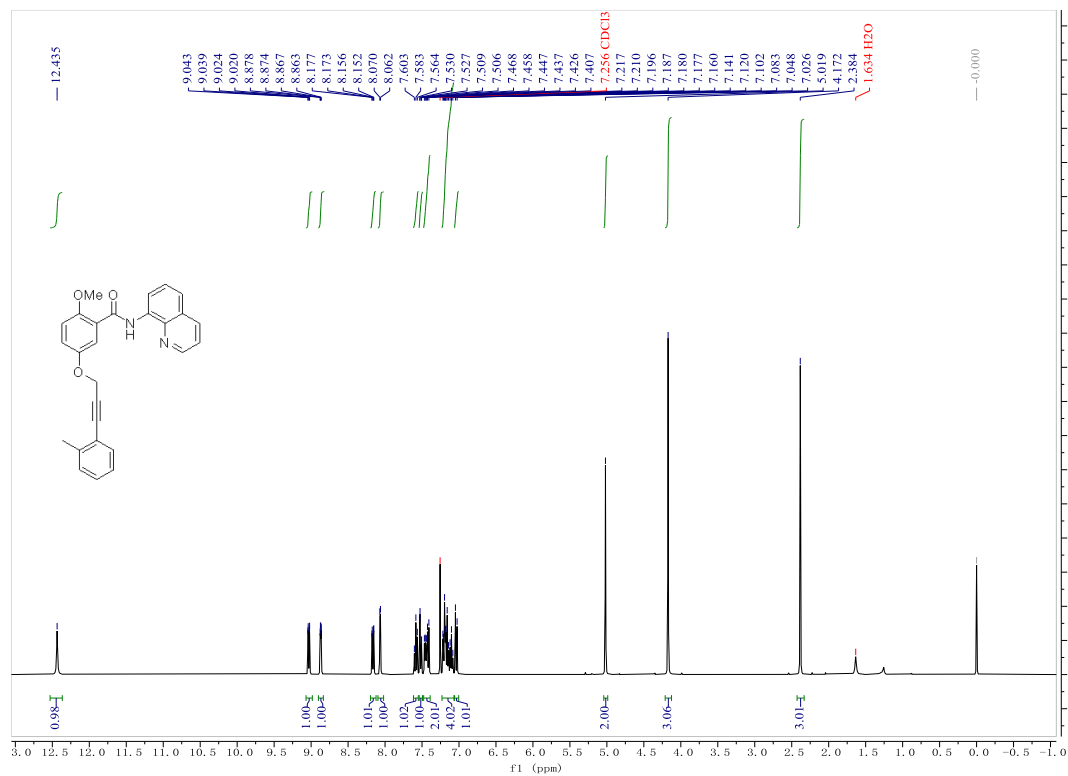


¹³C NMR (101 MHz, Chloroform-*d*)

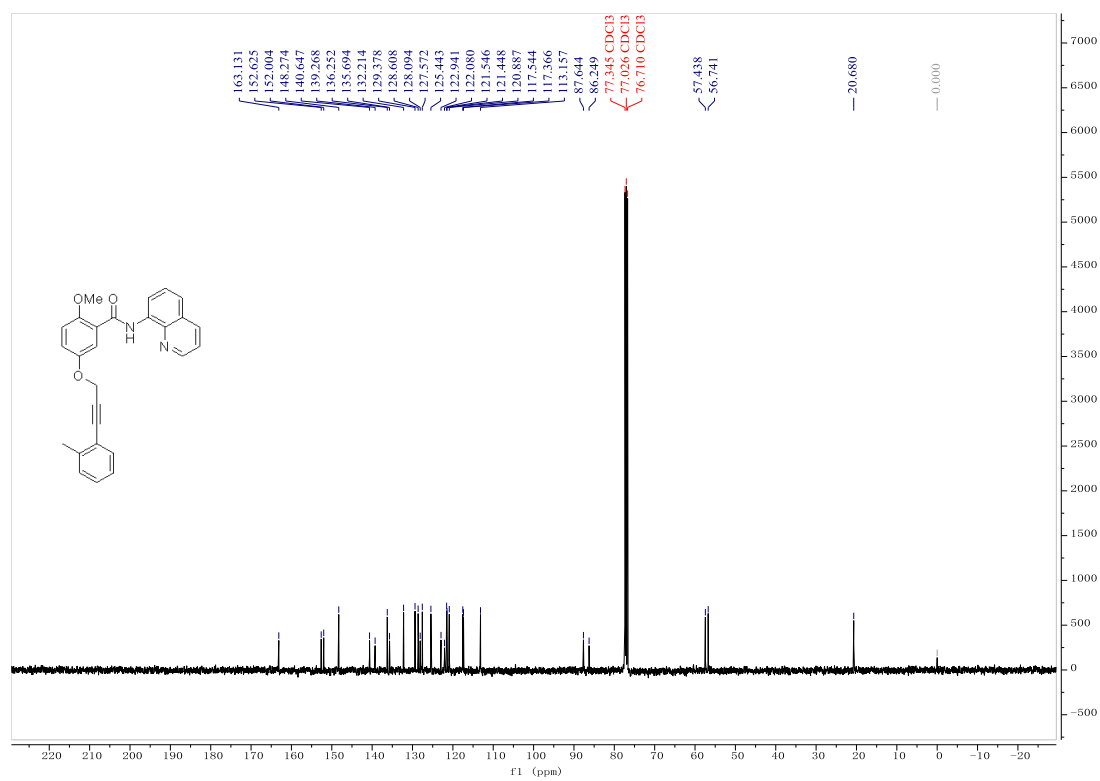


1j

¹H NMR (400 MHz, Chloroform-*d*)

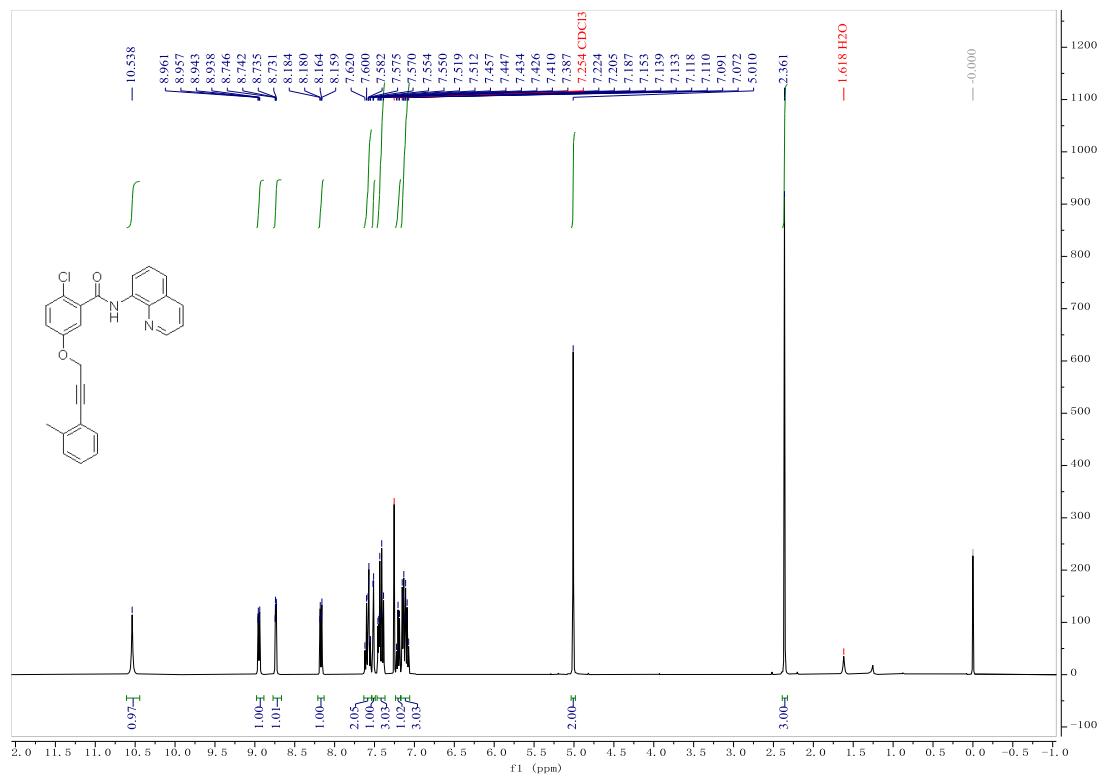


¹³C NMR (101 MHz, Chloroform-*d*)

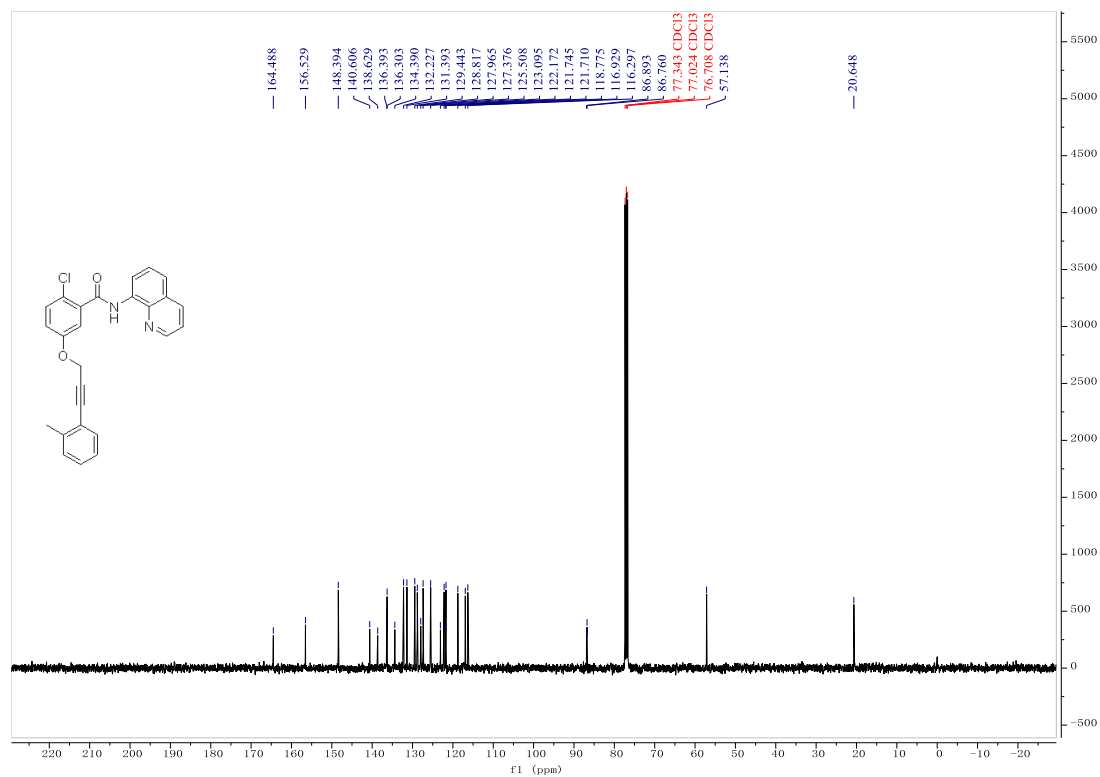


1k

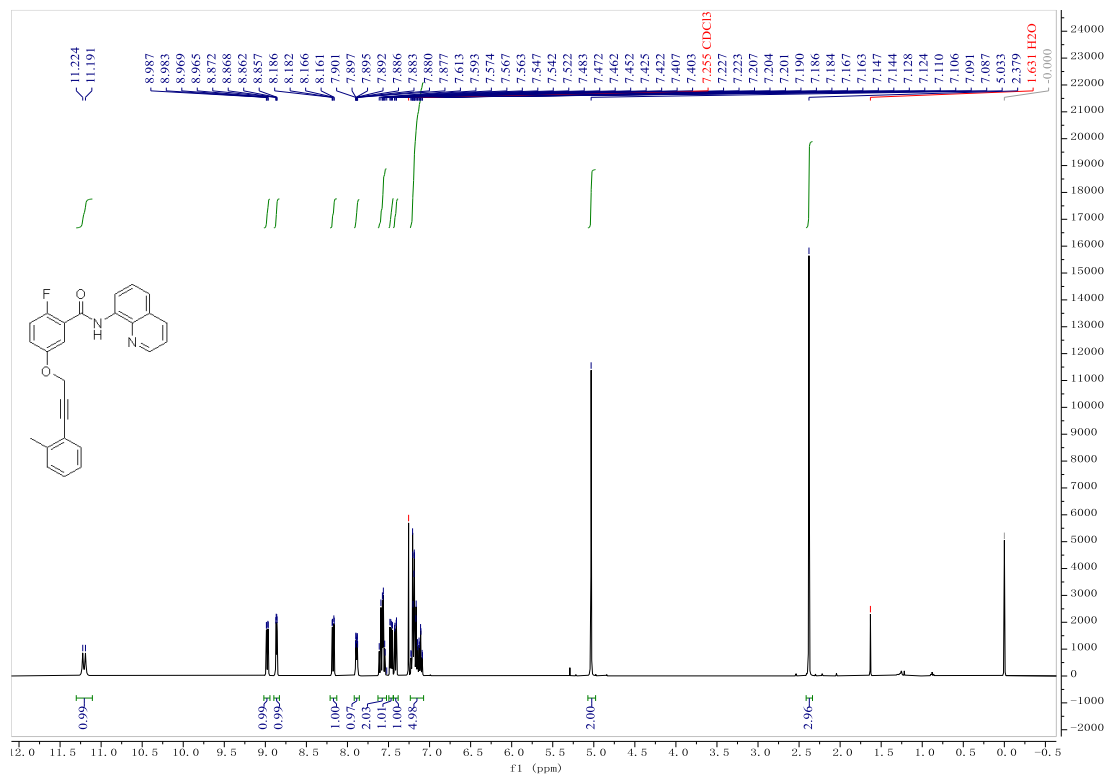
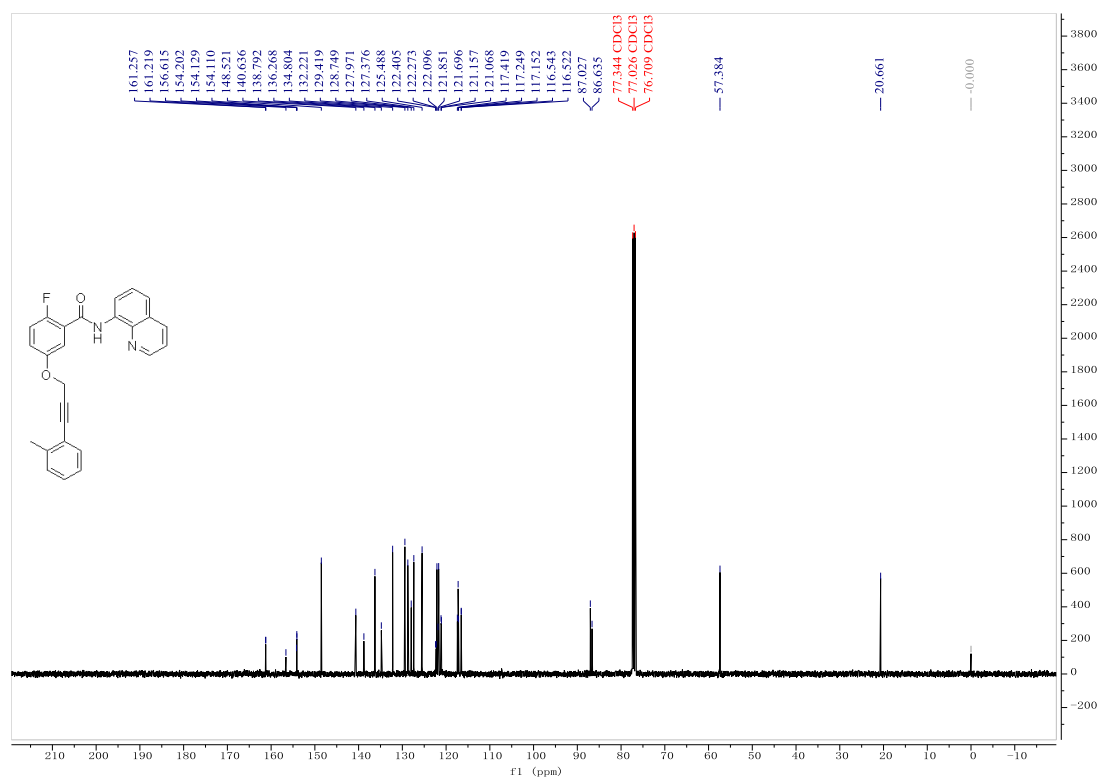
¹H NMR (400 MHz, Chloroform-*d*)



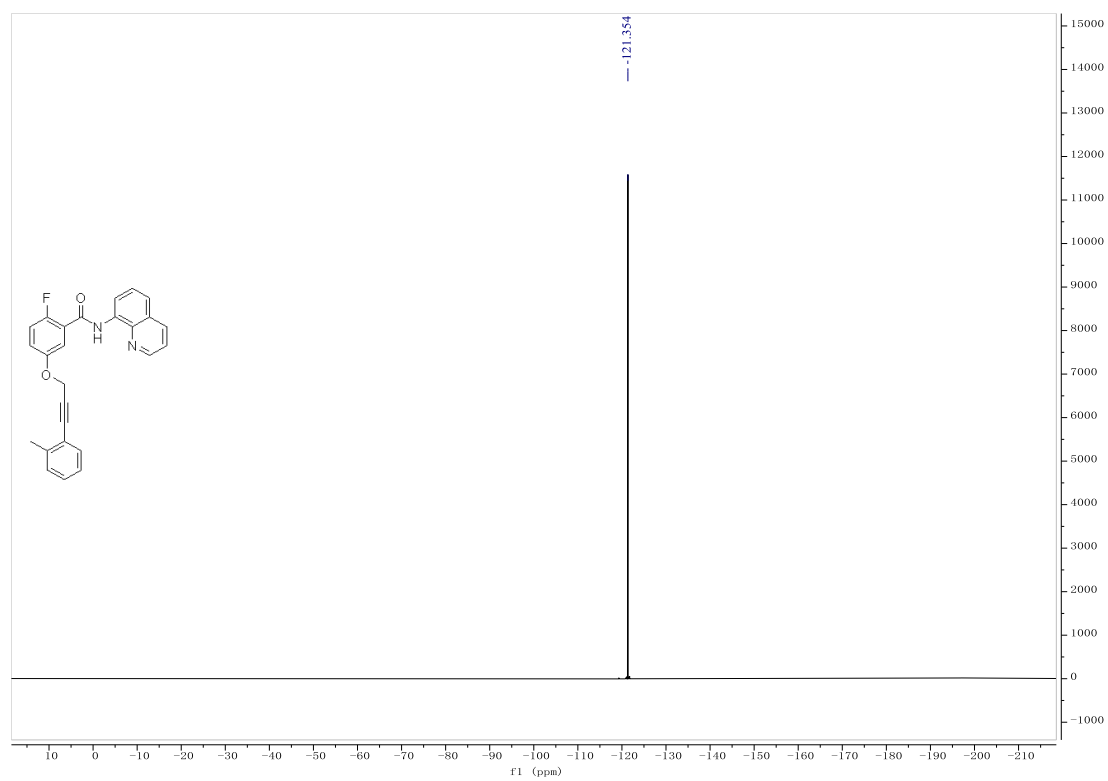
¹³C NMR (101 MHz, Chloroform-*d*)



11

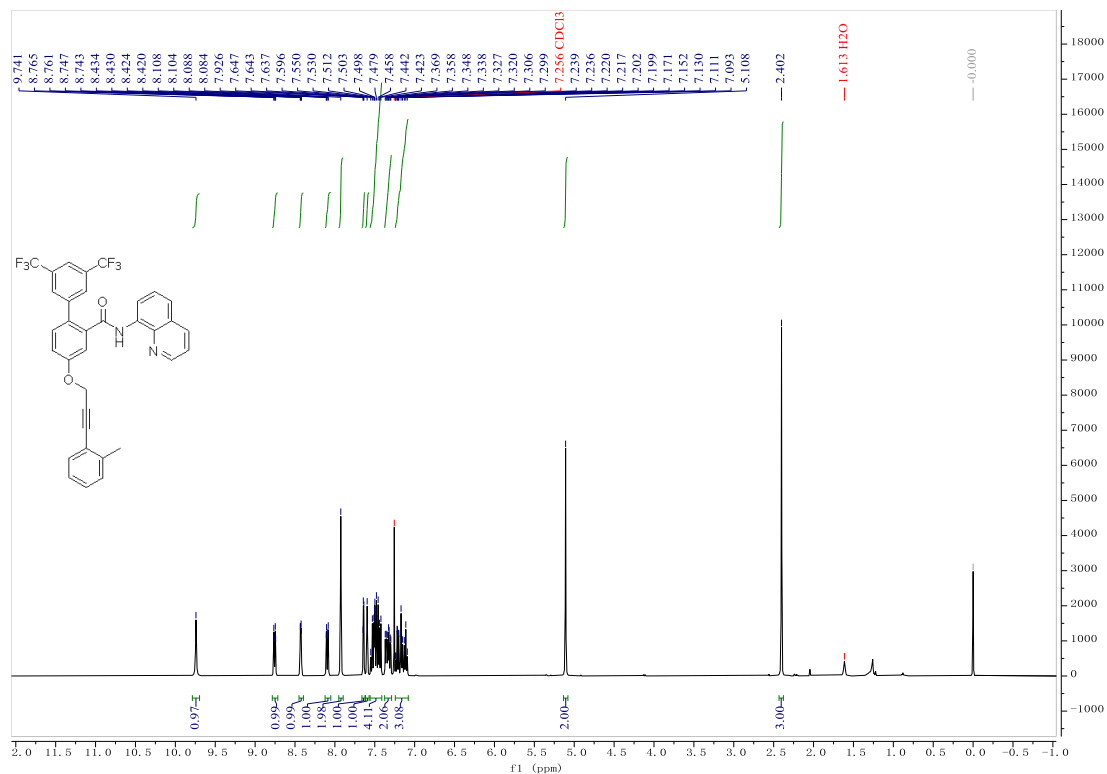
¹H NMR (400 MHz, Chloroform-*d*)¹³C NMR (101 MHz, Chloroform-*d*)

¹⁹F NMR (376 MHz, Chloroform-*d*)

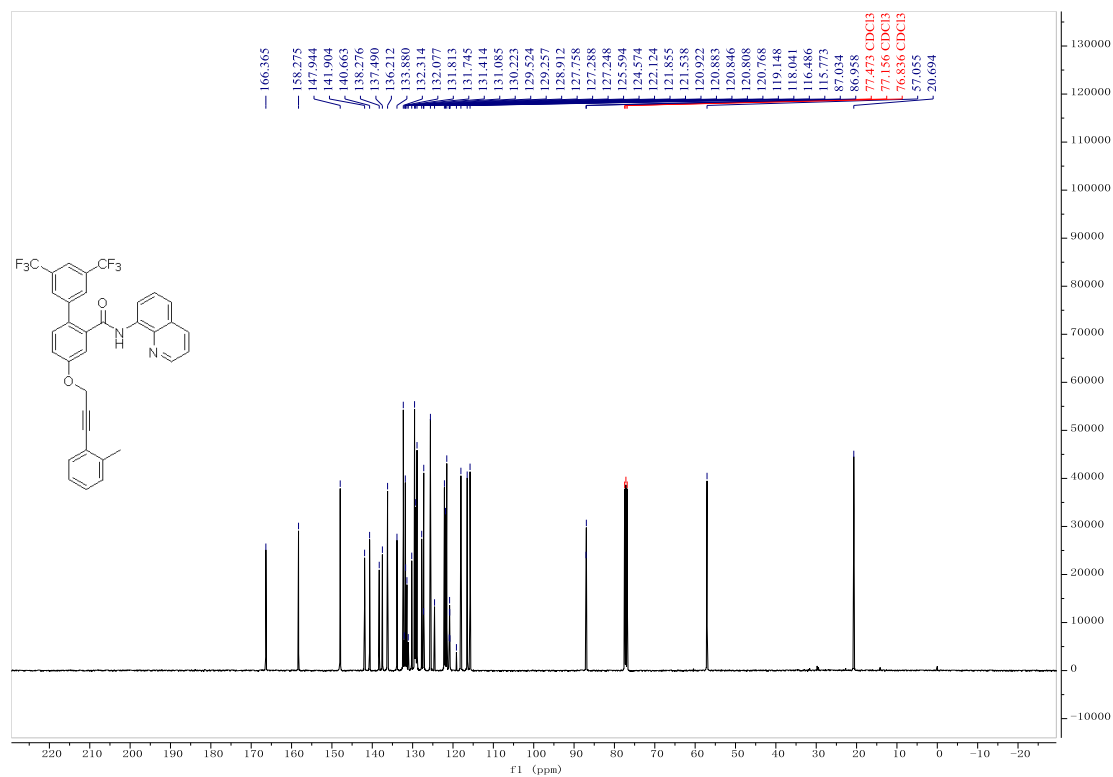


1m

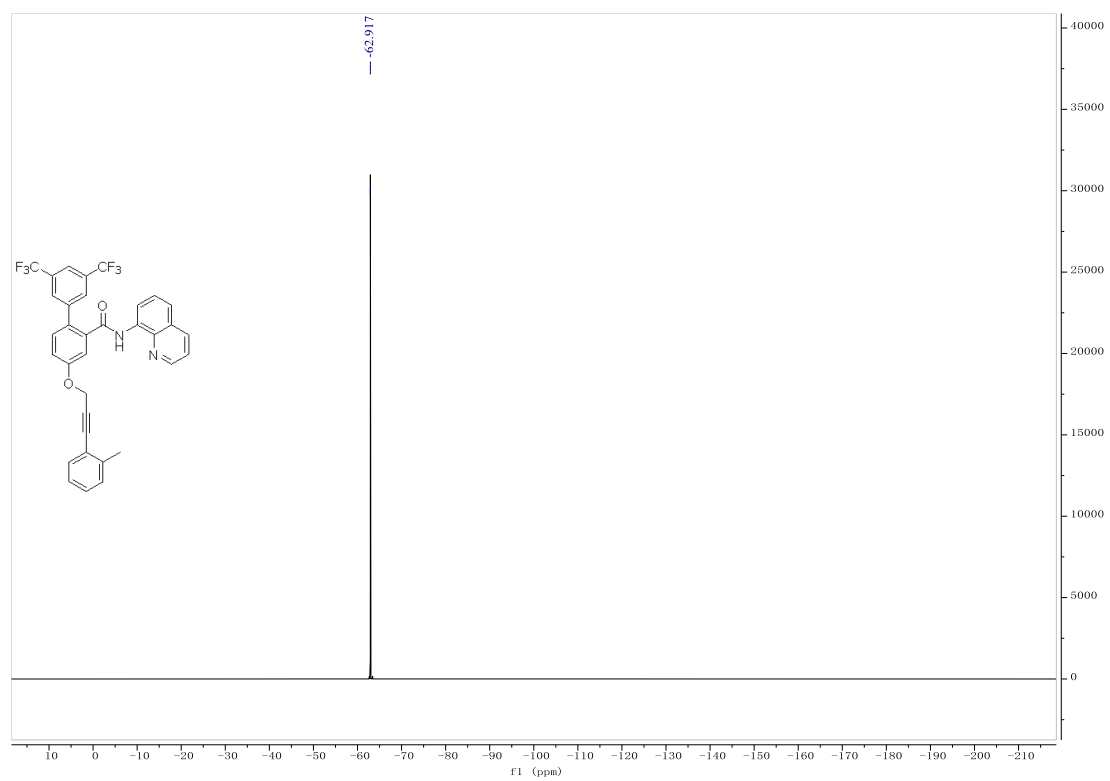
¹H NMR (400 MHz, Chloroform-*d*)



¹³C NMR (101 MHz, Chloroform-*d*)

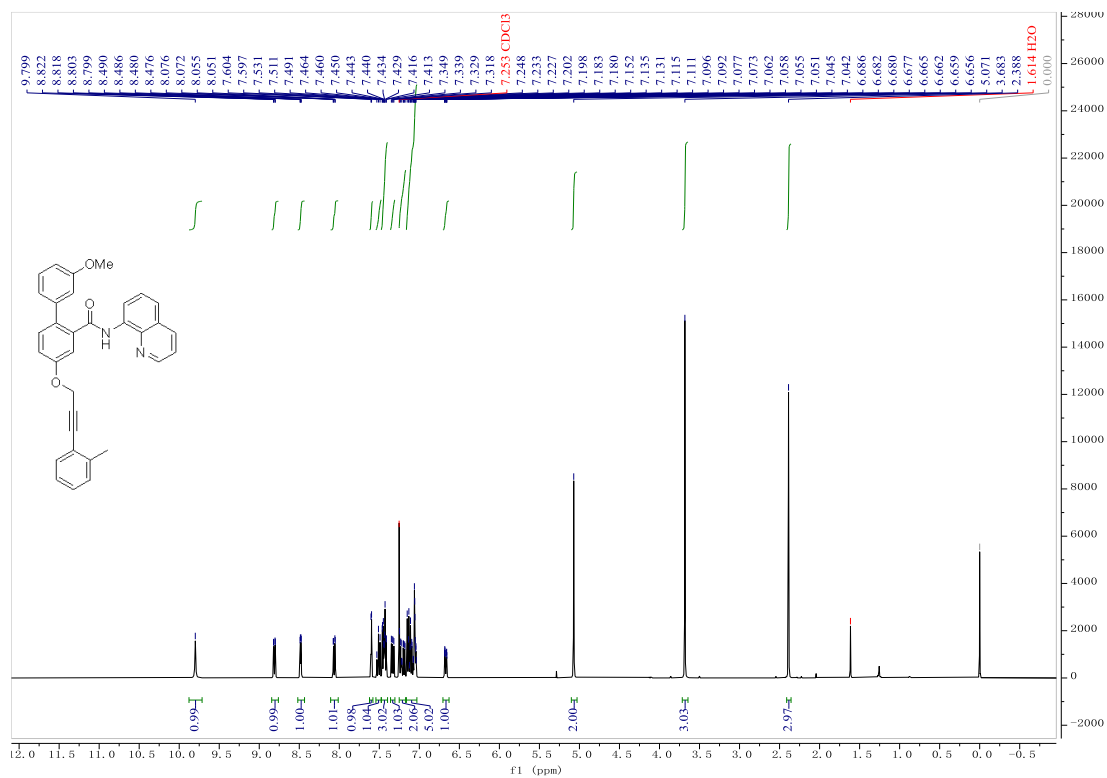


¹⁹F NMR (376 MHz, Chloroform-*d*)

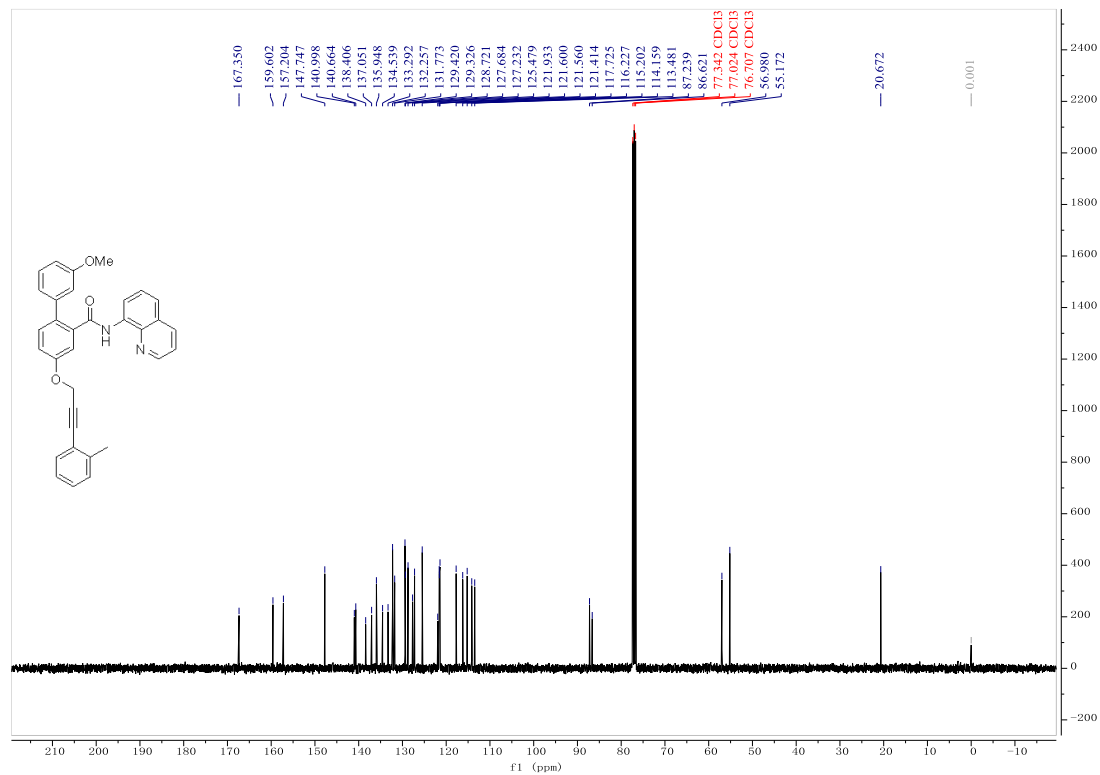


1n

¹H NMR (400 MHz, Chloroform-*d*)

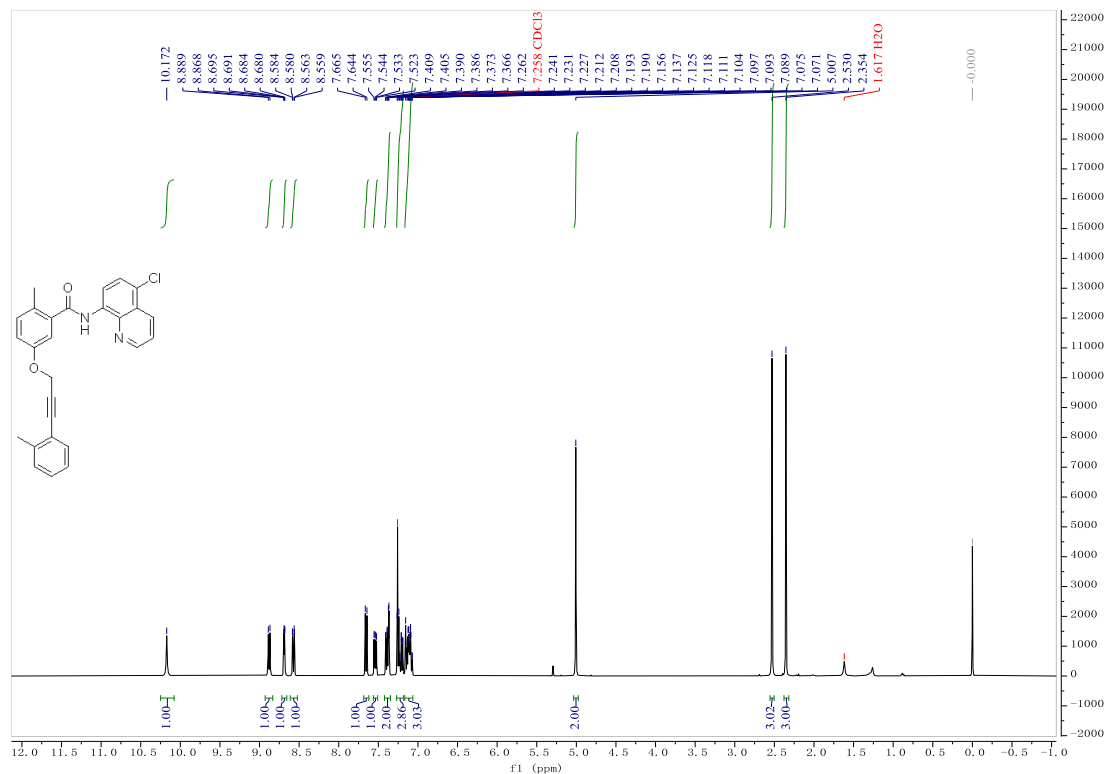


¹³C NMR (101 MHz, Chloroform-*d*)

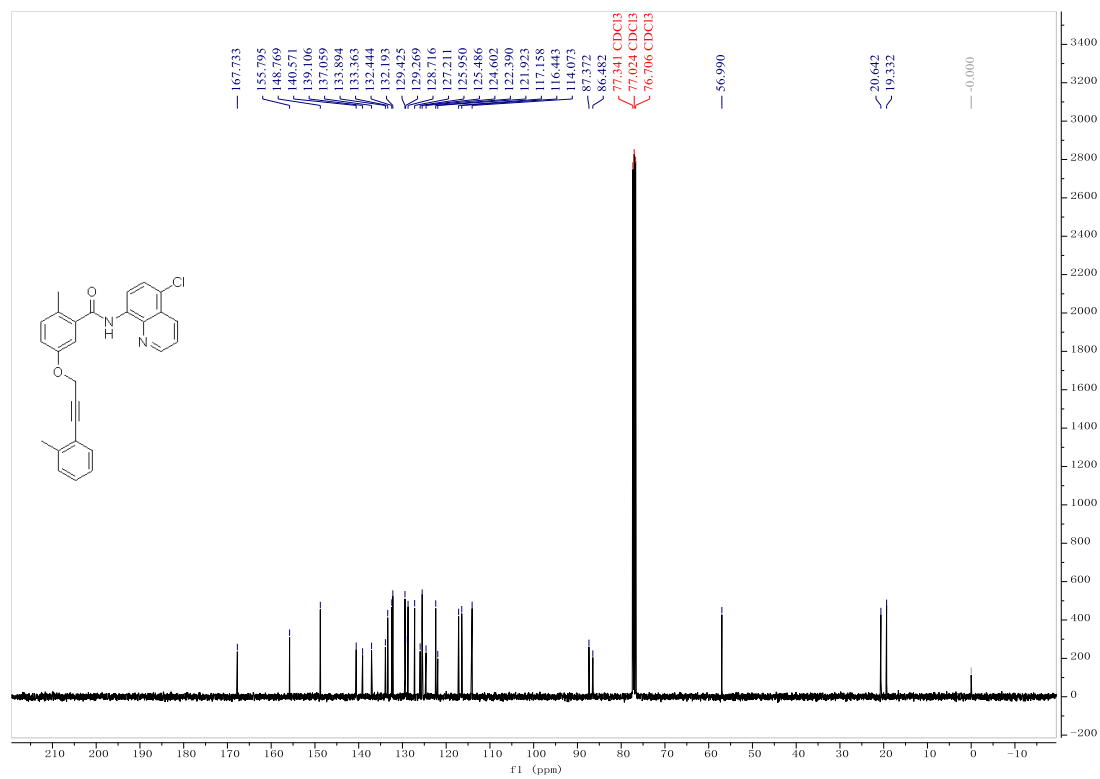


1o

¹H NMR (400 MHz, Chloroform-*d*)

