Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

Mechanochemical Release of *N*-Heterocyclic Carbenes from Flex-Activated Mechanophores

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I. General Information

^{1}H and ^{13}C NMR spectral data were recorded on Bruker Avance III 500 and Bruker Avance III 400 spectrometers. ^{1}H NMR chemical shifts for spectra collected in $CDCl_3$ or DMSO-d_6 are referenced to TMS ($\delta = 0.00$ ppm) or DMSO residual peak ($\delta = 2.50$ ppm), respectively. ^{13}C NMR chemical shifts of spectra collected in $CDCl_3$ or DMSO-d_6 are referenced to the shifts of the carbon in $CDCl_3$ ($\delta = 77.16$ ppm) or DMSO-d_6 ($\delta = 39.52$ ppm). ^{1}H resonance data are reported as the following format: chemical shift in ppm [multiplicity, coupling constant(s) (*J* in Hz), integration, and substructural assignment (e.g., =CHCH_aH_b)]. The protons in some complex structures are numbered to simplify the proton assignments.

High-resolution mass spectrometry (HRMS) was performed on Thermo Q Exactive™ Plus using electrospray ionization (ESI) or atmospheric solids analysis probe (ASAP-MS) method. Samples were injected as dilute solutions or directly analyzed as solids. UPLC/LC-MS data were measured on Acquity UPLC I-Class PLUS with an Acquity QDA MS detector (Waters) using an ACQUITY UPLC BEH C18 1.7 μm 2.1 X 50 mm column (Waters).

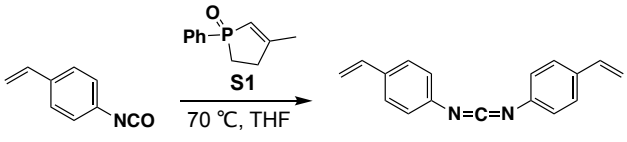
Reactions requiring anhydrous or air-free conditions were performed in the flame-dried glassware under nitrogen or argon atmosphere. Reported reaction temperatures are the temperature of the external heating bath. Triethylamine was distilled from CaH_2 and stored in a Schlenk flask. Anhydrous CH_2Cl_2 and THF were collected from a solvent purification system prior to use. 3-methyl-1-phenylphospholene oxide and di-*p*-tolylcarbodiimide were synthesized according to the reported methods.[1,2] Methyl acrylate and 1,6-hexanediol diacrylate were filtered through an activated basic alumina column to remove inhibitors before polymerizations. All other reagents were purchased from commercial sources and used as received unless otherwise specified.

The following instruments in the Paul Bender Chemistry Instrumentation Center was supported by: Thermo Q Exactive™ Plus by NIH 1S10 OD020022-1; Bruker Avance-500 by a generous gift from Paul J. and Margaret M. Bender; Bruker Avance-400 by NSF CHE-1048642 and the University of Wisconsin-Madison.

II. Preparation procedures and characterization data for all new compounds

a. Synthesis of NHC-CDI mechanophore 3

Bis(4-vinylphenyl)methanediimine (2)



1 2

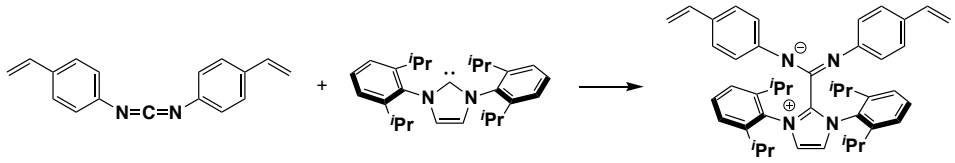
In a flame-dried flask under N_2 atmosphere, the stock solution of 3-methyl-1-phenylphospholene oxide **S1**[1] (2.6 mL, 1.2 mmol, 0.45 M in THF) was dropwise added to the solution of isocyanate **1** (3.9 g, 26.9 mmol) in THF (12 mL). The reaction mixture was stirred at 70 °C for 4 h before it was concentrated to 2 mL *in vacuo*. The crude product was purified by flash chromatography on silica gel (hexanes:EtOAc 20:1) to give carbodiimide **2** as a white solid (2.3 g, 70%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37 (d, *J* = 8.4 Hz, 4H, Ar-*H*), 7.13 (d, *J* = 8.4 Hz, 4H, Ar-*H*), 6.69 (dd, *J* = 17.6, 10.9 Hz, 2H, ArC*H*=CH_2), 5.71 (d, *J* = 17.6 Hz, 2H, ArCH=C*H*), 5.24 (d, *J* = 10.9 Hz, 2H, ArCH=C*H*).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.9, 136.1, 135.33, 135.27, 127.5, 124.5, and 114.0.

HRMS (ASAP-MS): Calcd for [$(C_{17}H_{15}N_2)^+$] [$(M+H)^+$] 247.1230; found: 247.1227.

NHC-CDI mechanophore 3



2 IPr 3

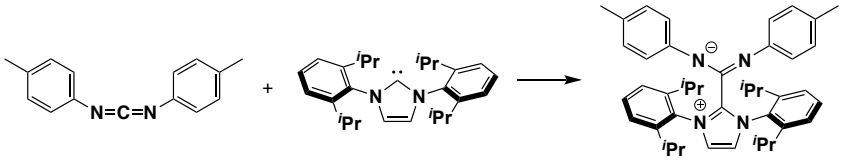
A flame-dried two-neck flask was loaded with a solution of carbodiimide **2** (364 mg, 1.48 mmol) in dry THF (3 mL) under an atmosphere of Ar. Subsequently, 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene (**IPr**) (605 mg, 1.56 mmol) was added to the solution while purging with Ar. The reaction mixture was stirred at room temperature for 1 h before it was concentrated to dryness. The residue was added 10 mL of hexane and put in the freezer for overnight. The resulting solids were washed with hexane 5 times and dried under vacuum to give NHC-CDI **3** as a yellow solid (893 mg, 95%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.45 [t, *J* = 7.8 Hz, 2H, Ar(NHC)-*H*], 7.26 [d, *J* = 7.8 Hz, 4H, Ar(NHC)-*H*], 7.12 (s, 2H, C*H*=C*H*), 6.66 [d, *J* = 8.4 Hz, 4H, Ar(CDI)-*H*], 6.36 (dd, *J* = 17.6, 10.8 Hz, 2H, ArC*H*=CH_2), 5.79 [d, *J* = 8.4 Hz, 4H, Ar(CDI)-*H*], 5.26 (dd, *J* = 17.6, 1.4 Hz, 2H, ArCH=C*H*), 4.76 (dd, *J* = 10.8, 1.4 Hz, 2H, ArCH=C*H*), 2.83 [hept, *J* = 6.8 Hz, 4H, C*H*$(CH_3)_2$], 1.28 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3)_2$], and 1.20 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3)_2$].

^{13}C NMR (126 MHz, $CDCl_3$) δ 151.3, 150.2, 145.6, 140.7, 137.8, 132.9, 130.5, 126.9, 125.0, 124.0, 121.4, 120.8, 107.9, 29.5, 25.3, and 23.1.

HRMS (ESI): Calcd for $[(C_{44}H_{51}N_4)^+]$ $[(M+H)^+]$ 635.4108; found: 635.4102.

b. Synthesis of control NHC-CDI 4



S2 **IPr** **4**

NHC-CDI **4** was prepared following the same procedure as for **3** from di-*p*-tolylcarbodiimide **S2**[2] (67 mg, 0.30 mmol) and **IPr** (122 mg, 0.31 mmol). Product **4** was obtained as a yellow solid (175 mg, 95%).

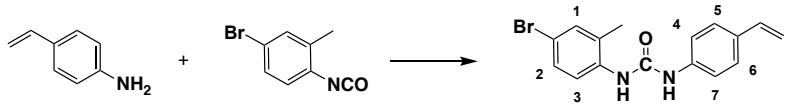
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.45 [t, *J* = 7.7 Hz, 2H, Ar(NHC)-*H*], 7.27 [d, *J* = 7.7 Hz, 4H, Ar(NHC)-*H*], 7.09 (s, 2H, C*H*=C*H*), 6.34 [d, *J* = 7.9 Hz, 4H, Ar(CDI)-*H*], 5.69 [d, *J* = 7.9 Hz, 4H, Ar(CDI)-*H*], 2.87 [hept, *J* = 6.8 Hz, 4H, C*H*$(CH_3)_2$], 1.97 (s, 6H, Ar-CH_3), 1.29 [d, *J* = 6.8 Hz, 12H, CH(C$H_3)_2$], and 1.19 [d, *J* = 6.8 Hz, 12H, CH(C$H_3)_2$].

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.8, 149.3, 145.7, 140.7, 133.1, 130.3, 127.0, 125.8, 123.9, 121.1, 120.8, 29.5, 25.2, 23.2, and 20.8.

HRMS (ESI): Calcd for $[(C_{42}H_{51}N_4)^+]$ $[(M+H)^+]$ 611.4108; found: 611.4108.

c. Synthesis of monofunctional NHC-CDI 8

1-(4-bromo-2-methylphenyl)-3-(4-vinylphenyl)urea (6)



S3 **S4** **6**

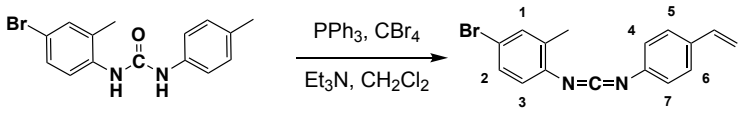
To a solution of 4-vinylaniline **S3** (298 mg, 2.50 mmol) in 10 mL of dry THF, under a nitrogen atmosphere, was added dropwise isocyanate **S4** (531 mg, 2.50 mmol) at room temperature. After stirring for overnight (ca. 12 h), the solids formed in the solution was filtered and washed with CH_2Cl_2 several times to give urea **6** (693 mg, 84%) as a white solid.

^{1}H NMR (DMSO-d_6, 400 MHz) δ 9.15 (s, 1H, N*H*CO), 8.00 (s, 1H, N*H*CO), 7.84 (d, *J* = 8.7 Hz, 1H, *H3*), 7.44 (d, *J* = 8.6 Hz, 2H, *H4* and *H7*), 7.42–7.37 (m, 3H, *H1*, *H5* and *H6*), 7.32 (dd, *J* = 8.7, 2.5 Hz, 1H, *H2*), 6.66 (dd, *J* = 17.7, 10.9 Hz, 1H, ArC*H*=CH_2), 5.70 (d, *J* = 17.7 Hz, 1H, ArCH=C*H*), 5.14 (d, *J* = 10.9 Hz, 1H, ArCH=C*H*), and 2.24 (s, 3H, Ar-CH_3).

^{13}C NMR (126 MHz, DMSO-d_6) δ 152.3, 139.4, 136.9, 136.2, 132.4, 130.9, 130.0, 128.8, 126.7, 122.4, 118.0, 114.2, 112.1, and 17.5.

HRMS (ESI): Calcd for $[(C_{16}H_{16}BrN_2O)^+]$ $[(M+H)^+]$ 331.0441; found: 331.0436.