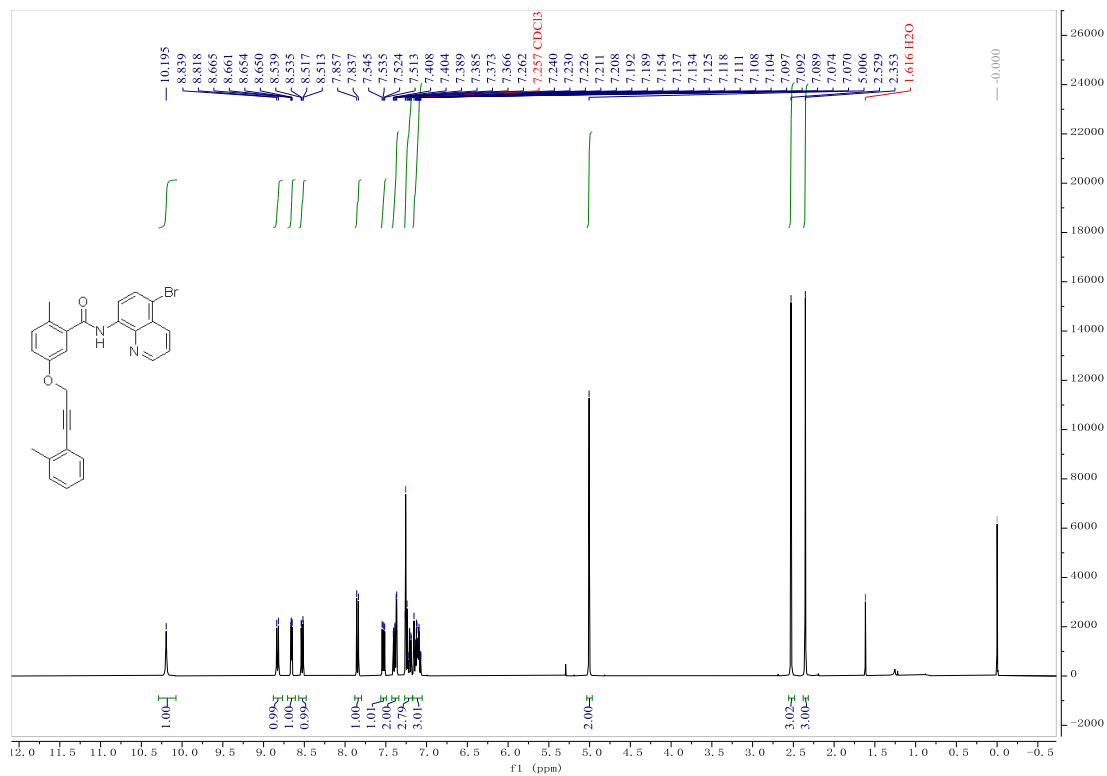


¹³C NMR (101 MHz, Chloroform-*d*)

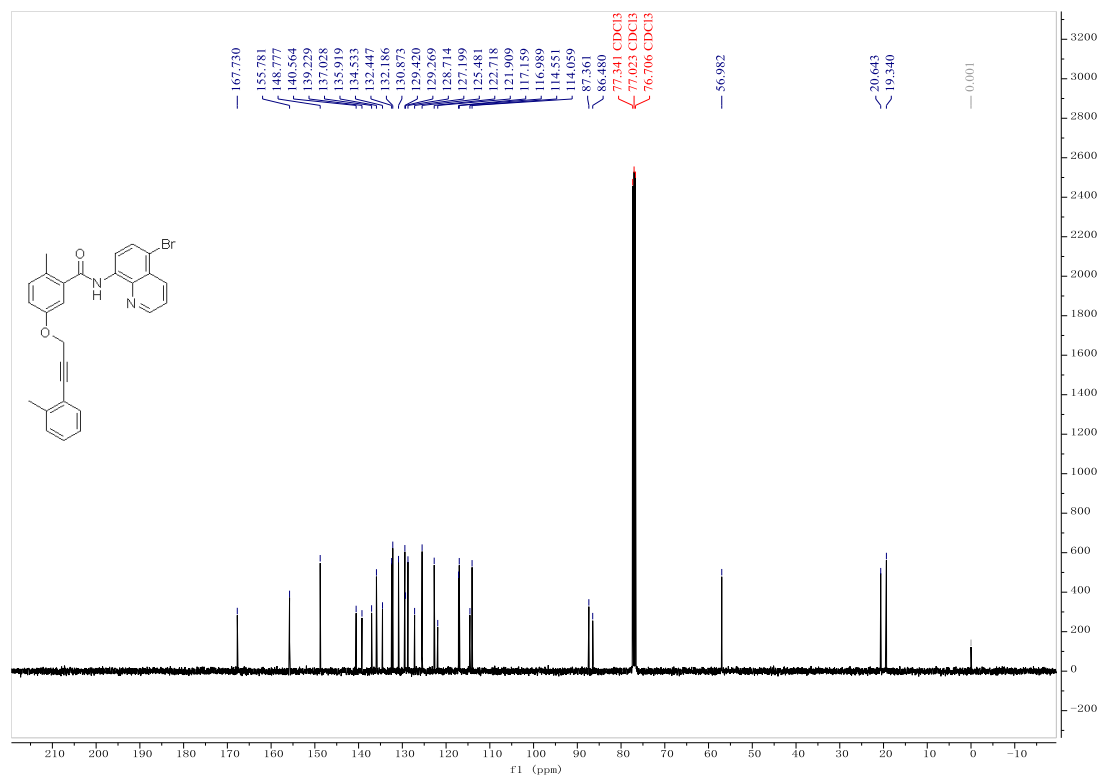


1p

¹H NMR (400 MHz, Chloroform-*d*)

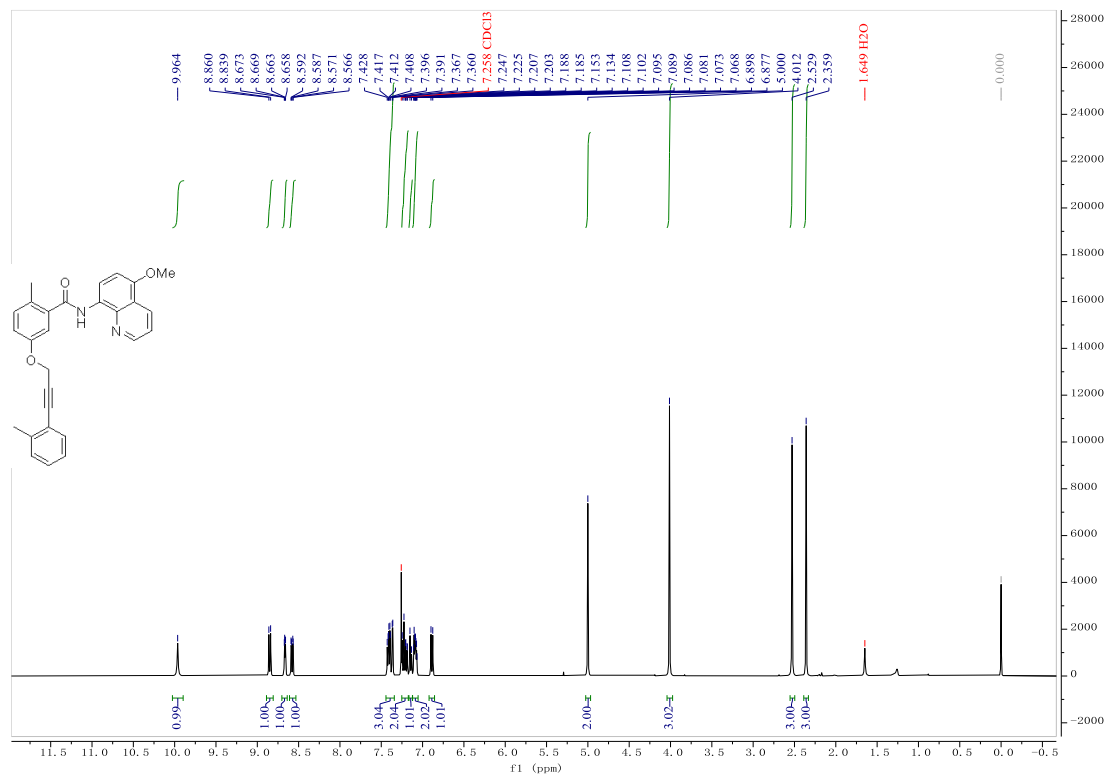


¹³C NMR (101 MHz, Chloroform-*d*)

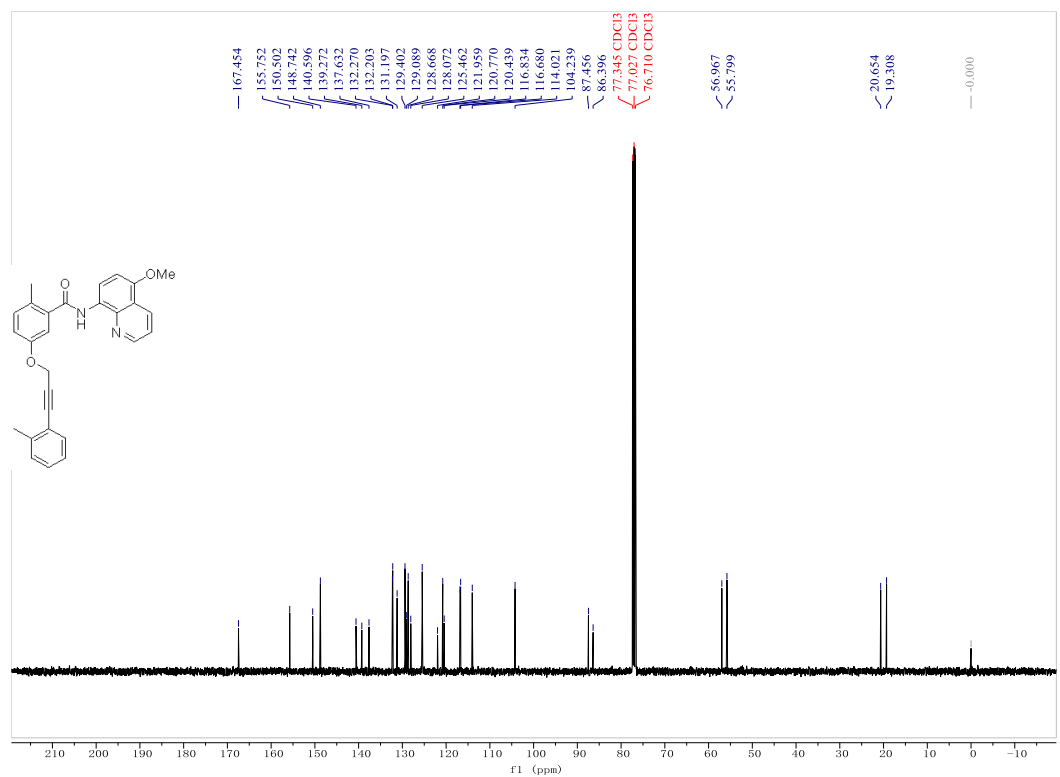


1q

¹H NMR (400 MHz, Chloroform-*d*)

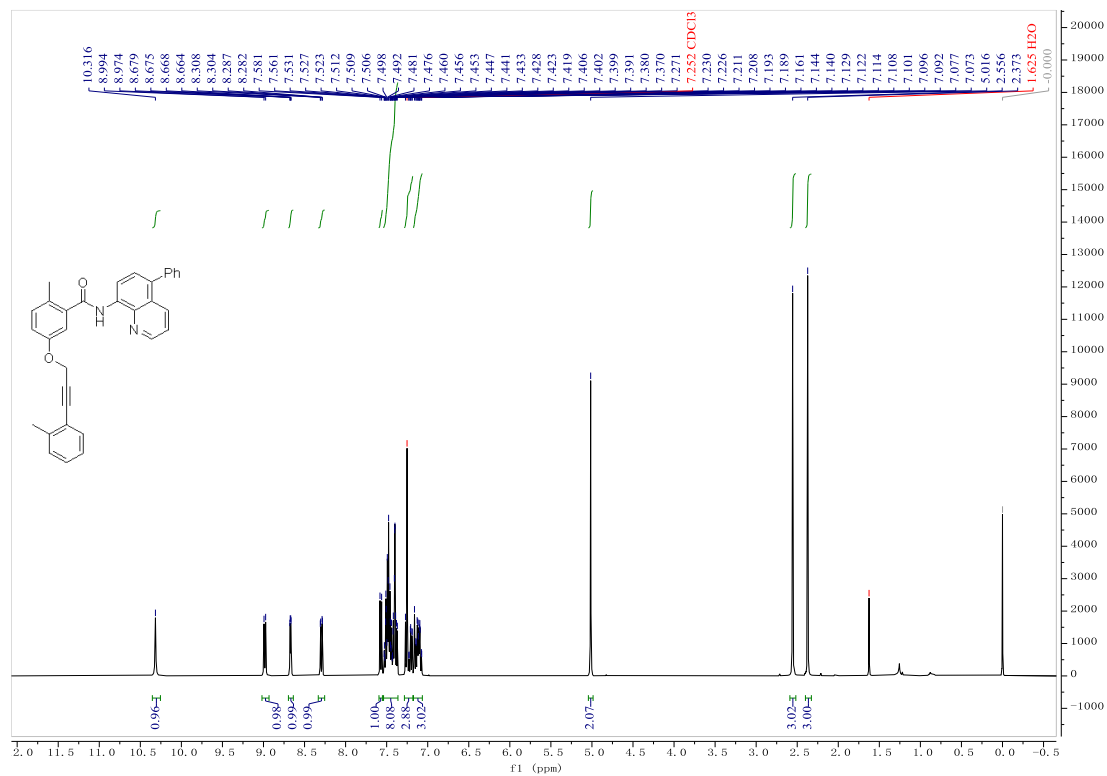


¹³C NMR (101 MHz, Chloroform-*d*)

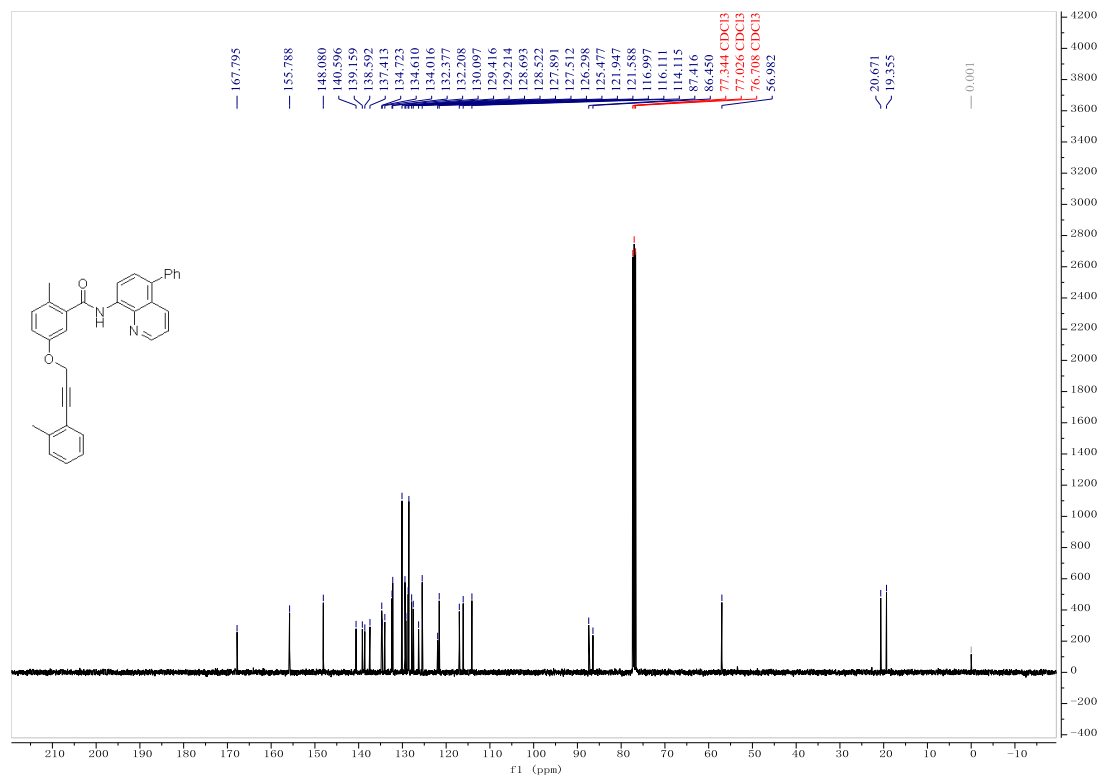


1r

¹H NMR (400 MHz, Chloroform-*d*)

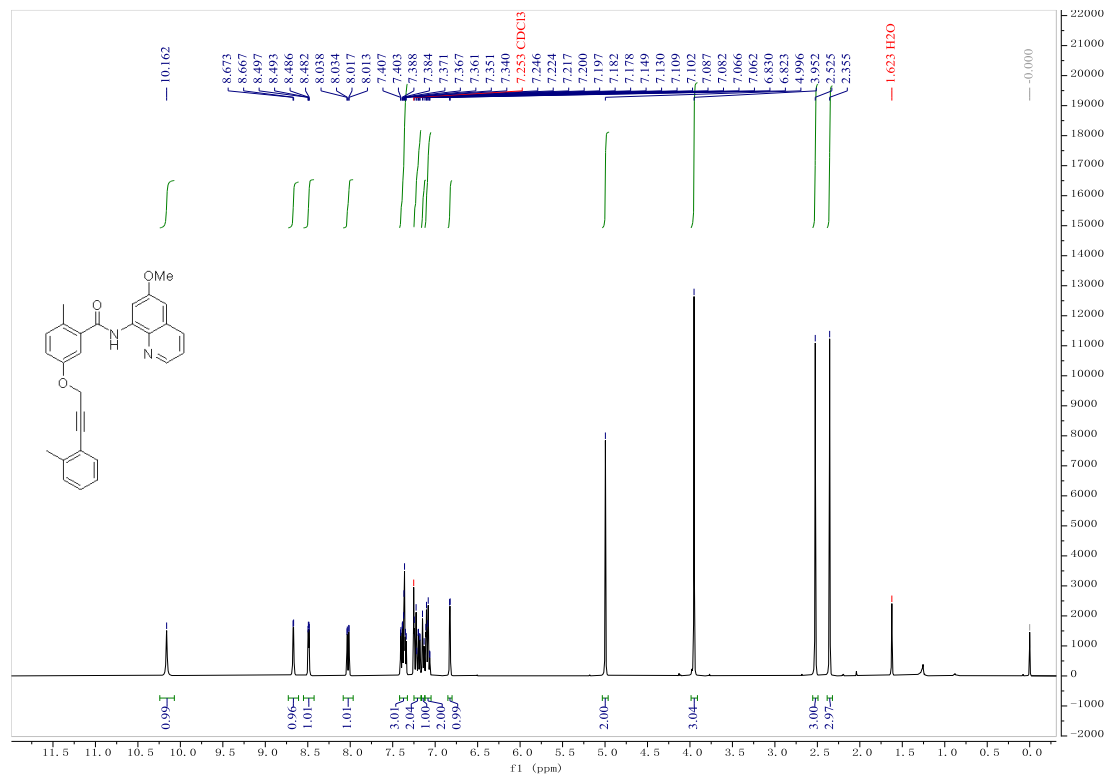


¹³C NMR (101 MHz, Chloroform-*d*)

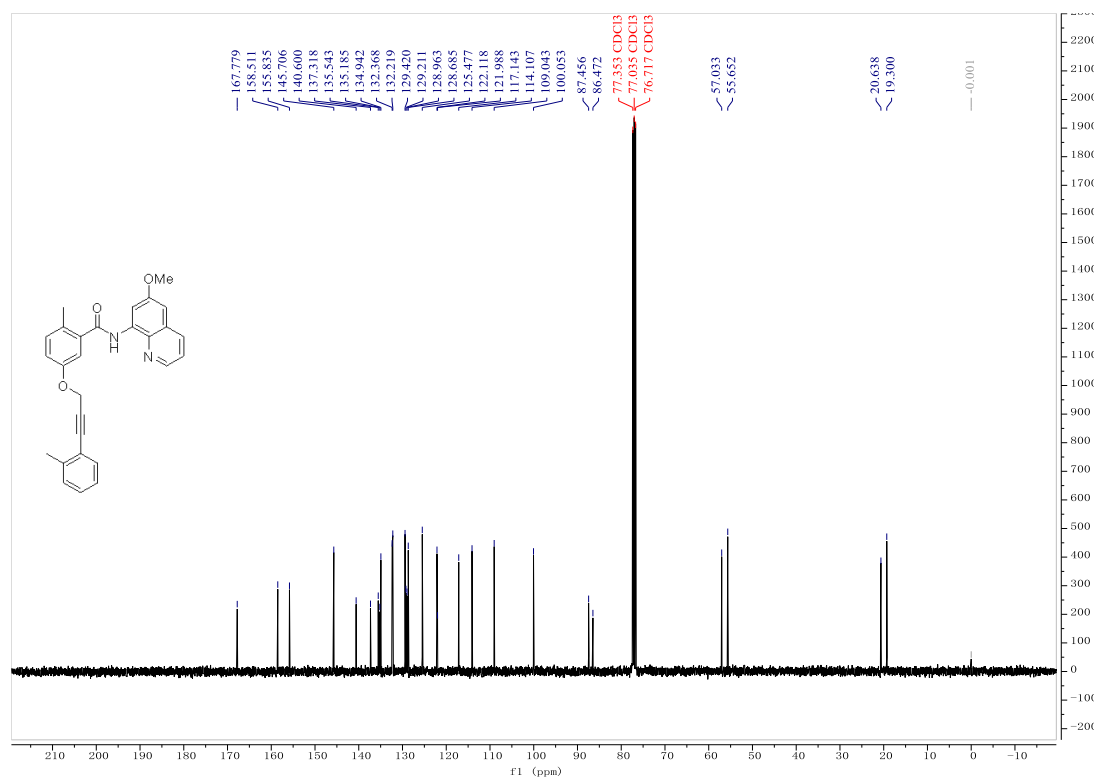


1s

¹H NMR (400 MHz, Chloroform-*d*)

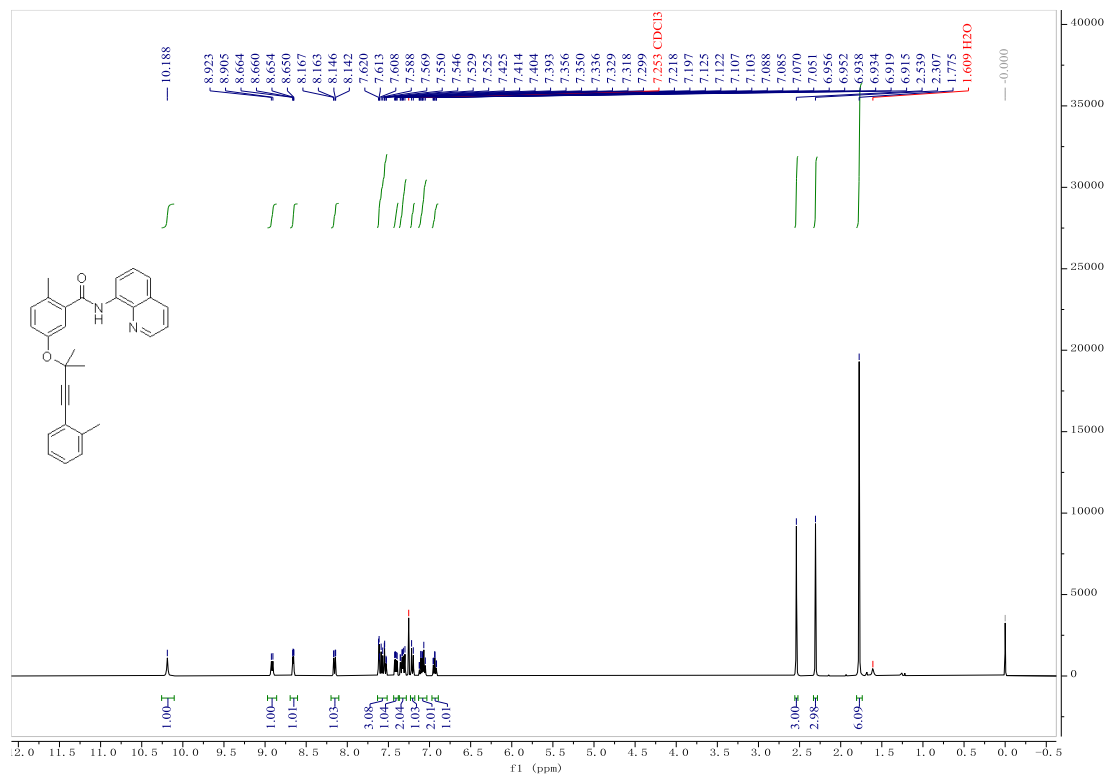


¹³C NMR (101 MHz, Chloroform-*d*)

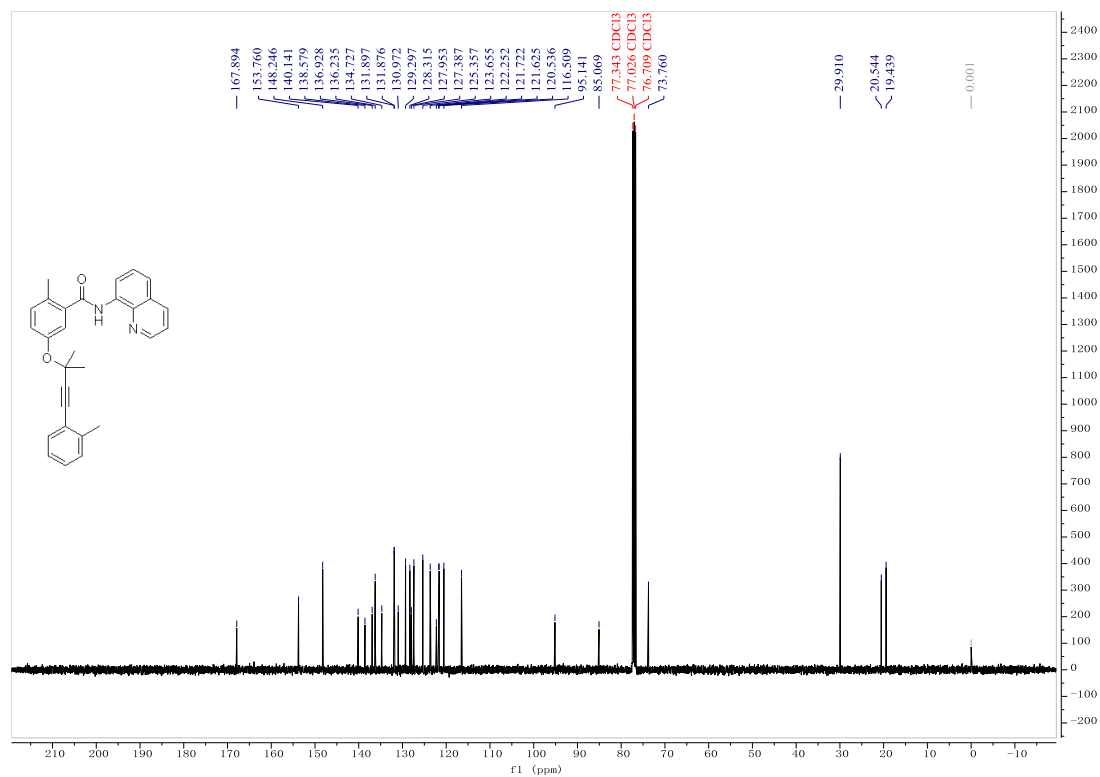


1t

¹H NMR (400 MHz, Chloroform-*d*)

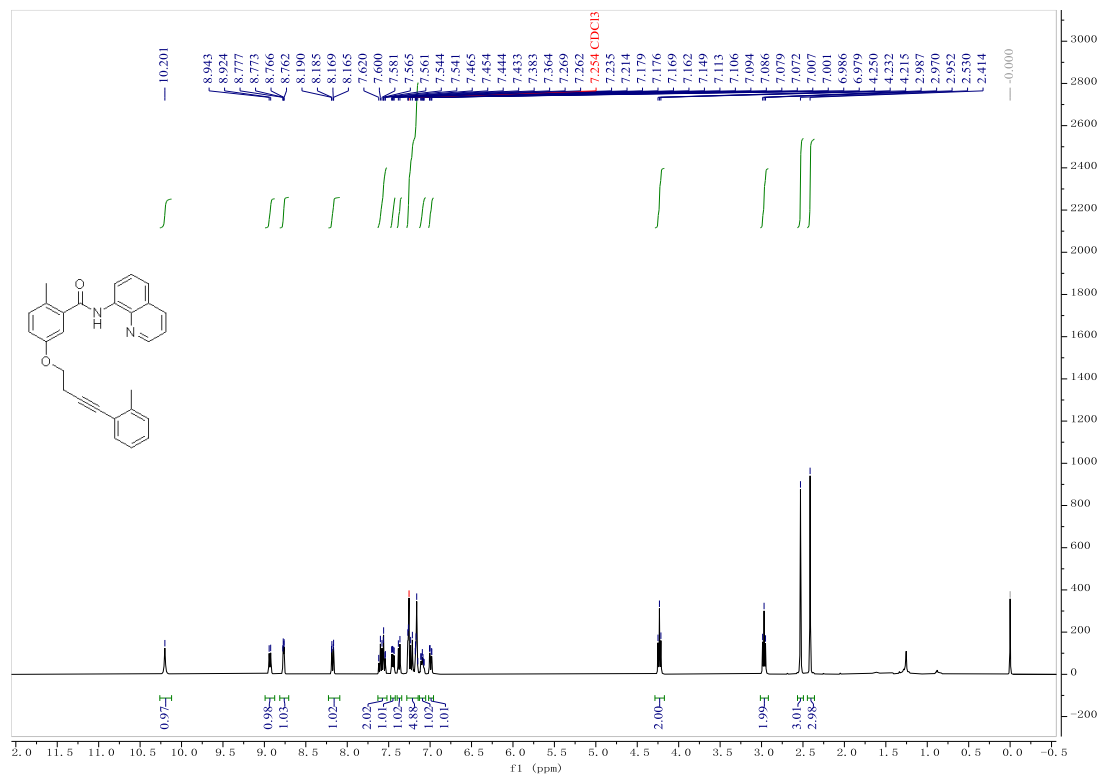


¹³C NMR (101 MHz, Chloroform-*d*)

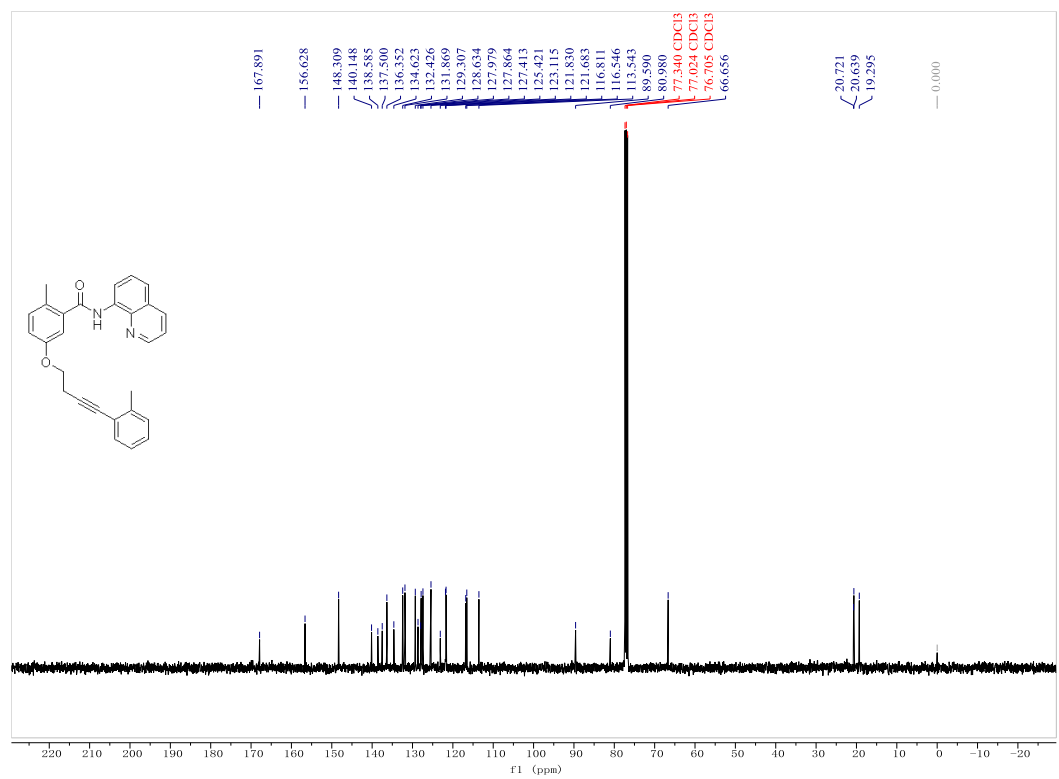


1u

¹H NMR (400 MHz, Chloroform-*d*)

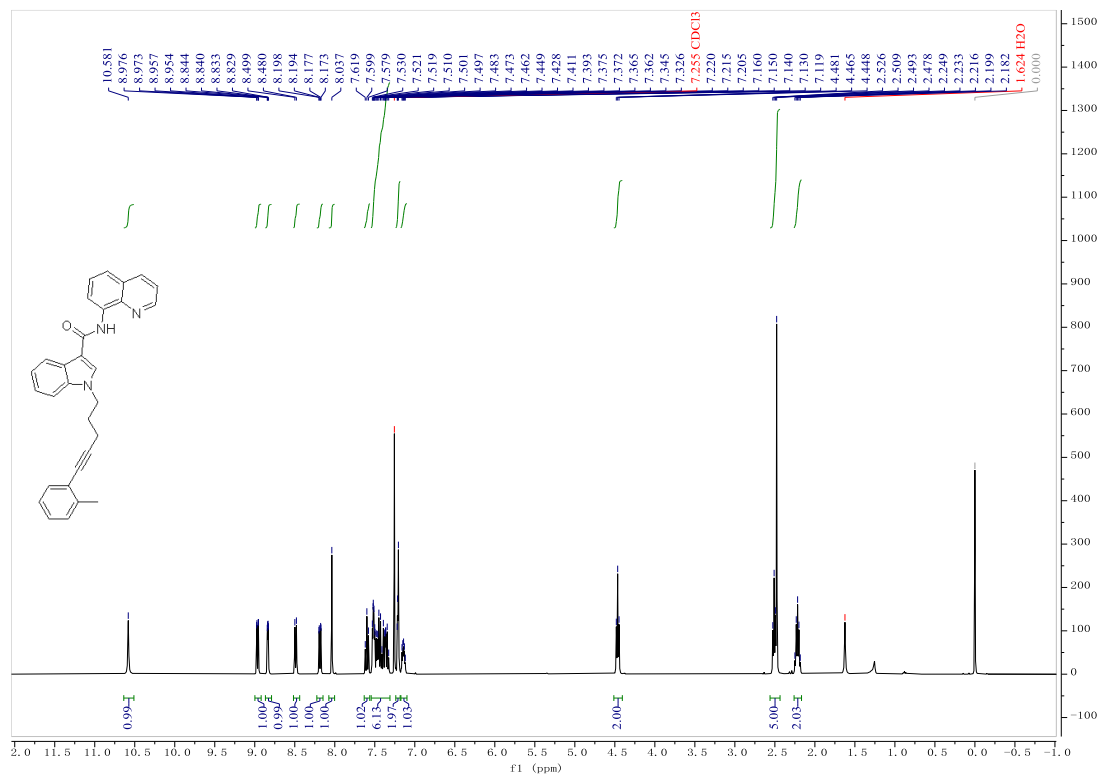


¹³C NMR (101 MHz, Chloroform-*d*)

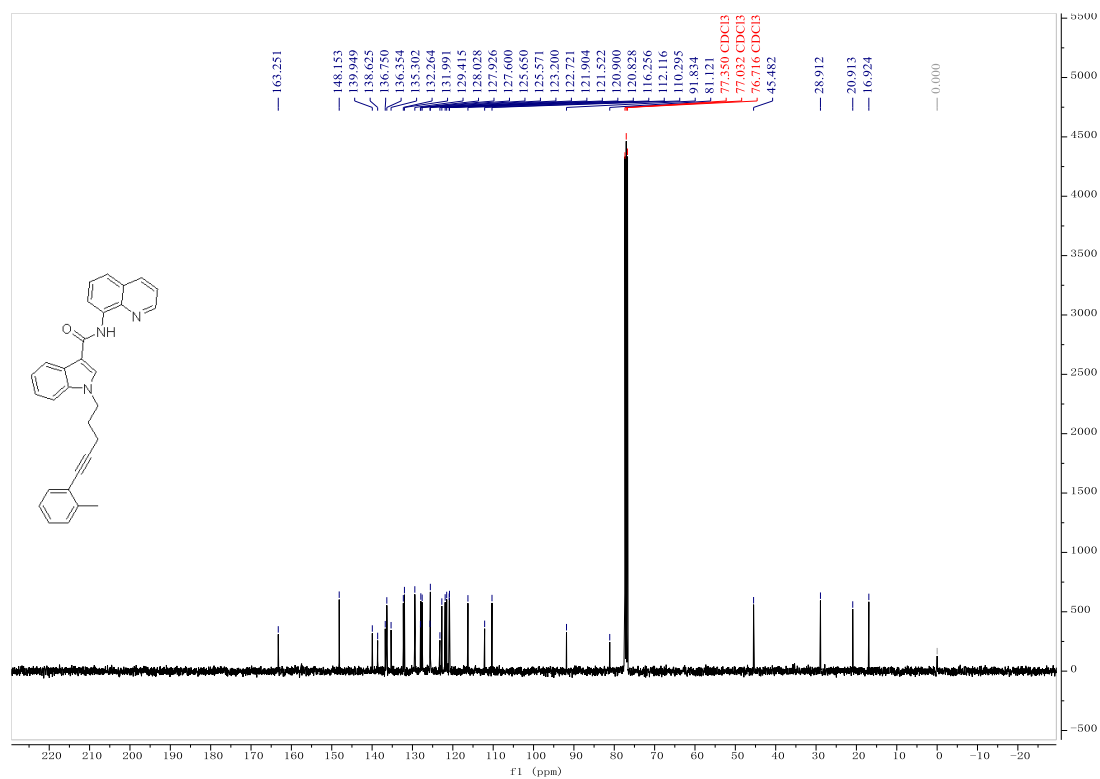


1v

¹H NMR (400 MHz, Chloroform-*d*)

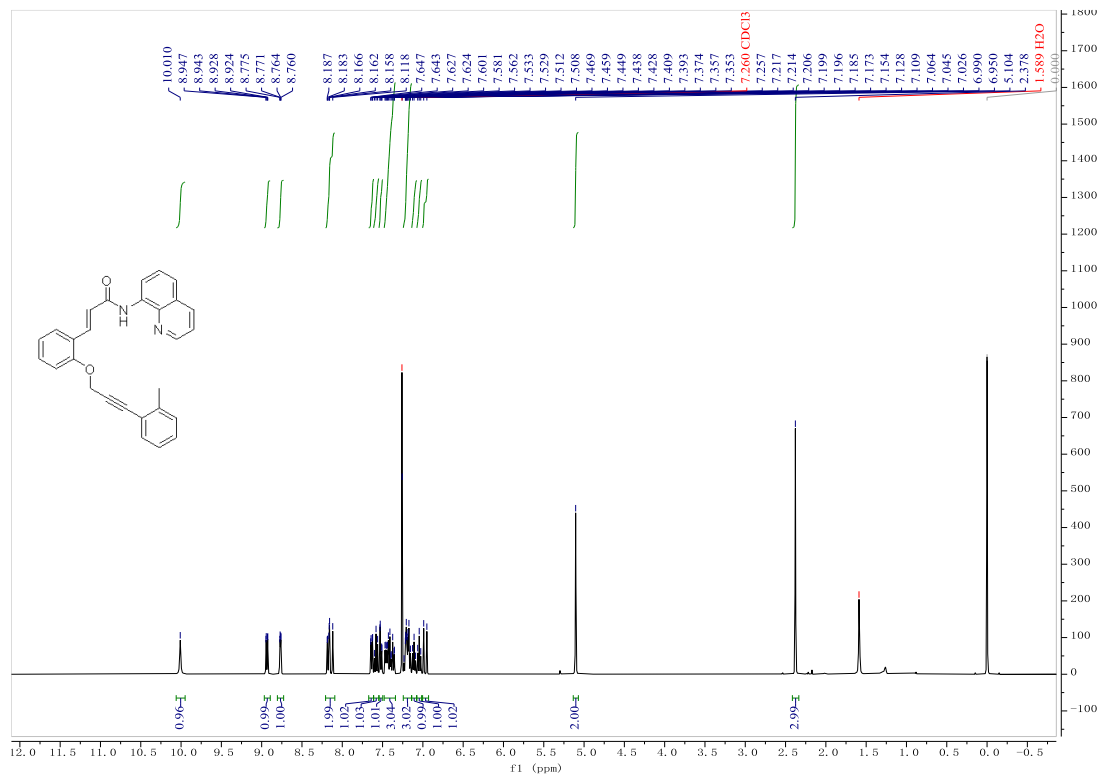


¹³C NMR (101 MHz, Chloroform-*d*)