N-(4-bromo-2-methylphenyl)-*N*-(4-vinylphenyl)methanediimine (7)



6 7

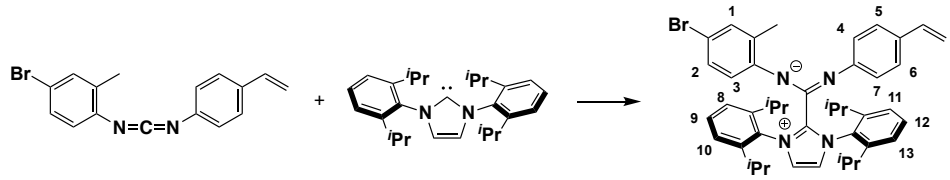
Et_3N (0.33 mL, 2.37 mmol), PPh_3 (472 mg, 1.80 mmol), and CBr_4 (518 mg, 1.56 mmol) were sequentially added to a stirred solution of urea **6** (400 mg, 1.21 mmol) in CH_2Cl_2 (10 mL) at 0 °C. After 5 h the reaction mixture was concentrated to about 1 mL. The residue was purified by flash flash chromatography (hexanes:EtOAc 40:1) to give carbodiimide **7** as a colorless oil (330 mg, 88%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37 [d, *J* = 8.4 Hz, 2H, *H4 (or H5)* and *H7 (or H6)*], 7.34 (d, *J* = 2.3 Hz, 1H, *H1*), 7.27 (dd, *J* = 8.4, 2.3 Hz, 1H, *H2*), 7.12 [d, *J* = 8.4 Hz, 2H, *H5 (or H4)* and *H6 (or H7)*], 7.03 (d, *J* = 8.4 Hz, 1H, *H3*), 6.68 (dd, *J* = 17.6, 10.9 Hz, 1H, ArC*H*=CH_2), 5.71 (d, *J* = 17.6 Hz, 1H, ArCH=C*H*), 5.24 (d, *J* = 10.9 Hz, 1H, ArCH=C*H*), and 2.34 (s, 3H, Ar-CH_3).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.9, 136.2, 136.1, 135.3, 134.9, 133.9, 133.7, 130.0, 127.5, 126.2, 124.4, 118.6, 114.0, and 18.3.

HRMS (ASAP-MS): Calcd for $[(C_{16}H_{14}BrN_2)^+]$ $[(M+H)^+]$ 313.0335; found: 313.0333.

Monofunctional NHC-CDI 8



7 8

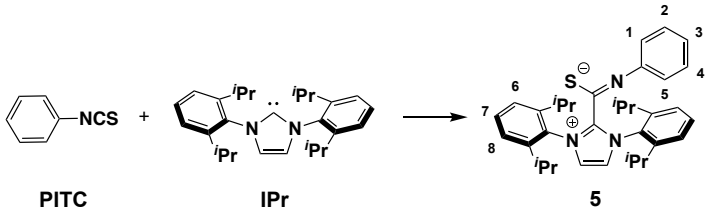
NHC-CDI **8** was prepared following the same procedure as for **3** from carbodiimide **7** (62 mg 0.20 mmol) and **IPr** (77 mg, 0.20 mmol). Product **8** was obtained as a yellow solid (126 mg, 91%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.46 (t, *J* = 7.8 Hz, 2H, *H9* and *H12*), 7.28 (d, *J* = 7.8 Hz, 4H, *H8*, *H10*, *H11* and *H13*), 7.12 (s, 2H, C*H*=C*H*), 6.65 (d, *J* = 2.4 Hz, 1H, *H1*), 6.61 [d, *J* = 8.4 Hz, 2H, *H5* (or *H4)* and *H6* (or *H7*)], 6.43 (dd, *J* = 8.5, 2.4 Hz, 1H, *H2*), 6.37 (dd, *J* = 17.5, 10.8 Hz, 1H, ArC*H*=CH_2), 5.70 [d, *J* = 8.4 Hz, 2H, *H4* (or *H5)* and *H7* (or *H6*)], 5.65 (d, *J* = 8.5 Hz, 1H, *H3*), 5.28 (dd, *J* = 17.5, 1.4 Hz, 1H, ArCH=C*H*), 4.78 (d, *J* = 10.8, 1.4 Hz, 1H, ArCH=C*H*), 2.87 [hept, *J* = 6.8 Hz, 4H, C*H*$(CH_3)_2$], 1.23 (s, 3H, Ar-CH_3), 1.28 [d, *J* = 6.8 Hz, 12H, CH(CH_3)$_2$], and 1.20 [d, *J* = 6.8 Hz, 12H, CH(CH_3)$_2$].

^{13}C NMR (126 MHz, $CDCl_3$) δ 151.2, 150.03, 149.95, 145.6, 140.6, 137.7, 133.1, 131.1, 130.6, 129.9, 127.1, 127.0, 124.8, 124.2, 121.8, 121.6, 120.7, 109.9, 108.2, 29.5, 25.2, 23.1, and 17.7.

HRMS (ESI): Calcd for $[(C_{43}H_{50}BrN_4)^+]$ $[(M+H)^+]$ 701.3213; found: 701.3216.

d. Synthesis of IPr-PITC adduct 5



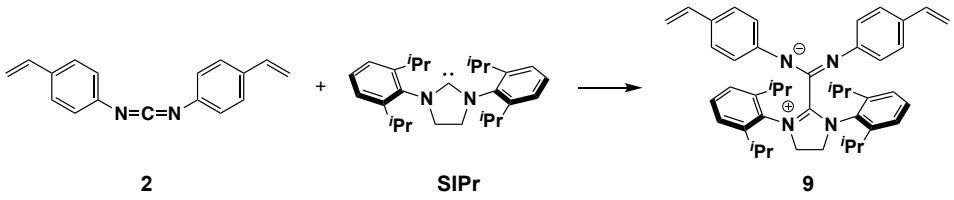
A flame-dried two-neck flask was loaded with a solution of phenyl isothiocyanate (23 µL, 0.19 mmol) in dry THF (1 mL) under an atmosphere of Ar. Subsequently, 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene (**IPr**) (77 mg, 0.20 mmol) was added to the solution while purging with Ar. The reaction mixture was stirred at room temperature for 1 h before it was concentrated to dryness. The residue was added 2 mL of hexane and put in the freezer for overnight. The resulting solids were washed with hexane 5 times and dried under vacuum to give IPr-PITC adduct **5** as a light-yellow solid (98 mg, 97%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48 (t, *J* = 7.8 Hz, 2H, *H7*), 7.29 (d, *J* = 7.8 Hz, 4H, *H6* and *H8*), 7.08 (s, 2H, C*H*=C*H*), 7.06 (dd, *J* = 7.8, 7.8 Hz, 2H, *H2* and *H4*), 6.79 (t, *J* = 7.5 Hz, 1H, *H3*), 6.50 (d, *J* = 7.8 Hz, 2H, *H1* and *H5*), 2.96 [hept, *J* = 6.8 Hz, 4H, C*H*$(CH_3)_2$], 1.35 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3)_2$], and 1.18 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3)_2$].

^{13}C NMR (126 MHz, $CDCl_3$) δ 164.4, 151.9, 147.9, 146.4, 131.5, 131.1, 128.2, 124.4, 122.2, 121.4, 121.1, 29.5, 25.8 and 23.1.

HRMS (ESI): Calcd for $[(C_{34}H_{42}N_3S)^+]$ $[(M+H)^+]$ 524.3094; found: 524.3092.

e. Synthesis of NHC-CDI mechanophore 9



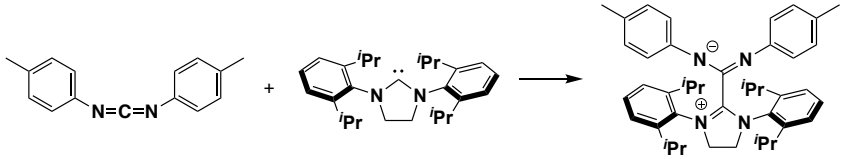
NHC-CDI **9** was prepared following the same procedure as for **3** from carbodiimide **2** (125 mg 0.51 mmol) and **SIPr** (208 mg, 0.53 mmol). Product **9** was obtained as a yellow solid (302 mg, 93%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36 [t, *J* = 7.8 Hz, 2H, Ar(NHC)-*H*], 7.20 [d, *J* = 7.8 Hz, 4H, Ar(NHC)-*H*], 6.62 [d, *J* = 8.4 Hz, 4H, Ar(CDI)-*H*], 6.34 (dd, *J* = 17.6, 10.8 Hz, 2H, ArC*H*=CH_2), 5.75 [d, *J* = 8.4 Hz, 4H, Ar(CDI)-*H*], 5.24 (dd, *J* = 17.6, 1.4 Hz, 2H, ArCH=C*H*), 4.75 (dd, *J* = 10.8, 1.4 Hz, 2H, ArCH=C*H*), 4.30 (s, 4H, CH_2–CH_2), 3.39 [hept, *J* = 6.8 Hz, 4H, C*H*$(CH_3)_2$], 1.35 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3)_2$], and 1.32 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3)_2$].

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.5, 151.3, 146.9, 141.0, 137.7, 132.1, 130.0, 127.0, 125.0, 124.4, 120.8, 108.0, 51.9, 29.6, 26.1, and 23.8.

HRMS (ESI): Calcd for [$(C_{44}H_{53}N_4)^+$] [$(M+H)^+$] 637.4265; found: 637.4261.

f. Synthesis of control NHC-CDI S5



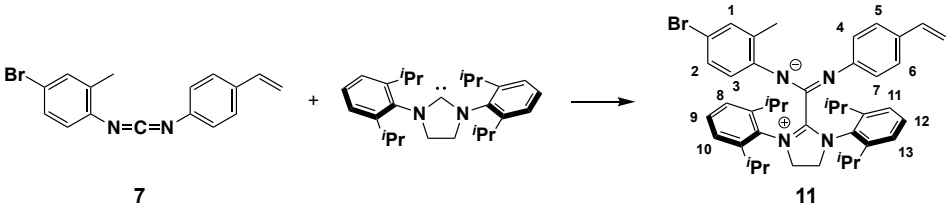
NHC-CDI **S5** was prepared following the same procedure as for **3** from carbodiimide **S2** (45 mg, 0.20 mmol) and **SIPr** (82 mg, 0.21 mmol). Product **S5** was obtained as a yellow solid (101 mg, 82%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36 [t, *J* = 7.7 Hz, 2H, Ar(NHC)-*H*], 7.21 [d, *J* = 7.7 Hz, 4H, Ar(NHC)-*H*], 6.30 [d, *J* = 8.0 Hz, 4H, Ar(CDI)-*H*], 5.63 [d, *J* = 8.0 Hz, 4H, Ar(CDI)-*H*], 4.28 (s, 4H, C*H*$_2$–C*H*$_2$), 3.40 [hept, *J* = 6.8 Hz, 4H, C*H*(CH_3)$_2$], 1.95 (s, 6H, Ar-C*H*$_3$), 1.36 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$], and 1.32 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$].

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.9, 149.2, 147.0, 140.9, 132.6, 129.7, 127.0, 125.8, 124.3, 121.0, 51.8, 29.6, 26.0, 23.9, and 20.7.

HRMS (ESI): Calcd for [$(C_{42}H_{53}N_4)^+$] [$(M+H)^+$] 613.4265; found: 613.4263.

g. Synthesis of monofunctional NHC-CDI 11



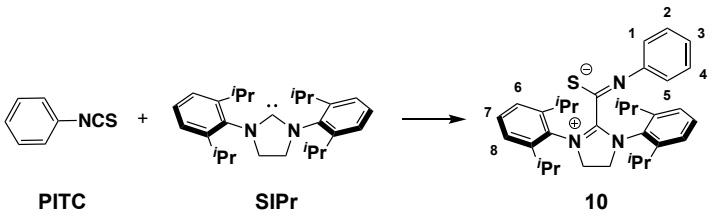
NHC-CDI **11** was prepared following the same procedure as for **3** from carbodiimide **7** (82 mg, 0.26 mmol) and **SIPr** (107 mg, 0.27 mmol). Product **11** was obtained as a yellow solid (172 mg, 93%).