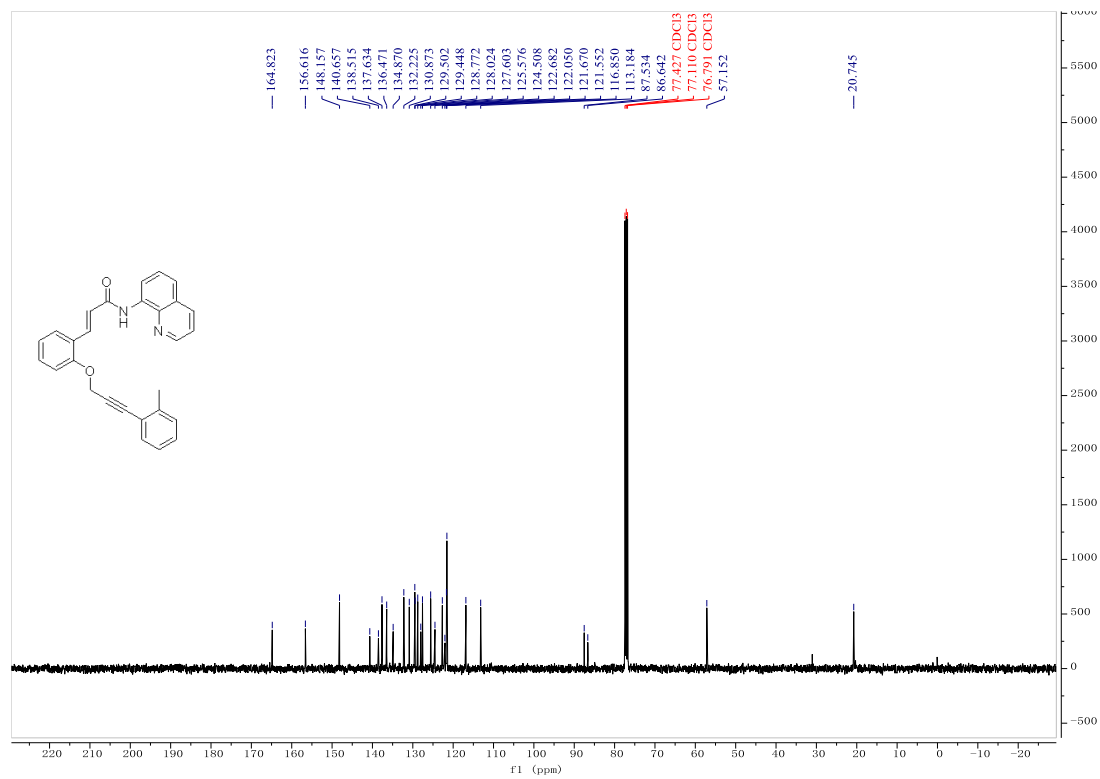


1w

¹H NMR (400 MHz, Chloroform-*d*)

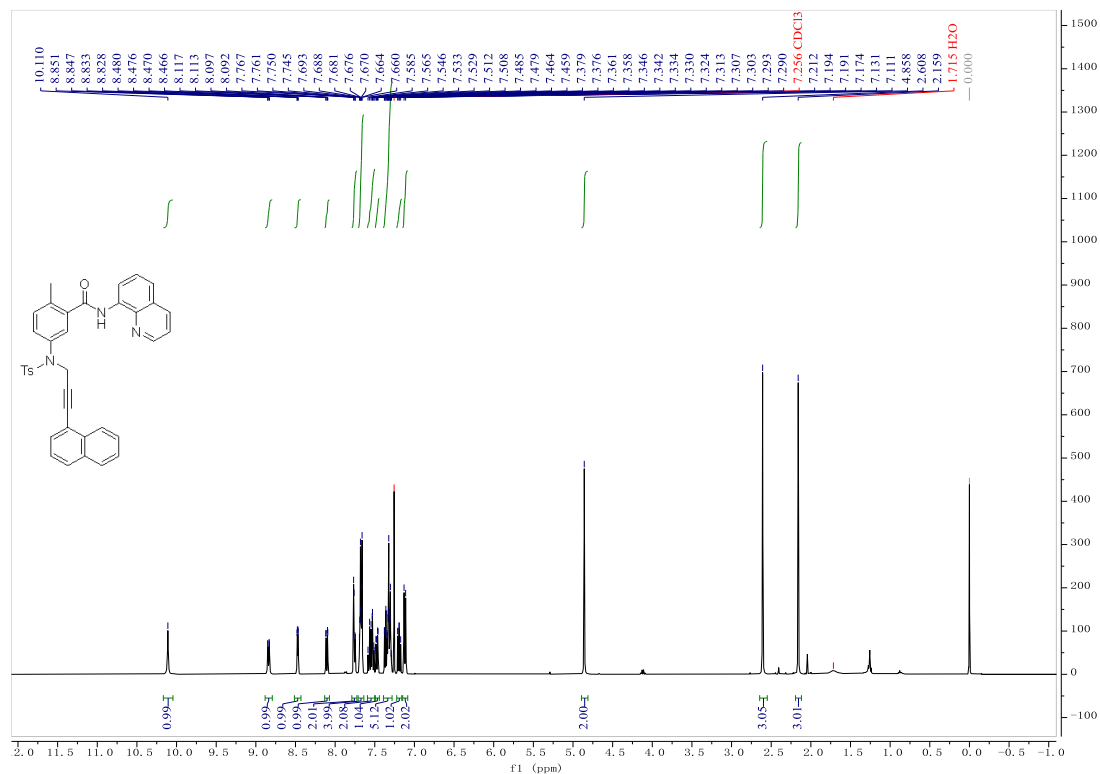


¹³C NMR (101 MHz, Chloroform-*d*)

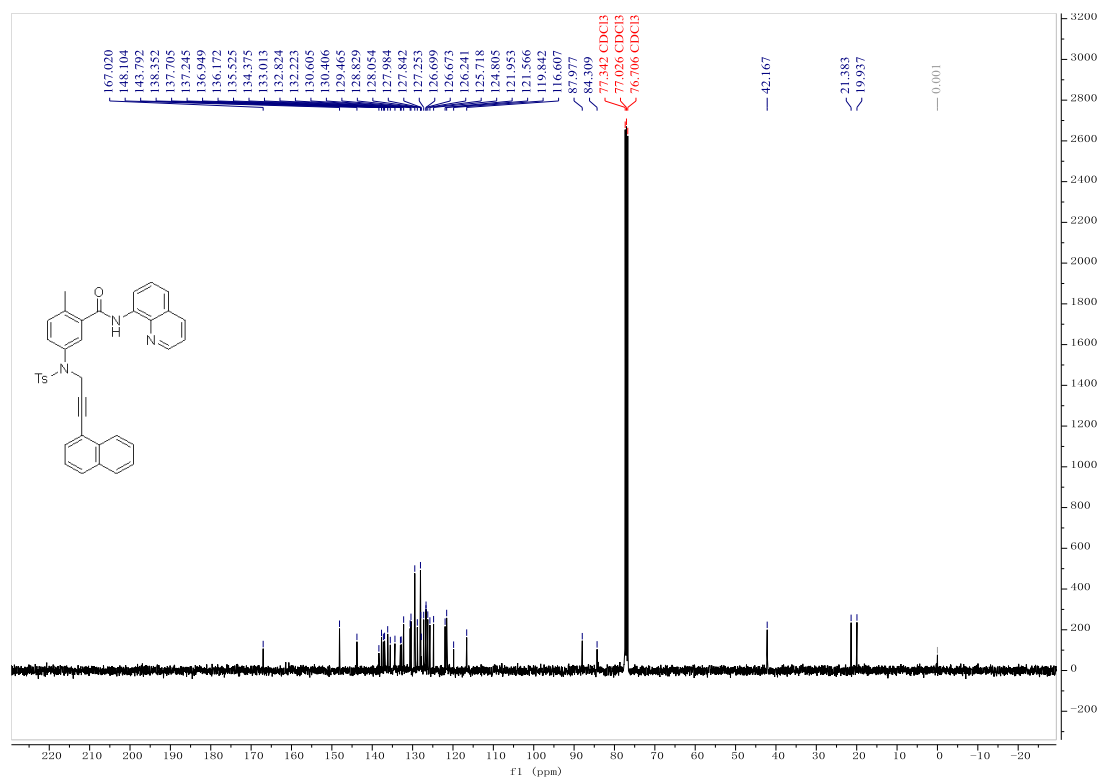


1x

¹H NMR (400 MHz, Chloroform-*d*)

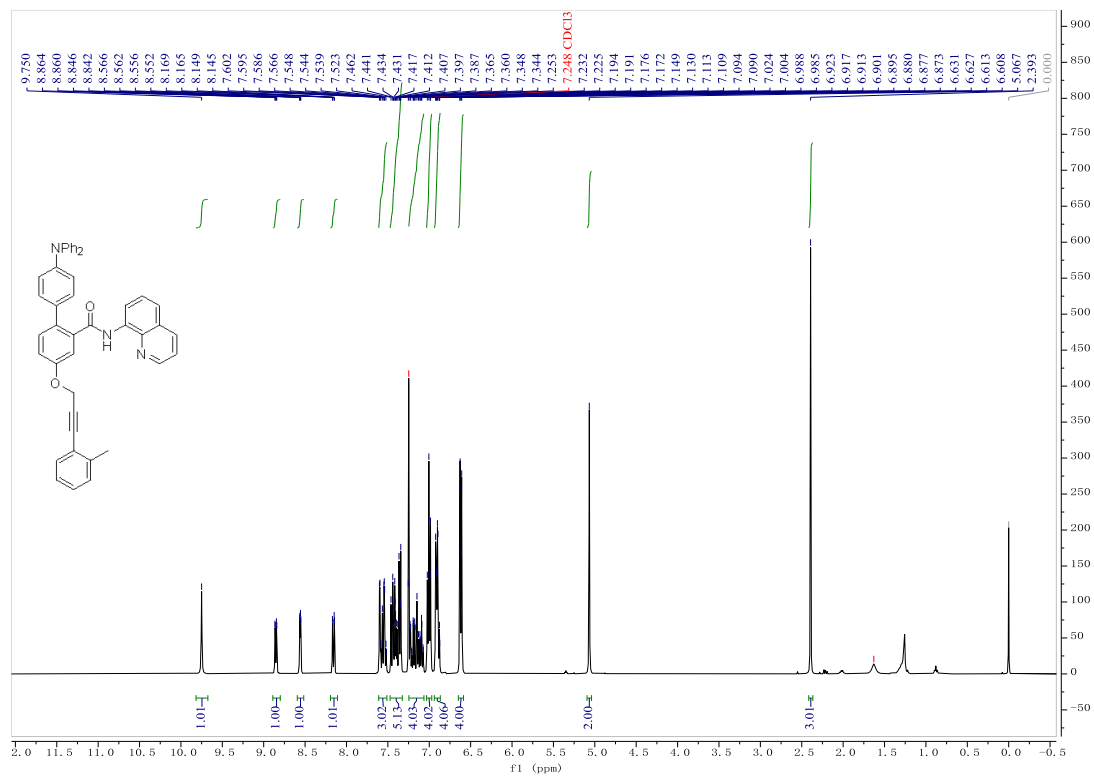


¹³C NMR (101 MHz, Chloroform-*d*)

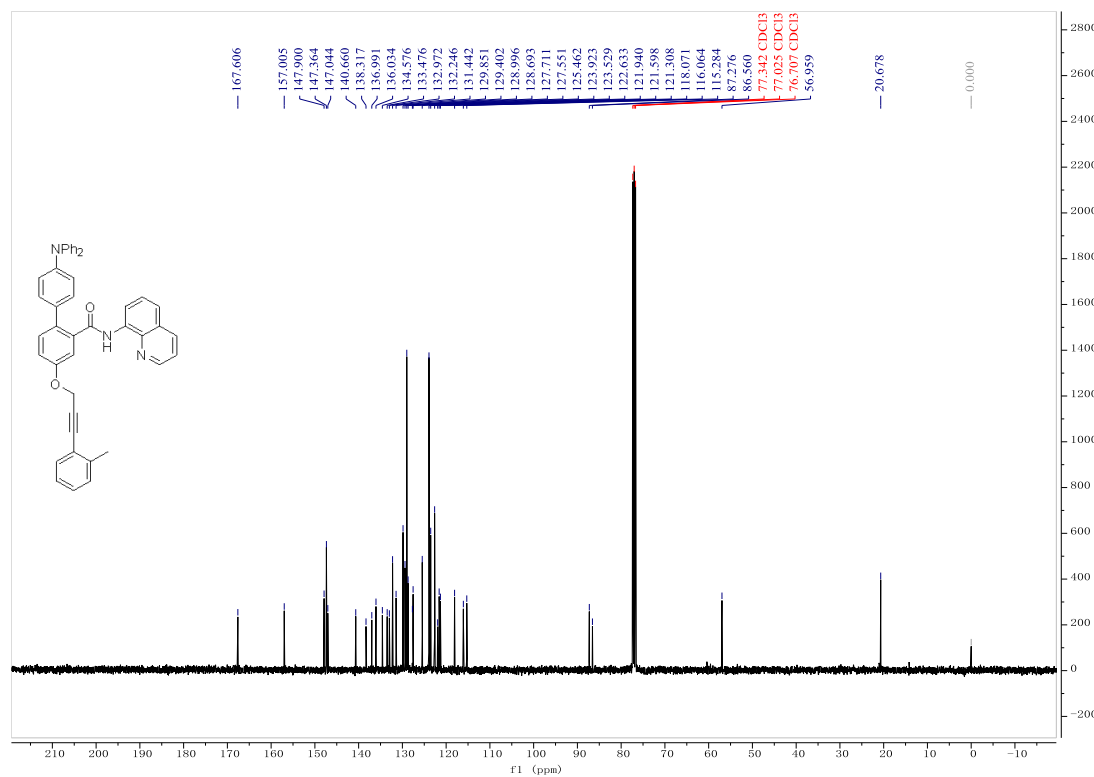


1y

¹H NMR (400 MHz, Chloroform-*d*)

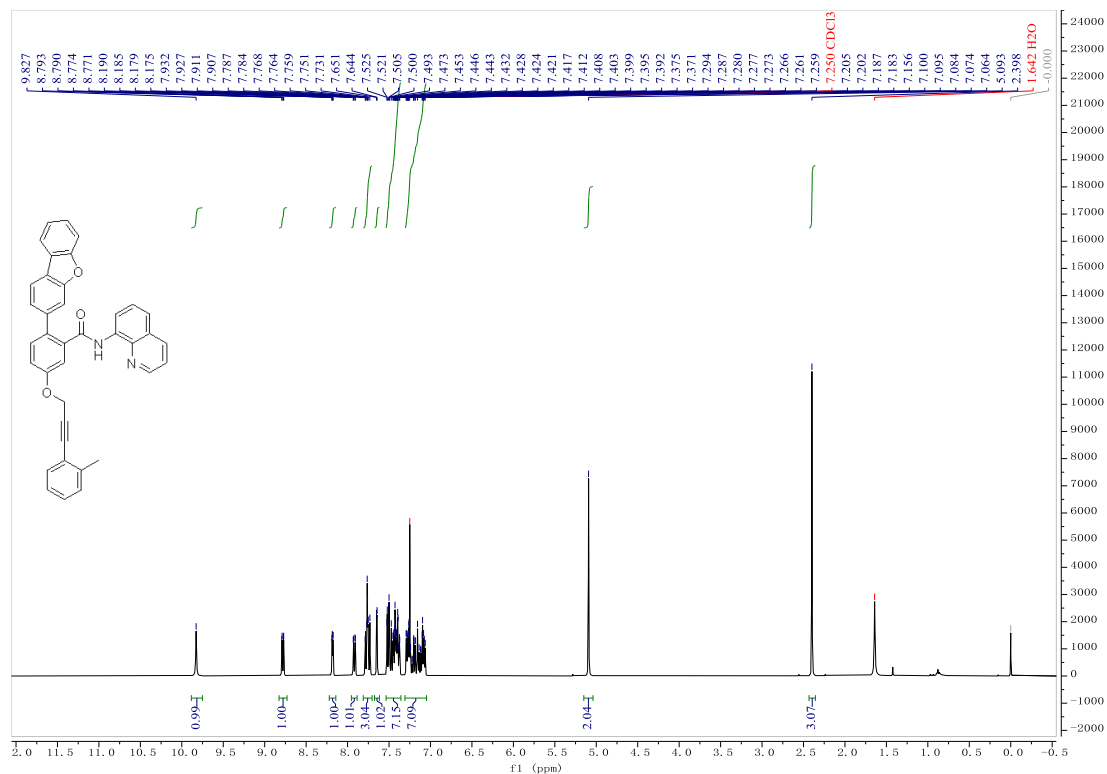


¹³C NMR (101 MHz, Chloroform-*d*)

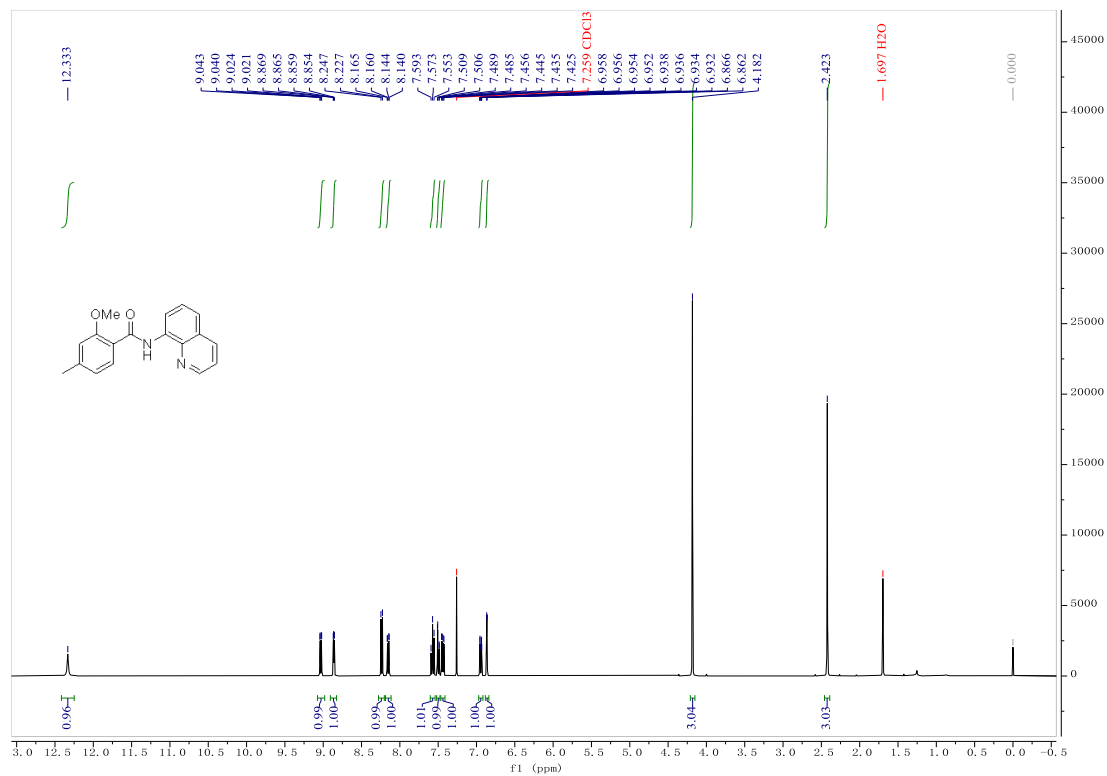
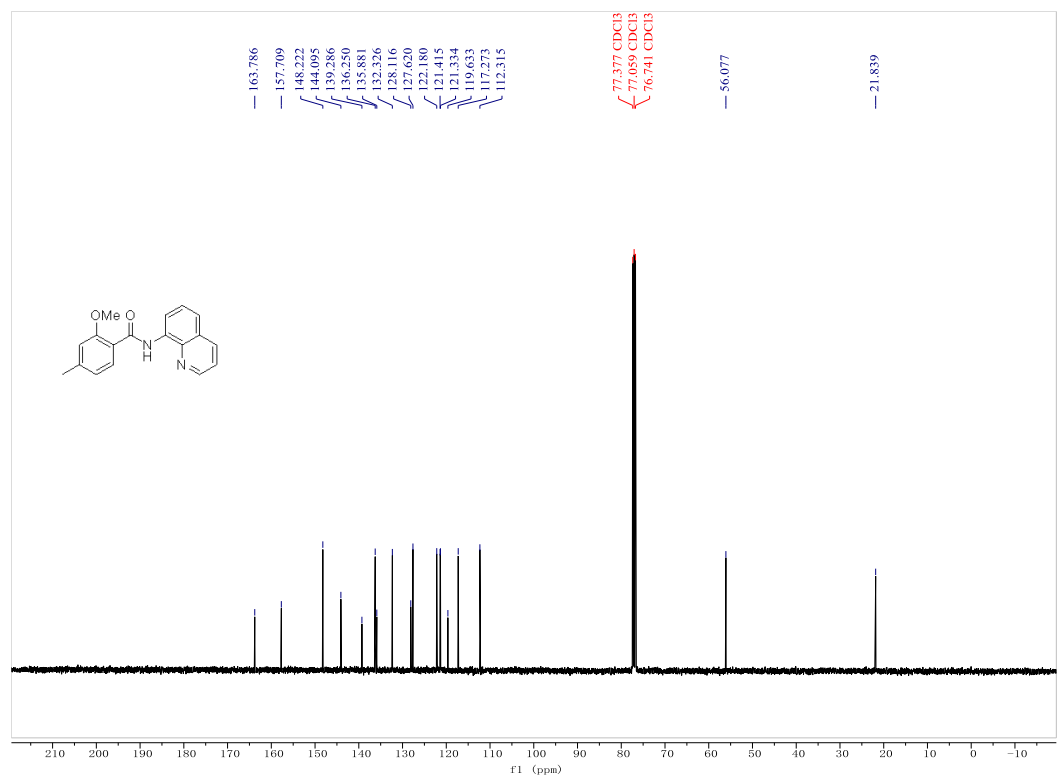


1z

¹H NMR (400 MHz, Chloroform-*d*)

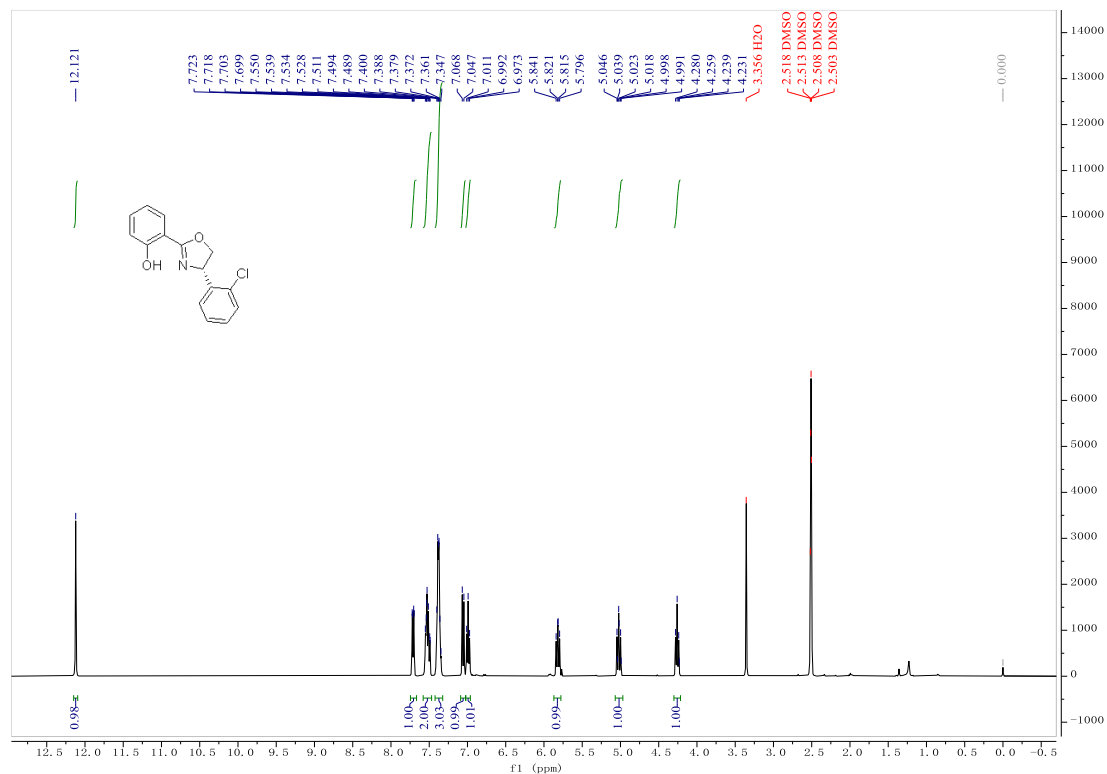


3

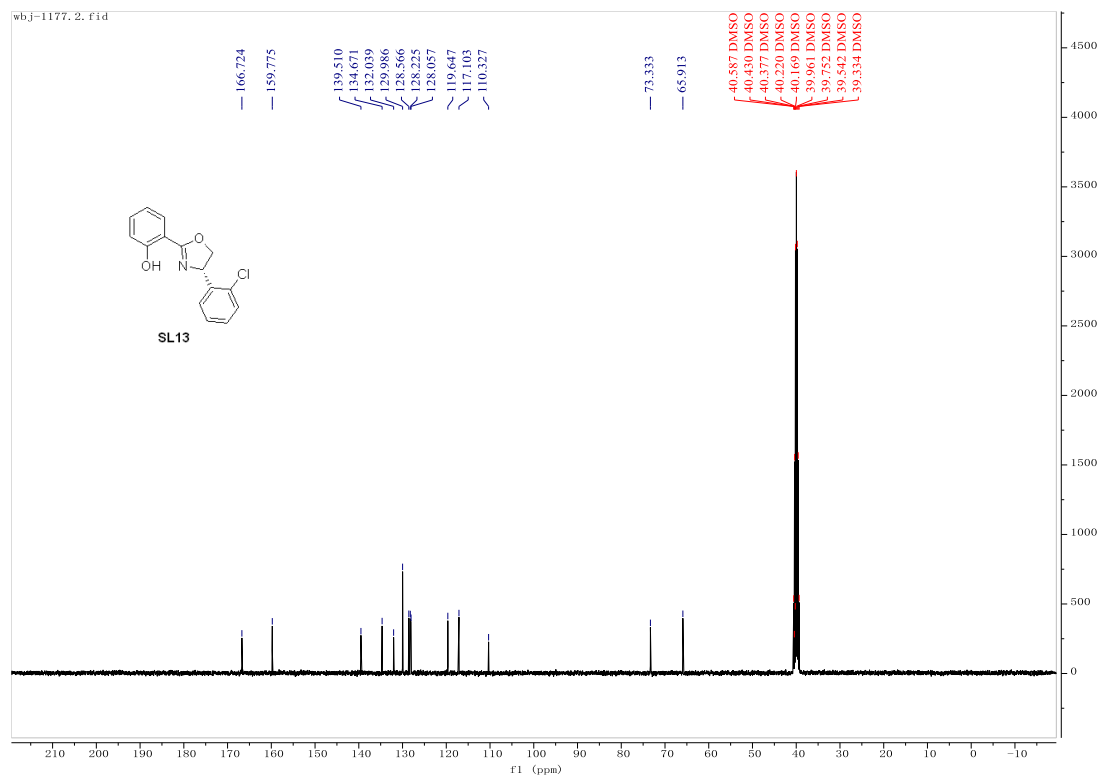
 ^1H NMR (400 MHz, Chloroform-*d*) ^{13}C NMR (101 MHz, Chloroform-*d*)

L6

¹H NMR (400 MHz, Chloroform-*d*)

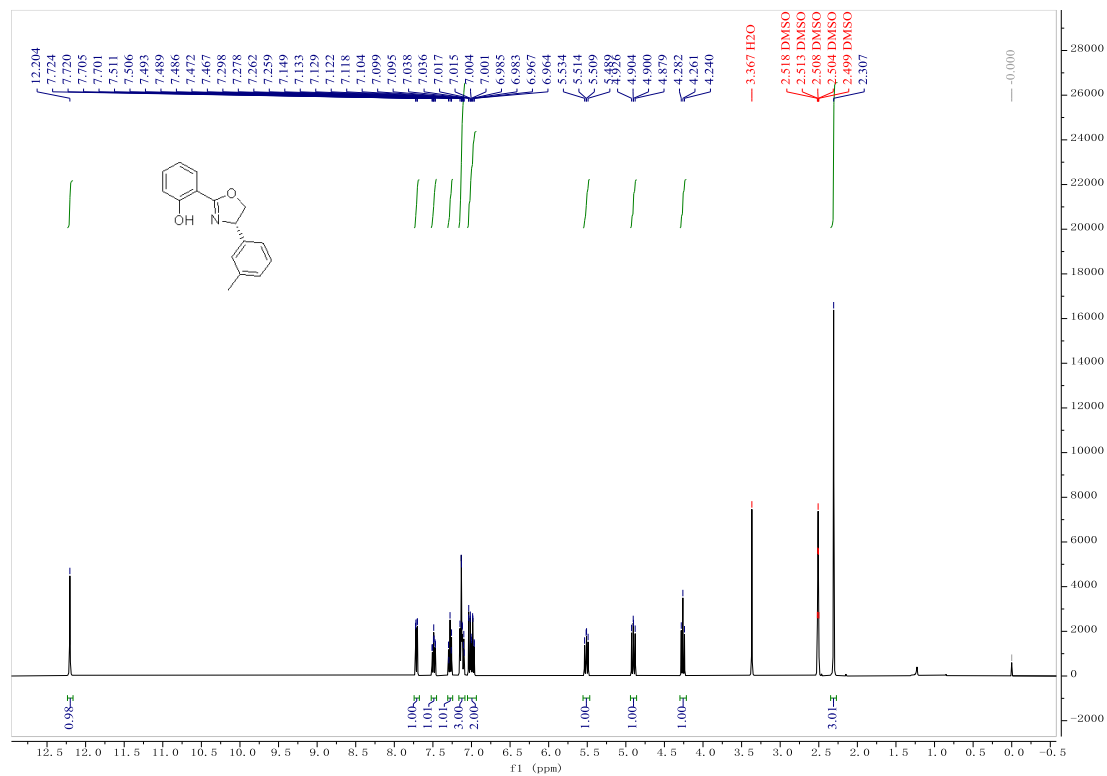


¹³C NMR (101 MHz, Chloroform-*d*)

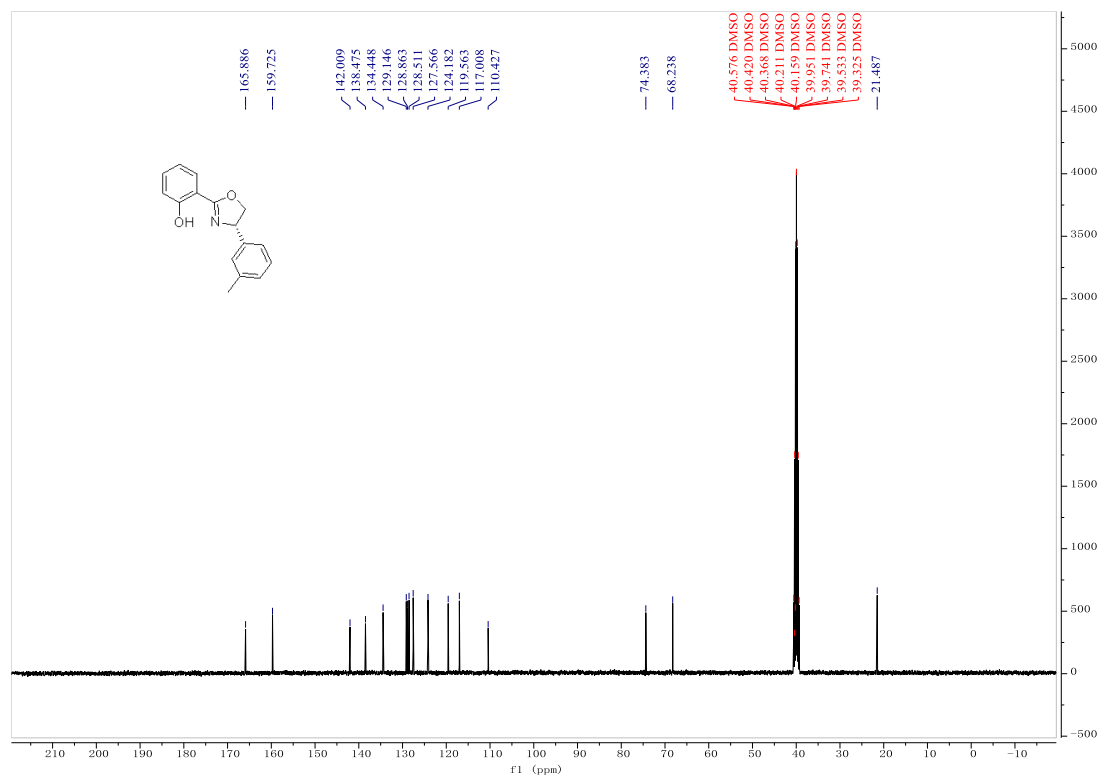


L7

^1H NMR (400 MHz, Chloroform-*d*)

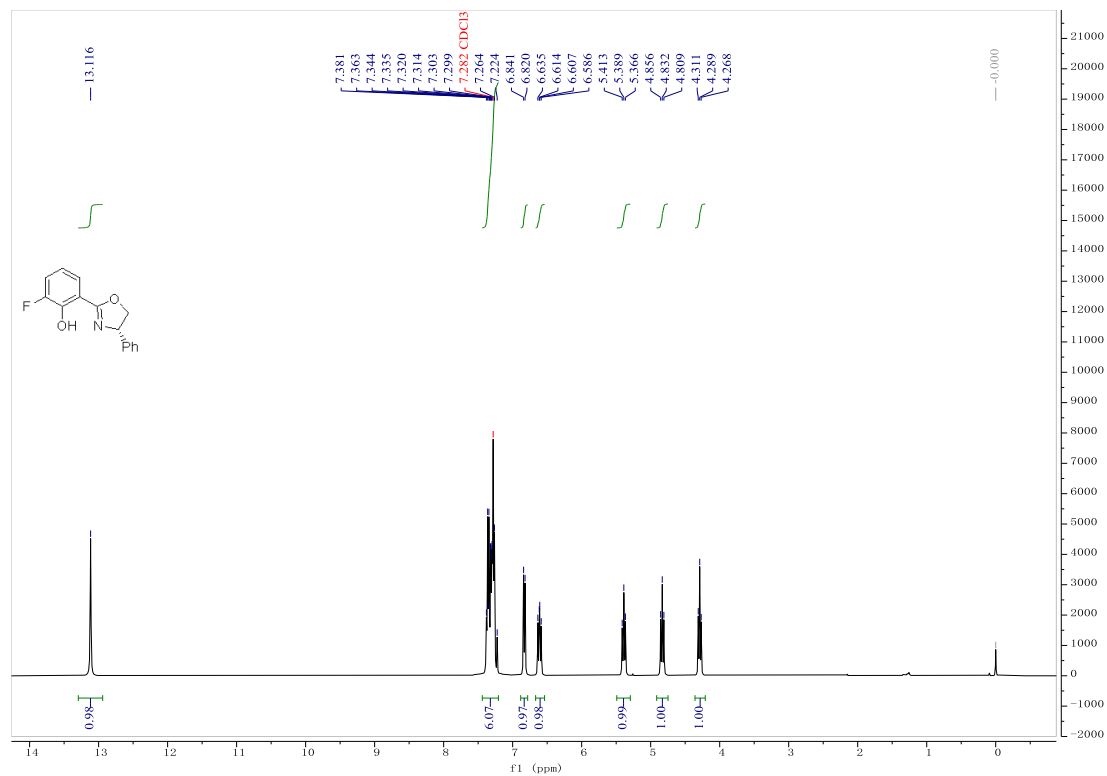


^{13}C NMR (101 MHz, Chloroform-*d*)

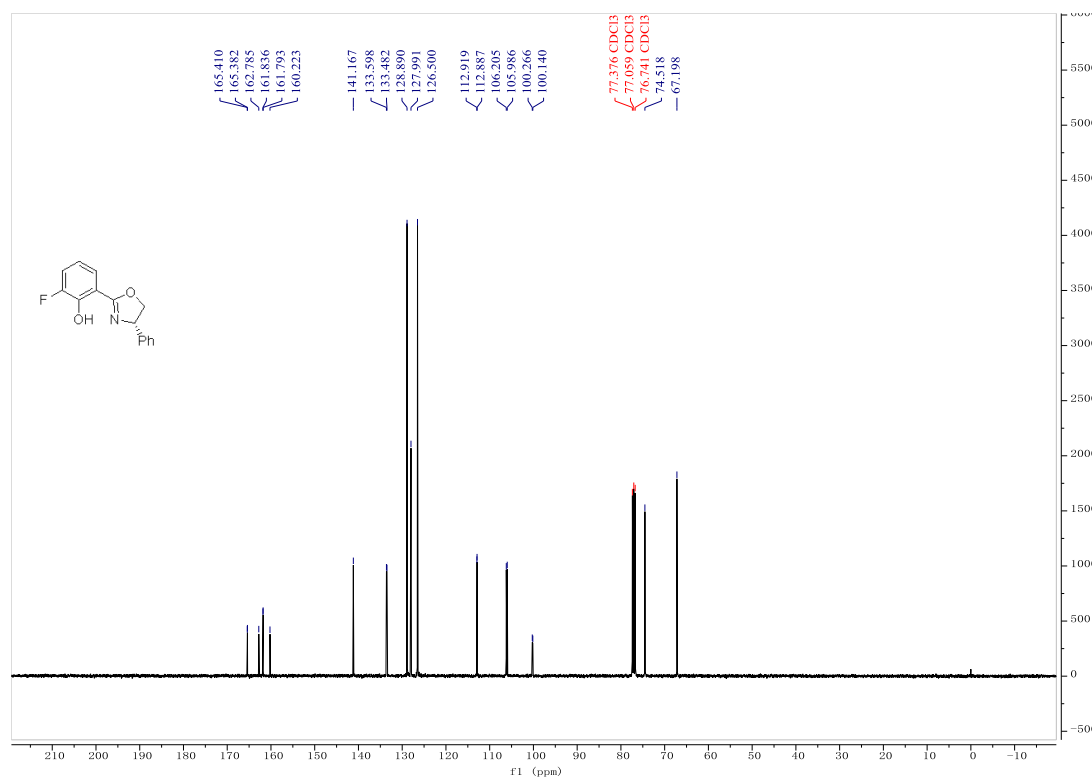


L9

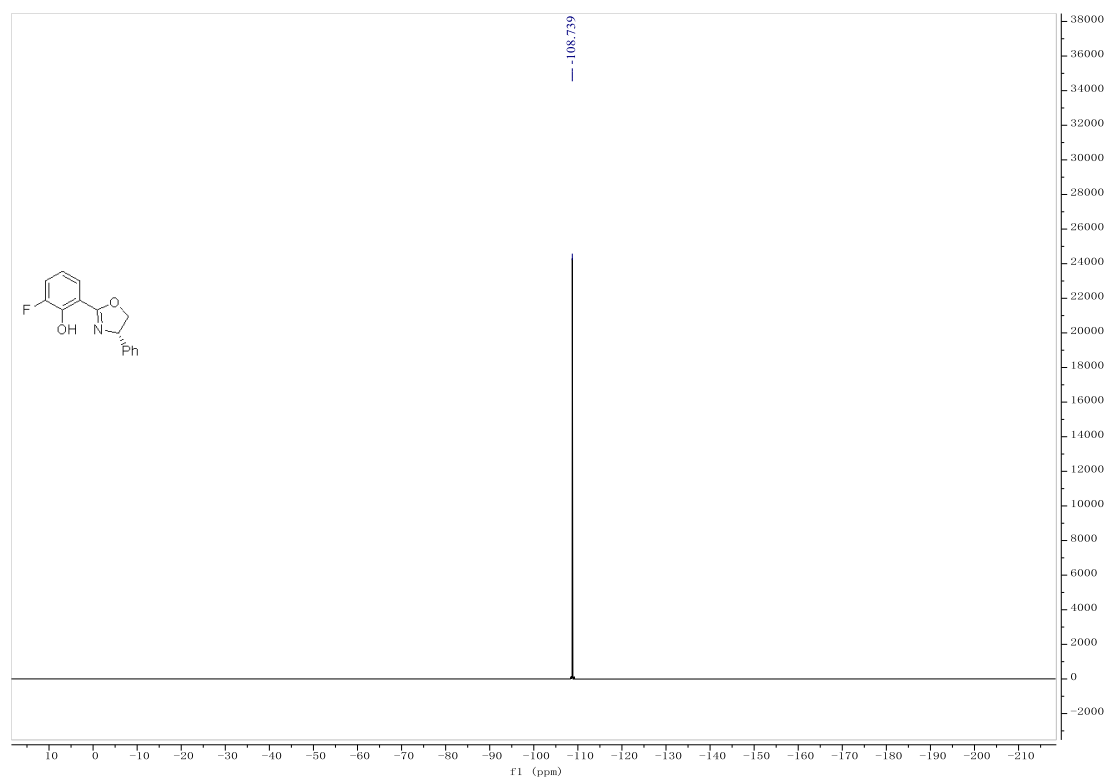
^1H NMR (400 MHz, Chloroform-*d*)