^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.37 (t, *J* = 7.7 Hz, 2H, *H9* and *H12*), 7.22 (d, *J* = 7.7 Hz, 4H, *H8*, *H10*, *H11* and *H13*), 6.58–6.55 [m, 3H, *H1*, *H5 (*or *H4)* and *H6 (*or *H7)*], 6.44 (dd, *J* = 8.5, 2.5 Hz, 1H, *H*2), 6.35 (dd, *J* = 17.5, 10.8 Hz, 1H, ArC*H*=CH_2), 5.65 [d, *J* = 8.4 Hz, 2H, *H4 (or H5)* and *H7 (or H6)*], 5.62 (d, *J* = 8.5 Hz, 1H, *H3*), 5.26 (dd, *J* = 17.5, 1.4 Hz, 1H, ArCH=C*H*), 4.77 (dd, *J* = 10.8, 1.4 Hz, 1H, ArCH=C*H*), 4.30 (s, 4H, C*H*$_2$–C*H*$_2$), 3.40 [hept, *J* = 6.8 Hz, 4H, C*H*(CH_3)$_2$], 1.35 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$], 1.33 [d, *J* = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$], and 1.06 (s, 3H, Ar-C*H*$_3$).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 151.0, 150.1, 146.9, 140.6, 137.7, 132.5, 131.1, 130.1, 130.0, 127.11, 127.08, 124.65, 124.58, 122.2, 121.0, 110.2, 108.2, 52.0, 29.6, 26.1, 23.8, and 17.5.

HRMS (ESI): Calcd for $[(C_{43}H_{52}BrN_4)^+]$ $[(M+H)^+]$ 703.3370; found: 703.3365.

h. Synthesis of SIPr-PITC adduct 10



SIPr-PITC **10** was prepared following the same procedure as for **5** from phenyl isothiocyanate PITC (21 μL, 0.18 mmol) and **SIPr** (72 mg, 0.18 mmol). The product was further recrystallized to give SIPr-PITC **10** as a light-yellow solid (69 mg, 75%).

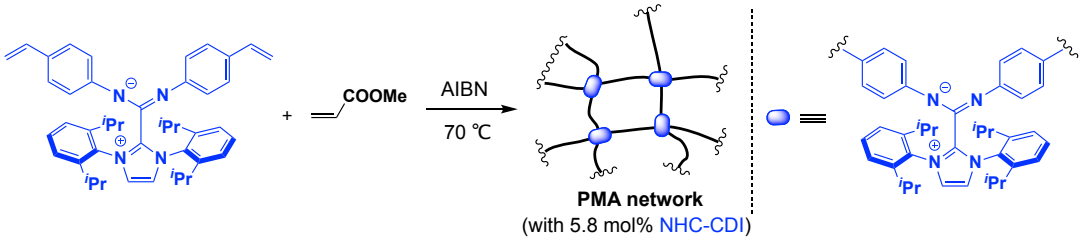
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39 (t, *J* = 7.8 Hz, 2H, *H7*), 7.23 (d, *J* = 7.8 Hz, 4H, *H6* and *H8*), 7.02 (dd, *J* = 7.8, 7.8 Hz, 2H, *H2* and *H4*), 6.77 (t, *J* = 7.5 Hz, 1H, *H3*), 6.36 (dd, *J* = 7.8, 1.4 Hz, 2H, *H1* and *H5*), 4.29 (s, 4H, CH_2–CH_2), 3.48 [hept, *J* = 6.8 Hz, 4H, $CH(CH_3)_2$], 1.40 [d, *J* = 6.8 Hz, 12H, $CH(CH_3)_2$], and 1.31 [d, *J* = 6.8 Hz, 12H, $CH(CH_3)_2$].

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 162.6, 151.5, 147.5, 131.3, 130.4, 128.2, 124.8, 122.1, 121.4, 51.8, 29.5, 26.4, and 23.9.

HRMS (ESI): Calcd for $[(C_{34}H_{44}N_3S)^+]$ $[(M+H)^+]$ 526.3250; found: 526.3244.

III. Synthesis of PMA networks

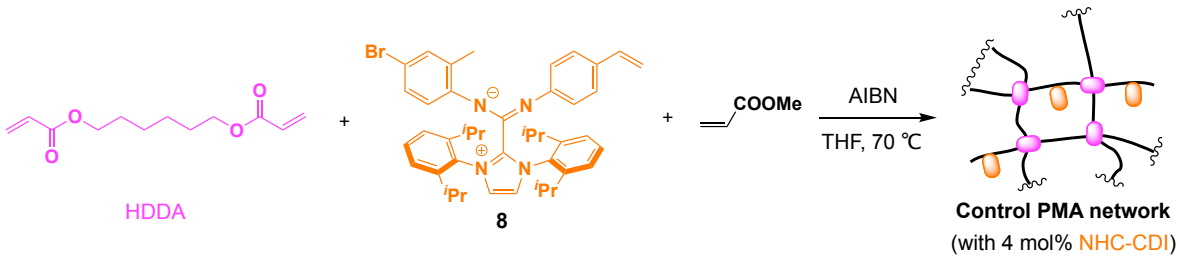
a. Synthesis of the PMA network that contains NHC-CDI mechanophore 3



In a scintillation vial, azobisisobutyronitrile AIBN (4 mg, 0.02 mmol) was added to the solution of NHC-CDI **3** (80 mg, 0.13 mmol) in methyl acrylate (0.26 mL, 2.87 mmol). The mixture was degassed by two freeze-pump-thaw cycles and backfilled with Ar. With being firmly sealed with a Teflon-lined screw cap, the vial was put in an oil bath that had been pre-equilibrated to 70 °C. After 12 h, the vial was cooled down to room temperature and solvent mixture of CH_2Cl_2 with $CDCl_3$ (V: V = 1: 3) was added. During the soaking process, the solids were gently squeezed into small pieces by a spatula, before the soaking solution was removed by a pipette and replaced with a fresh portion of solvents. This soaking process was repeated until no reactants were observed by ^{1}H NMR, and the remaining solids were dried *in vacuo* to give the desired PMA network as a red

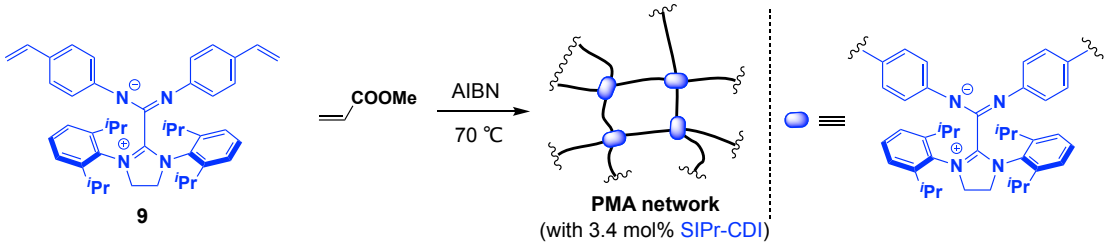
solid (126 mg). The final loading of **3** within the PMA network was determined by ^{1}H NMR analysis of the combined soaking solutions and determined to be 5.8 mol%.

b. Synthesis of the PMA network that contains monofunctional NHC-CDI 8



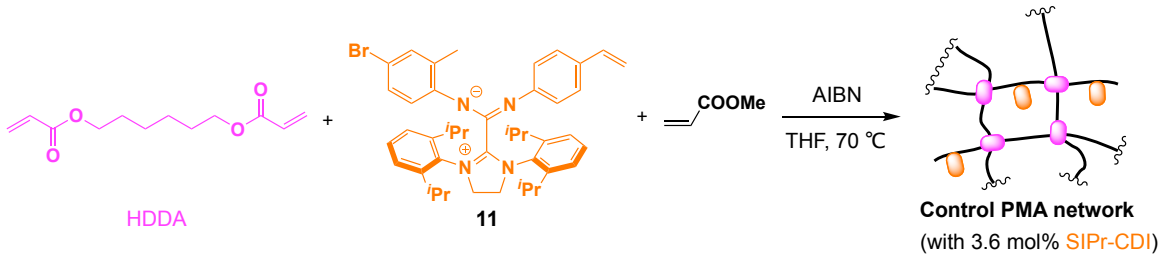
In a scintillation vial, AIBN (3 mg, 0.02 mmol) was added to the mixture of NHC-CDI **8** (63 mg, 0.09 mmol), 1,6-hexanediol diacrylate HDDA (20 μL, 0.09 mmol), and methyl acrylate (0.23 mL, 2.5 mmol) in dry THF (0.15 mL). The mixture was degassed by two freeze-pump-thaw cycles and backfilled with Ar. With being firmly sealed with a Teflon-lined screw cap, the vial was put in an oil bath that had been pre-equilibrated to 70 °C. After 14 h, the vial was cooled down to room temperature and a solvent mixture of CH_2Cl_2 with $CDCl_3$ (v:v = 1:3) was added. The solids were gently broken into small pieces by a spatula before the soaking solution was removed by a pipette and replaced with a fresh portion of solvent. This soaking process was repeated until no reactants were observed by ^{1}H NMR, and the remaining solids were dried *in vacuo* to give the desired PMA network as a red-orange solid (140 mg). The final loading of **8** within the PMA network was determined by ^{1}H NMR analysis of the combined soaking solutions and determined to be 4.0 mol%. The final loading of HDDA was determined to be 4.0 mol%.

c. Synthesis of the PMA network that contains SIPr-CDI mechanophore 9



PMA network containing mechanophore **9** was prepared following the same procedure as for the PMA network containing **3** from SIPr-CDI **9** (56 mg, 0.09 mmol), methyl acrylate (0.27 mL, 2.98 mmol) and AIBN (4 mg, 0.02 mmol). The final PMA network was obtained as an orange solid (118 mg). The loading of **9** within the PMA network was determined to be 3.4 mol%.

d. Synthesis of the PMA network that contains NHC-CDI mechanophore 11



The control PMA network containing SIPr-CDI **11** was prepared following the same procedure as for the control PMA network containing **8** from SIPr-CDI **11** (84 mg, 0.12 mmol), methyl acrylate (0.26 mL, 2.87 mmol), HDDA (27 μL, 0.12 mmol) and AIBN (4 mg, 0.02 mmol). The final PMA network was obtained as a red-orange solid (184 mg). The loading of **11** within the PMA network was determined to be 3.6 mol% and the final loading of HDDA was determined to be 4.1 mol%.

IV. General procedure for building calibration curves

Different amounts of NHC-PITC (or SIPr-PITC) adduct were added to six-2 mL vials. After dispensing 985 μL of MeOH and 15 μL of internal standard 9-methylanthracene solution (1.04 mM in MeOH) to each of the 2 mL vials, the resulting solutions were analyzed by LC-MS. The UV absorption spectra at 330 nm were extracted, and the peak area ratios of NHC-PITC to internal standard were recorded. Each sample was prepared in triplicate and the calibration curve was made by plotting the averaged area ratio of NHC-PITC to internal standard versus the concentration of NHC-PITC. As shown in the Figure S1 and Figure S2 below, the relationship between averaged area ratio and concentration provided a good linear relationship. The error bars were also incorporated into each averaged point.

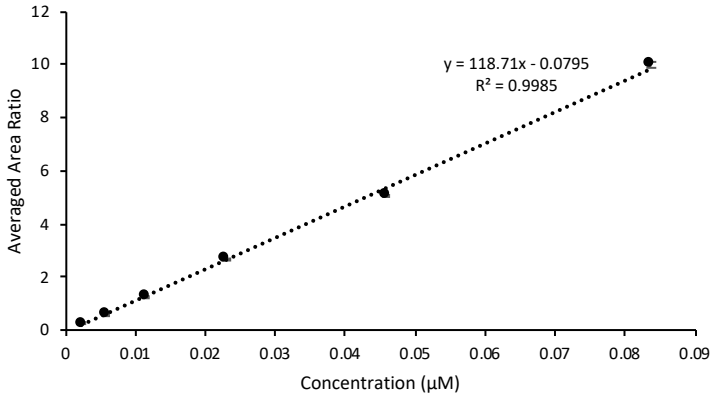


Figure S1. Calibration curve for NHC-PITC **5**.

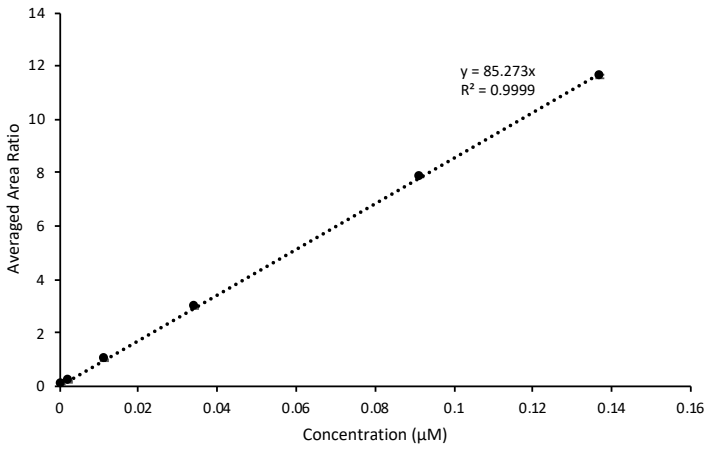


Figure S2. Calibration curve for SIPr-PITC **10**.

V. Activation of NHC-CDI mechanophores by compression

a. General procedure for compression studies

The stock solution of phenyl isothiocyanate PITC (0.09~0.11 mL, 0.021~0.025 mmol, 0.23 M in CH_2Cl_2) was slowly added to a sample of PMA network (18~20 mg), letting PITC solution to be fully absorbed before subsequent additions. The CH_2Cl_2 in the sample was removed by gently applying reduced pressure (~15 torr) for 8 min via rotary evaporation before the sample was further dried under high vacuum for another 10 min. Then, the sample was loaded into a standard KBr pellet die, and the desired pressure (calculated by dividing the load by area of the pellet die surface, 6.5 mm radius) was applied via a Specac hydraulic press with attached manometer. After the sample was compressed for 10 min, it was transferred to a vial and the pellet die was washed with 2 mL of CH_2Cl_2 which was added to the vial. The resulting mixture was stirred for 15 min, followed by adding polymer-bound benzylamine (45 mg, 4.0 mmol/g loading, purchased from Sigma-Aldrich). After 1 h, the mixture was filtered through a 0.45 micron PTFE syringe filter, and the remaining polymer was washed with CH_2Cl_2 several times until no NHC-PITC adduct was detected by GC-MS. The combined CH_2Cl_2 solution was concentrated to dryness. Subsequently, 985 μL of MeOH and 15 μL of 9-methylanthracene solution (1.04 mM in MeOH) were added to the vial. The resulting solution was filtered through a 0.45 micron PTFE syringe filter again and analyzed by LC-MS. The activation percentage was calculated by dividing the detected NHC-PITC adduct (determined from the calibration curve) by the total amount of NHC-CDI present in the sample.

For successive compression cycles, the sample was folded between each 10 min cycle. The same compression procedure was repeated for desired times and the final sample was transferred to a vial to go through the same work up procedure as described above.

b. Results of compression studies for the PMA network containing NHC-CDI 3

All of the compression experiments were performed following the general compression procedure described above, using 18 mg of PMA network containing NHC-CDI **3** and 0.1 mL of PITC solution (0.23 M in CH_2Cl_2). The results were summarized in Table S1.

Table S1. Raw data for the plots in Figure 5 and Figure 6 of the main text.

Entry	Pressure (MPa)	Compression Cycles	Activation Percentage (%)	Average (%)	Std. Dev.
1	740	1	0.45	0.41	0.058
2	740	1	0.39		
3	740	1	0.37		
4	740	1	0.34		
5	740	1	0.50		
6	740	1	0.43		
7	370	1	0.29	0.29	0.015
8	370	1	0.31		
9	370	1	0.28		
10	74	1	0.22	0.22	0.006
11	74	1	0.21		
12	74	1	0.22		
13	0	1	0	0	0
14	740	2	0.71	0.74	0.093
15	740	2	0.84		
16	740	2	0.66		
17	740	3	1.03	1.01	0.017
18	740	3	1.00		
19	740	3	1.00		
20	740	4	1.07	1.06	0.101
21	740	4	0.95		
22	740	4	1.15		

c. Results of compression studies about the control PMA network containing NHC-CDI 8

All of the compression experiments were performed following the general compression procedure described above, using 20 mg of control PMA network containing NHC-CDI **8** and 0.11 mL of PITC solution (0.23 M in CH_2Cl_2). The results were summarized in Table S2.

Table S2. Raw data for control experiments using NHC-CDI **8**.

Entry	Pressure (MPa)	Compression Cycle	Activation Percentage (%)	Average (%)
1	740	1	0.036	0.03
2	740	1	0.020	
3	740	1	0.025	

d. Results of compression studies for the PMA network containing SIPr-CDI 9

All of the compression experiments were performed following the general compression procedure described above, using 18 mg of PMA network containing SIPr-CDI **9** and 0.09 mL of PITC solution (0.23 M in CH_2Cl_2). The results were summarized in Table S3.

Table S3. Raw data for compression experiments on activation of SIPr-CDI **9**.

Entry	Pressure (MPa)	Compression Cycle	Activation Percentage (%)	Average (%)
1	740	1	0.47	0.46
2	740	1	0.42	
3	740	1	0.48	

e. Results of compression studies for the control PMA network containing SIPr-CDI 11

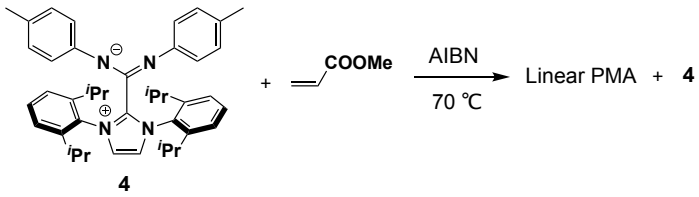
All of the compression experiments were performed following the general compression procedure described above, using 18 mg of control PMA network containing SIPr-CDI **11** and 0.09 mL of PITC solution (0.23 M in CH_2Cl_2). The results were summarized in Table S4.

Table S4. Raw data for control experiments using SIPr-CDI **11**.

Entry	Pressure (MPa)	Compression Cycles	Activation Percentage (%)	Average (%)
1	740	1	0.001	0.003
2	740	1	0.008	
3	740	1	0.001	

VI. Examining stability of NHC-CDI and SIPr-CDI

a. Examining stability of NHC-CDI



In a scintillation vial, 1,2,4,5-tetramethylbenzene (11 mg, 0.08 mmol) and AIBN (2 mg, 0.01 mmol) were sequentially added to the solution of NHC-CDI **4** (35 mg, 0.06 mmol) in methyl acrylate (0.25 mL, 2.76 mmol). The mixture was degassed by two freeze-pump-thaw cycles and backfilled with Ar. With being firmly sealed with a Teflon-lined screw cap, the vial was put in an oil bath that had been pre-equilibrated to 70 °C. After 15 h, the vial was cooled down to room temperature and 1.5 mL of $CDCl_3$ was added. An aliquot of the solution was diluted by $CDCl_3$ and analyzed by ^1H NMR. By comparing the aromatic peaks of CDI, 90% of NHC-CDI **4** was recovered. As shown in Figure S3, there are no obvious other peaks other than NHC-CDI **4**, linear PMA and left methyl acrylate.

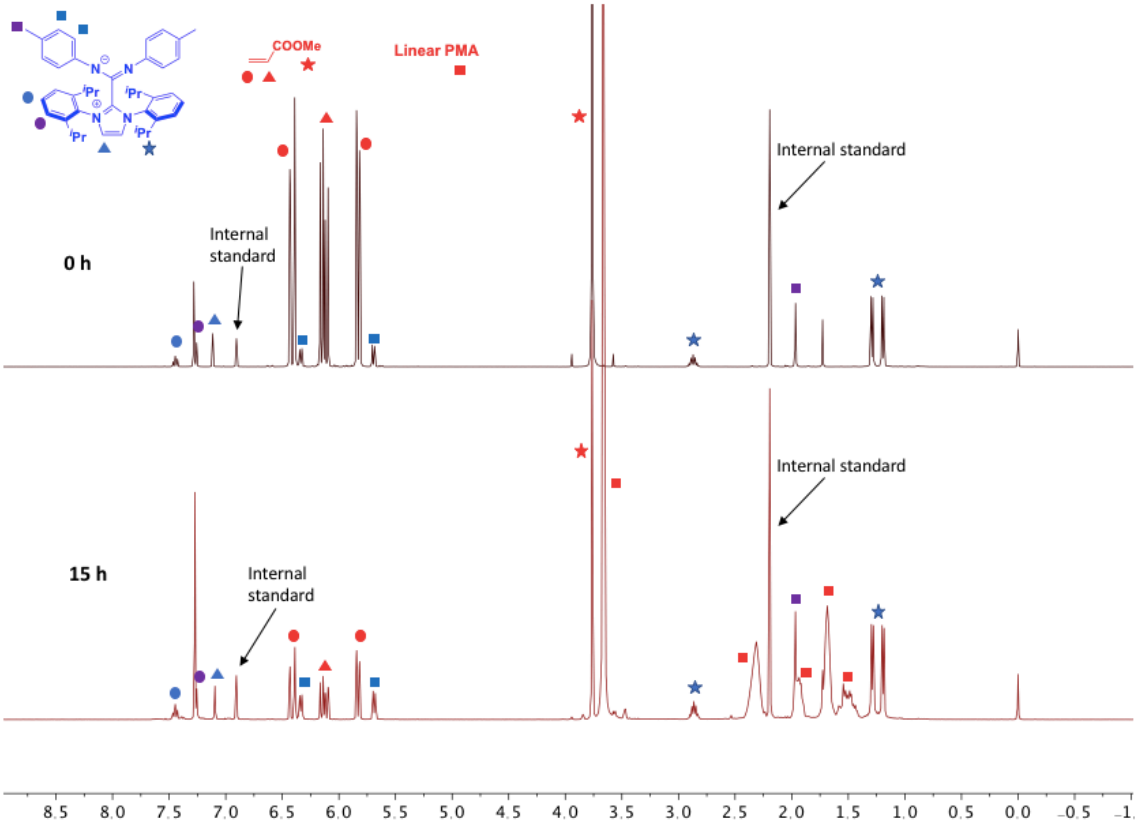
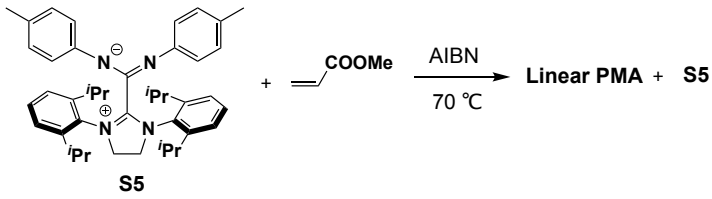


Figure S3. Examining stability of NHC-CDI **4** under polymerization conditions. The peaks that are marked by blue and purple rectangle, circle, triangle as well as star are the peaks of NHC-CDI. The peaks that are marked by red circle, triangle and star are the peaks of methyl acrylate. The peaks that are marked by red rectangle are the peaks of linear PMA.

b. Examining stability of SIPr-CDI



In a scintillation vial, 1,2,4,5-tetramethylbenzene (11 mg, 0.08 mmol) and AIBN (2 mg, 0.01 mmol) were sequentially added to the solution of SIPr-CDI **S5** (20 mg, 0.03 mmol) in methyl acrylate (0.34 mL, 3.75 mmol). The mixture was degassed by two freeze-pump-thaw cycles and backfilled with Ar. With being firmly sealed with a Teflon-lined screw cap, the vial was put in an oil bath that had been pre-equilibrated to 70 °C. After 15 h, the vial was cooled down to room temperature and 1.5 mL of $CDCl_3$ was added. An aliquot of the solution was diluted by $CDCl_3$ and analyzed by ^1H NMR. By comparing the aromatic peaks of CDI, 92% of SIPr-CDI **S5** was recovered. As shown in Figure S4, there are no obvious other peaks other than SIPr-CDI **S5**, linear PMA and left methyl acrylate.