^{13}C NMR (101 MHz, Chloroform-*d*)

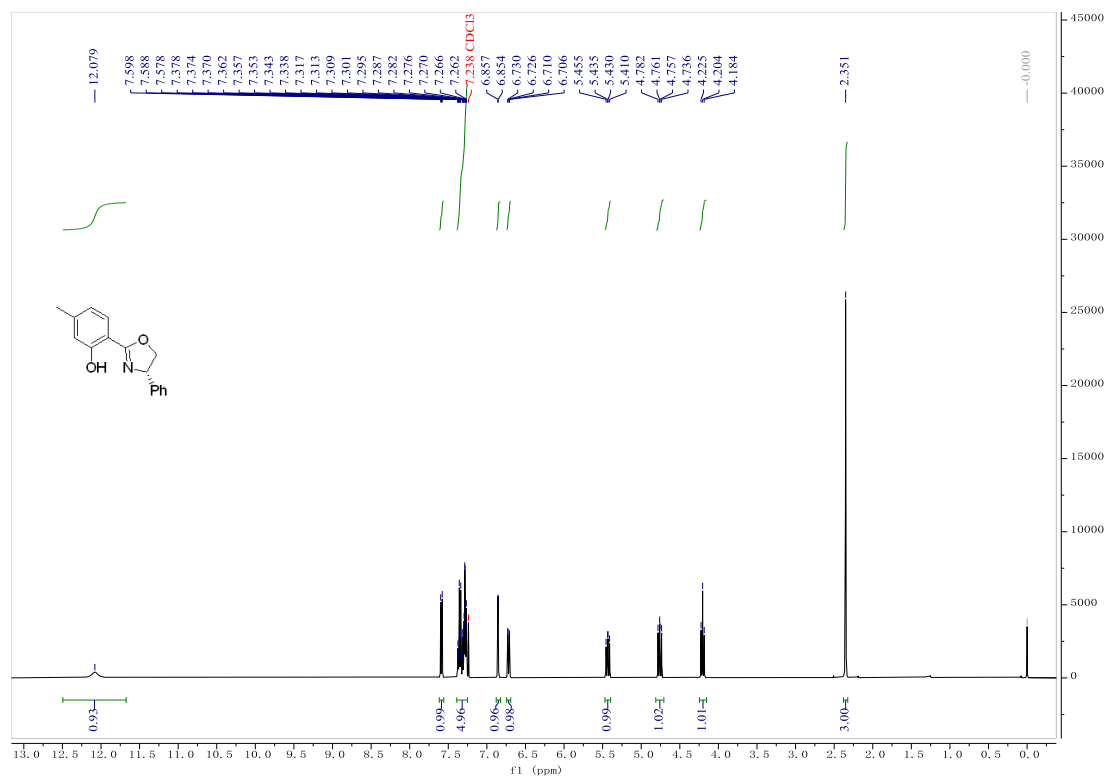


¹⁹F NMR (376 MHz, Chloroform-*d*)

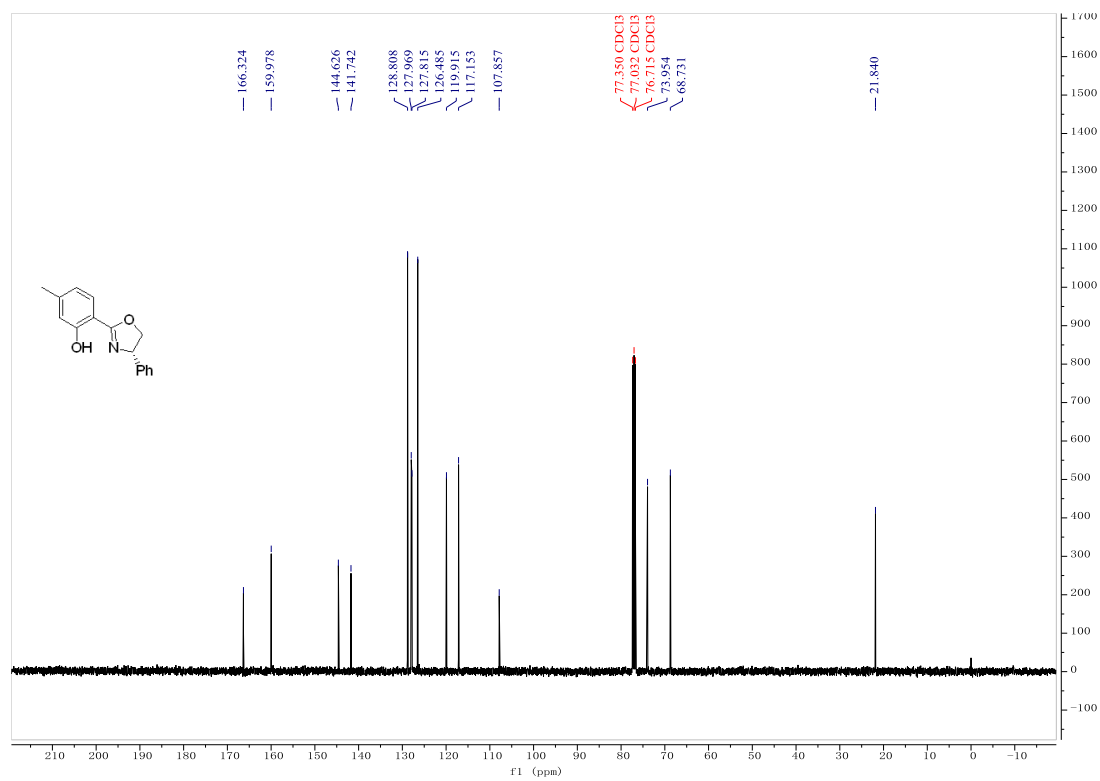


L10

¹H NMR (400 MHz, Chloroform-*d*)

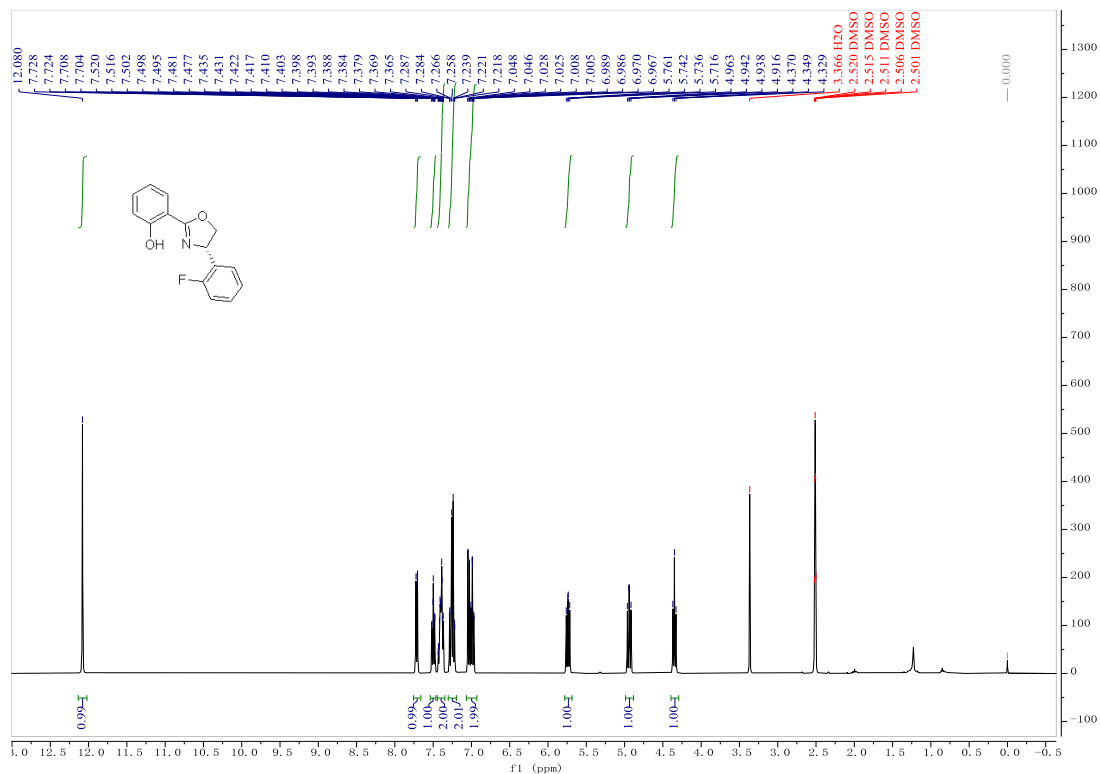


¹³C NMR (101 MHz, Chloroform-*d*)

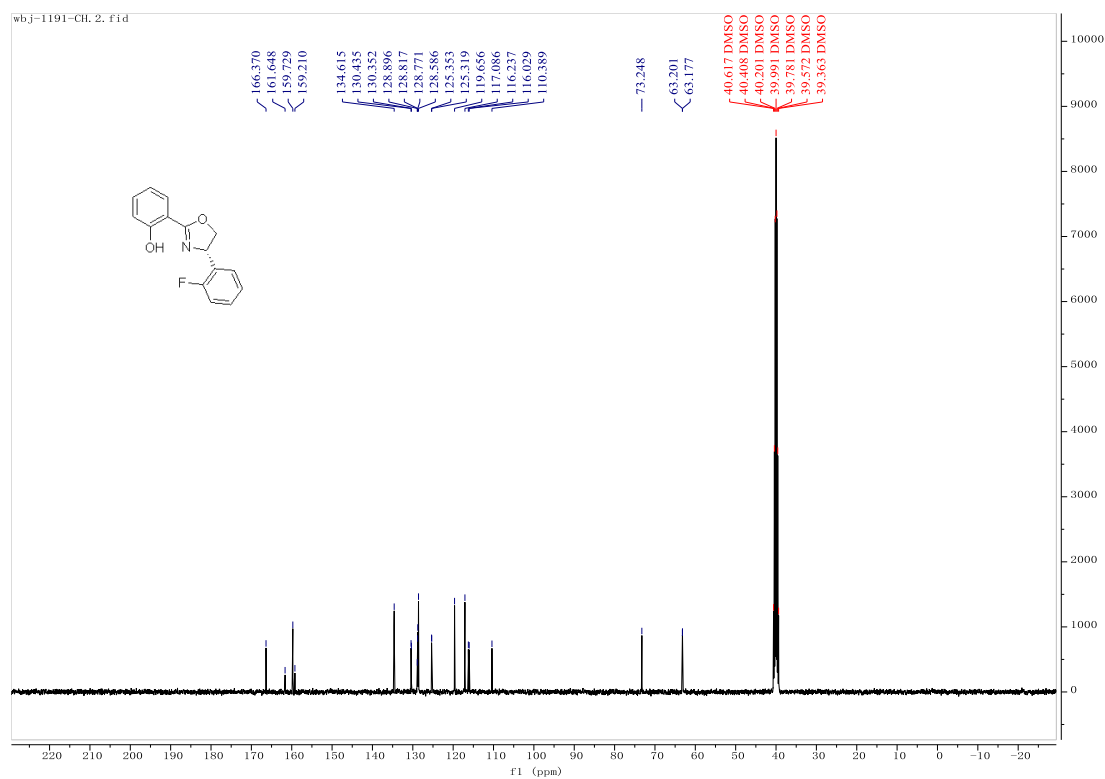


L15

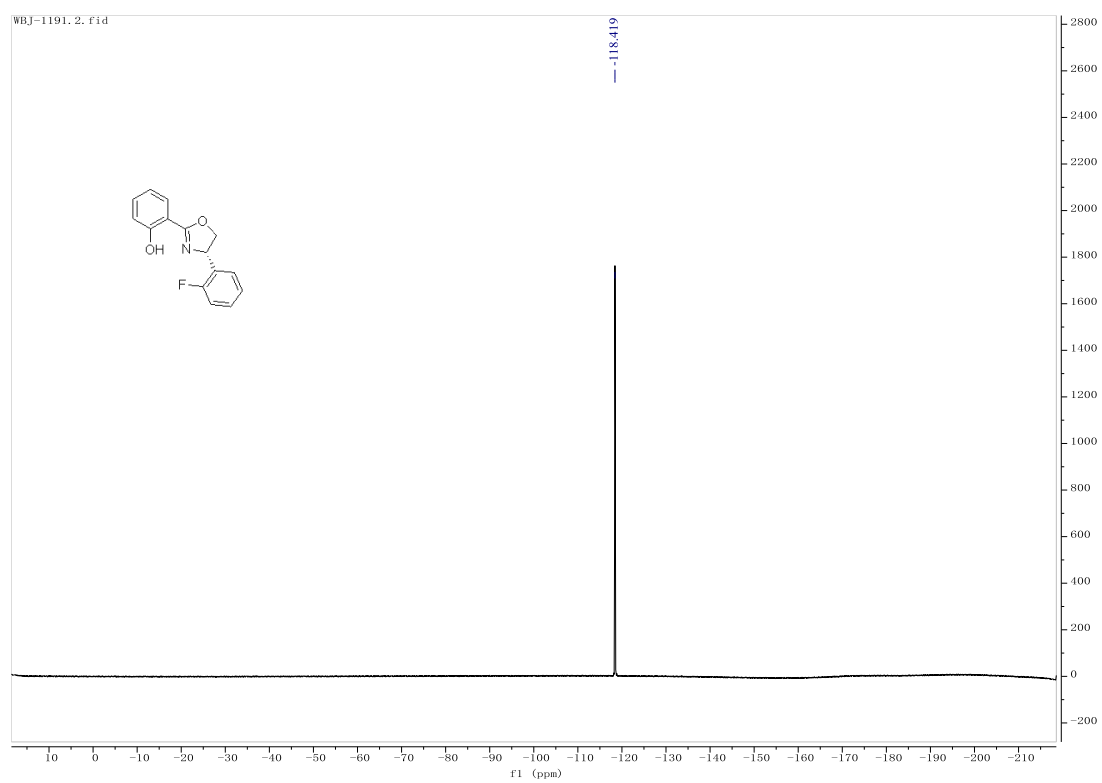
¹H NMR (400 MHz, Chloroform-*d*)



¹³C NMR (101 MHz, Chloroform-*d*)

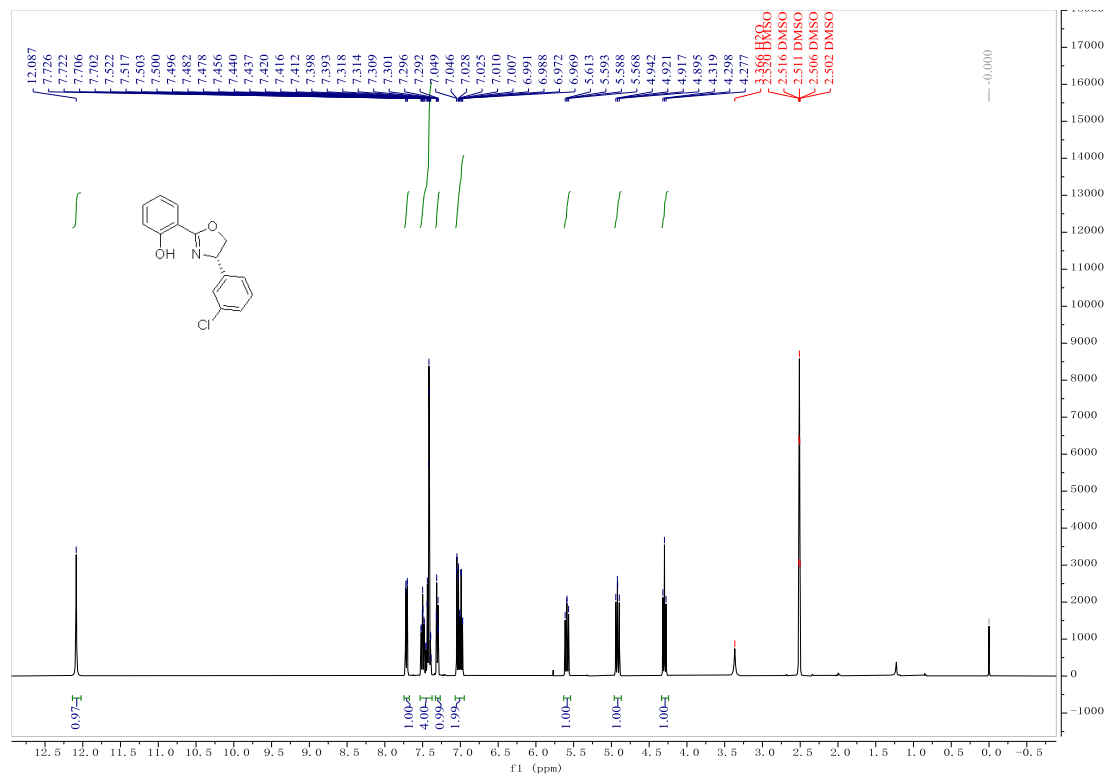


¹⁹F NMR (376 MHz, Chloroform-*d*)

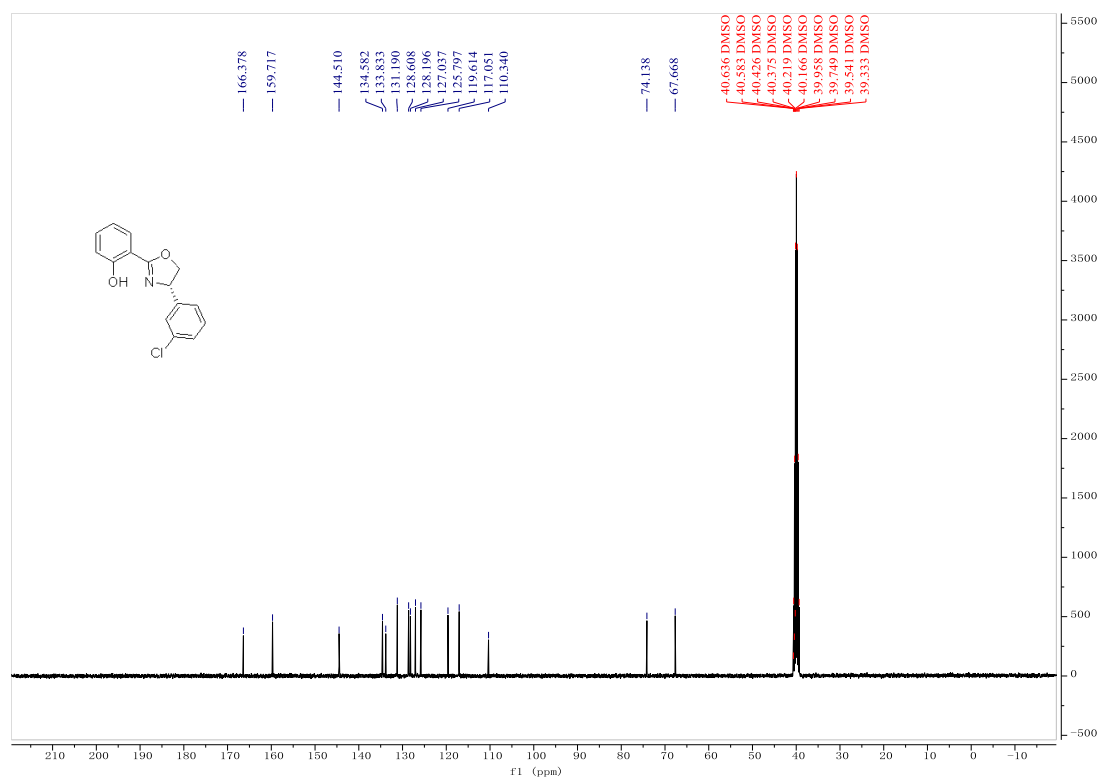


L16

¹H NMR (400 MHz, Chloroform-*d*)

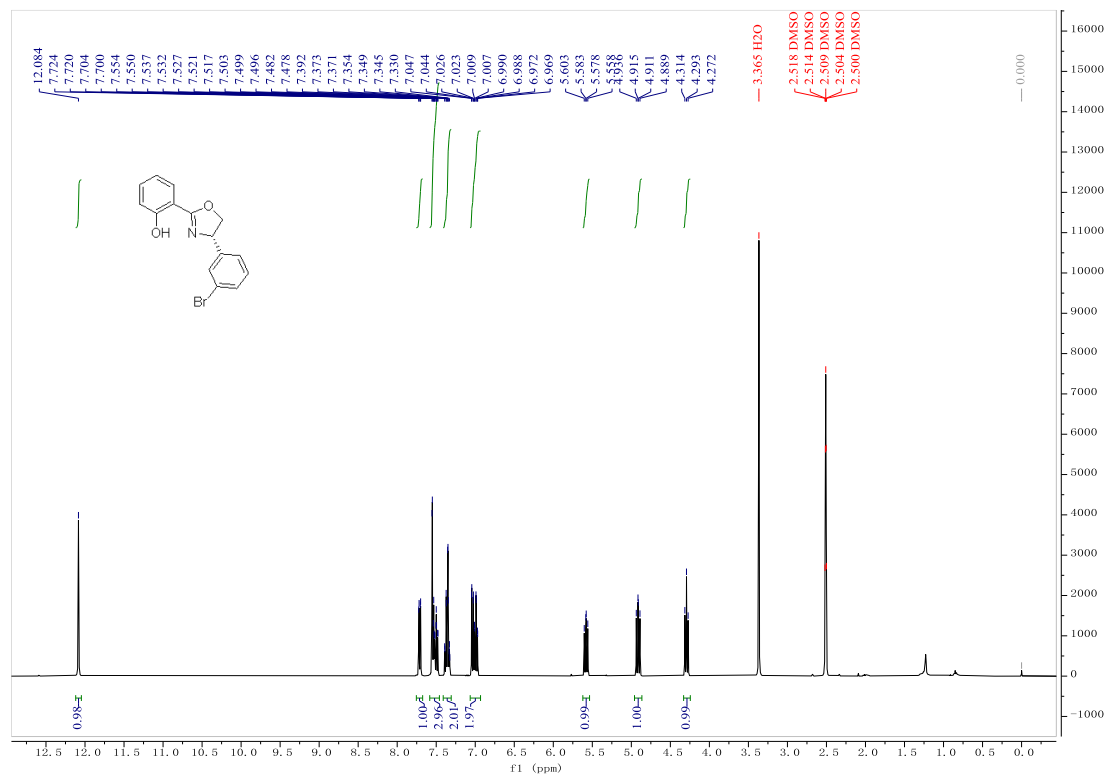


¹³C NMR (101 MHz, Chloroform-*d*)

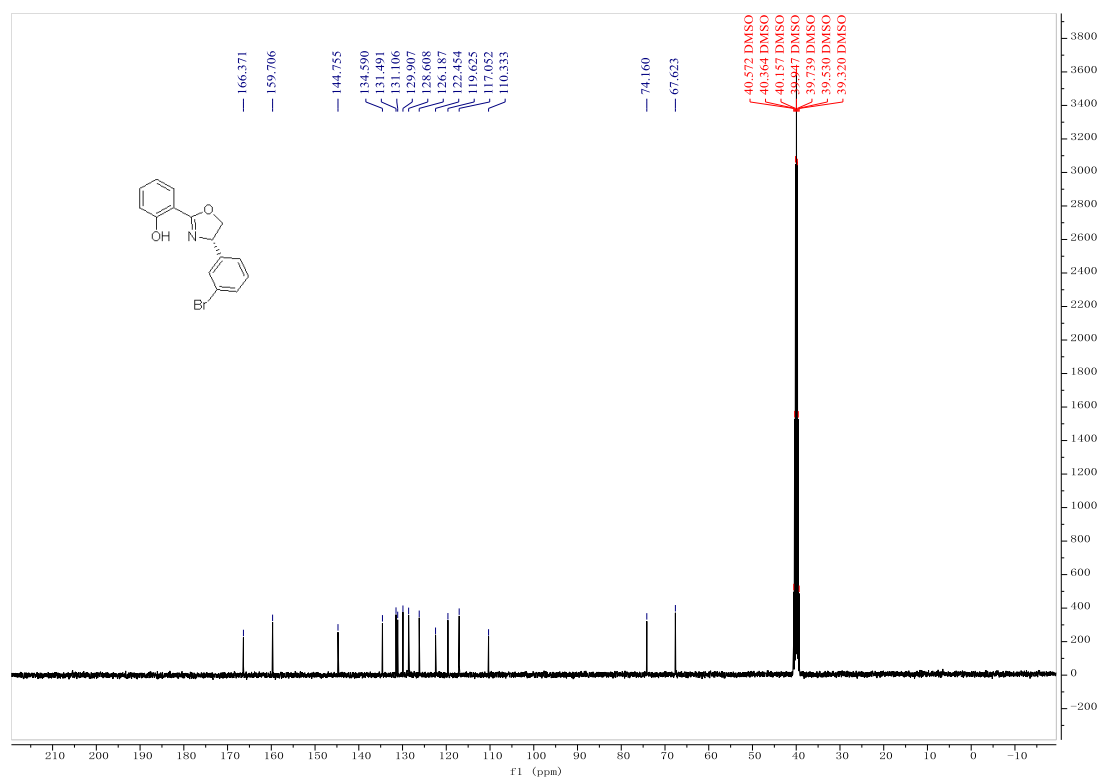


L17

¹H NMR (400 MHz, Chloroform-*d*)

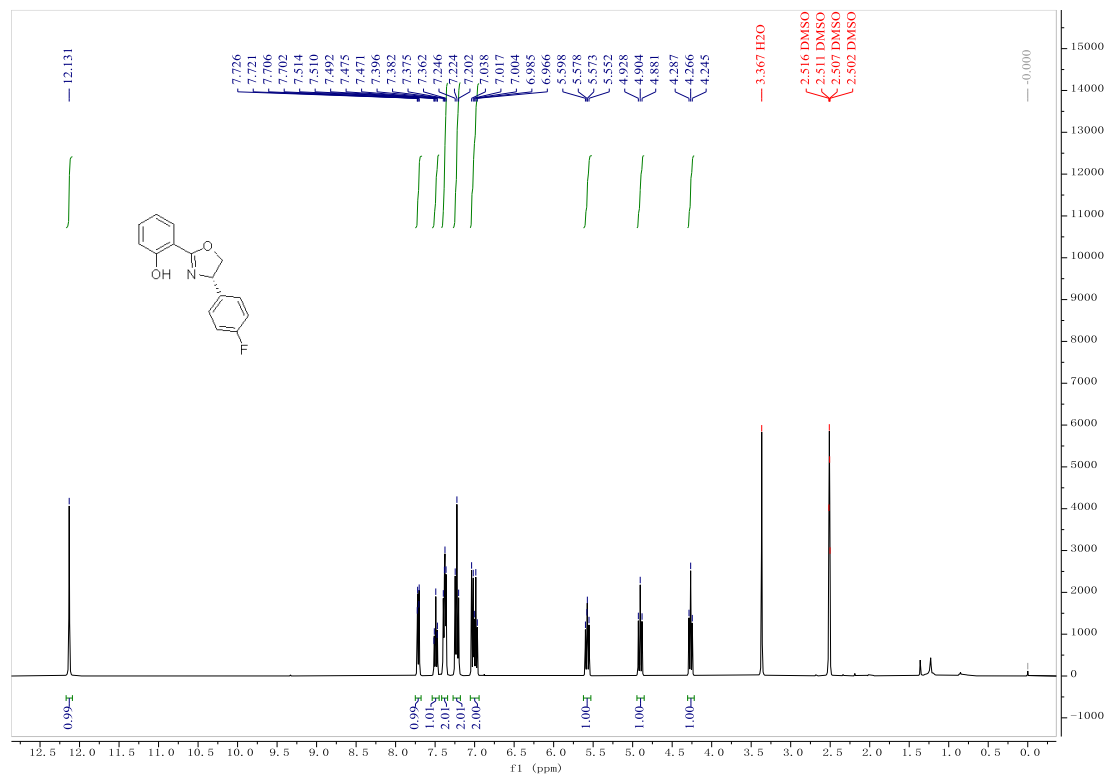


¹³C NMR (101 MHz, Chloroform-*d*)

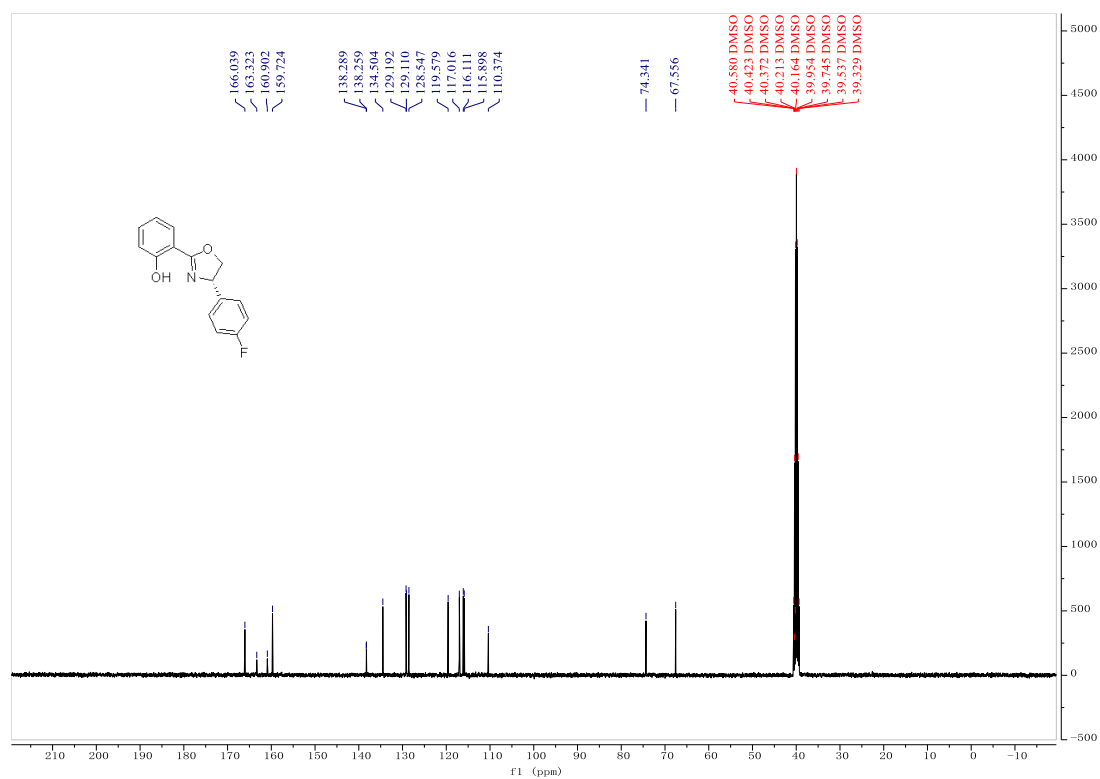


L18

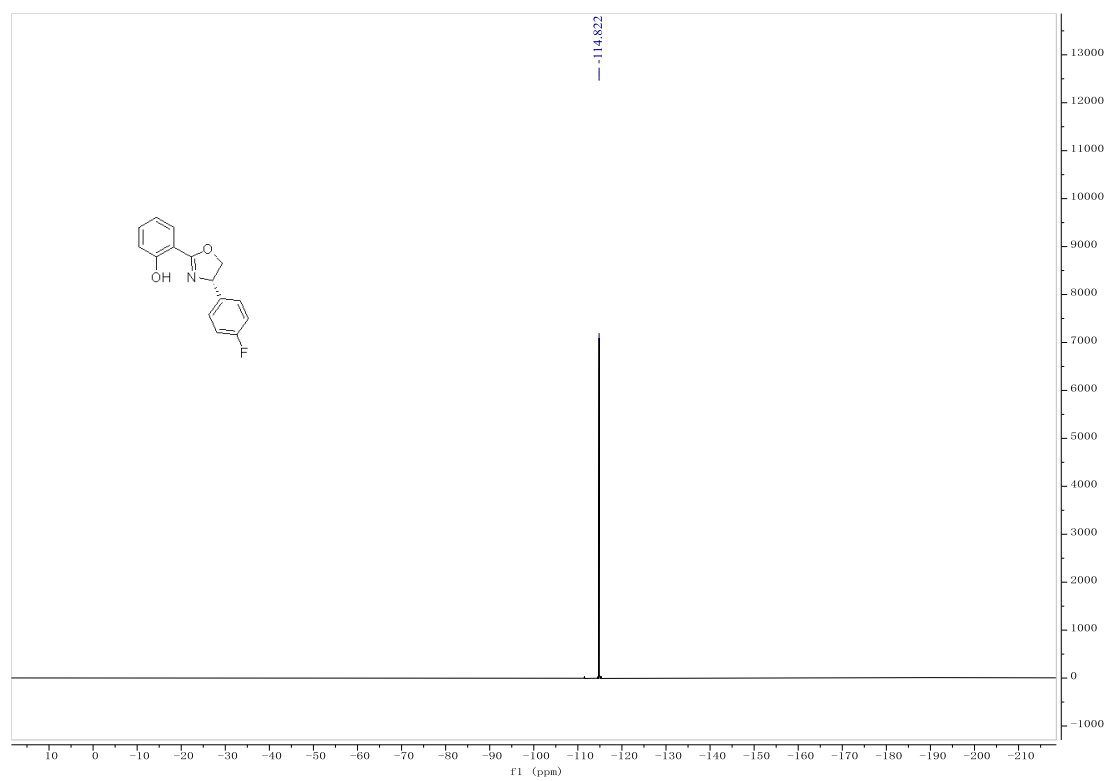
¹H NMR (400 MHz, Chloroform-*d*)



¹³C NMR (101 MHz, Chloroform-*d*)

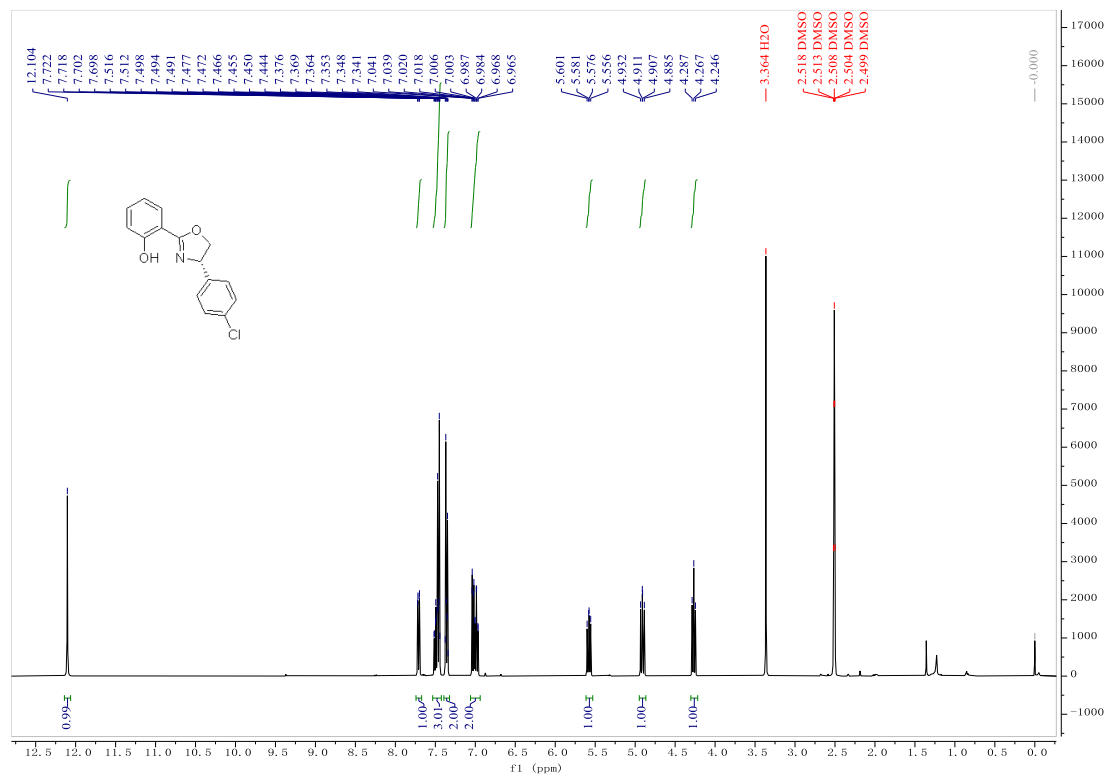


¹⁹F NMR (376 MHz, Chloroform-*d*)

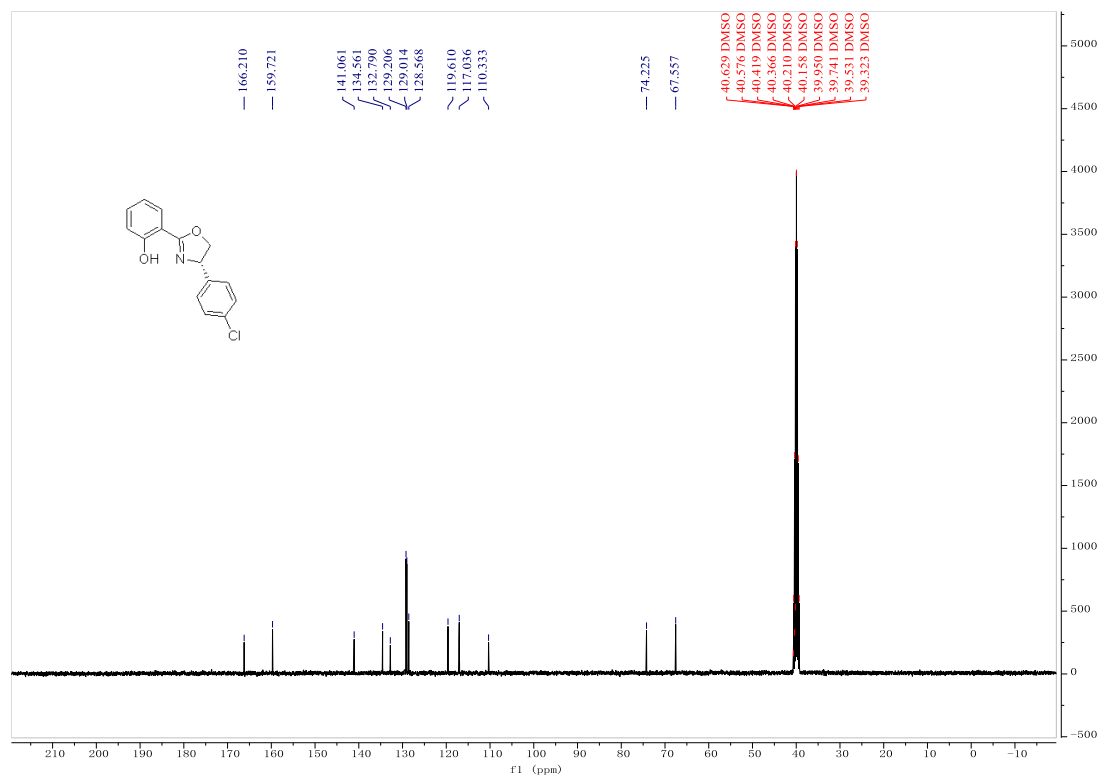


L19

¹H NMR (400 MHz, Chloroform-*d*)