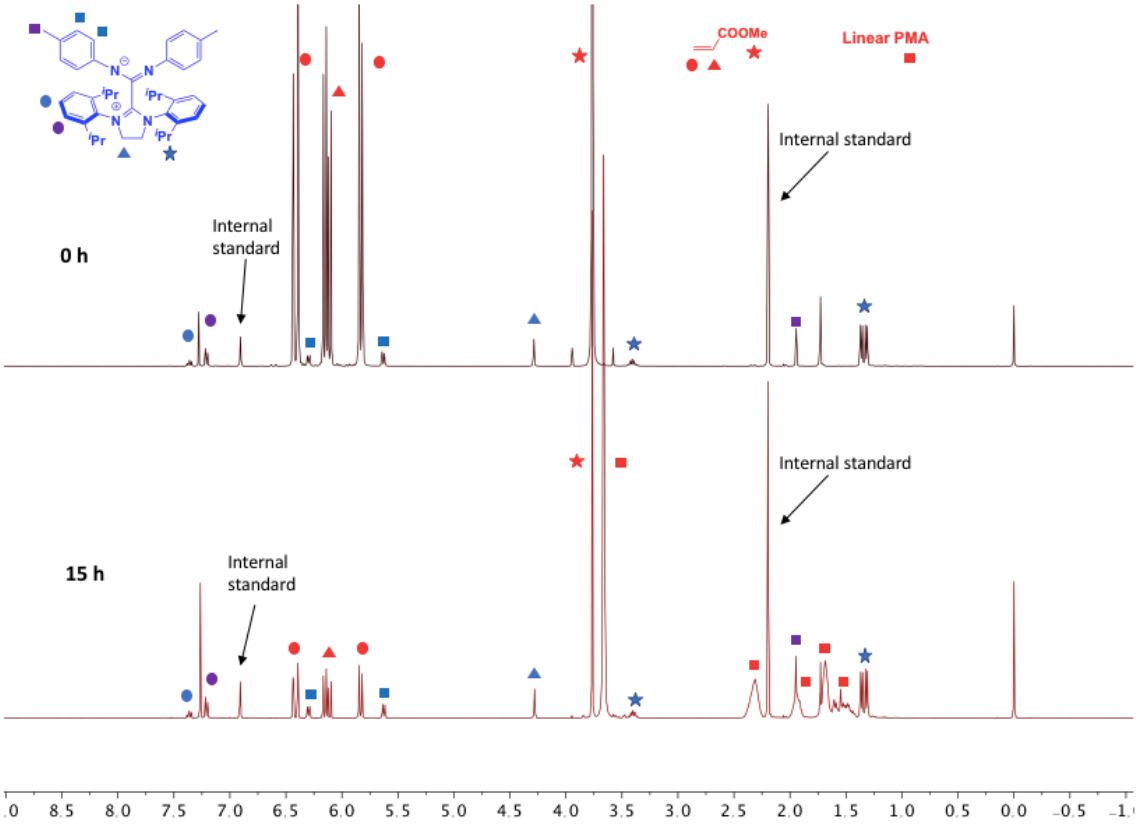


Figure S4. Examining stability of SIPr-CDI **S5** under polymerization conditions. The peaks that are marked by blue and purple rectangle, circle, triangle as well as star are the peaks of SIPr-CDI **S5**. The peaks that are marked by red circle, triangle and star are the peaks of methyl acrylate. The peaks that are marked by red rectangle are the peaks of linear PMA.

VII. Computational details

Density functional theory simulations were performed using the B3LYP[3–5] level of theory and the LANL2DZ basis set[6–8] as implemented in the Q-Chem 5.0 software package.[9] The force functionality[10] of Growing String Method (GSM)[11–13] was used to calculate transition states (TSs), reaction paths (RPs), and product geometries for mechanophore activation at specific magnitudes of applied force. Constant tensile forces were applied to the terminal carbons in the model to simulate experimental conditions, where the structures were fully optimized under the mechanical load. GSM was converged to an RMS gradient tolerance of 0.0005 Ha/Å. Energies reported in the text are gas-phase electronic energies. As discussed in prior work,[10] GSM simulations are highly useful for mechanophore characterization due to their ability to locate precise transition states (saddle points on the force-biased potential energy surface), and therefore provide accurate activation energies.

The models for the mechanophores consist of the core mechanophore unit along with terminal methyl groups to represent the connections to the polymer chain. Previous studies[10] have indicated small to negligible effects of polymer truncations, supporting the validity of small mechanophore/polymer models. In order to arrive at reaction pathways under tensile load, the reactant state was first optimized under each force value (0 to 4 nN), starting from an initial structure that was optimized under the maximum force (4 nN). This ensures that the conformation of the chain is consistent across the range of forces, and represents an equilibrium condition for the initial mechanophore geometry.

Optimized Cartesian Coordinates of Selected Structures – B3LYP/LANL2DZ

4 nN Reactant
96
0.000000
C -0.386469 2.948288 -0.949391
C -0.207350 1.489208 -0.442045
N -1.260358 0.610500 -0.289227
N 0.919153 0.780682 -0.076154
C -0.781247 -0.633539 0.138775
C 0.558032 -0.524142 0.293471
C 2.297951 1.229526 0.066654
C 2.584925 2.174035 1.089202
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H -3.859090 1.964665 3.633270
H -2.642773 2.980777 2.841606
H -2.180941 1.911275 4.179948
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H 1.283412 -1.319391 0.645623
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H 3.761358 1.262734 -6.881095
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H 4.718074 2.700778 -6.478009
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C 2.001347 2.727667 -5.610526
C 3.371842 2.702270 -5.270953
C 3.669955 3.117304 -3.952354
C 2.684063 3.534621 -3.039743
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3.5 nN Product

96

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C 3.771308 2.337257 1.191939
C 4.785718 1.890403 0.343818
C 3.196937 0.424477 -0.806967
C 4.493538 0.950699 -0.639056
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C -3.323279 0.753247 1.110053
C -4.694554 1.055089 1.117199
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C -3.441566 0.427670 -1.336988
N -1.004918 4.774311 -0.431514
N 0.338843 4.222624 -2.378228
C 1.304120 3.746107 -3.255210
C -2.020244 5.144698 0.437842
C 0.966623 3.444641 -4.593684
C 1.938989 3.016227 -5.508340
C 3.294442 2.868149 -5.151864
C 3.618703 3.166459 -3.811399
C 2.659835 3.596302 -2.883393

C -1.745356 6.012603 1.520967
C -2.748433 6.389186 2.422776
C -4.077331 5.930241 2.304540
C -4.340254 5.067099 1.221287
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H 4.647471 3.062864 -3.475638
H 2.955314 3.816583 -1.863598
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C -2.561175 0.755972 2.437764
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C 3.047159 -0.582308 -1.961140
H 5.277376 0.618891 -1.313877
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C 1.373163 1.380811 3.321445
H 1.202816 0.333970 3.046939
H 0.576691 1.685953 4.011488
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H 0.427780 2.225993 1.569424
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H 0.666125 4.086939 3.072761
H 1.636693 4.434698 1.633093
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H 0.917743 -1.049755 -2.185949
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H 1.407099 0.461479 -2.972388
C 3.402386 -2.023624 -1.514933
H 3.822955 -0.282265 -2.679883
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H -4.065937 -0.356269 3.585808
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H -1.497285 0.626417 2.222132
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H -1.455358 -1.935029 0.631007
H 1.293176 -1.674265 0.825302
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H -0.065142 3.554734 -4.909156
H 3.898538 1.969889 -7.048716
H 5.053682 1.701976 -5.728350
H 4.957568 3.285103 -6.512559
H -0.733841 6.383268 1.647178
H -6.024542 5.672688 3.258544
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C 4.648706 1.078053 -0.568531
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C 1.562234 2.316734 -5.183907
C 2.937360 2.405408 -4.892225
C 3.263236 2.855181 -3.596771
C 2.286136 3.144699 -2.634510
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C -2.804410 5.818677 2.436626
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C -4.268367 5.226467 0.646845
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H 5.436616 0.698113 -1.211478
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H 4.200357 3.193502 2.035111

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H 1.122105 -1.080383 -2.127483
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C 3.020493 2.452496 -4.876440
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H 1.338104 -1.416130 0.669122
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C 2.444128 1.843712 1.162306
C 3.702703 2.452958 1.272688
C 4.729321 2.159949 0.375064
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C 1.387063 2.113078 2.237348
H 3.881152 3.158992 2.074157
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H -2.636546 1.155134 -3.370988
H -1.611516 0.004308 -4.259538
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C -1.886410 -2.189936 -2.602887
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H -0.943463 -2.068141 -2.066246
H -1.650635 -2.484043 -3.633036
H -2.441049 -3.012980 -2.135878
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H 3.391055 2.645969 -6.729017	H -1.674918 4.765392 2.599785	H -4.421732 8.681727 3.266152

VIII. References for supplementary information

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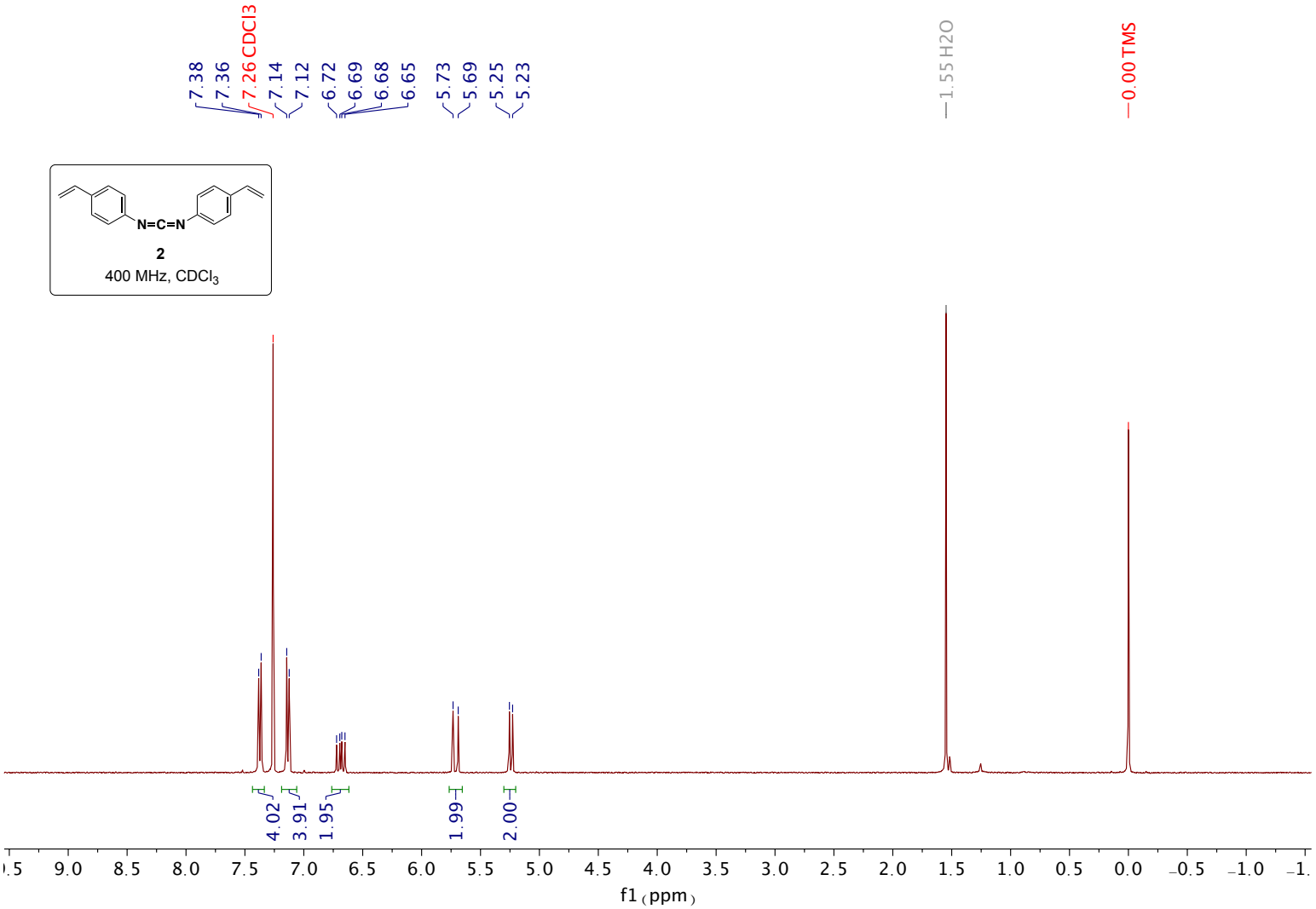
IX. Copies of ^{1}H and ^{13}C NMR spectra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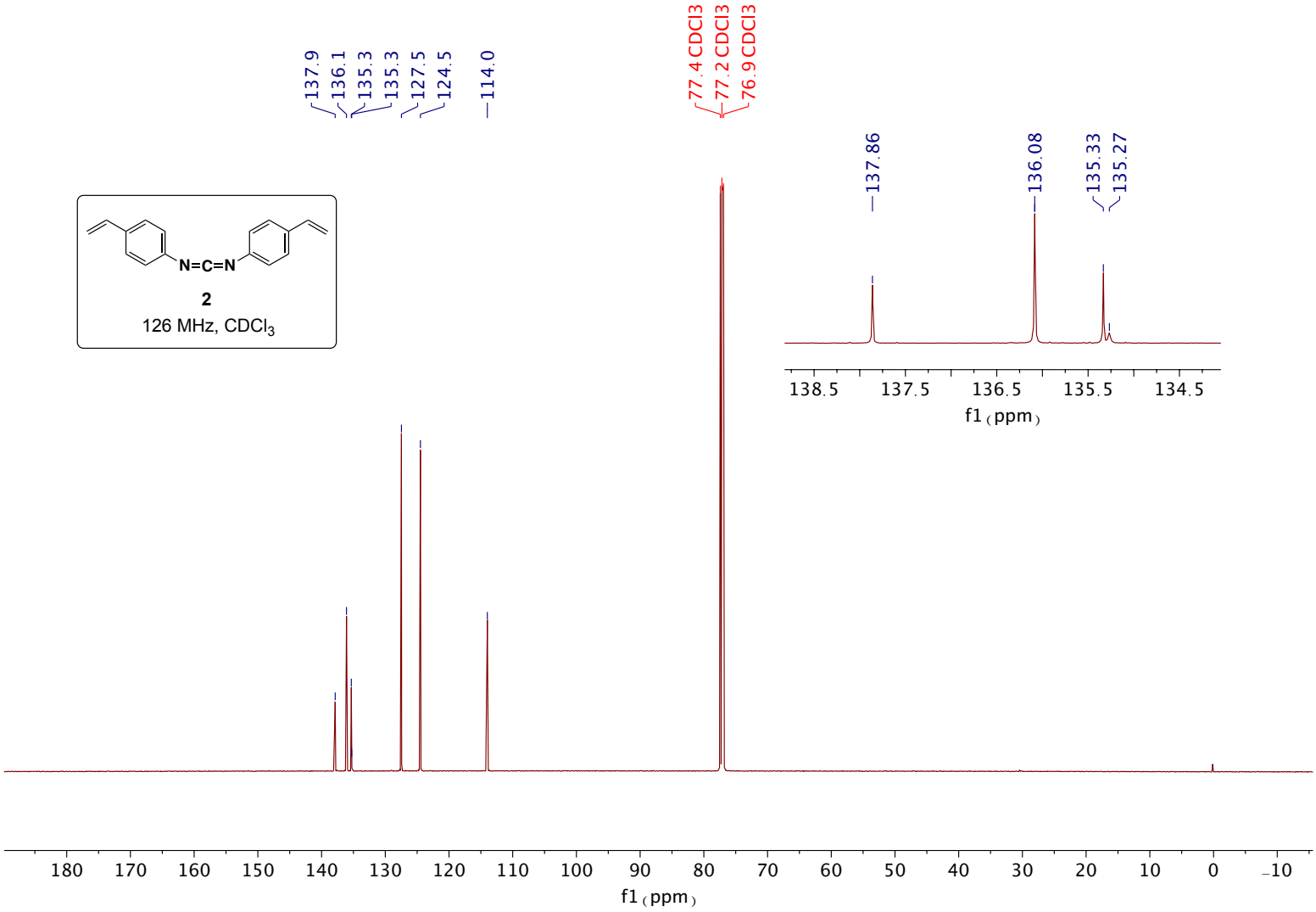
7.36
7.26 CDCl3
7.14
7.12
6.72
6.69
6.68
6.65
5.73
5.69
5.25
5.23
1.55 H2O
0.00 TMS
N=C=N
2
400 MHz, CDCl3
4.02
3.91
1.95
1.99
2.00
f1 (ppm)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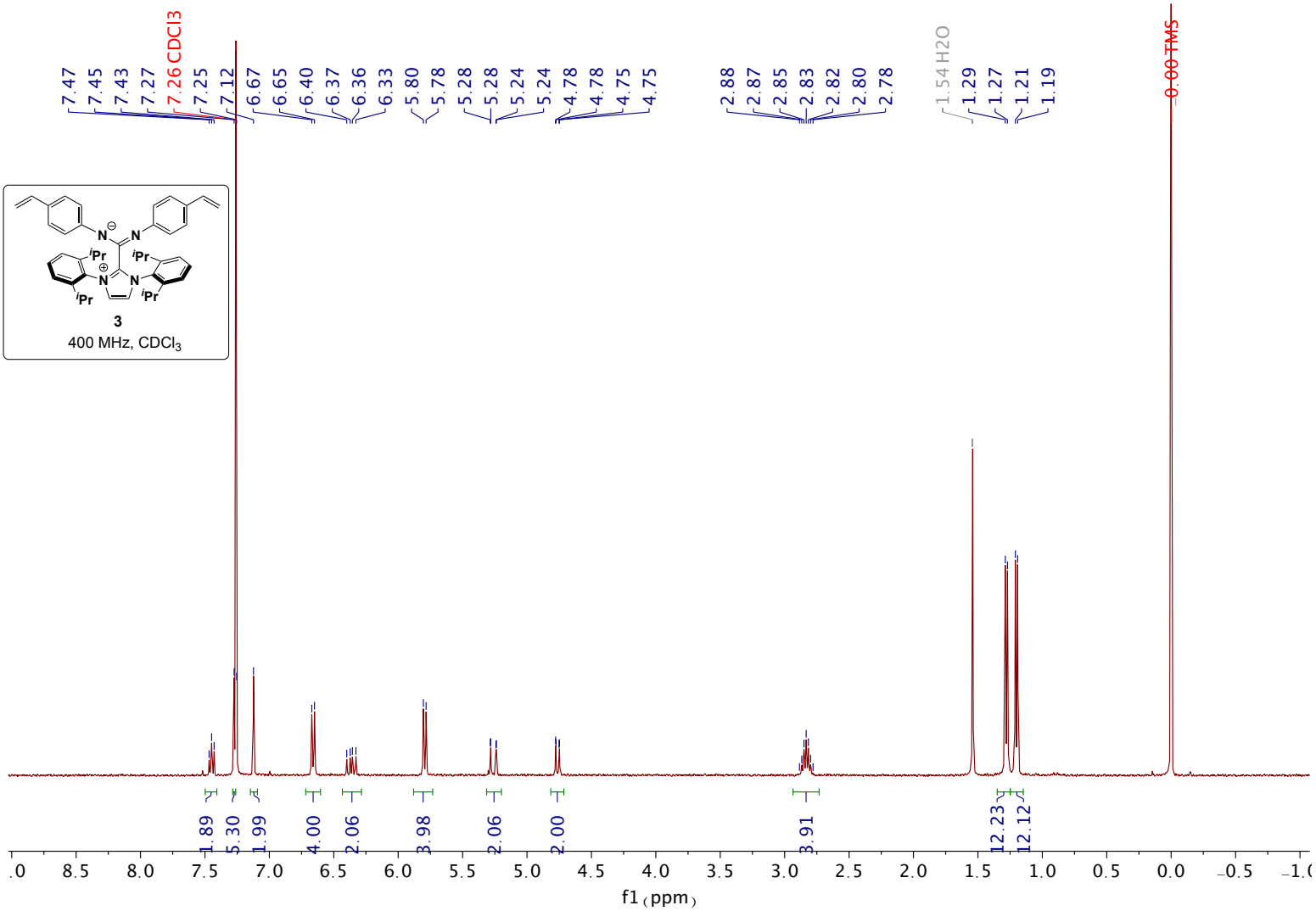
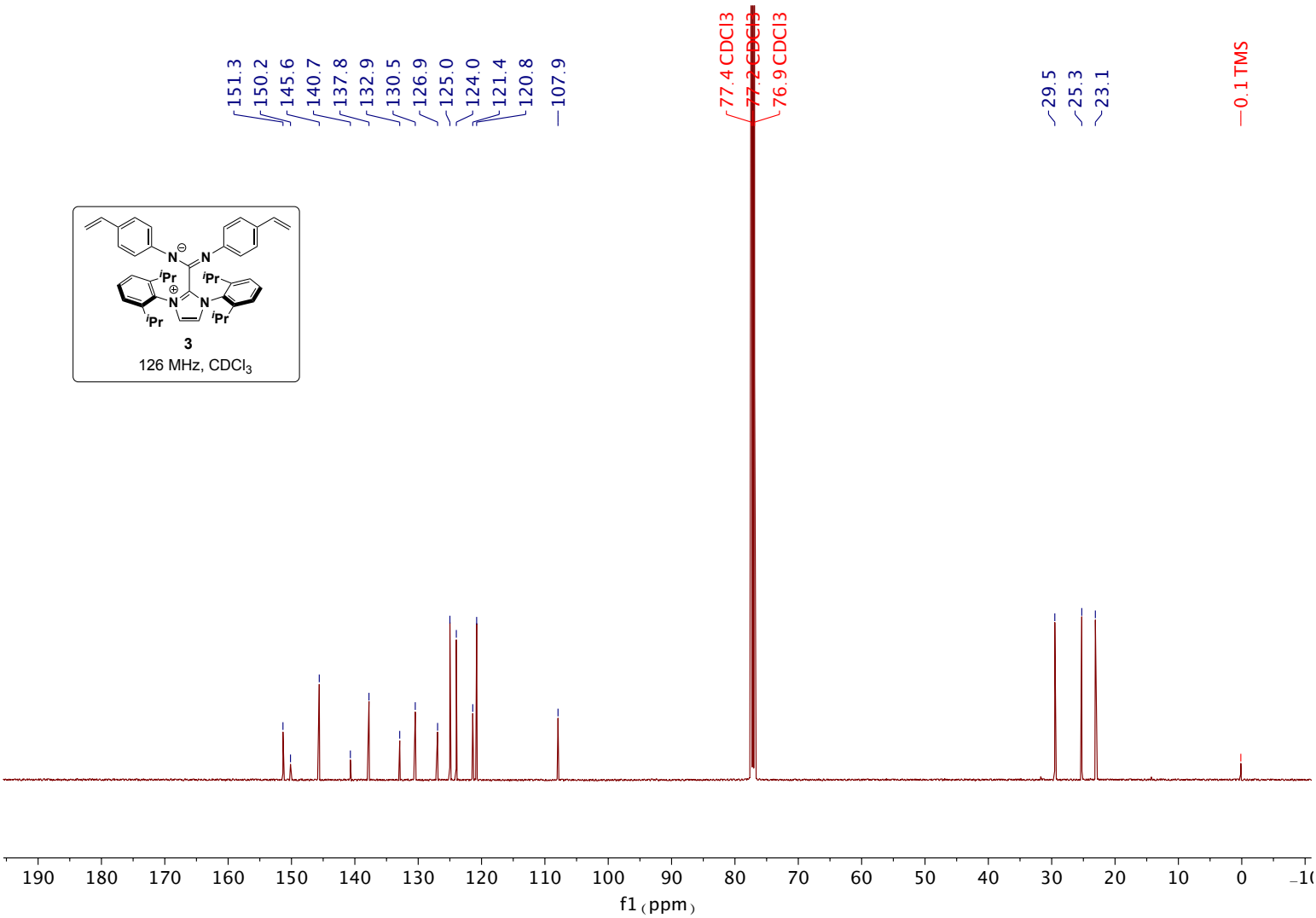
136.1
135.3
135.3
127.5
124.5
114.0
77.4 CDCl3
77.2 CDCl3
76.9 CDCl3
N=C=N
2
126 MHz, CDCl3
137.86
136.08
135.33
135.27
138.5
137.5
136.5
135.5
134.5
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)