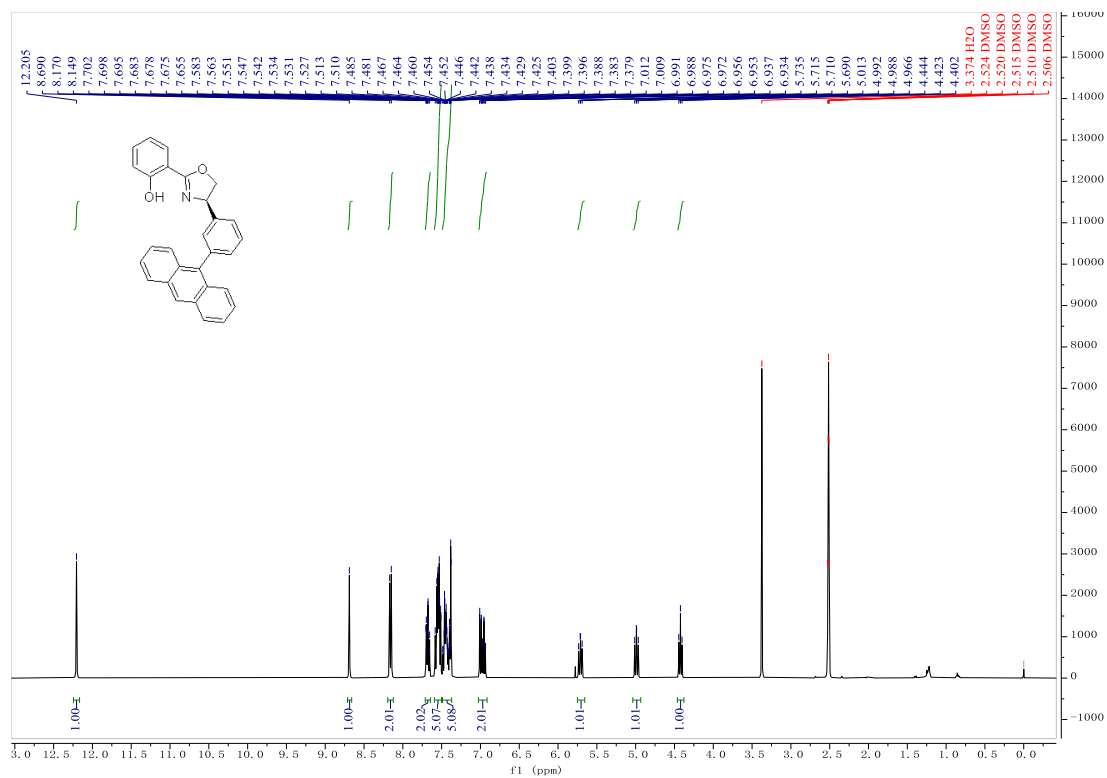


¹³C NMR (101 MHz, Chloroform-*d*)

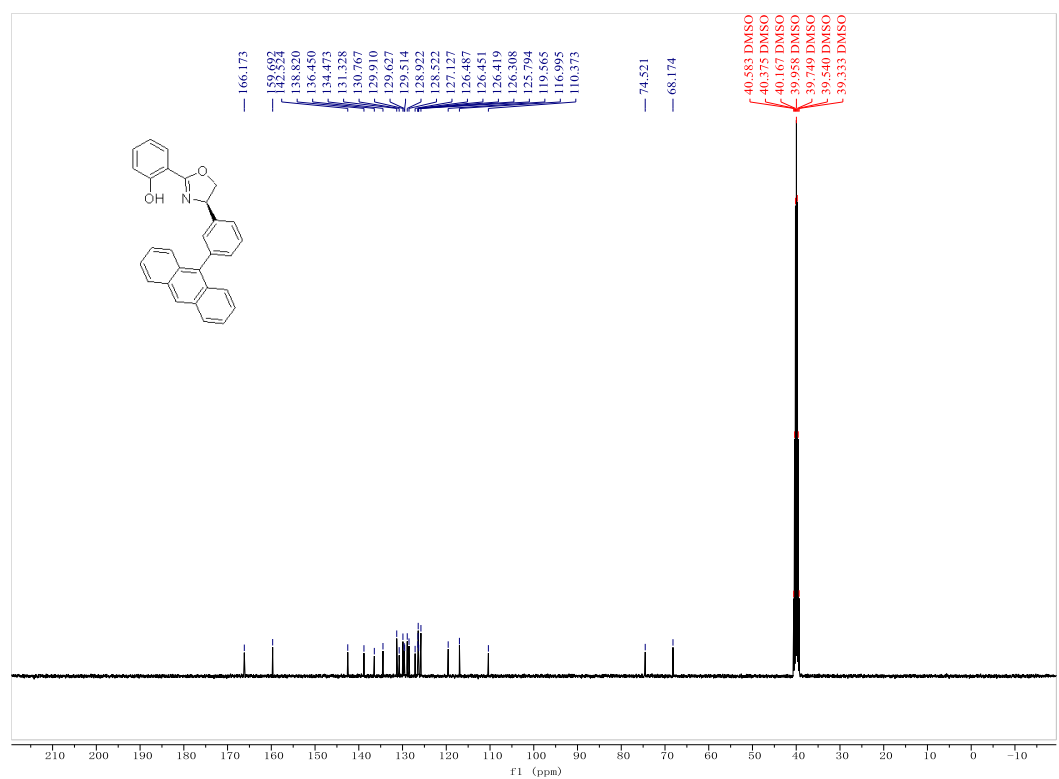


L20

^1H NMR (400 MHz, Chloroform-*d*)

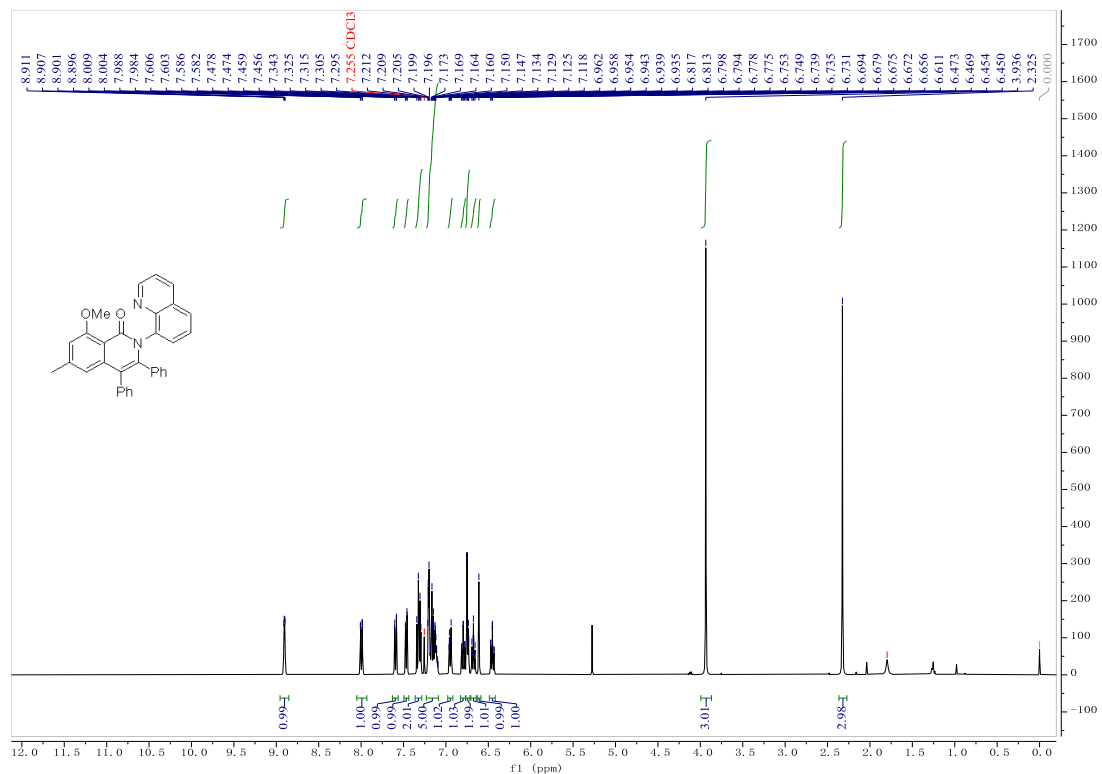


^{13}C NMR (101 MHz, Chloroform-*d*)

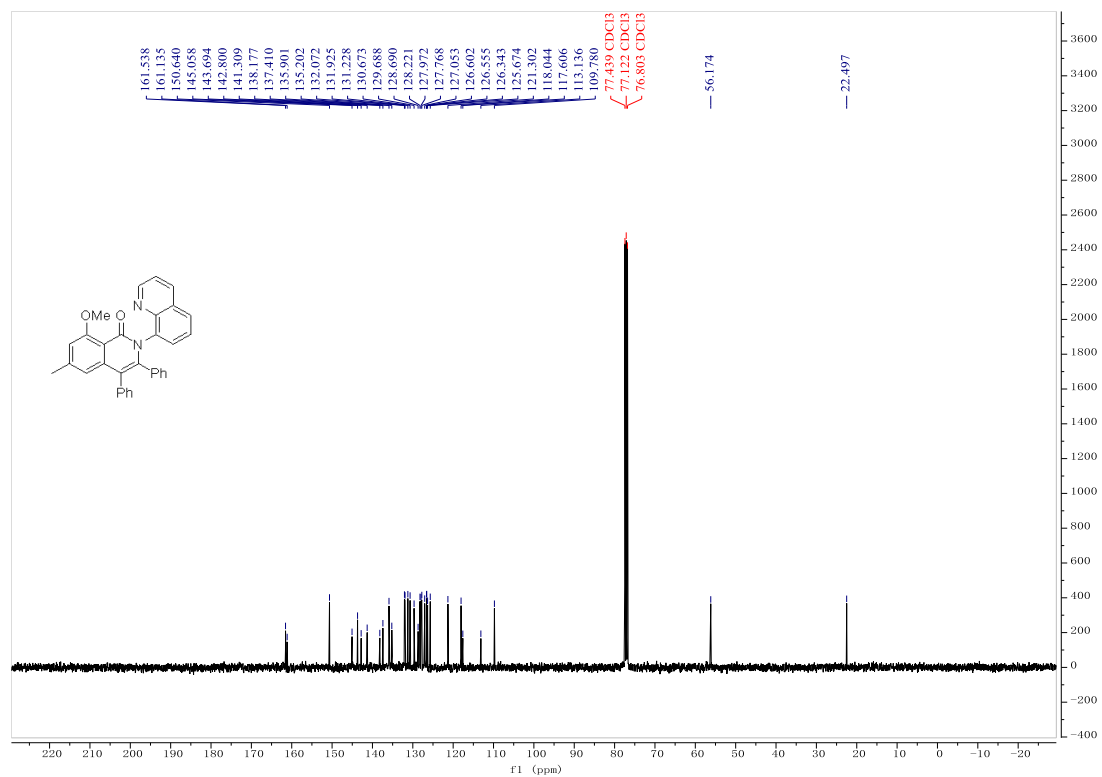


5a

¹H NMR (400 MHz, Chloroform-*d*)

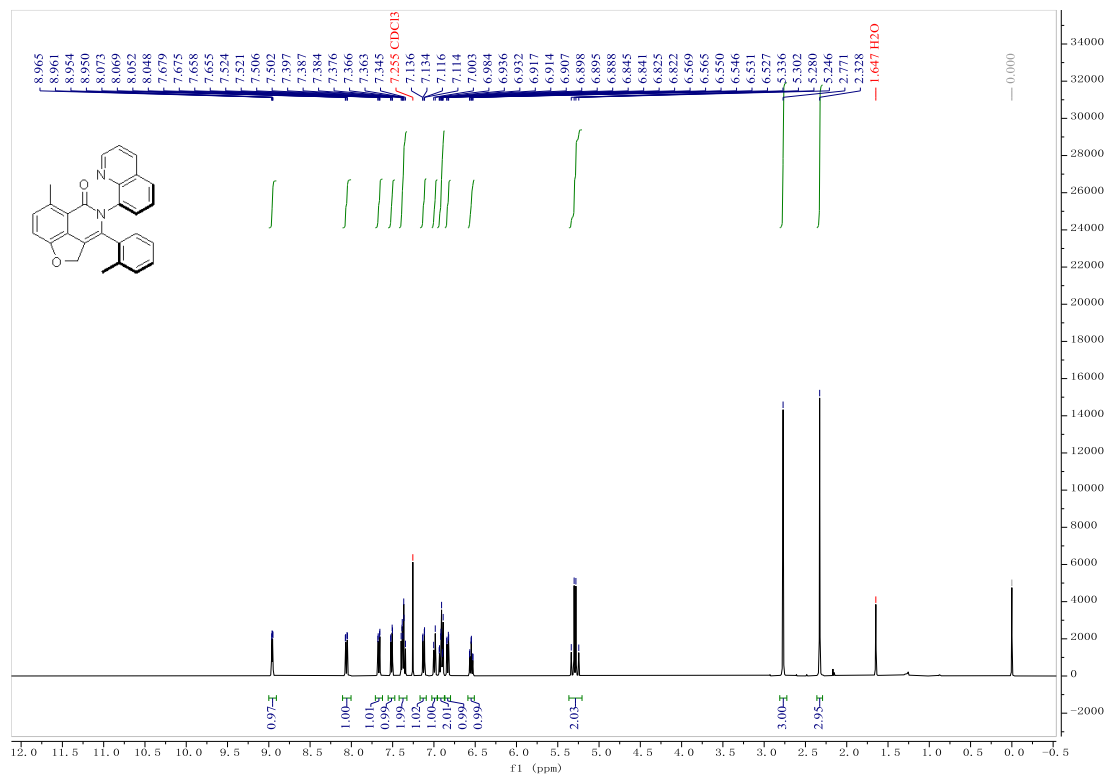


¹³C NMR (101 MHz, Chloroform-*d*)

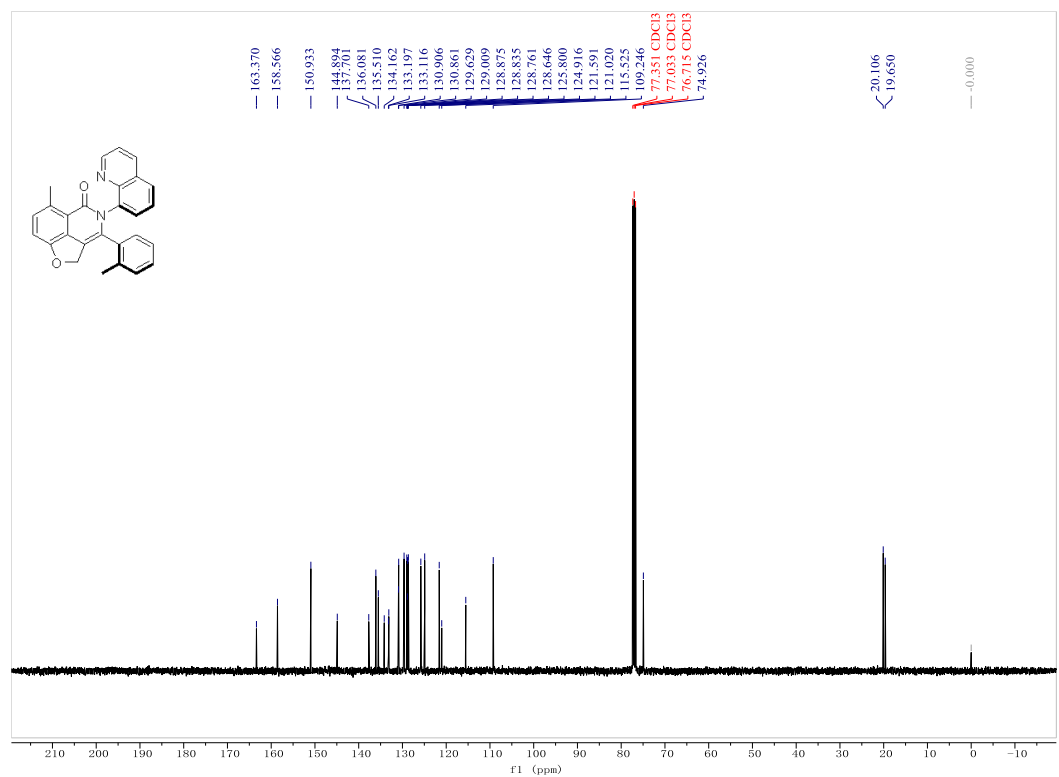


2a

¹H NMR (400 MHz, Chloroform-*d*)

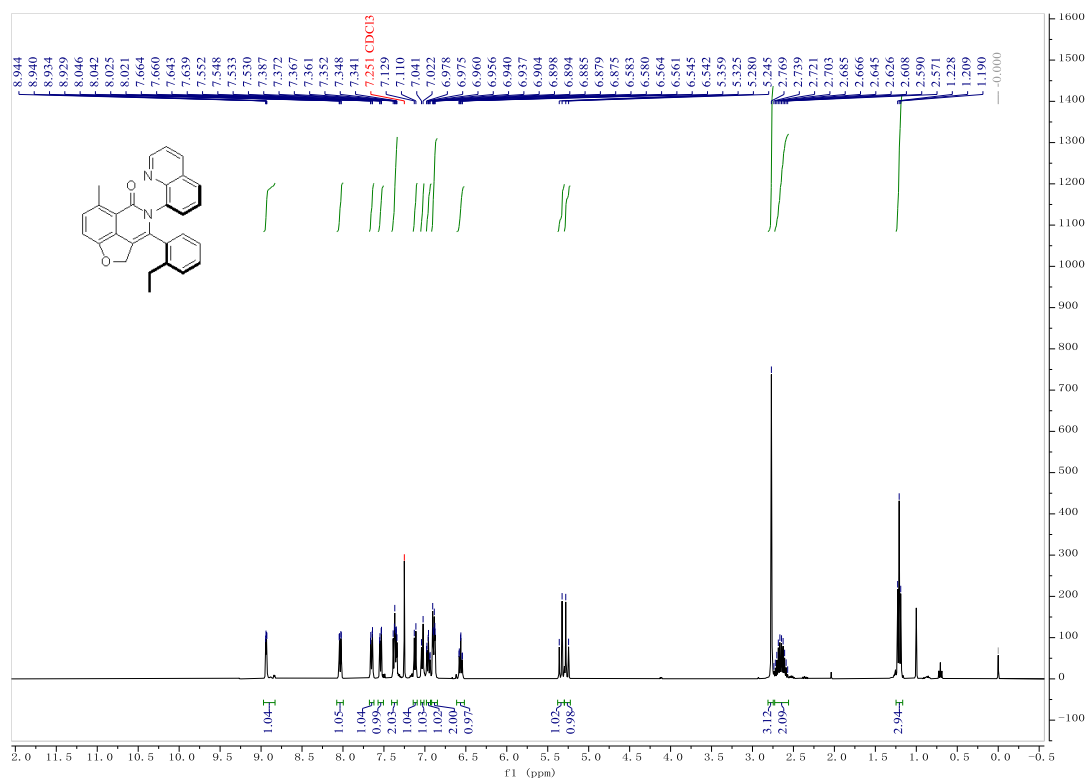


¹³C NMR (101 MHz, Chloroform-*d*)

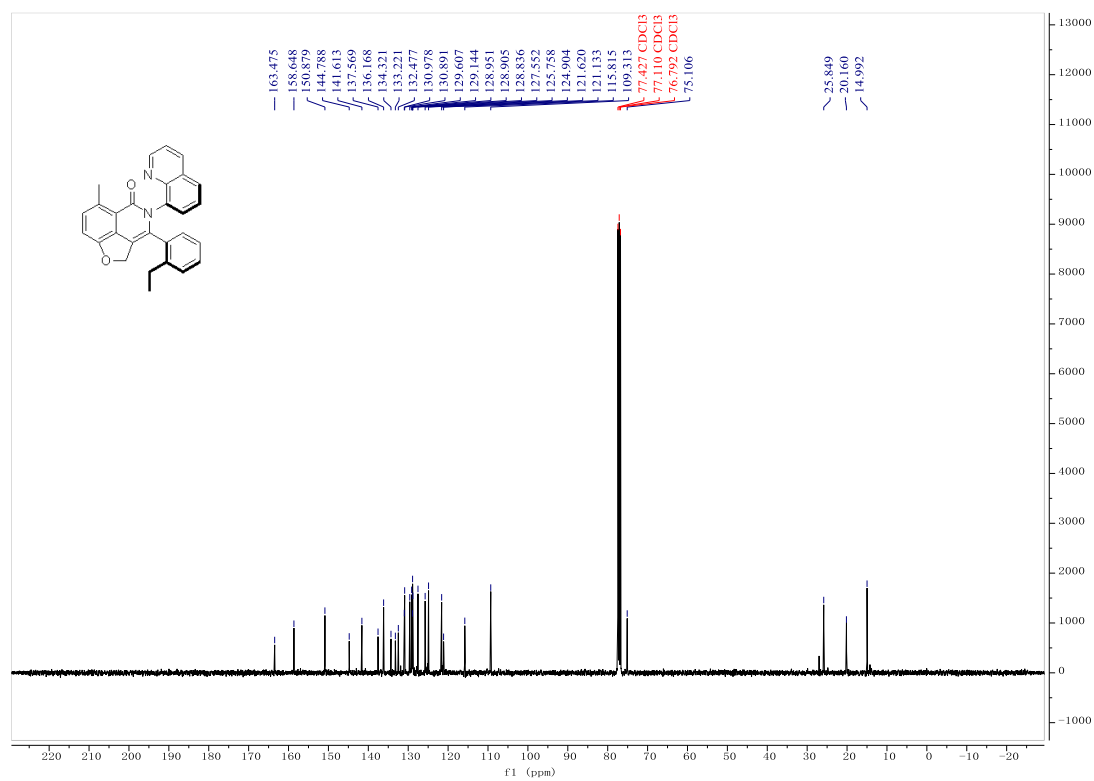


2b

¹H NMR (400 MHz, Chloroform-*d*)

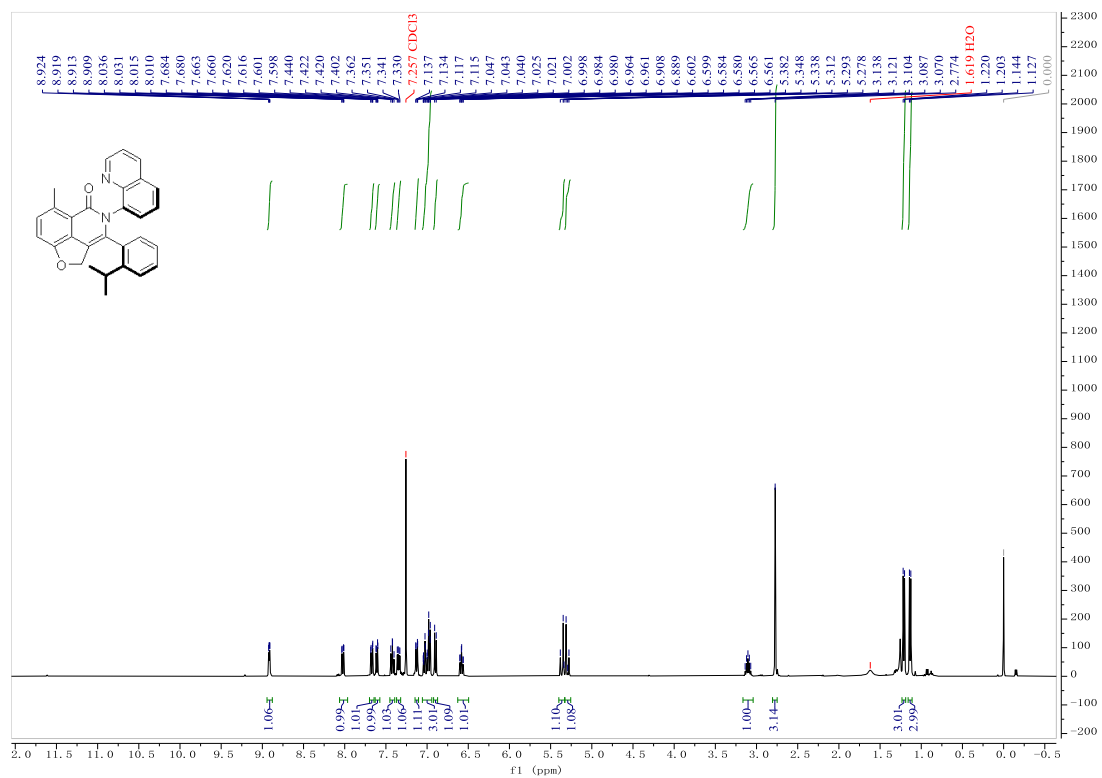


¹³C NMR (101 MHz, Chloroform-*d*)

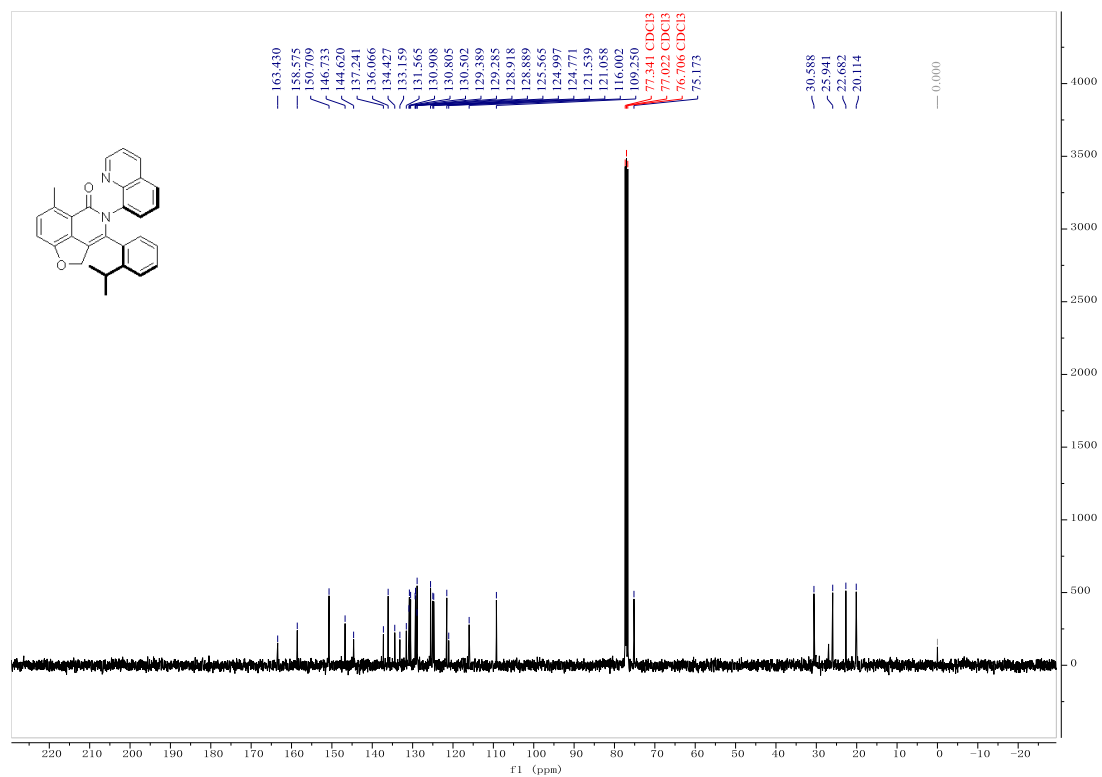


2c

¹H NMR (400 MHz, Chloroform-*d*)

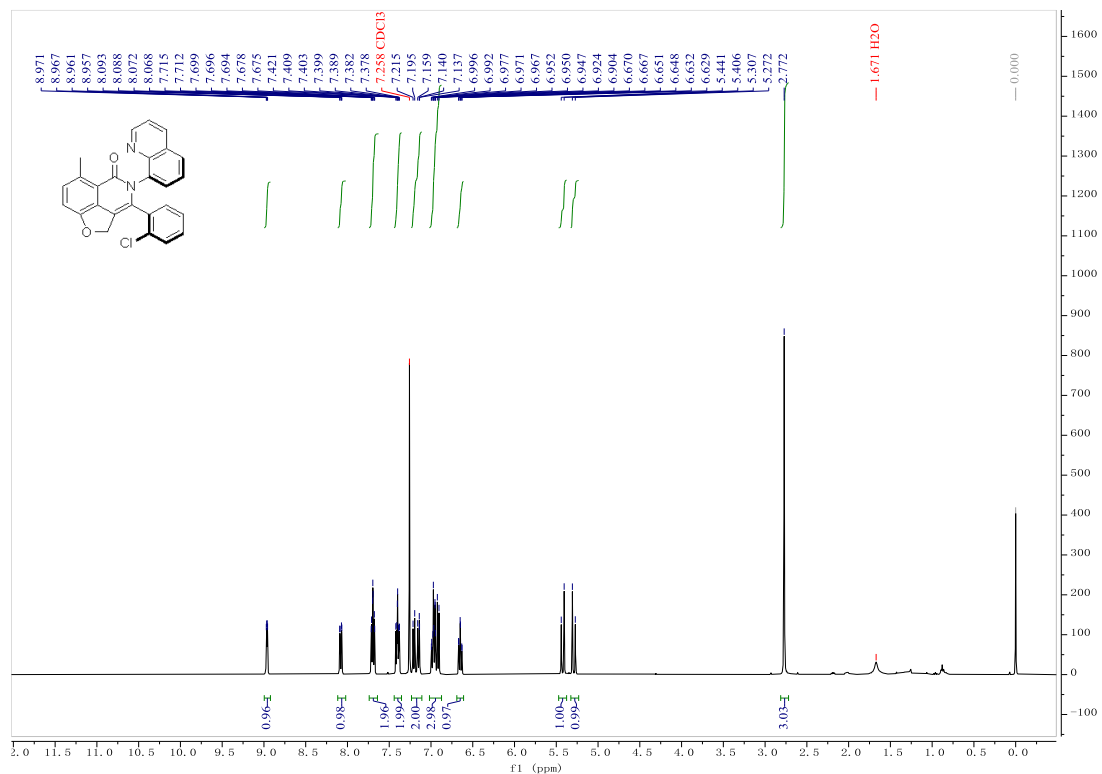


¹³C NMR (101 MHz, Chloroform-*d*)

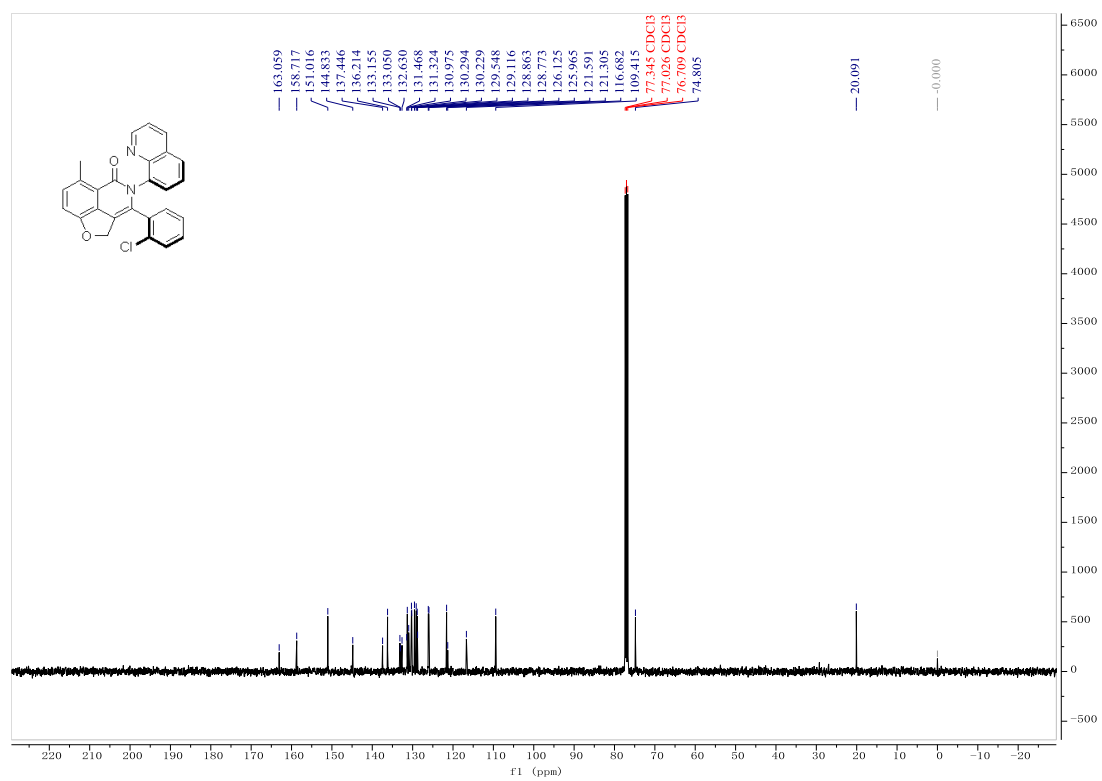


2d

¹H NMR (400 MHz, Chloroform-*d*)

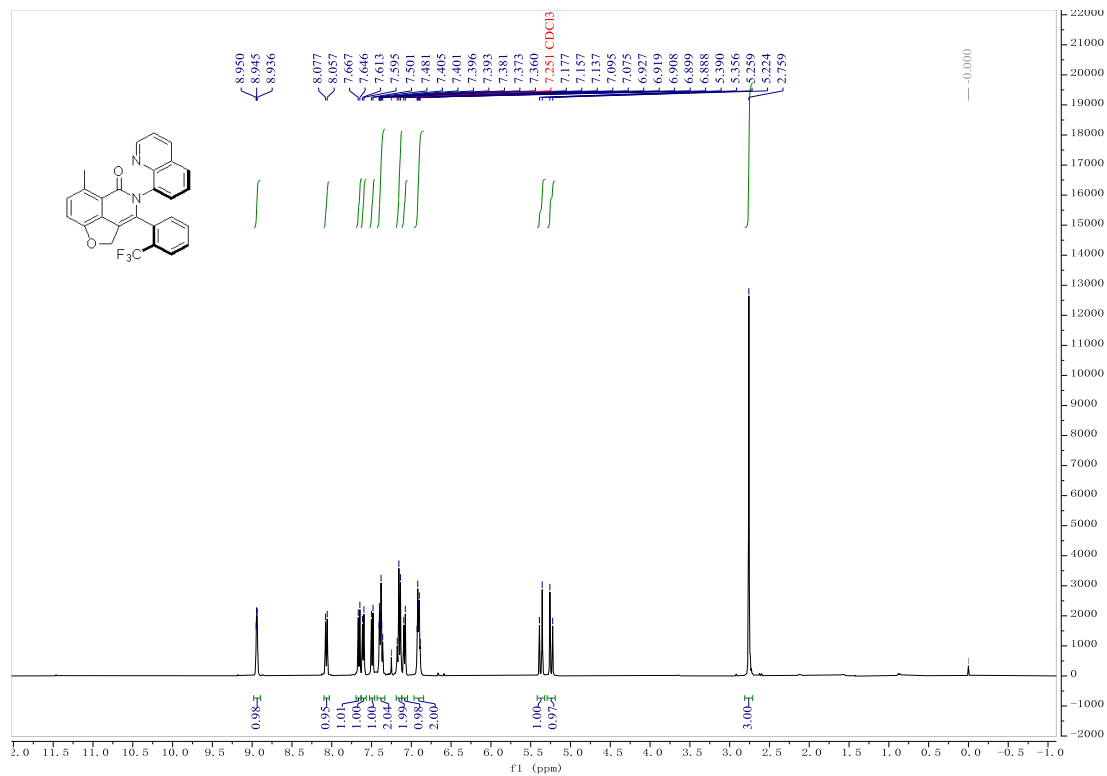


¹³C NMR (101 MHz, Chloroform-*d*)

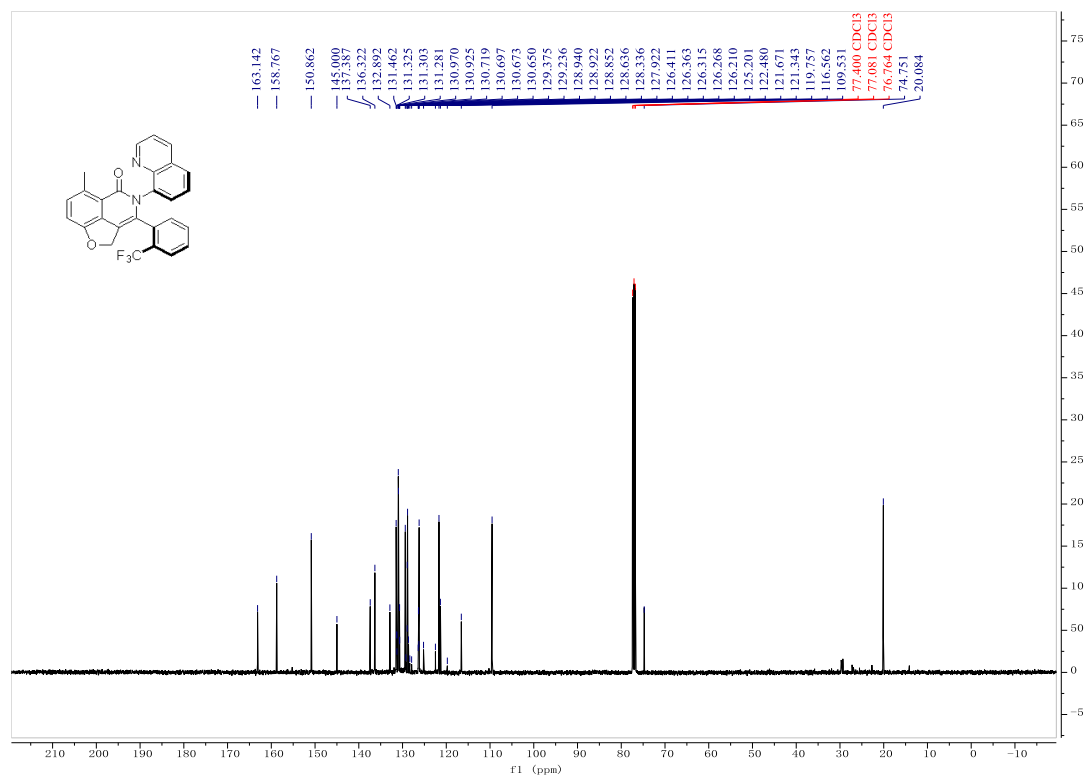


2e

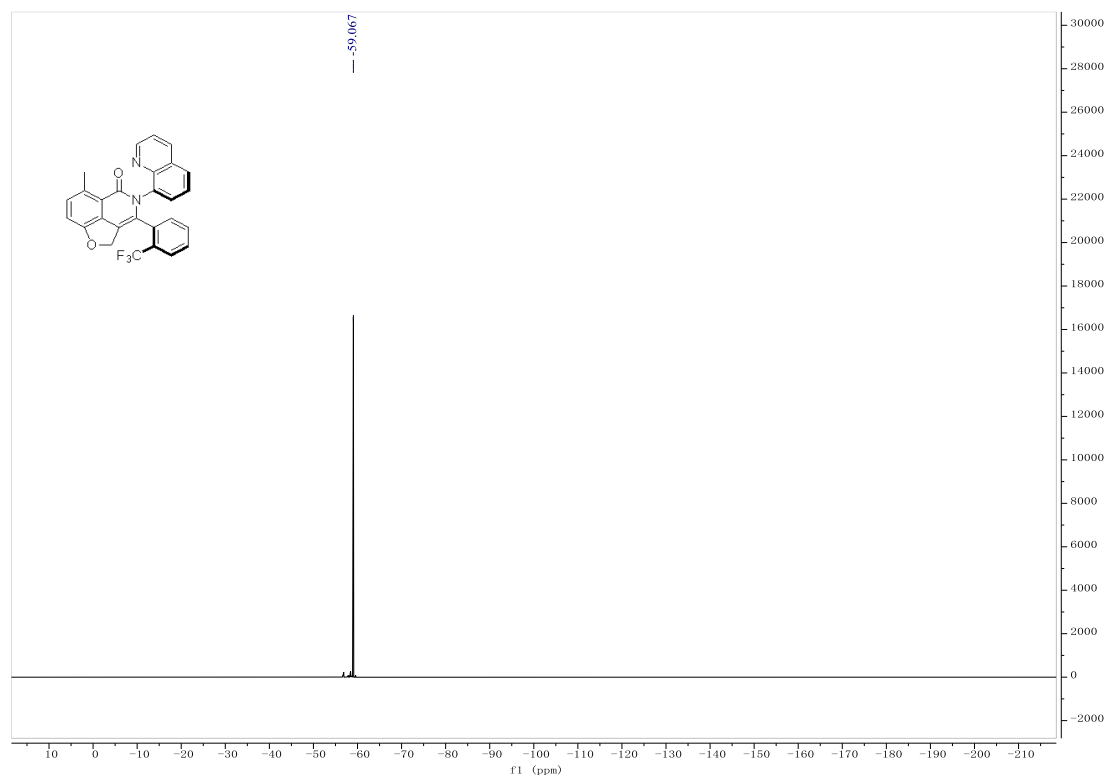
¹H NMR (400 MHz, Chloroform-*d*)



¹³C NMR (101 MHz, Chloroform-*d*)

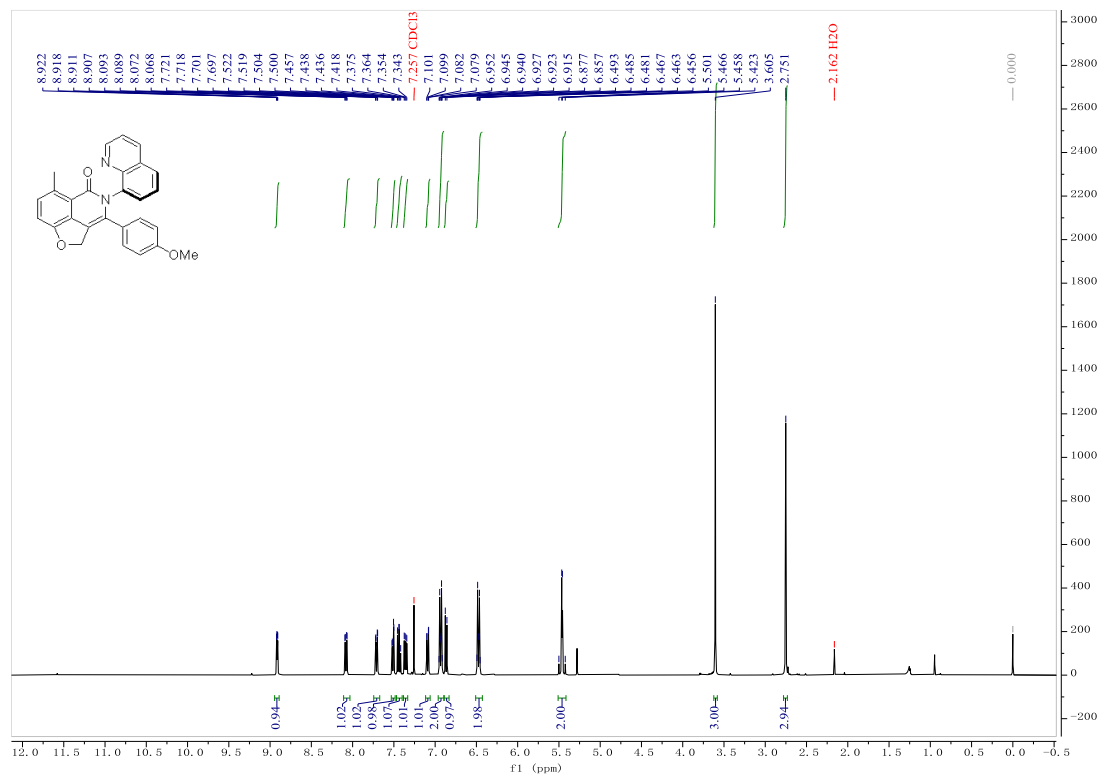


¹⁹F NMR (376 MHz, Chloroform-*d*)

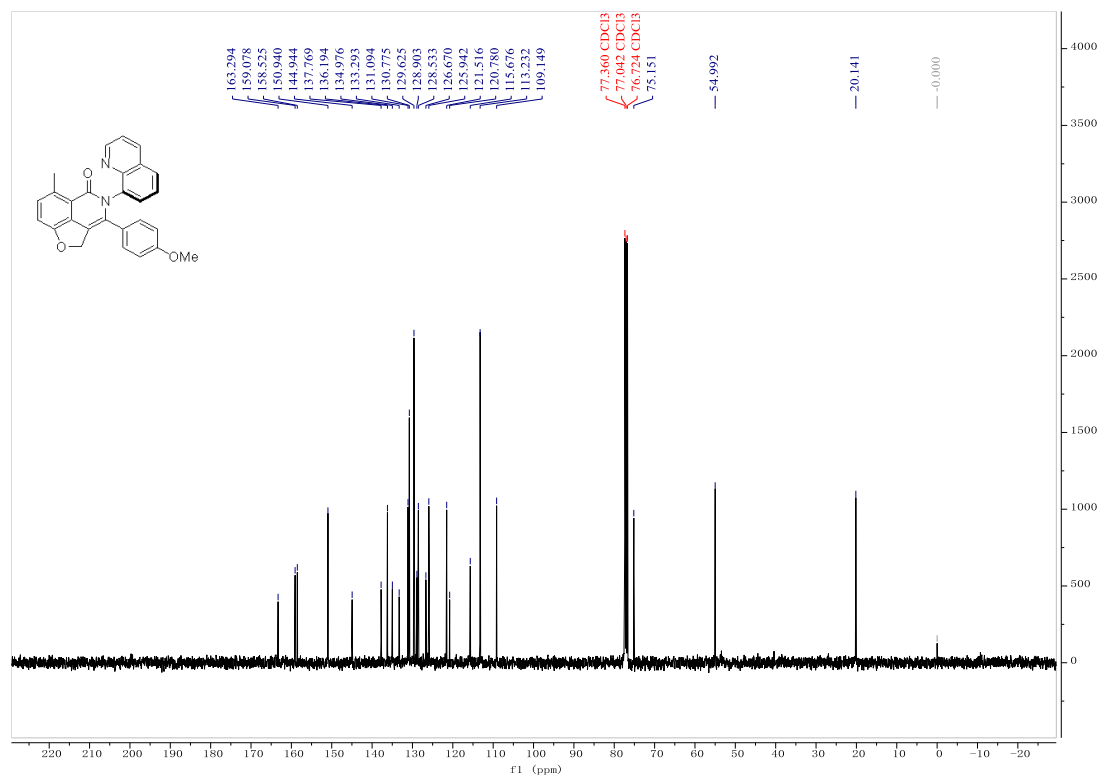


2f

¹H NMR (400 MHz, Chloroform-*d*)

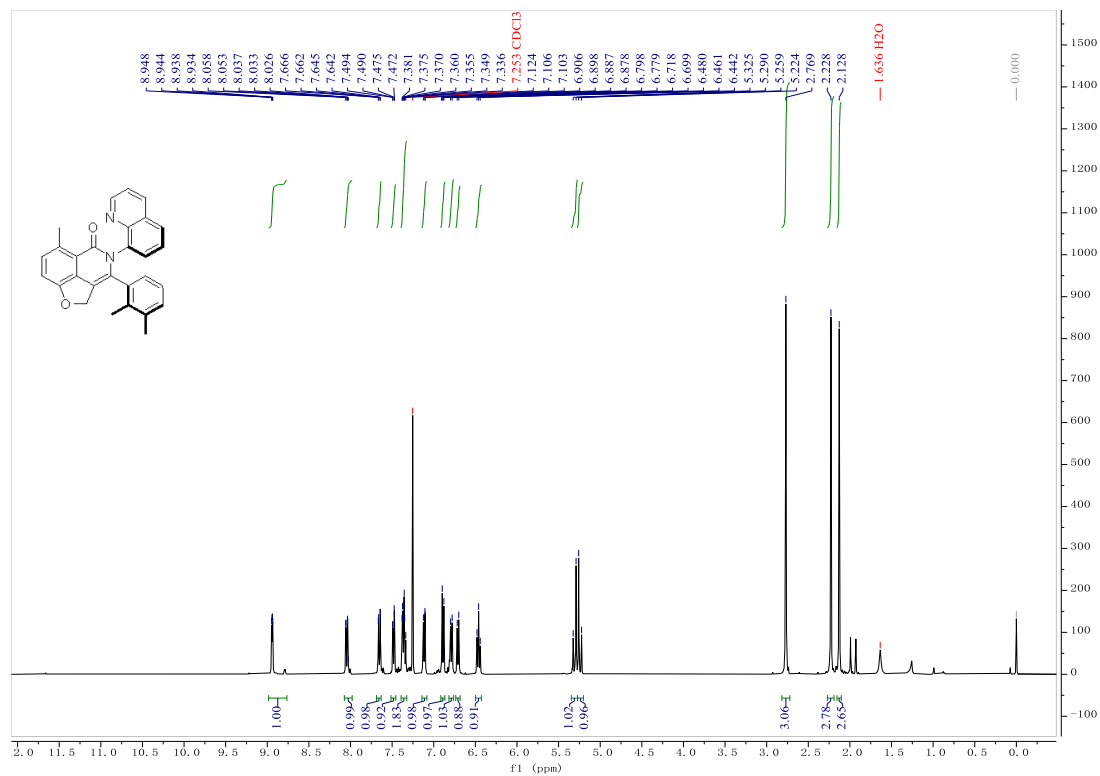


¹³C NMR (101 MHz, Chloroform-*d*)

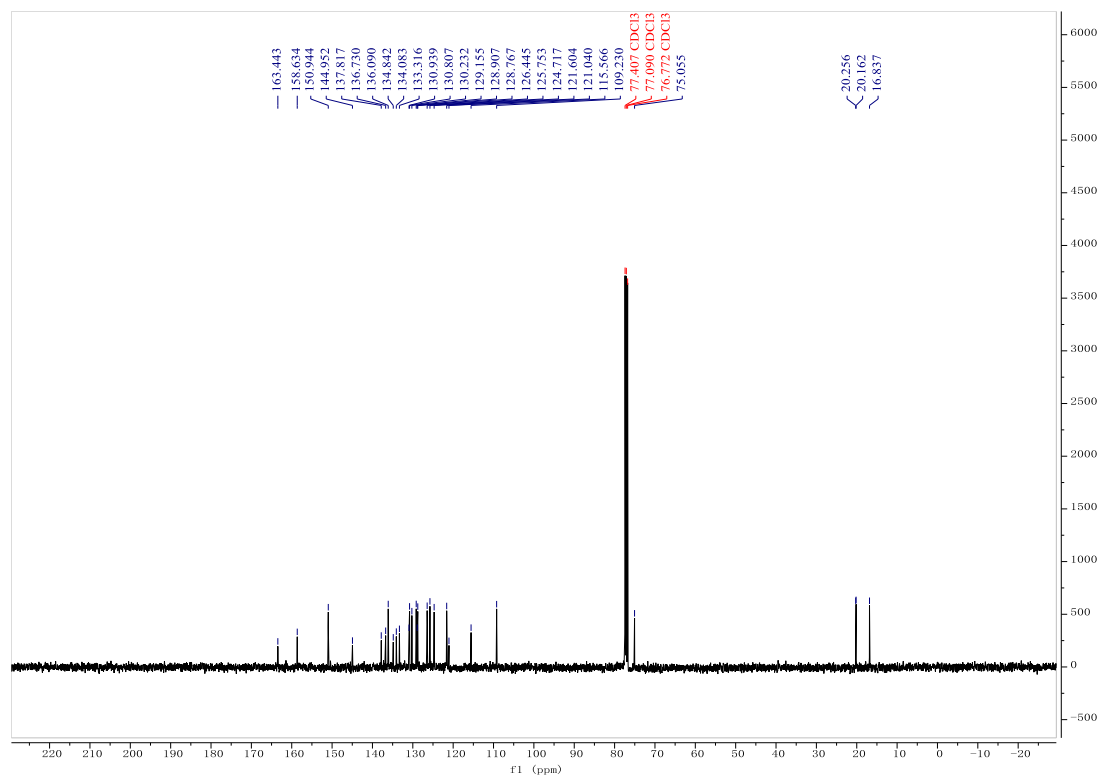


2g

¹H NMR (400 MHz, Chloroform-*d*)

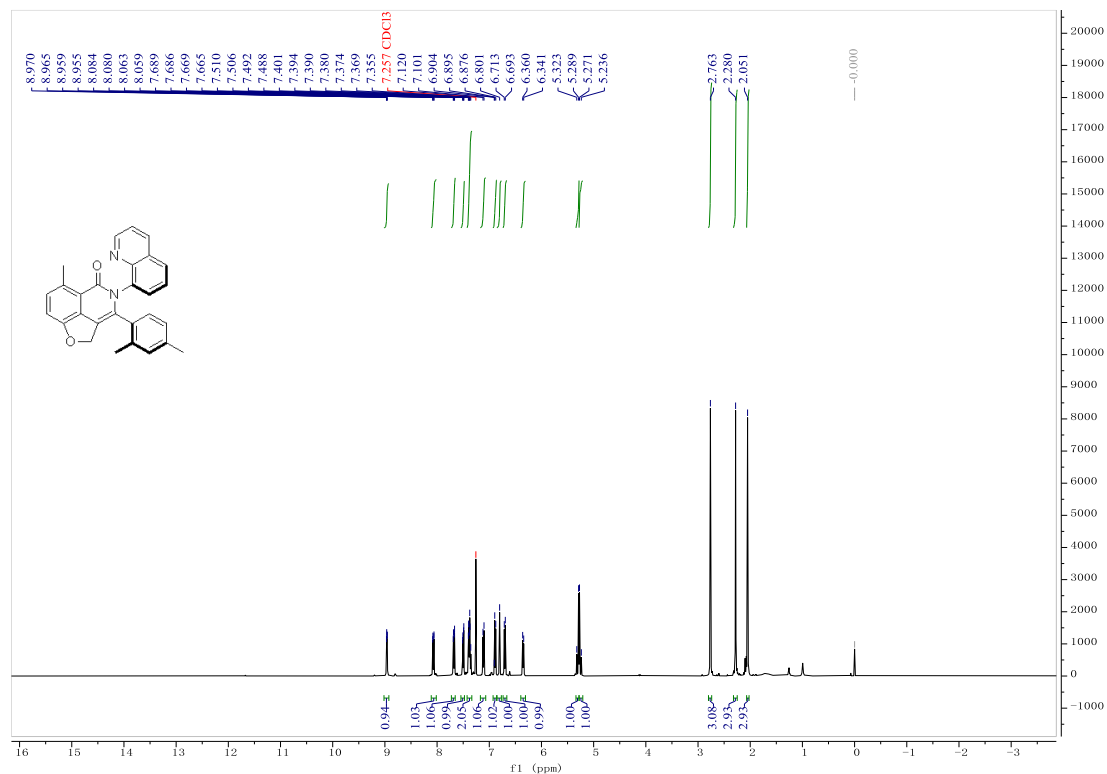


¹³C NMR (101 MHz, Chloroform-*d*)

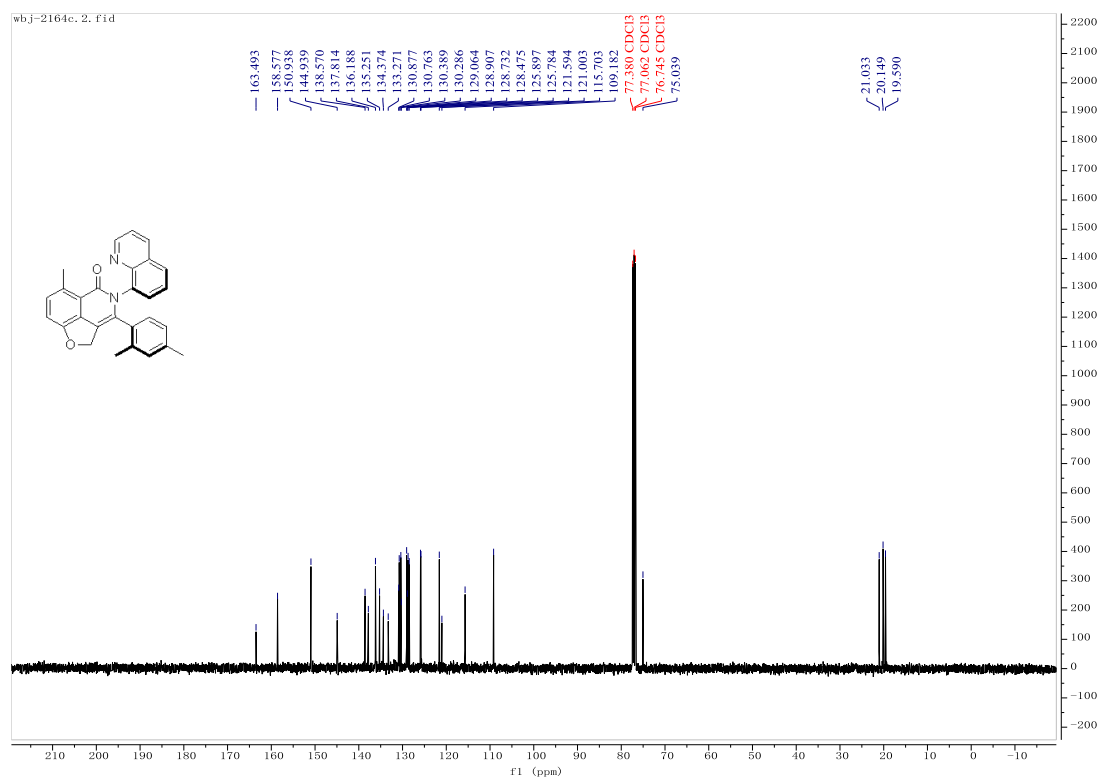


2h

¹H NMR (400 MHz, Chloroform-*d*)

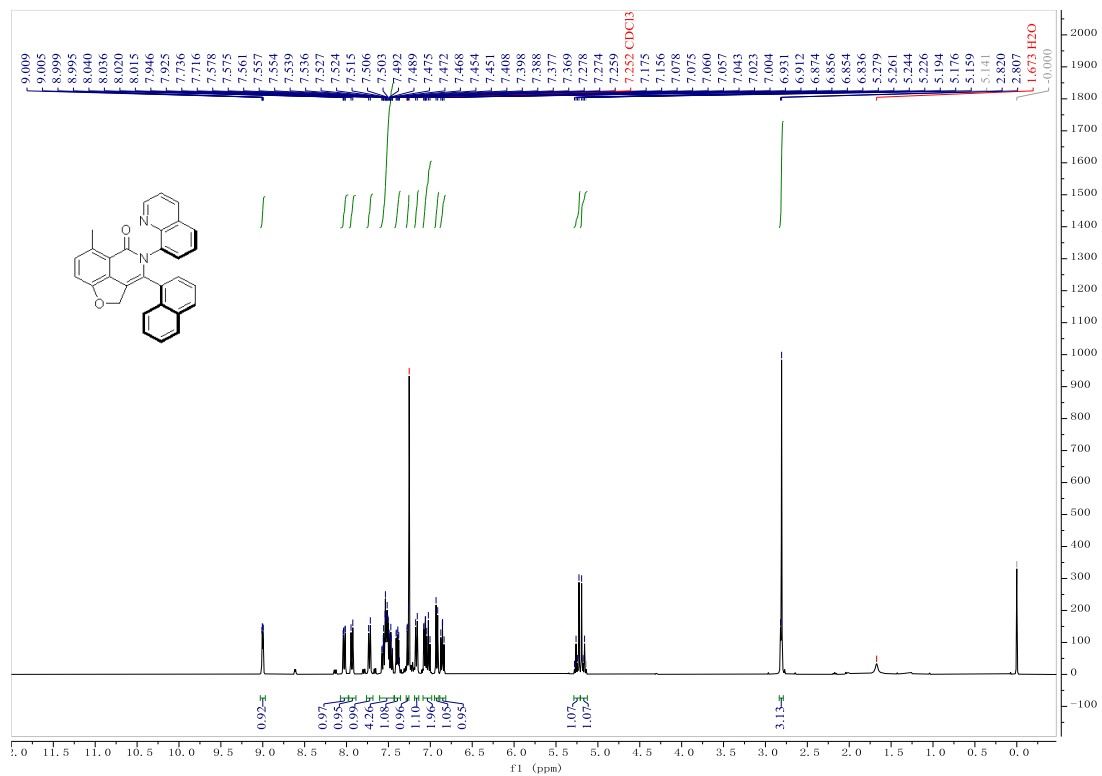


¹³C NMR (101 MHz, Chloroform-*d*)

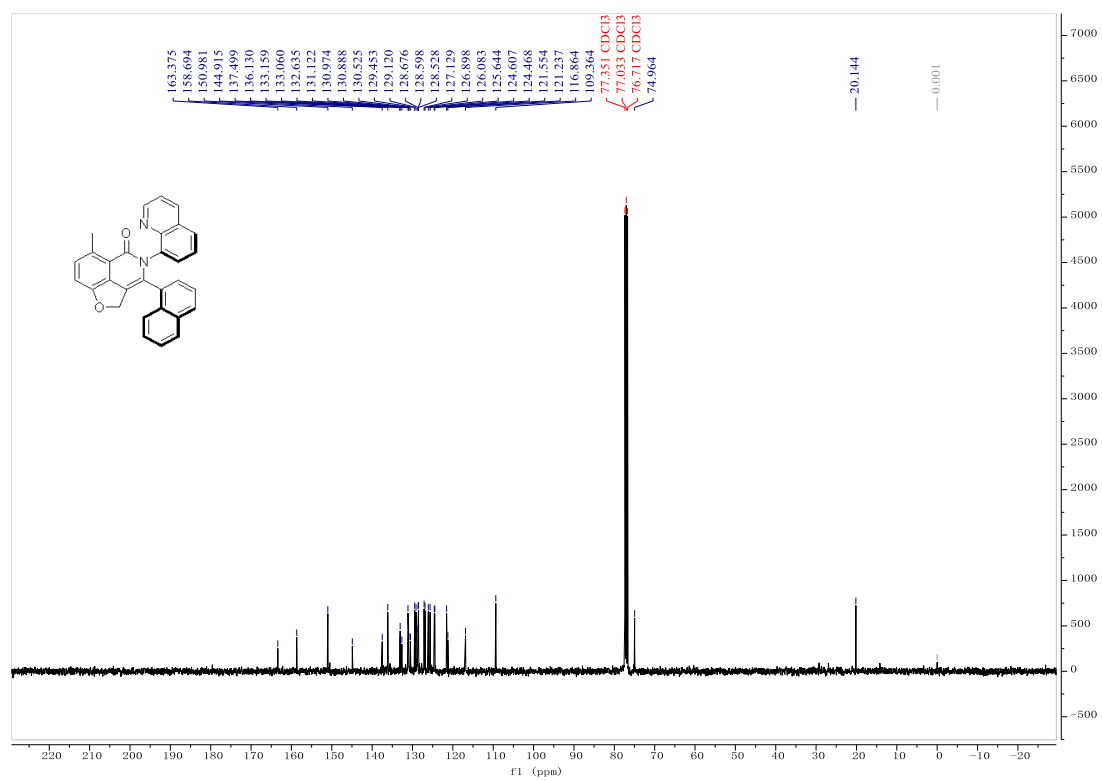


2i

^1H NMR (400 MHz, Chloroform-*d*)

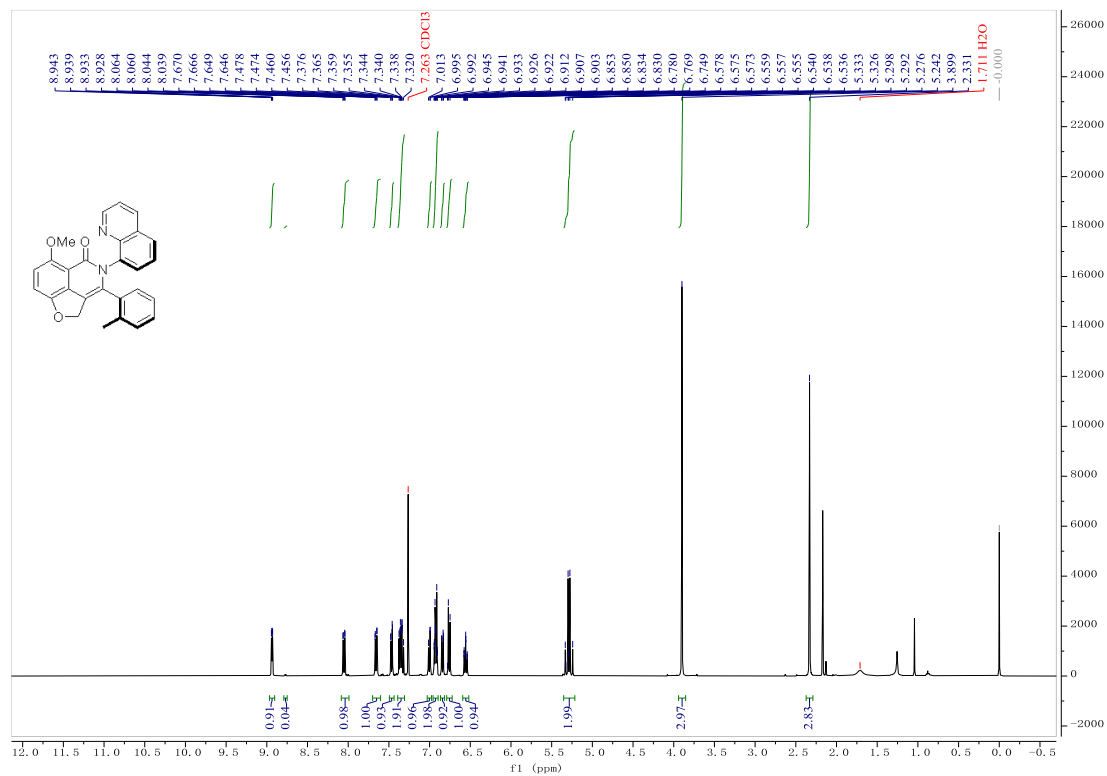


^{13}C NMR (101 MHz, Chloroform-*d*)

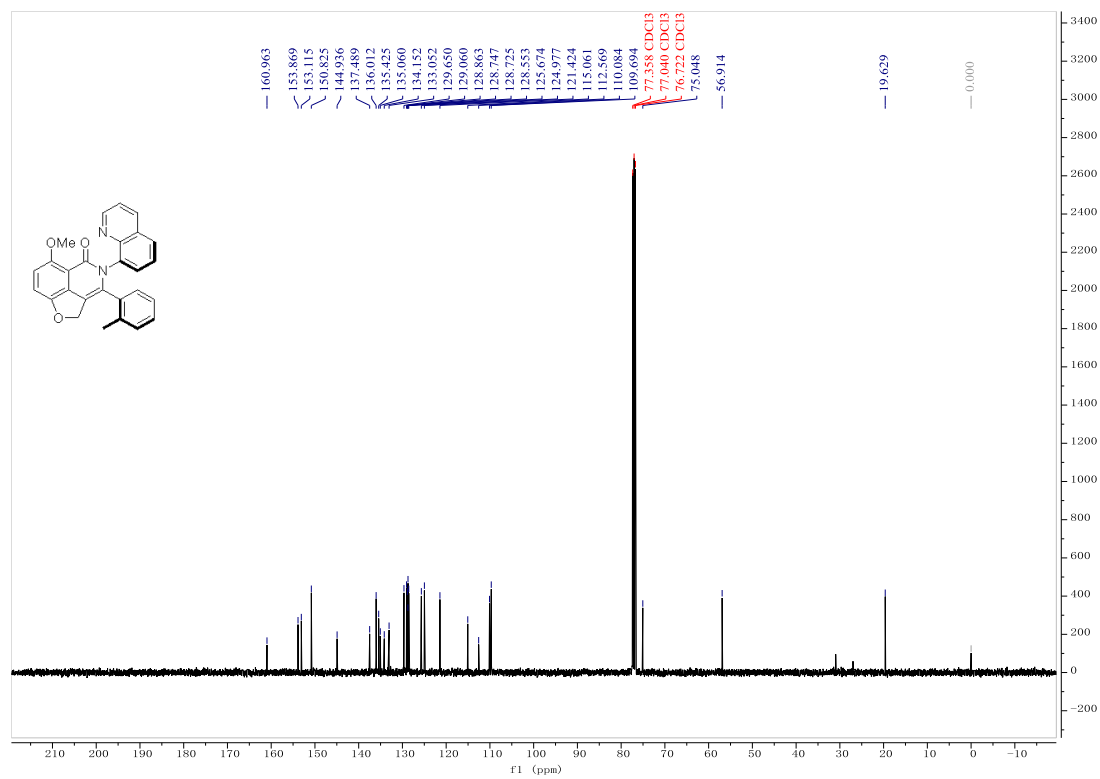


2j

¹H NMR (400 MHz, Chloroform-*d*)

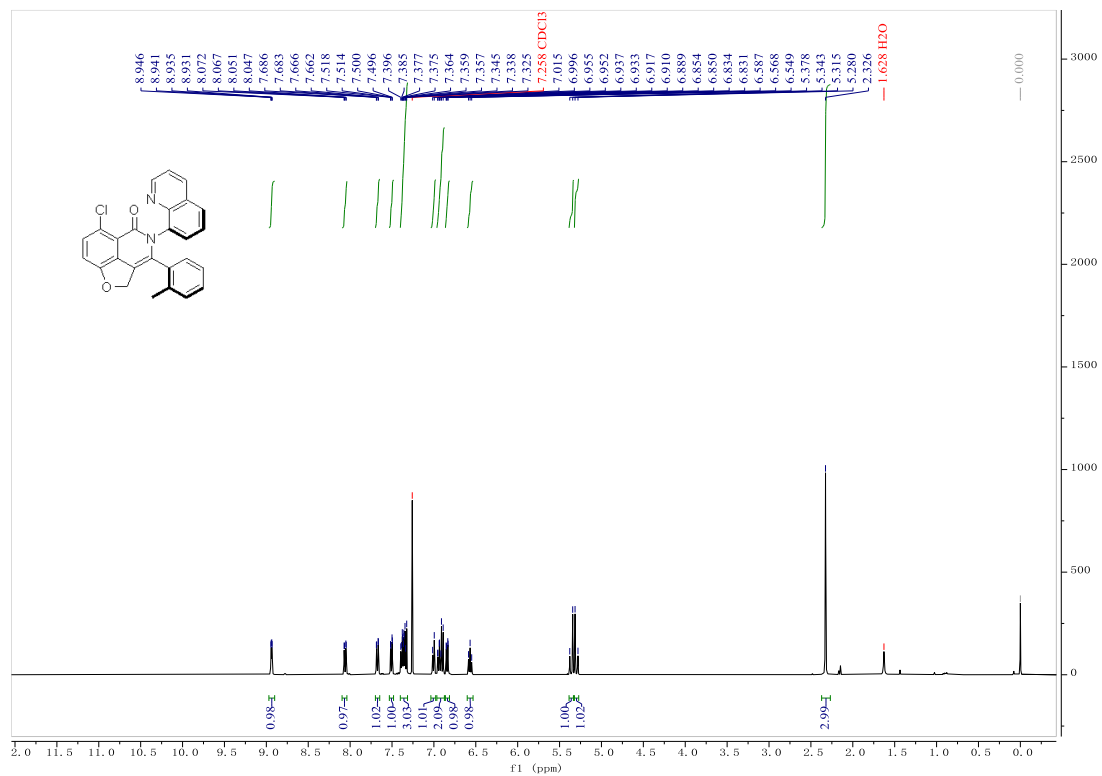


¹³C NMR (101 MHz, Chloroform-*d*)

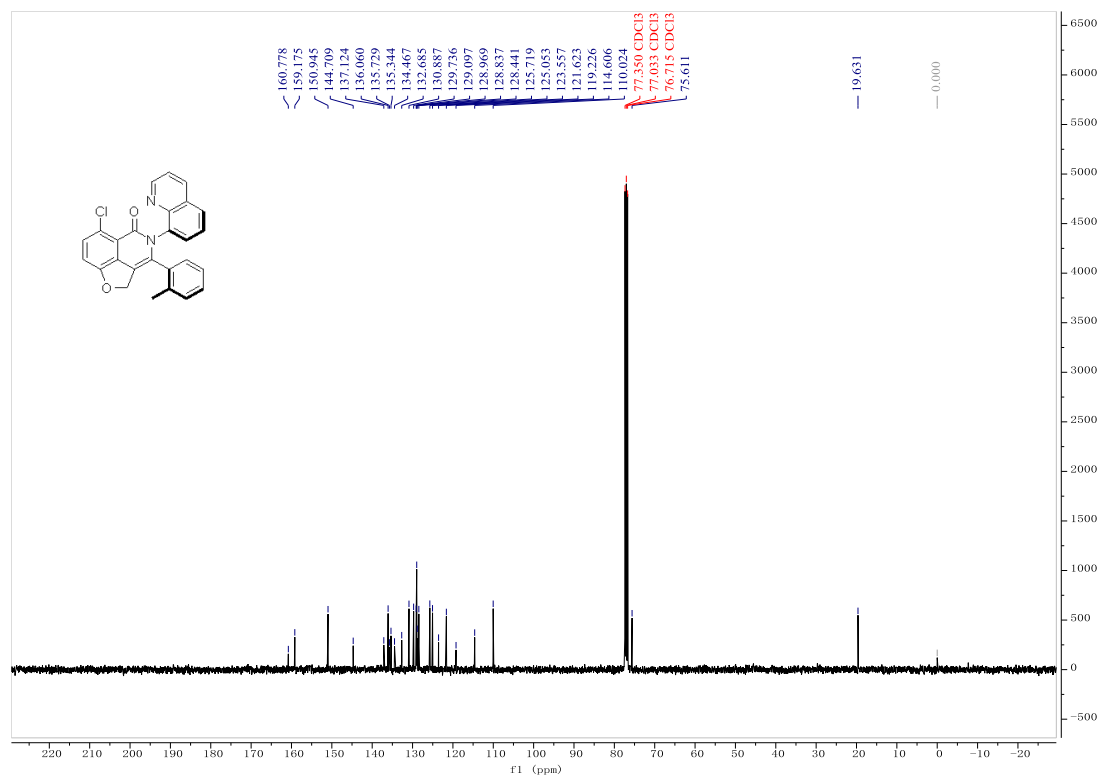


2k

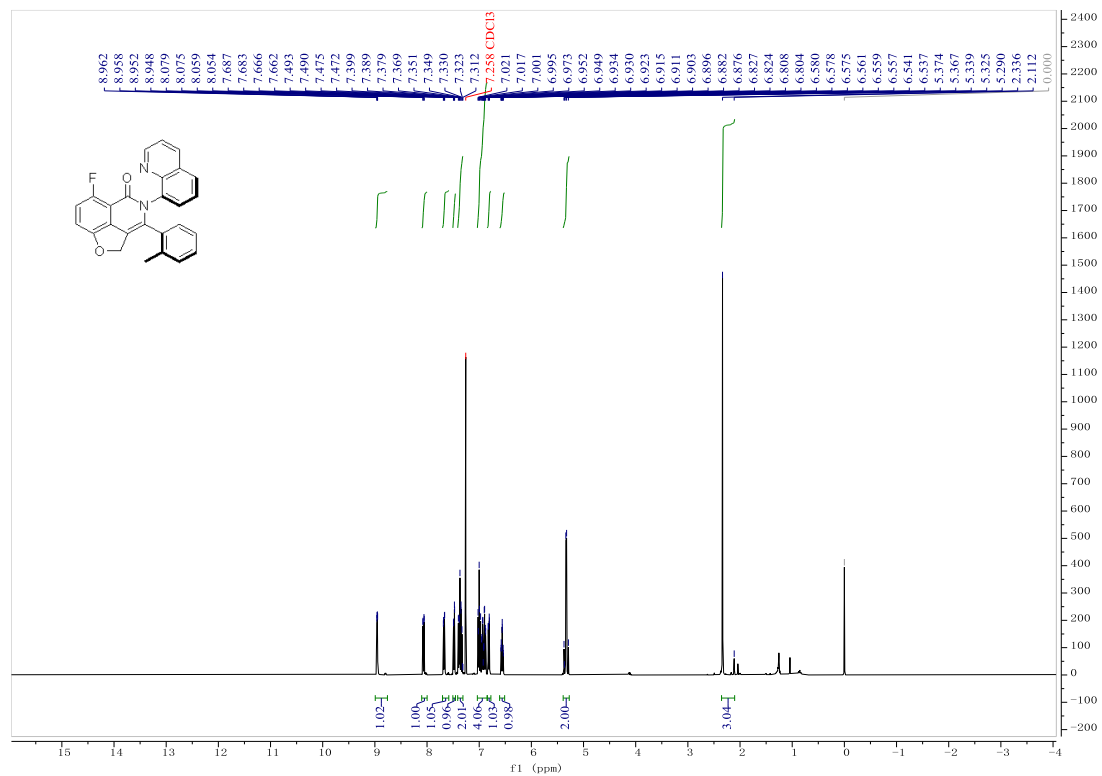
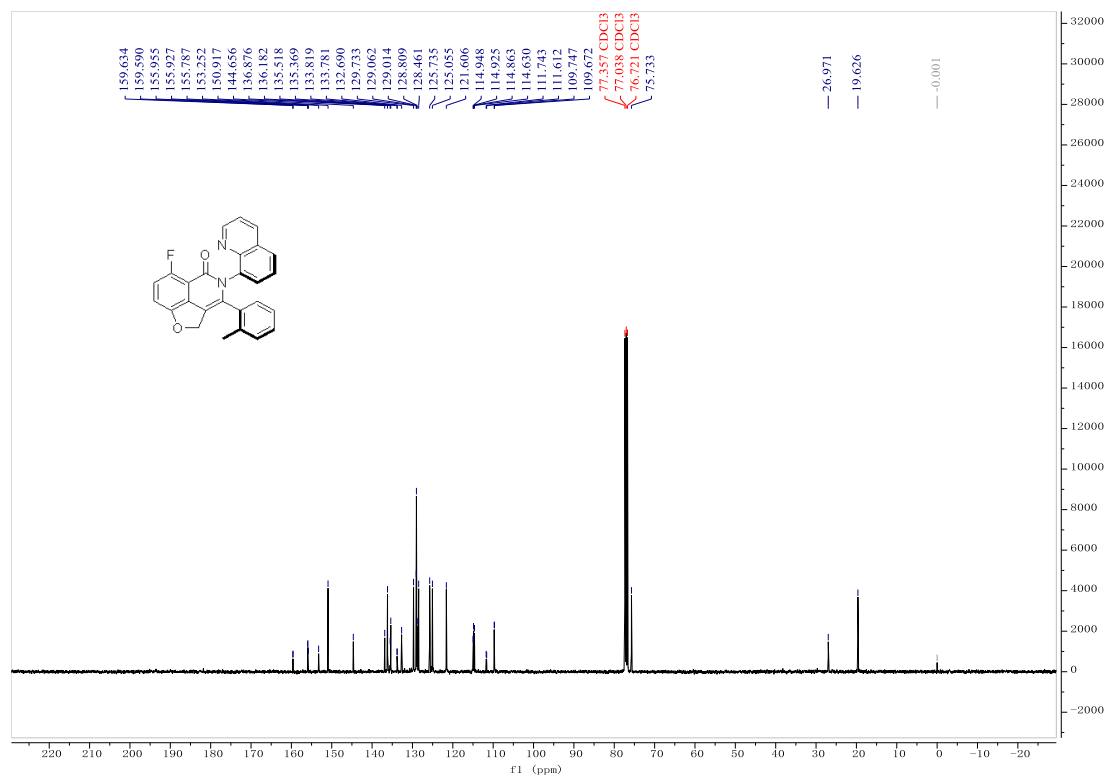
¹H NMR (400 MHz, Chloroform-*d*)