3

400 MHz, $CDCl_3$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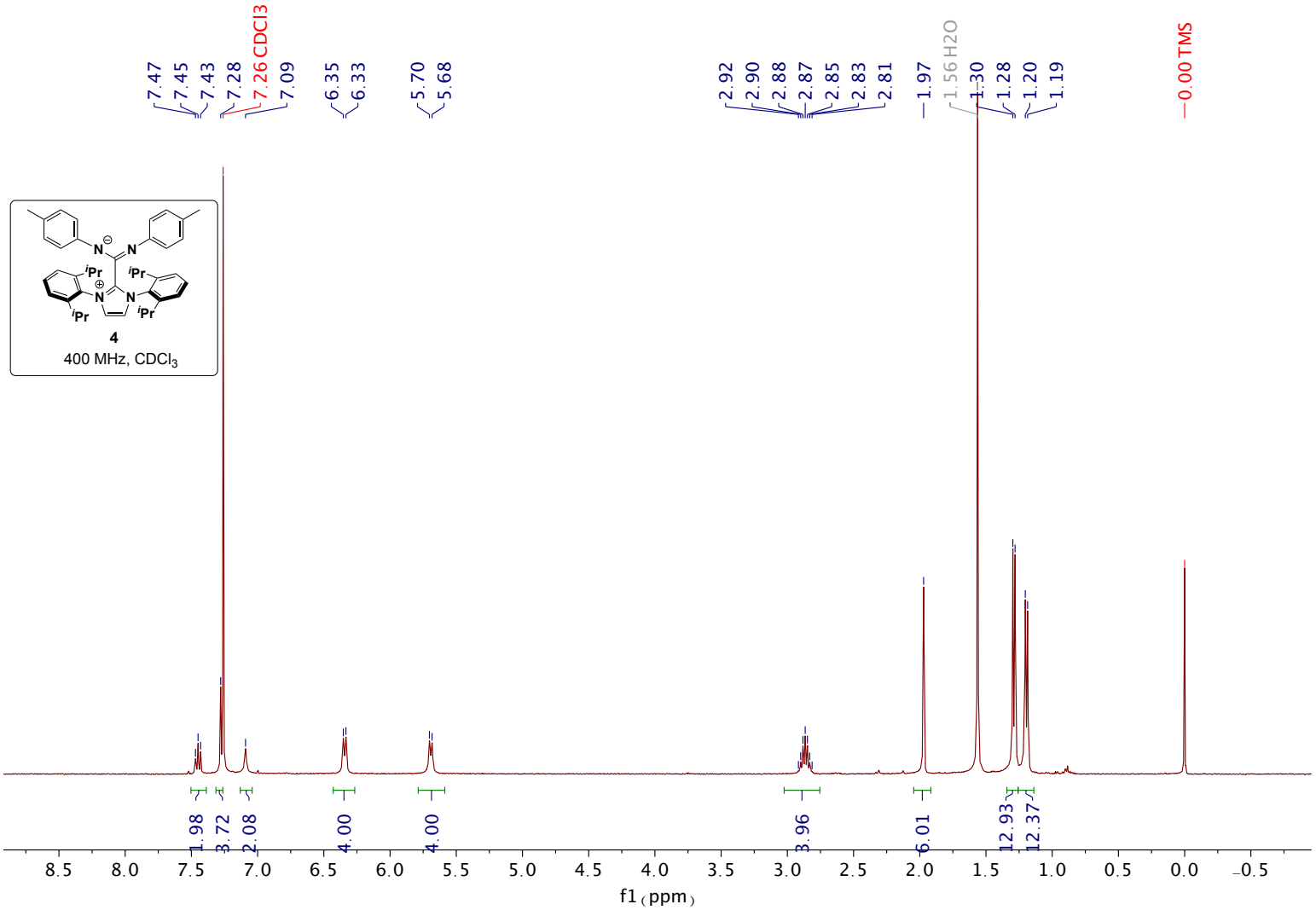
140.7
137.8
132.9
130.5
126.9
125.0
124.0
121.4
120.8
107.9
77.4 CDCl3
77.2 CDCl3
76.9 CDCl3
29.5
25.3
23.1
0.1 TMS
3
126 MHz, CDCl3
f1 (ppm)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7.45
7.43
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7.26 CDCl3
7.09
6.35
6.33
5.70
5.68
2.92
2.90
2.88
2.87
2.85
2.83
2.81
1.97
1.56 H2O
1.30
1.28
1.20
1.19
0.00 TMS
4
400 MHz, CDCl3
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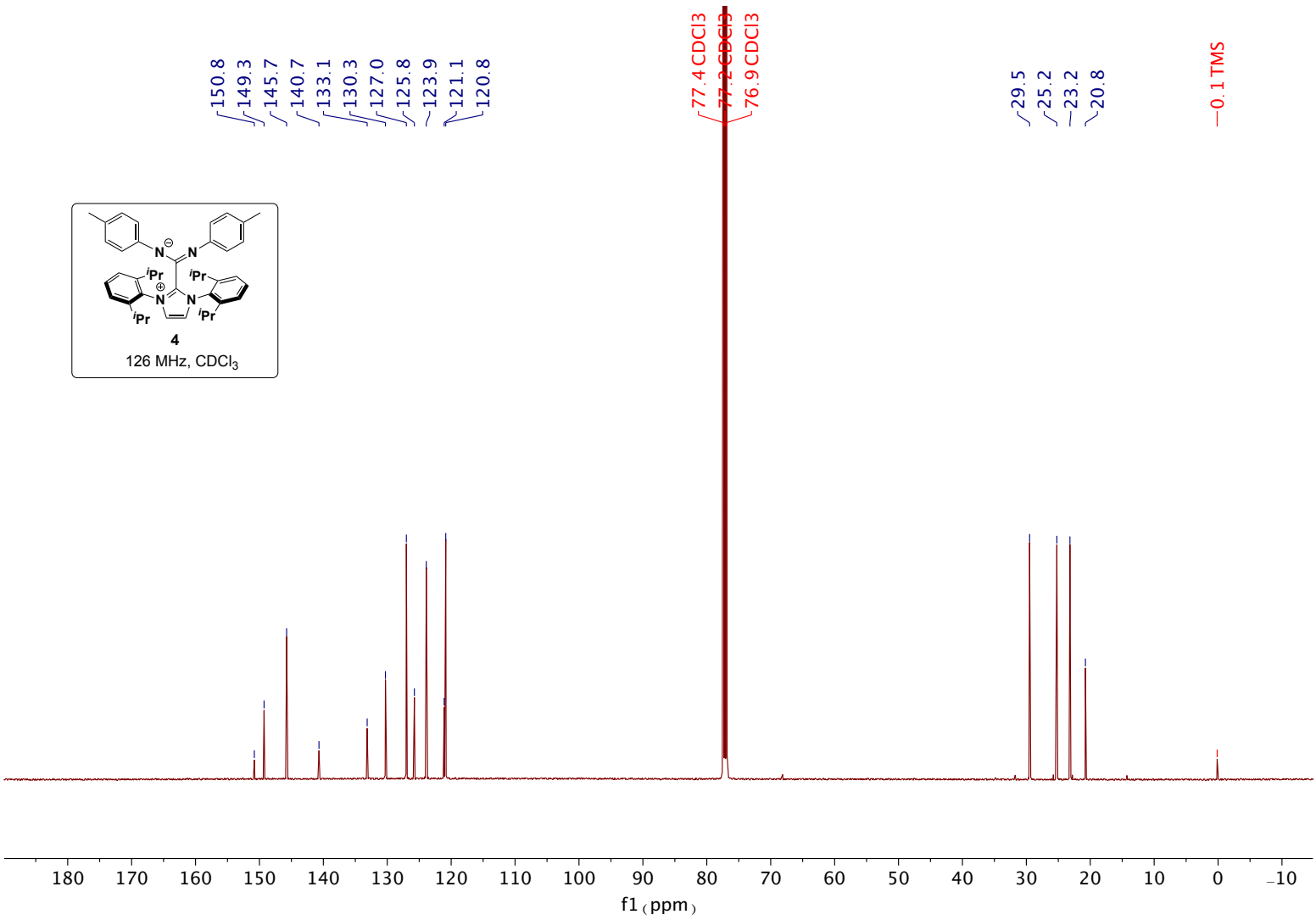
3.72
2.08
4.00
4.00
3.96
6.01
12.93
12.37
f1 (ppm)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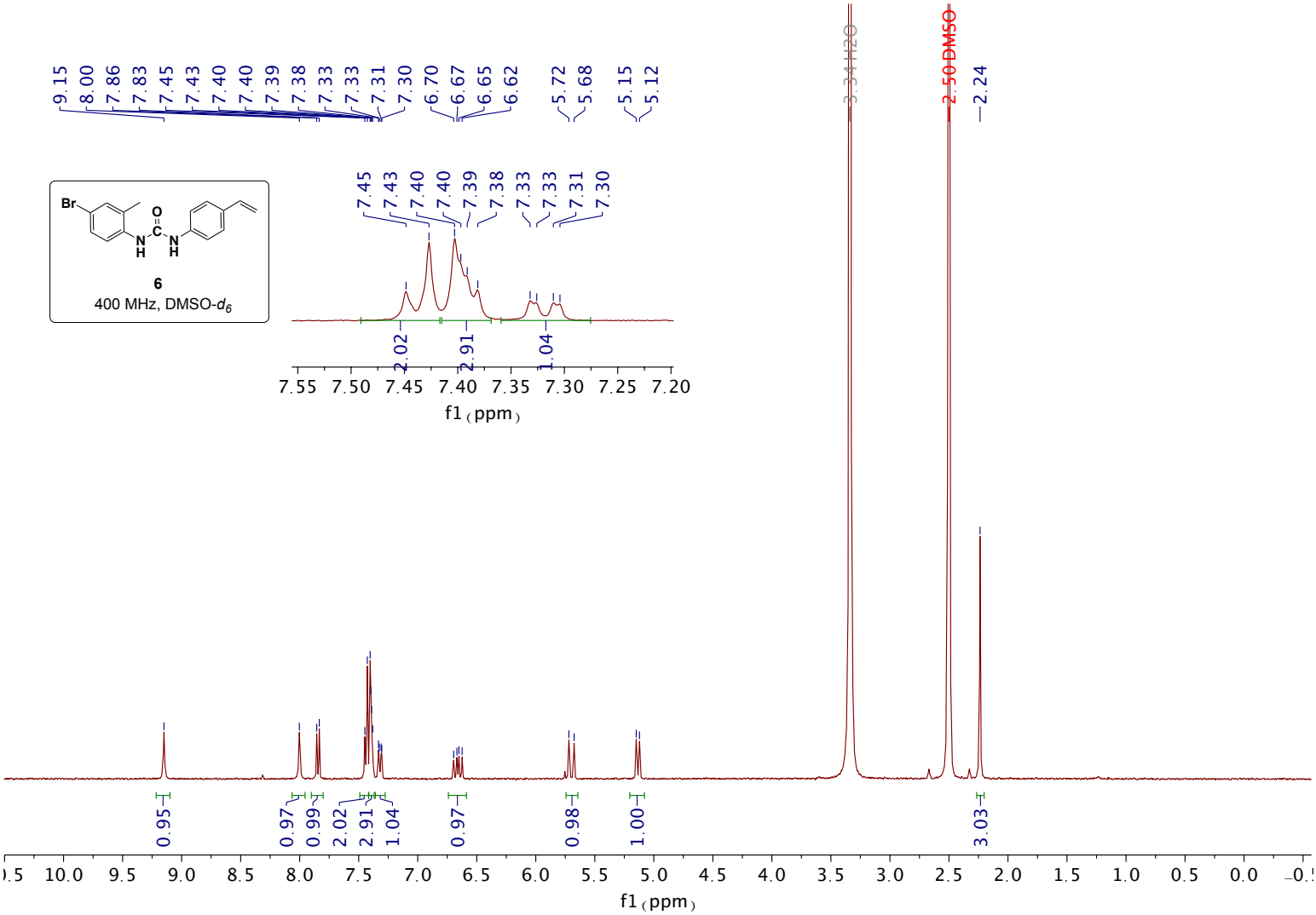
145.7
140.7
133.1
130.3
127.0