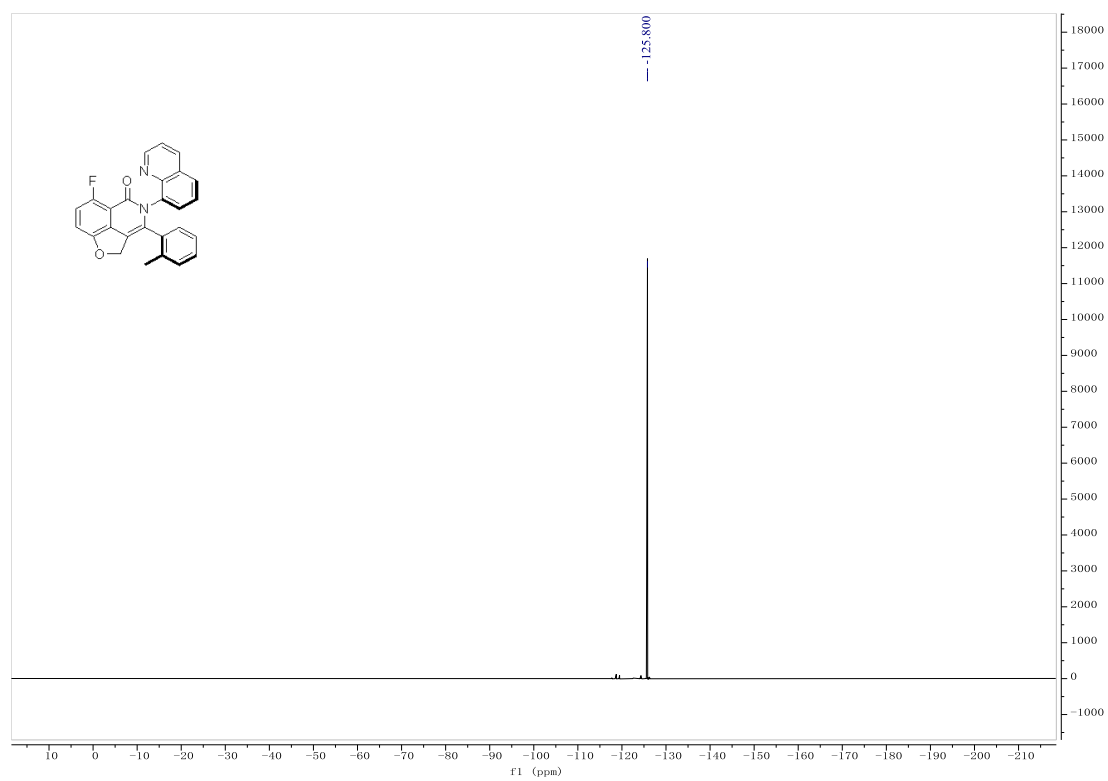
¹³C NMR (101 MHz, Chloroform-*d*)



21

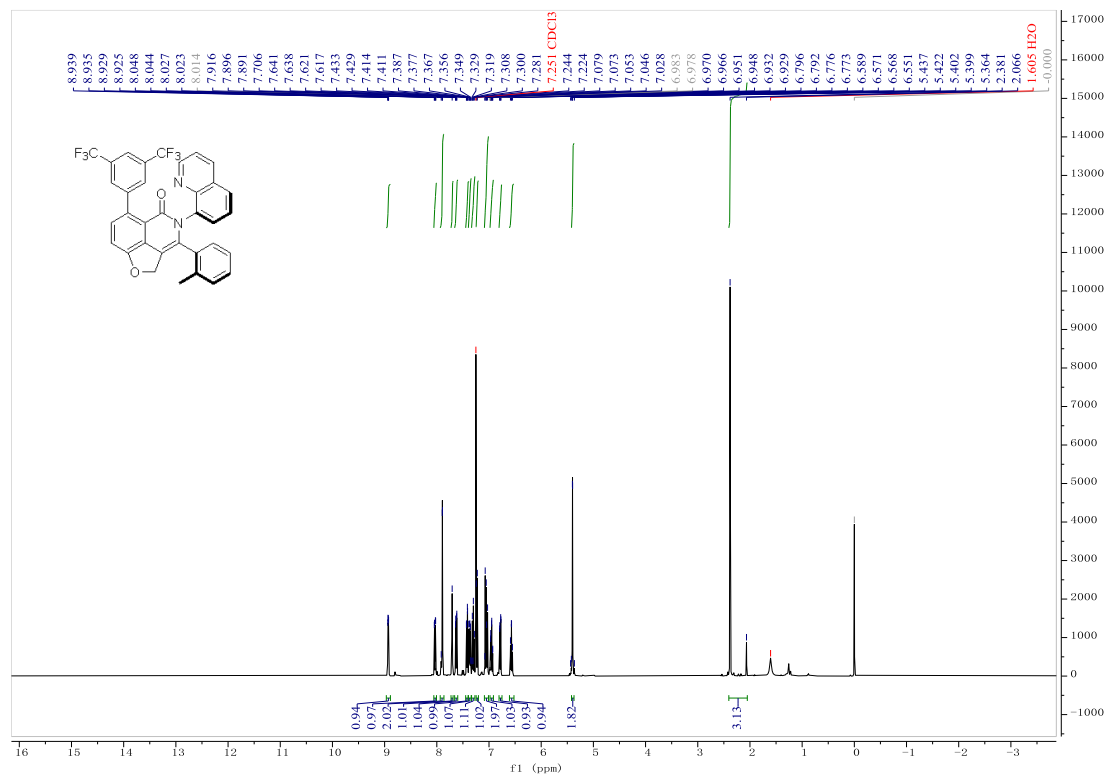
 ^1H NMR (400 MHz, Chloroform-*d*) ^{13}C NMR (101 MHz, Chloroform-*d*)

¹⁹F NMR (376 MHz, Chloroform-*d*)

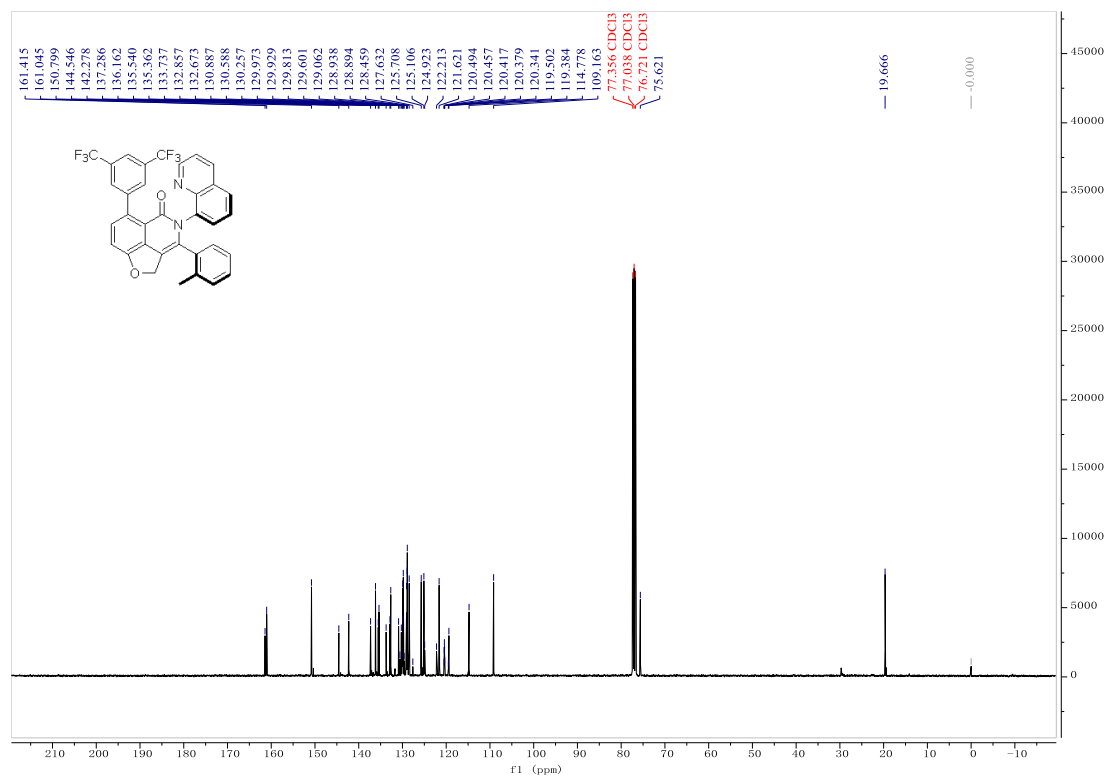


2m

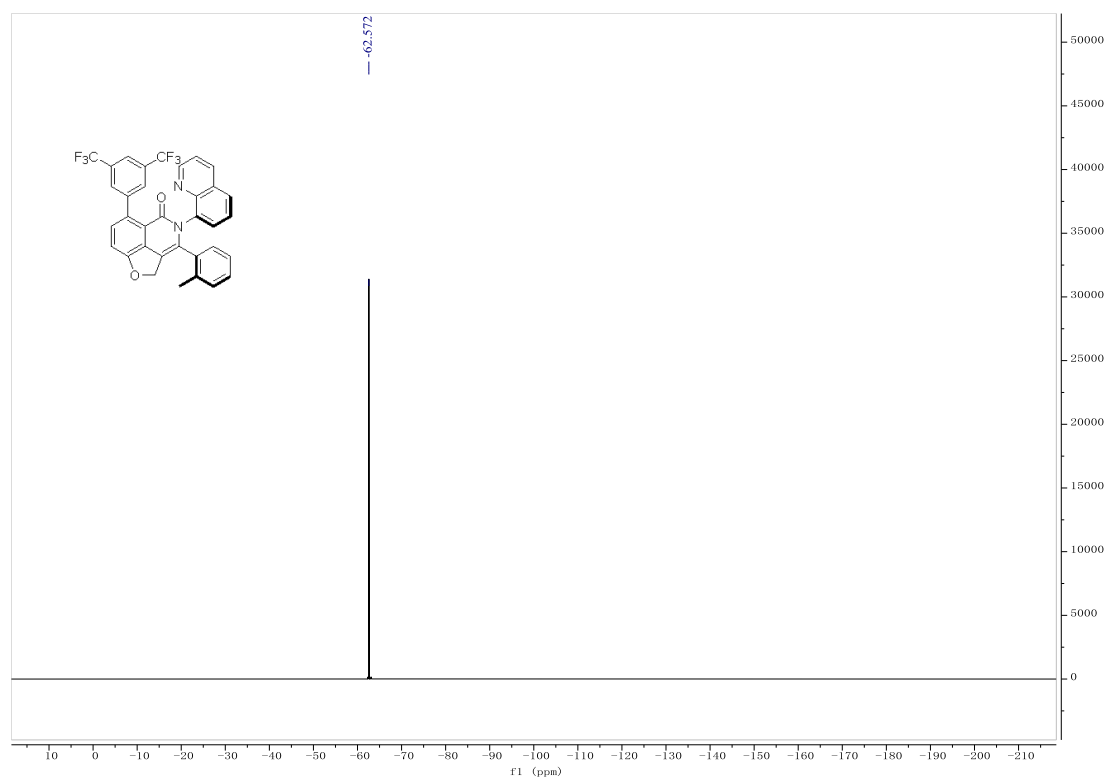
¹H NMR (400 MHz, Chloroform-*d*)



¹³C NMR (101 MHz, Chloroform-*d*)

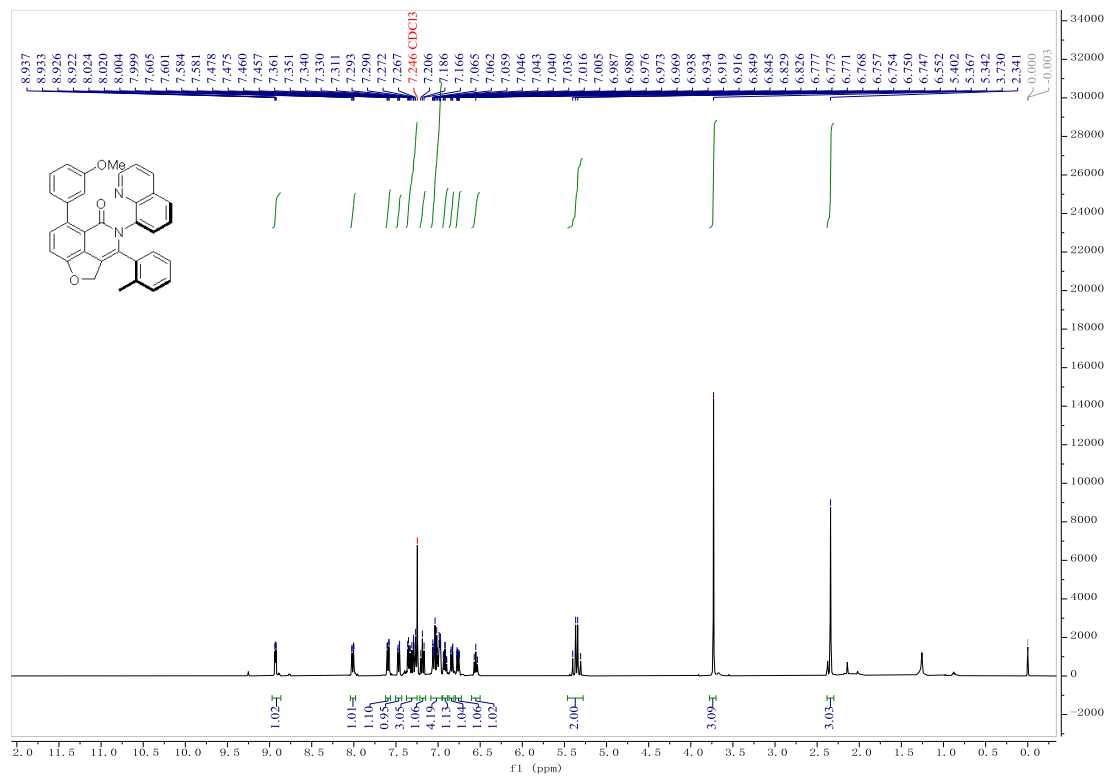


¹⁹F NMR (376 MHz, Chloroform-*d*)

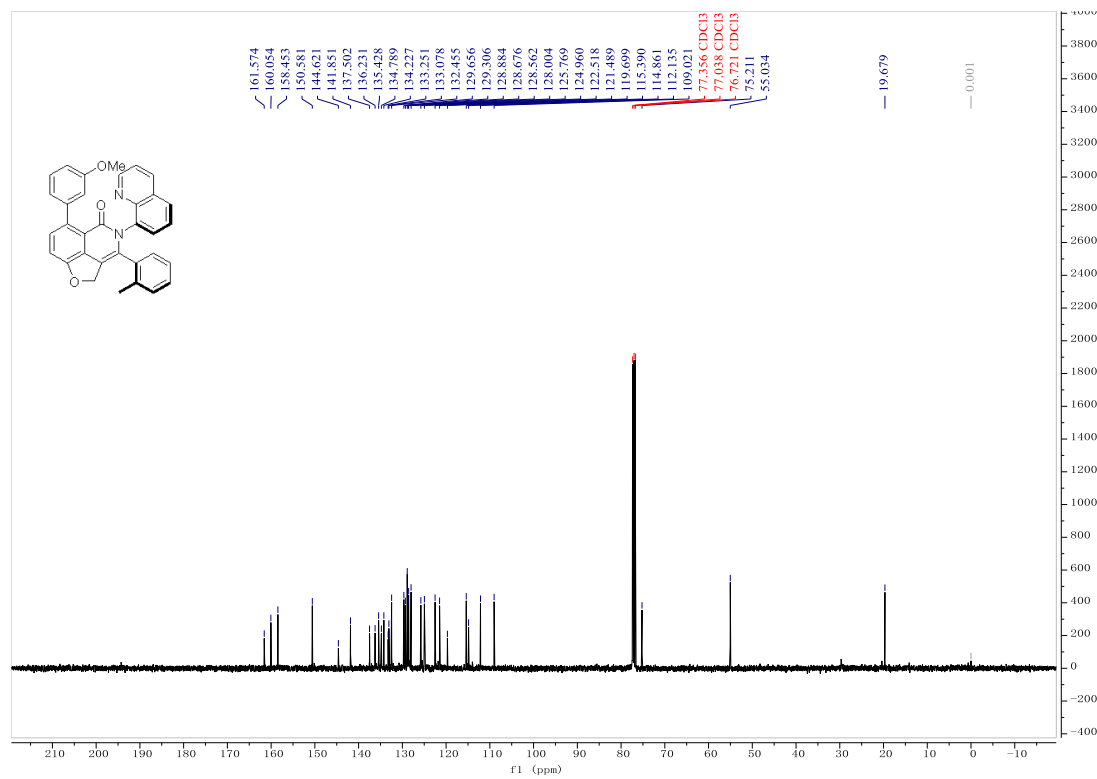


2n

¹H NMR (400 MHz, Chloroform-*d*)

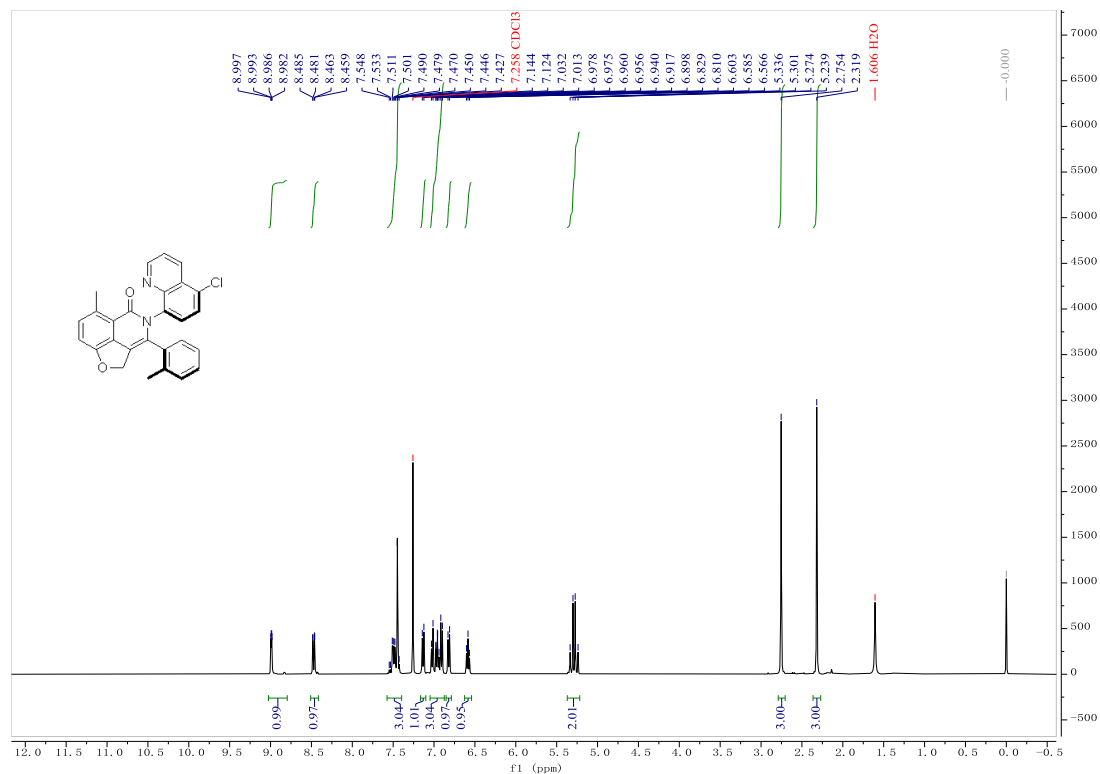


¹³C NMR (101 MHz, Chloroform-*d*)

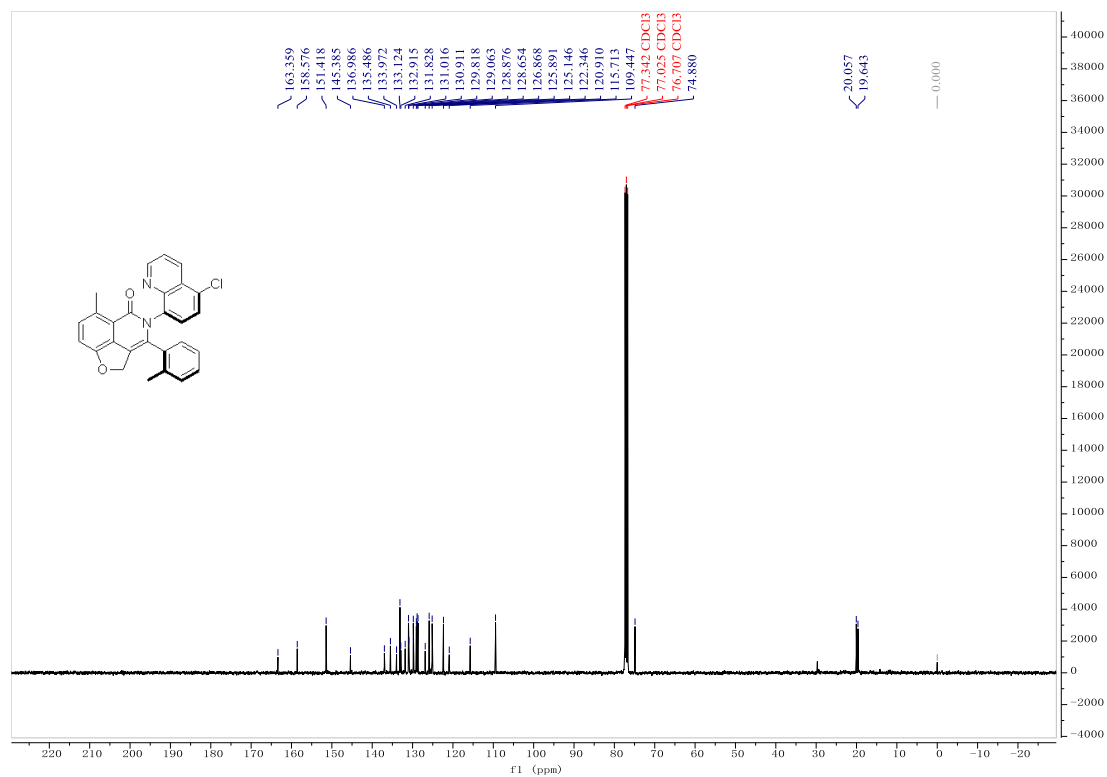


2o

¹H NMR (400 MHz, Chloroform-*d*)

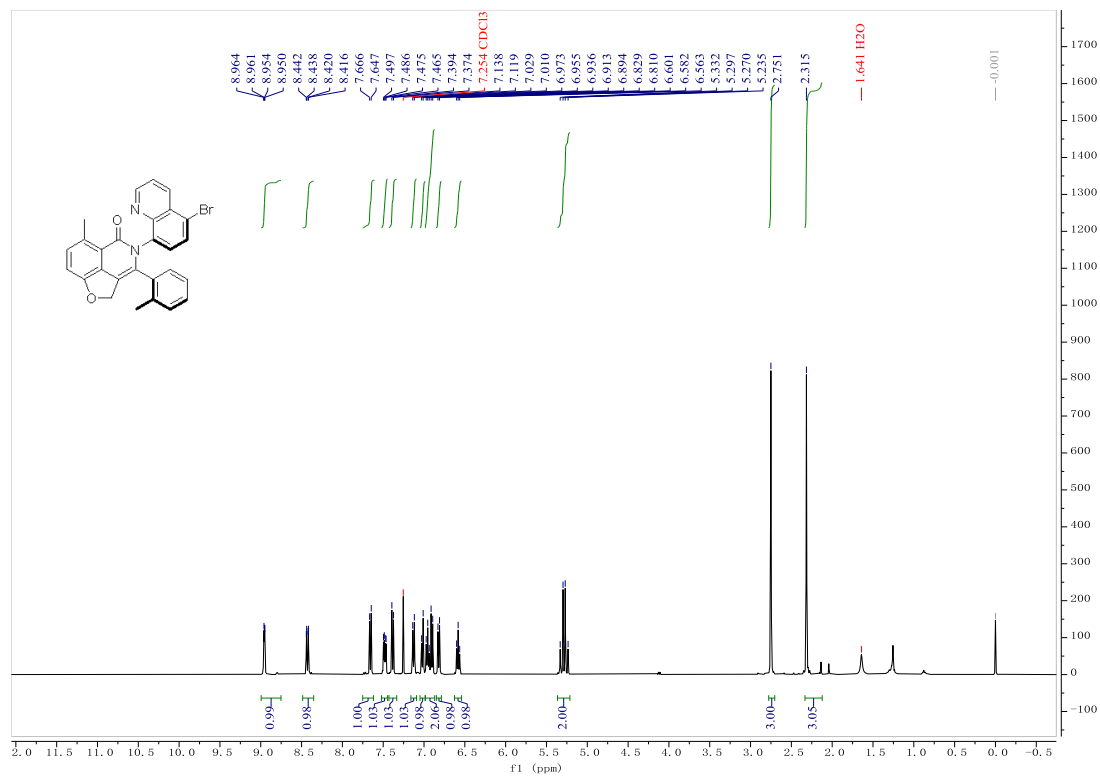


¹³C NMR (101 MHz, Chloroform-*d*)

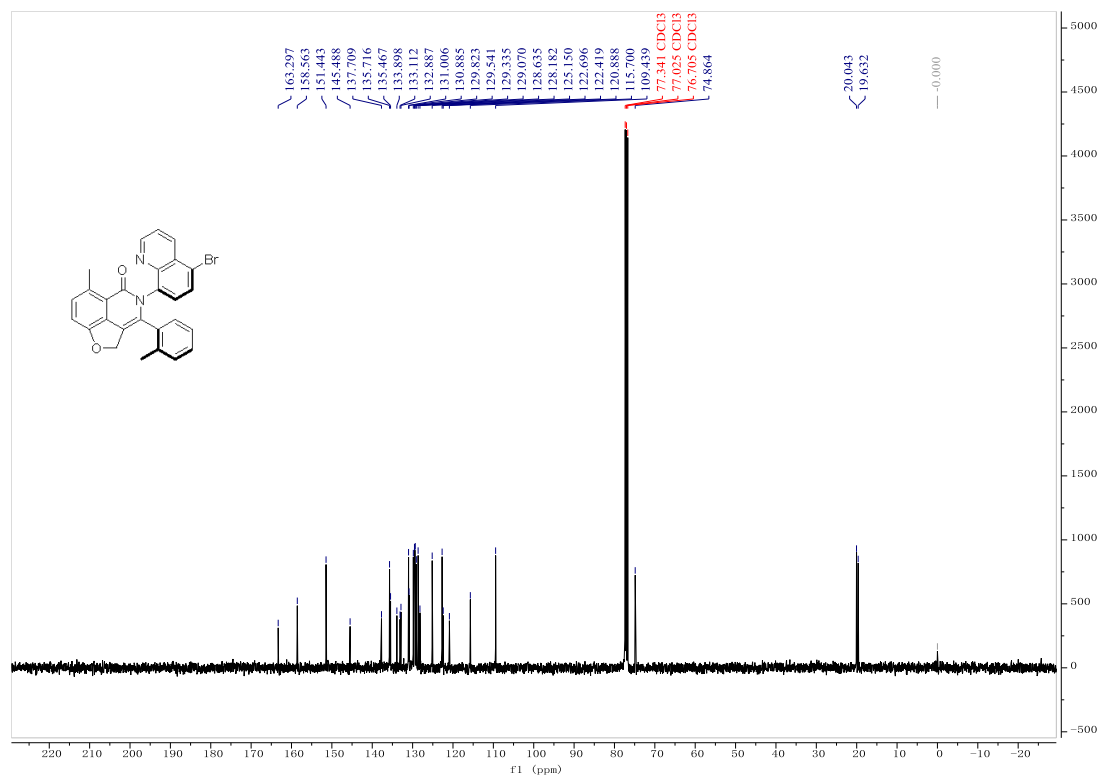


2p

¹H NMR (400 MHz, Chloroform-*d*)

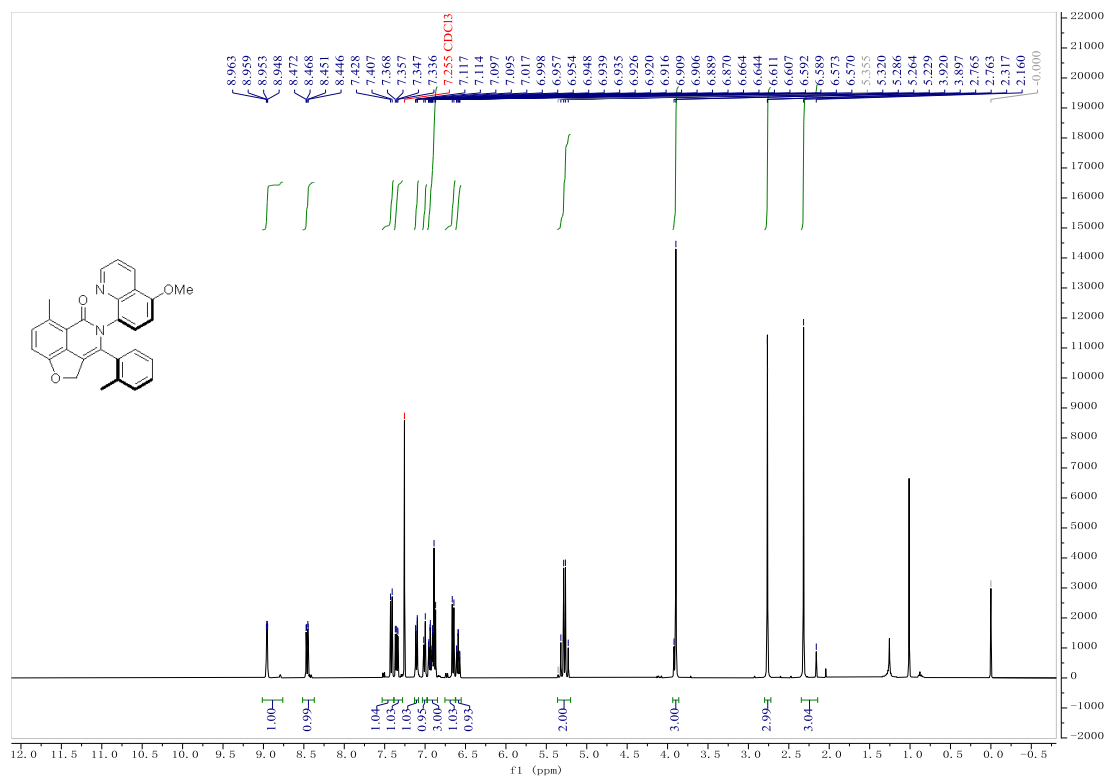


¹³C NMR (101 MHz, Chloroform-*d*)

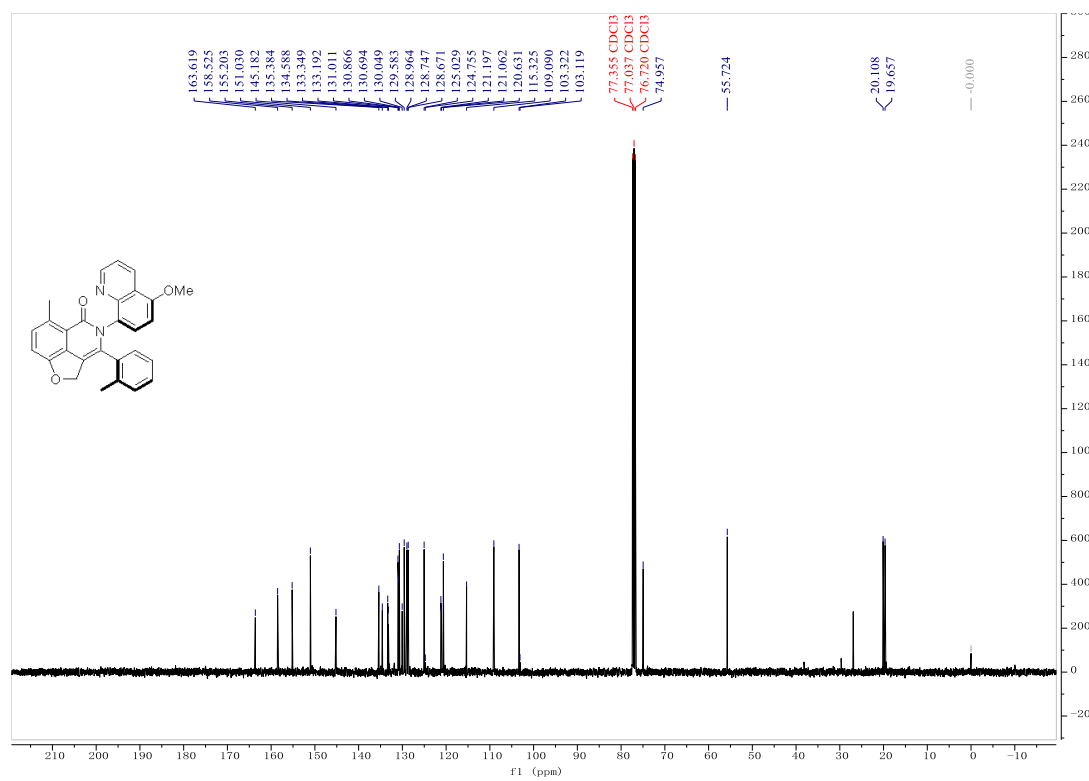


2q

¹H NMR (400 MHz, Chloroform-*d*)

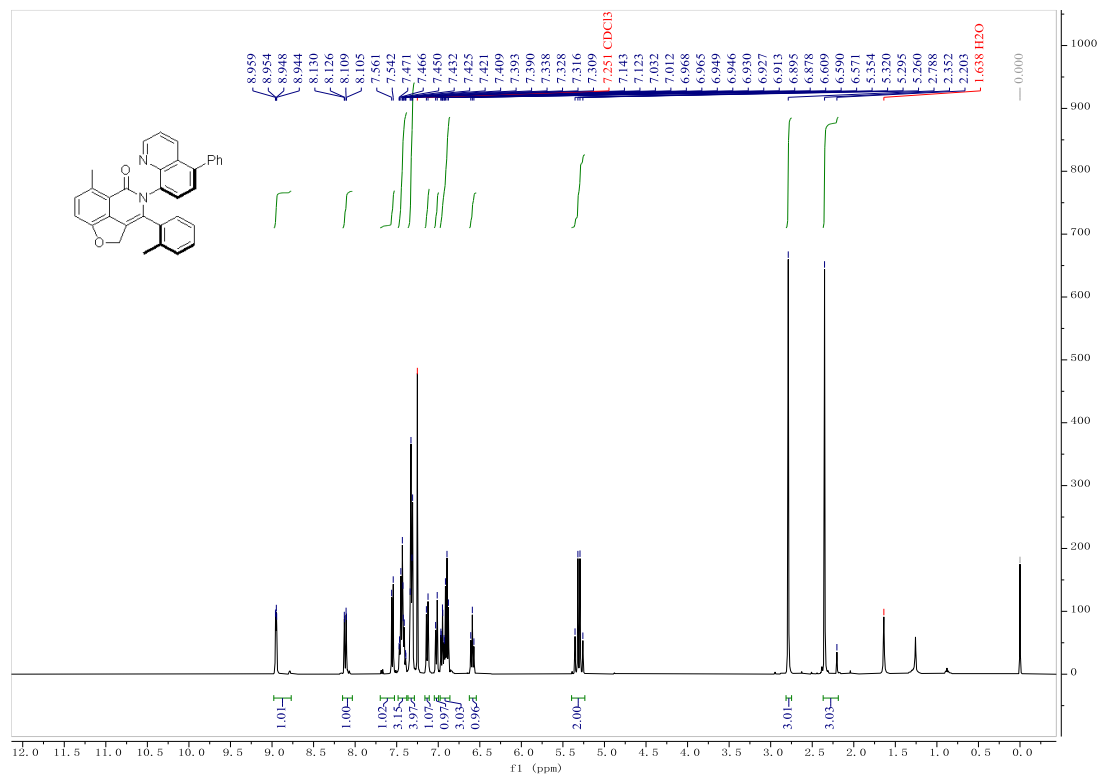


¹³C NMR (101 MHz, Chloroform-*d*)

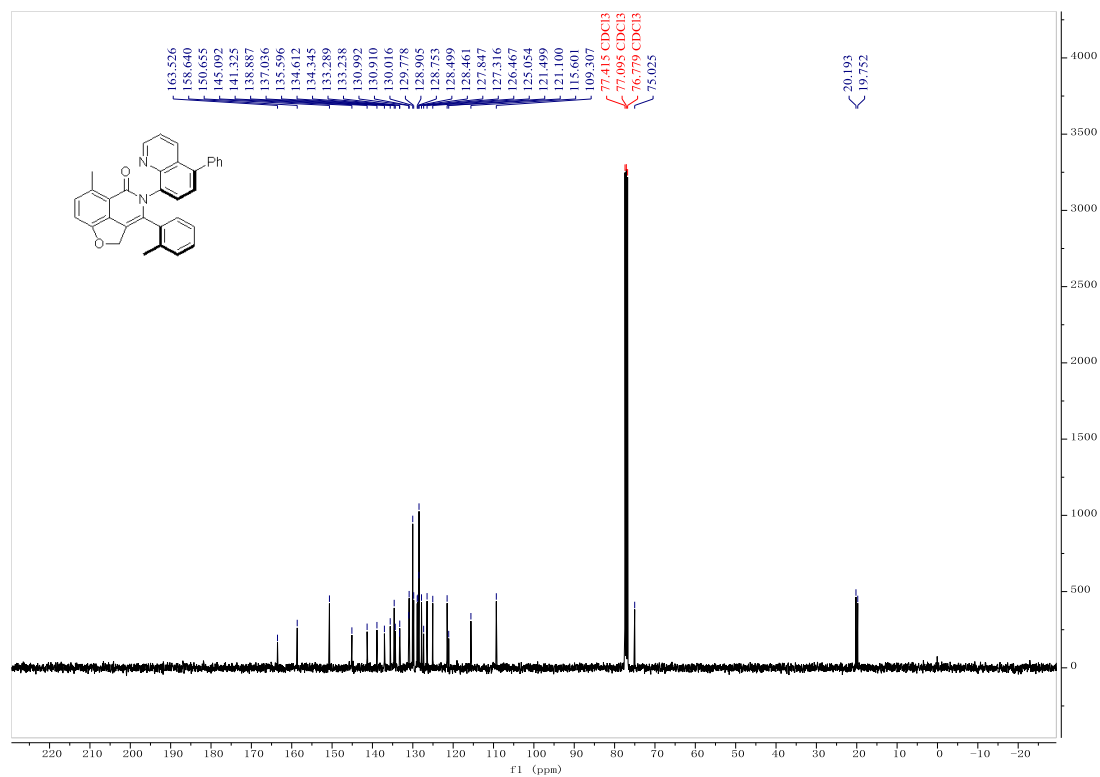


2r

¹H NMR (400 MHz, Chloroform-*d*)

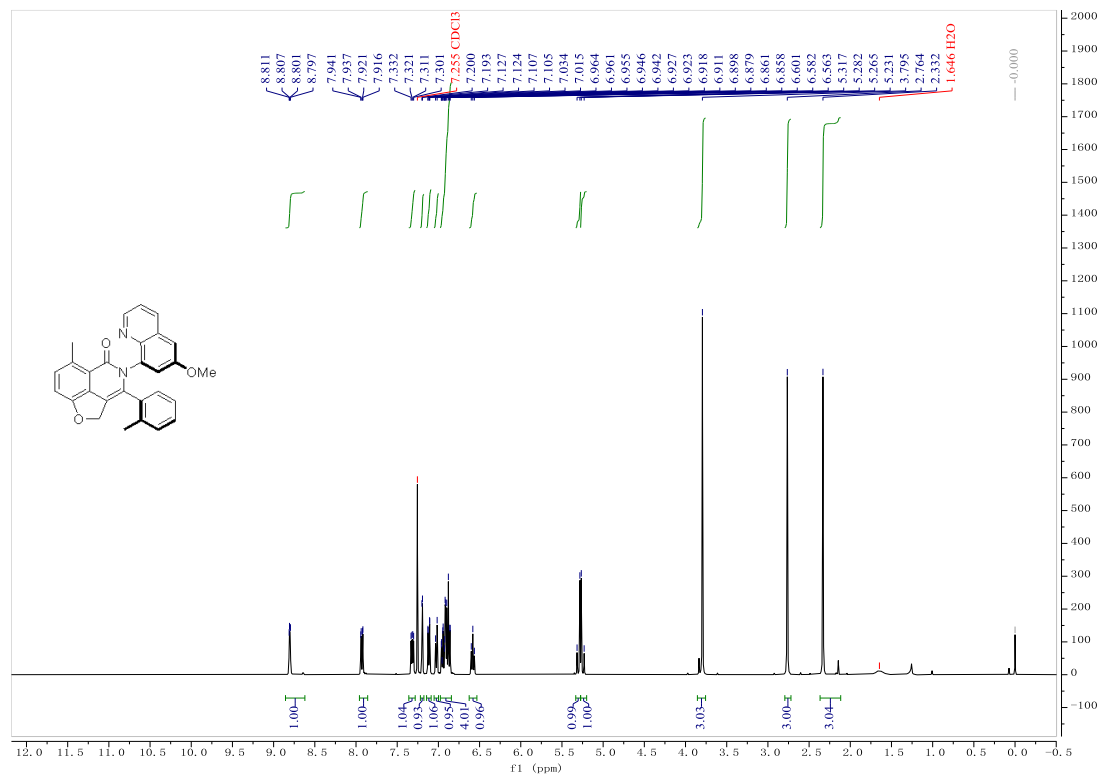


¹³C NMR (101 MHz, Chloroform-*d*)

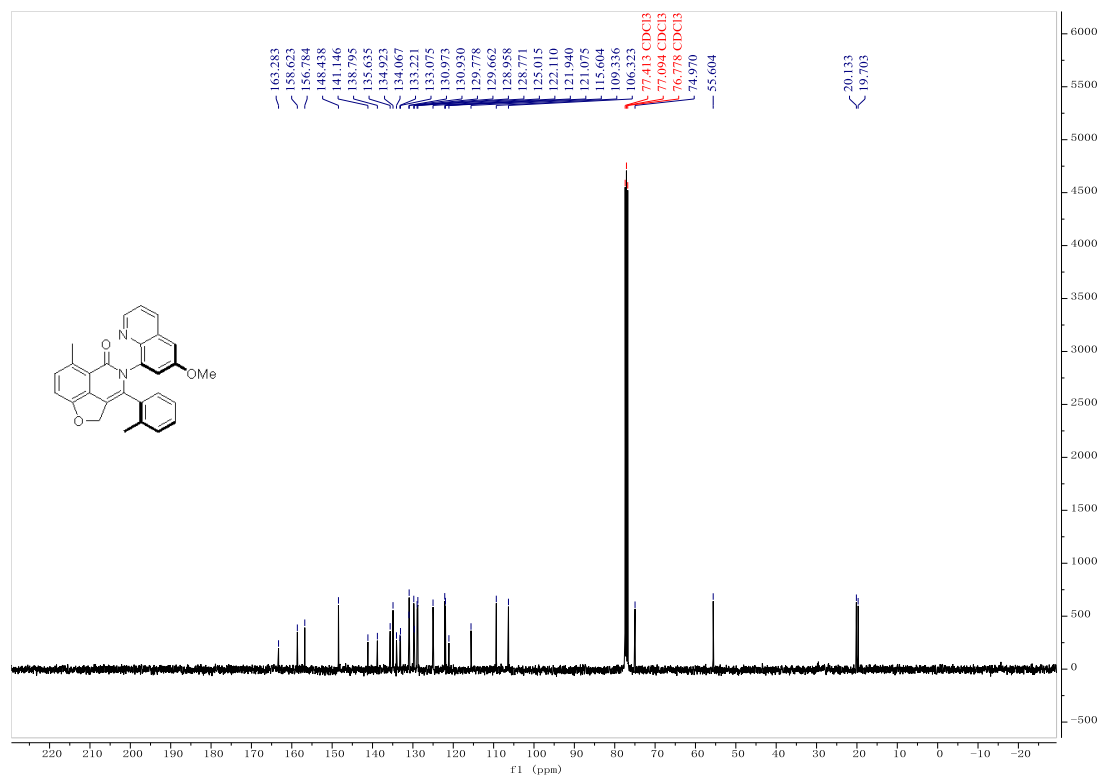


2s

^1H NMR (400 MHz, Chloroform-*d*)

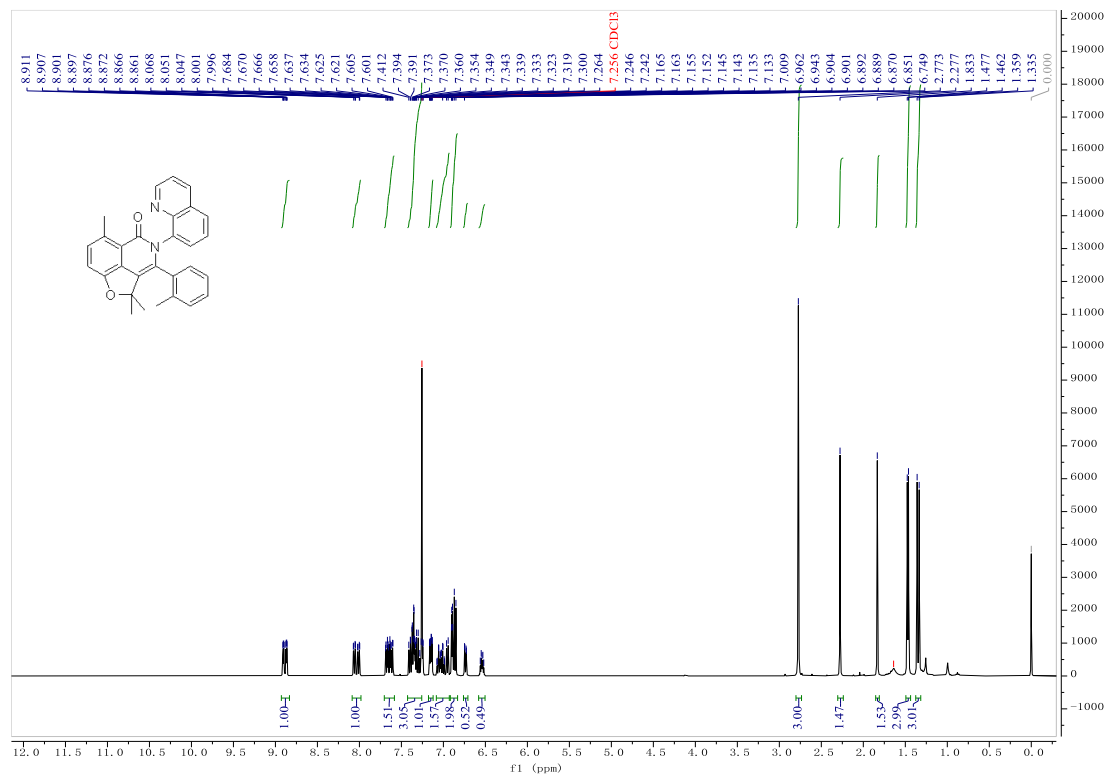


^{13}C NMR (101 MHz, Chloroform-*d*)

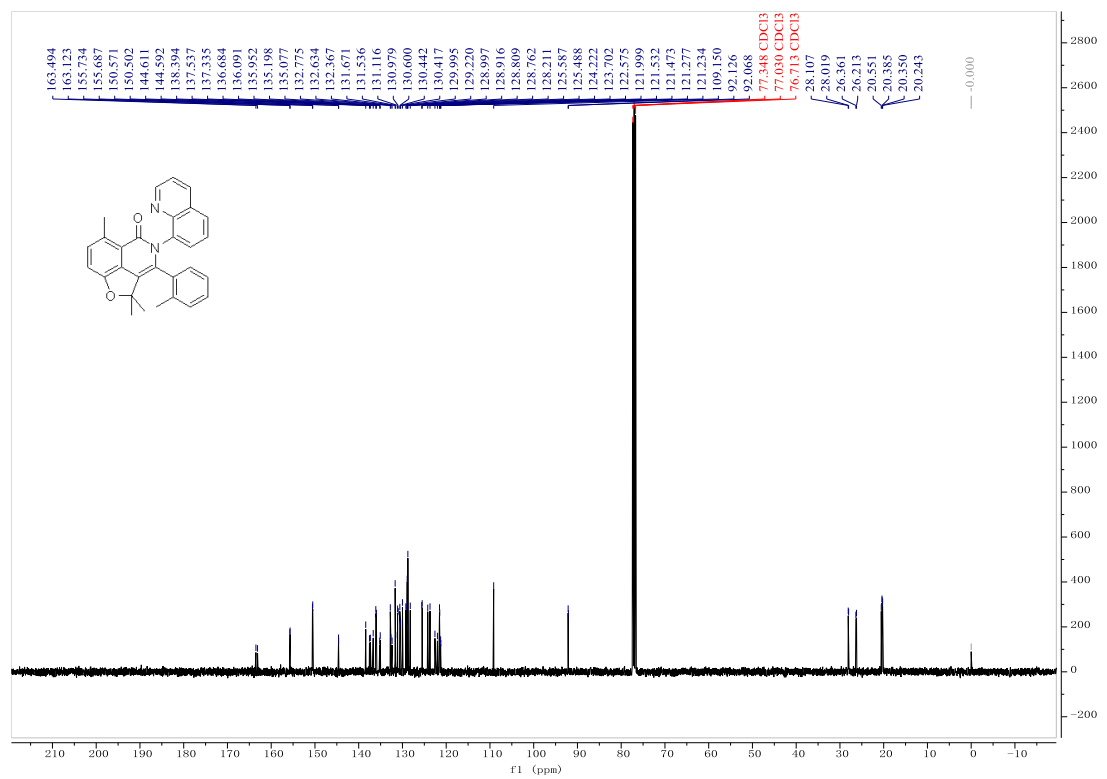


2t

¹H NMR (400 MHz, Chloroform-*d*)

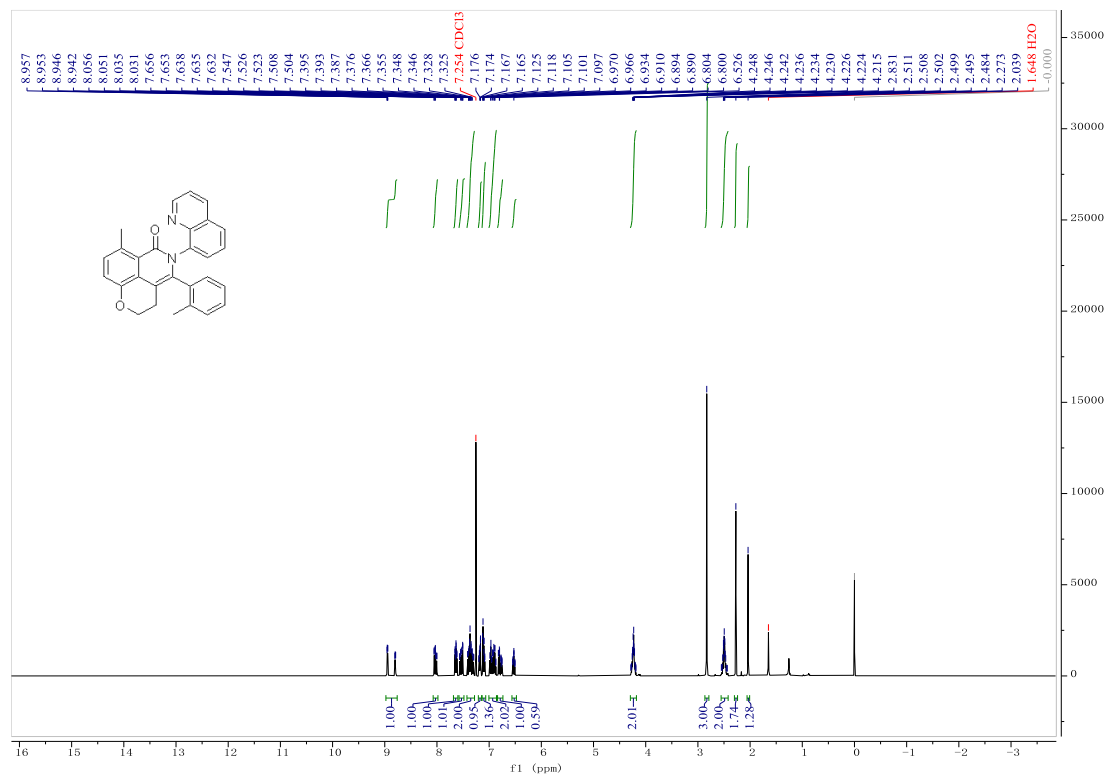


¹³C NMR (101 MHz, Chloroform-*d*)

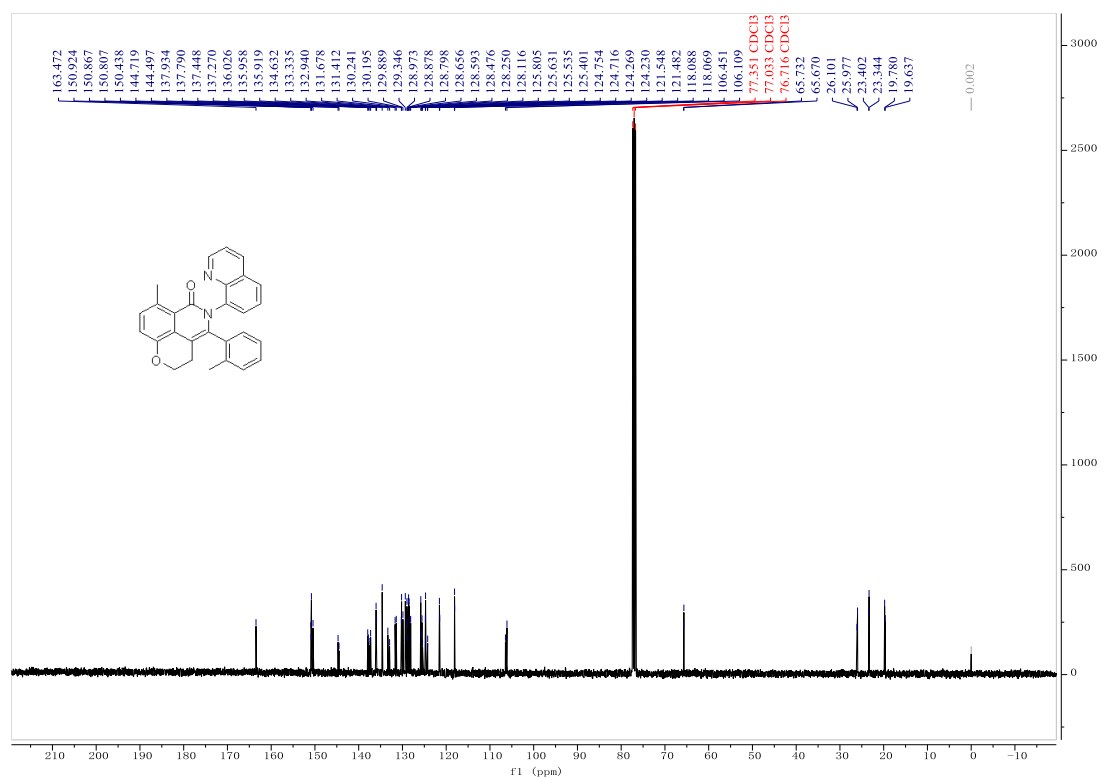


2u

¹H NMR (400 MHz, Chloroform-*d*)

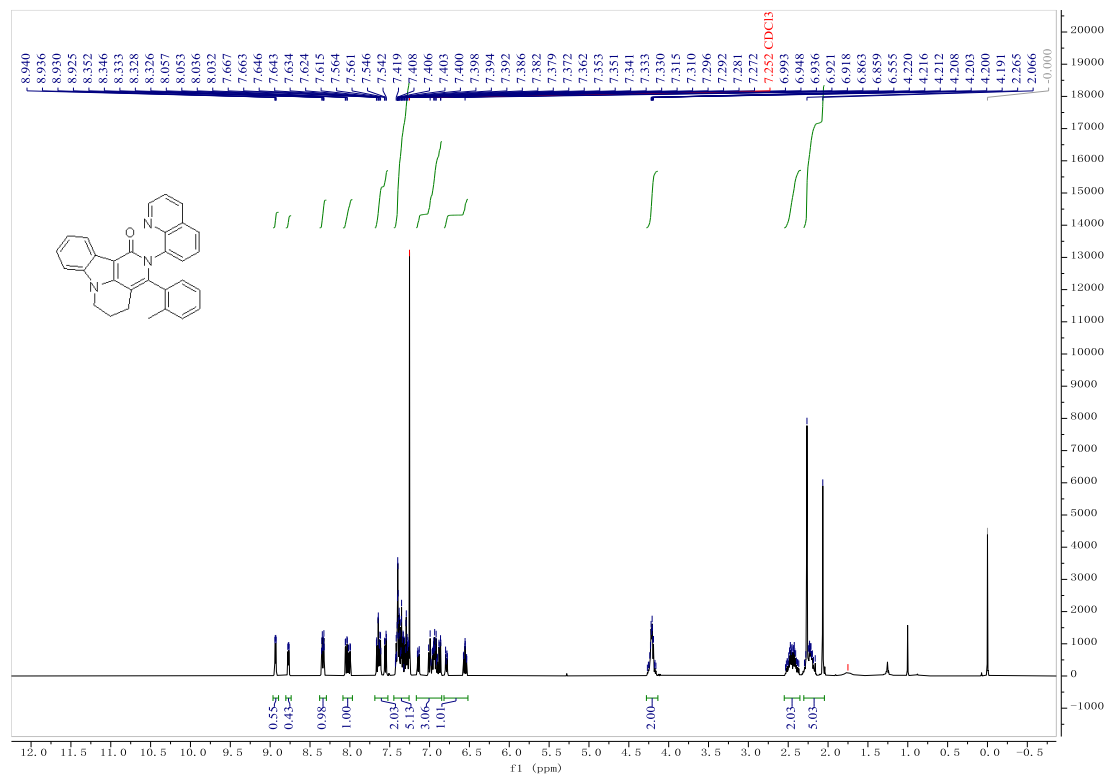


¹³C NMR (101 MHz, Chloroform-*d*)

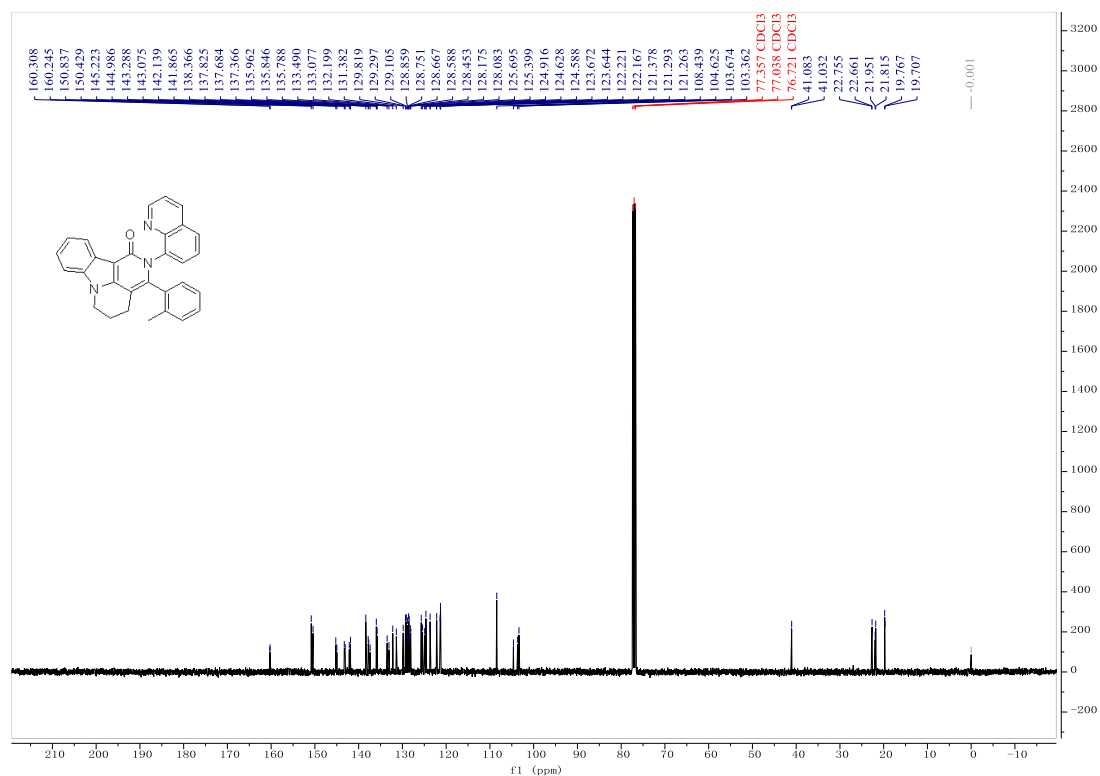


2v

¹H NMR (400 MHz, Chloroform-*d*)

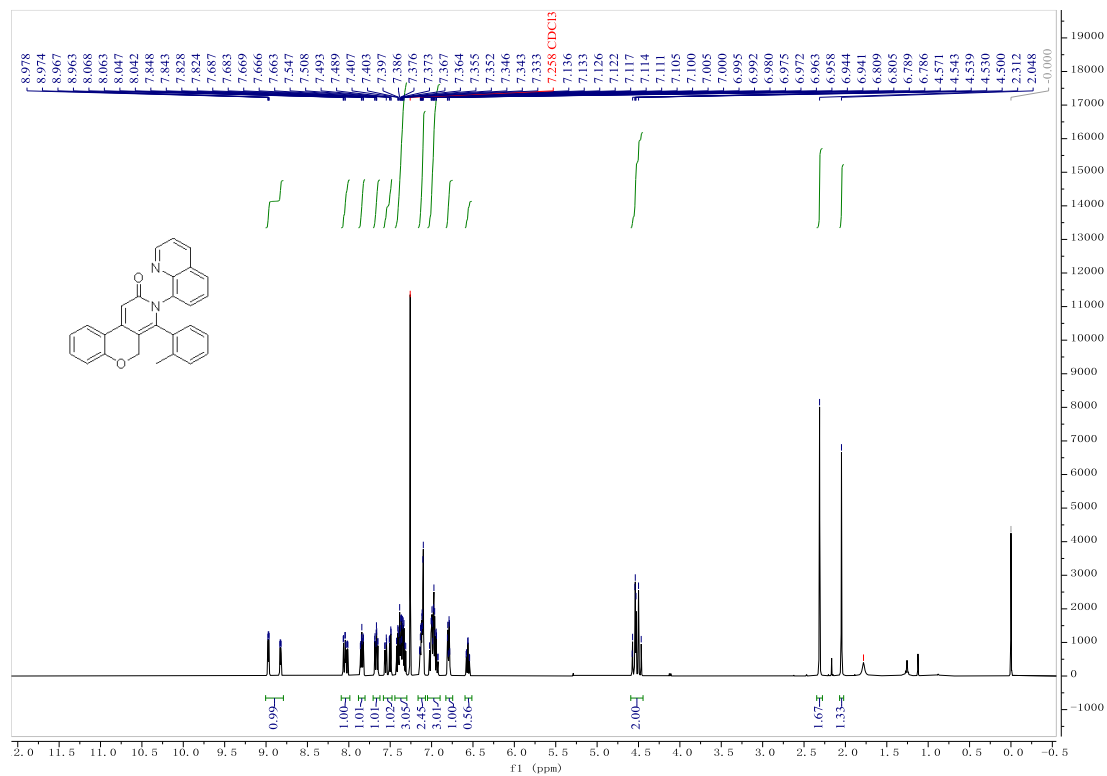


¹³C NMR (101 MHz, Chloroform-*d*)

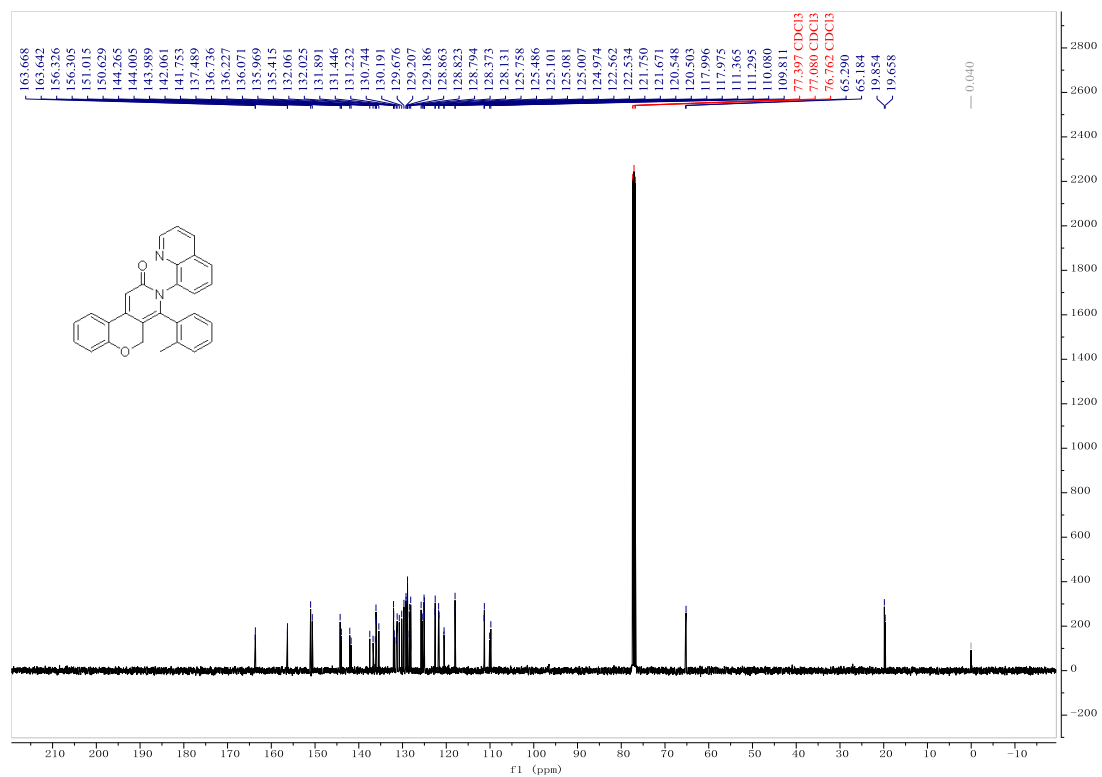


2w

¹H NMR (400 MHz, Chloroform-*d*)

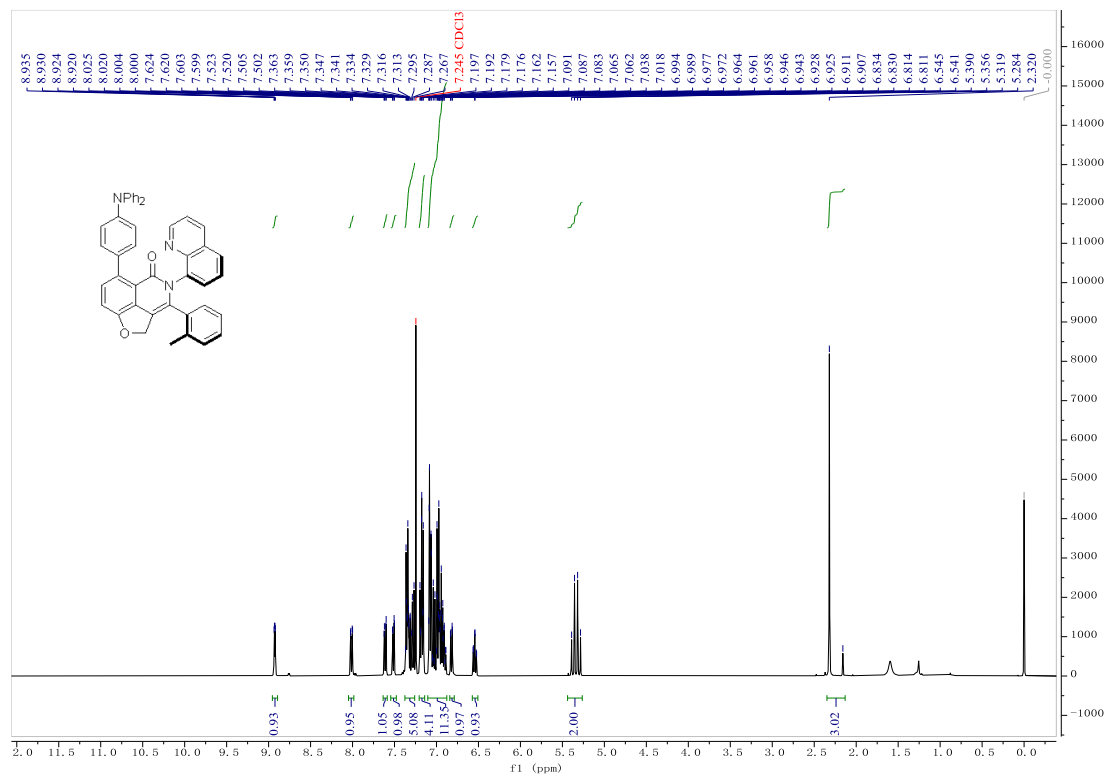


¹³C NMR (101 MHz, Chloroform-*d*)



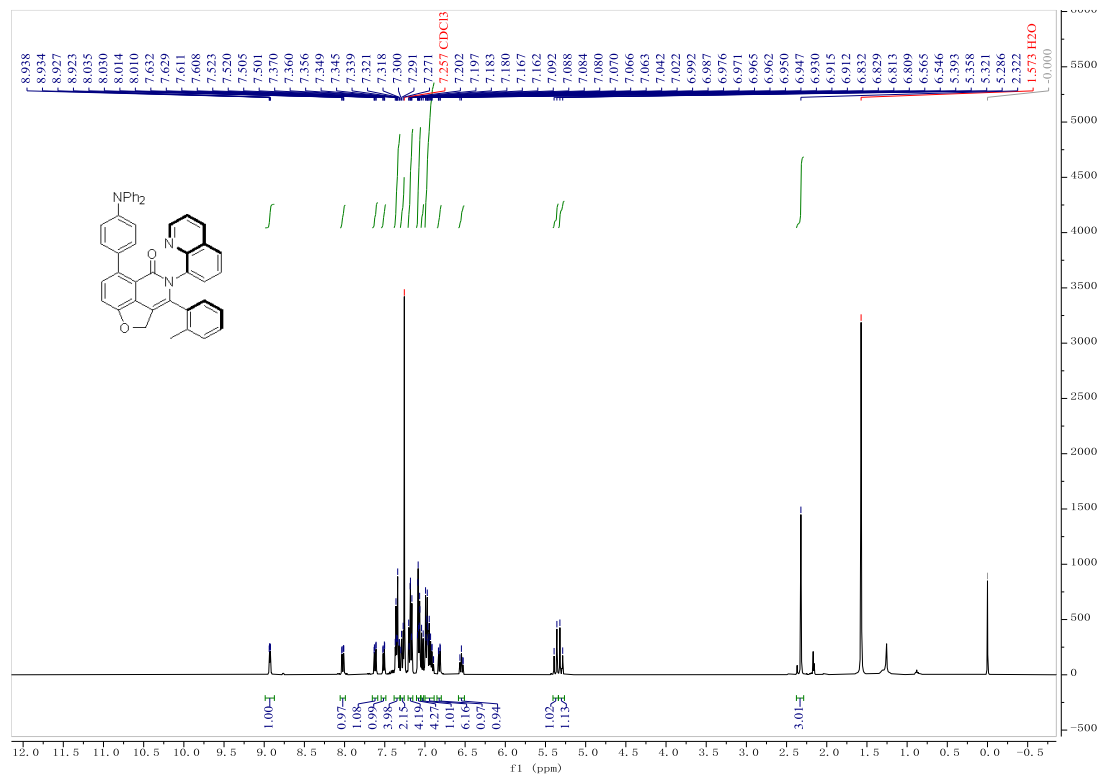
2y

¹H NMR (400 MHz, Chloroform-*d*)



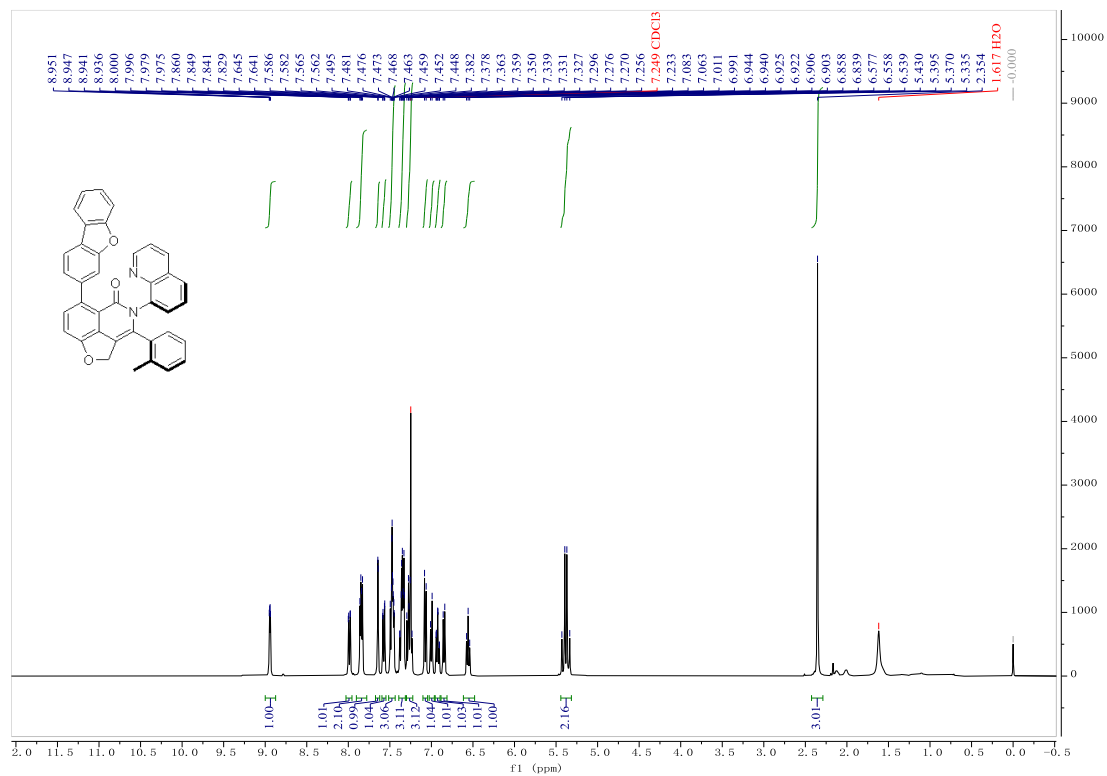
2y-ent

¹H NMR (400 MHz, Chloroform-*d*)

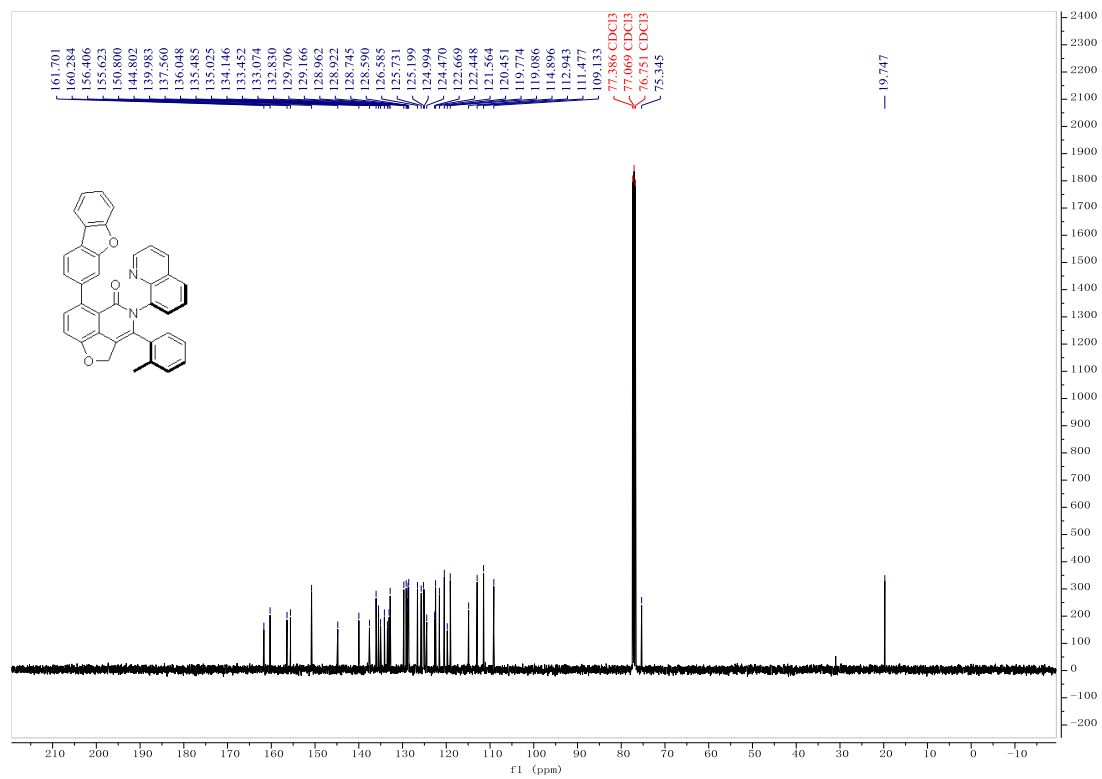


2z

¹H NMR (400 MHz, Chloroform-*d*)



¹³C NMR (101 MHz, Chloroform-*d*)



2z-ent

¹H NMR (400 MHz, Chloroform-*d*)