125.8
123.9
121.1
120.8
77.4 CDCl3
77.2 CDCl3
76.9 CDCl3
29.5
25.2
23.2
20.8
0.1 TMS
4
126 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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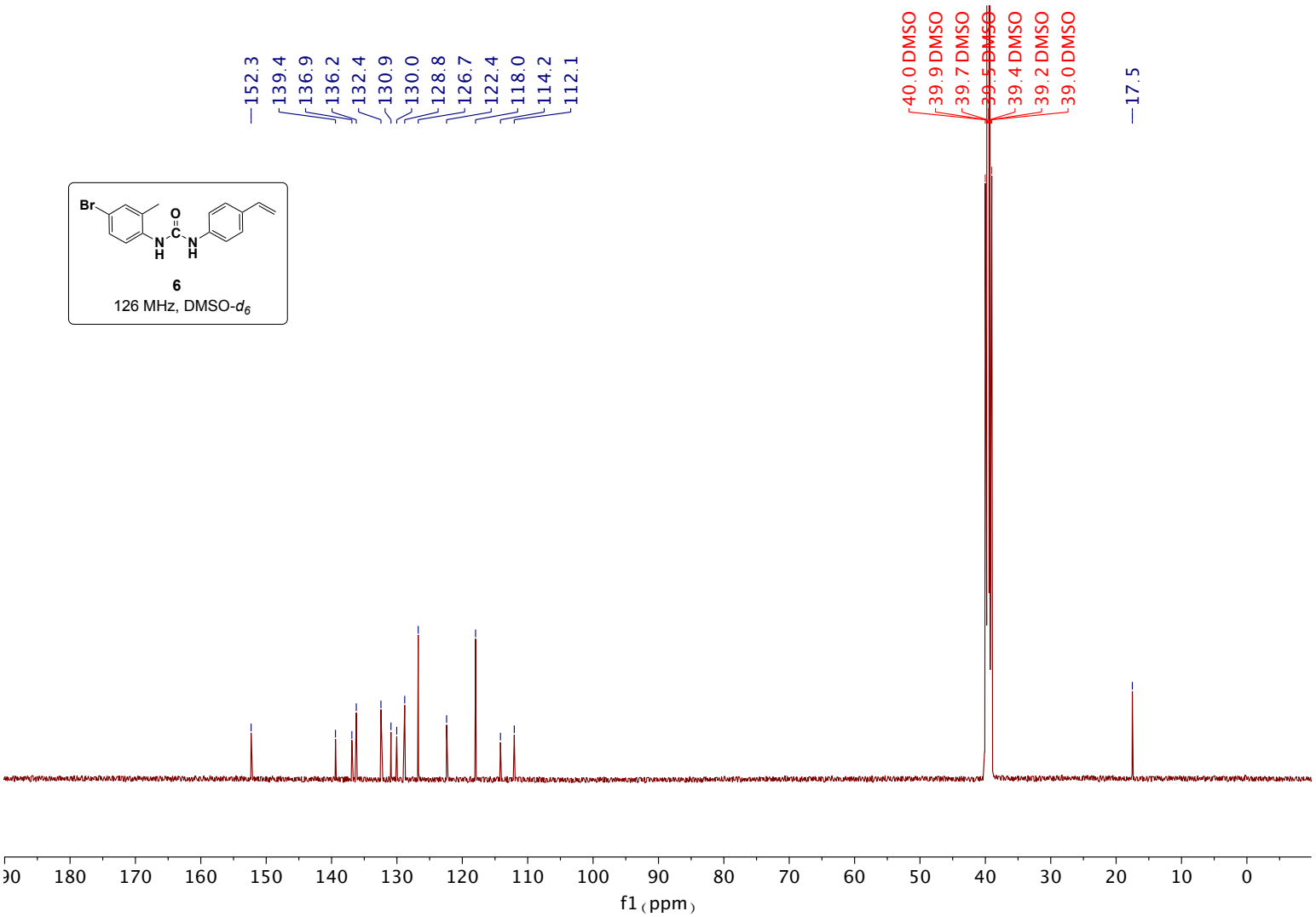
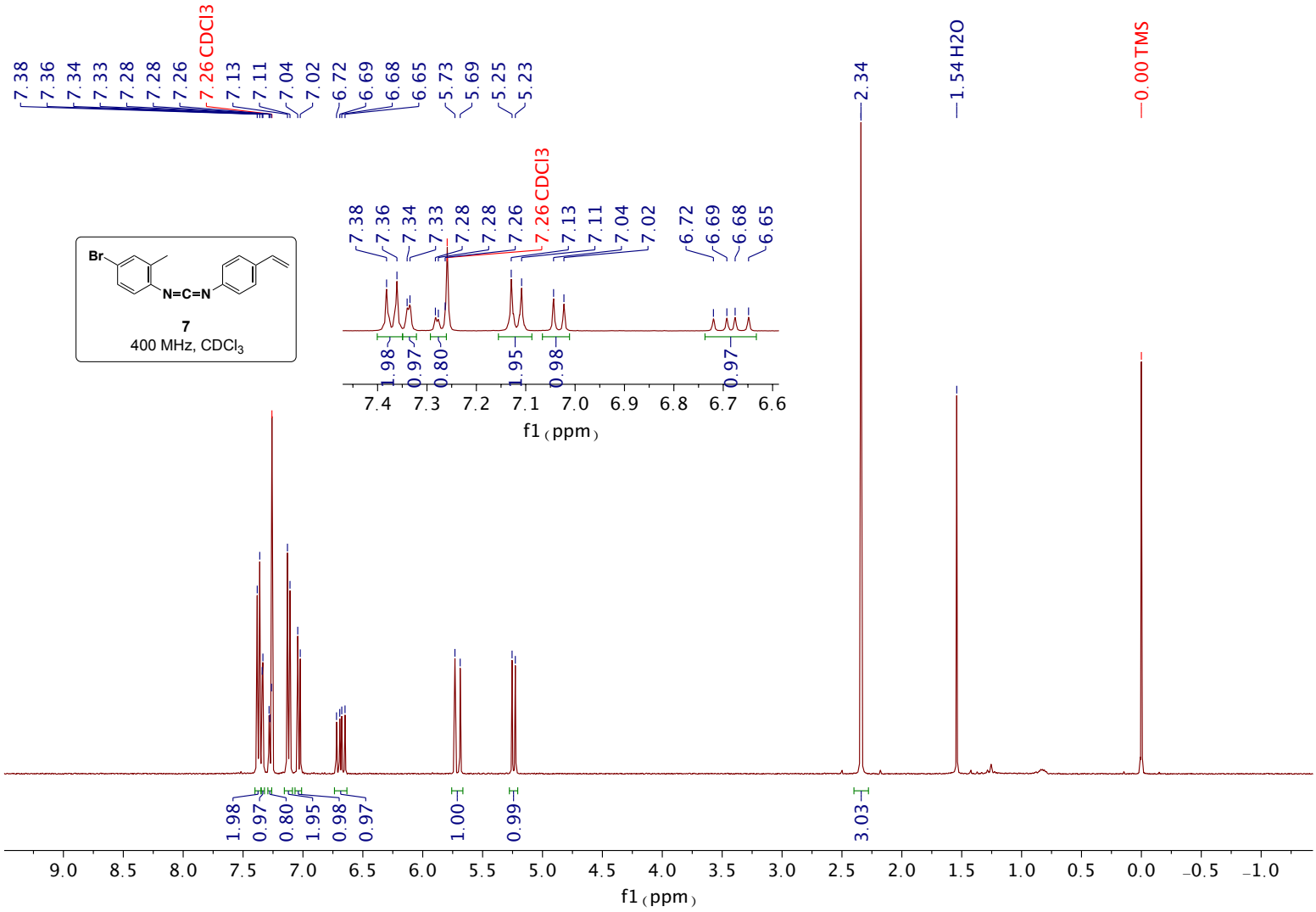
8.00
7.86
7.83
7.45
7.43
7.40
7.40
7.39
7.38
7.33
7.33
7.31
7.30
6.70
6.67
6.65
6.62
5.72
5.68
5.15
5.12
3.34 H2O
2.50 DMSO
2.24
Br
O
N
H
C
N
H
6
400 MHz, DMSO-d6
2.02
2.91
1.04
f1 (ppm)
0.95
0.97
0.99
2.02
2.91
1.04
0.97
0.98
1.00
3.03
f1 (ppm)


152.3
139.4
136.9
136.2
132.4
130.9
130.0
128.8
126.7
122.4
118.0
114.2
112.1
40.0 DMSO
39.9 DMSO
39.7 DMSO
39.5 DMSO
39.4 DMSO
39.2 DMSO
39.0 DMSO
17.5
Br
O
N
H
C
N
H
6
126 MHz, DMSO-d_6
f1 (ppm)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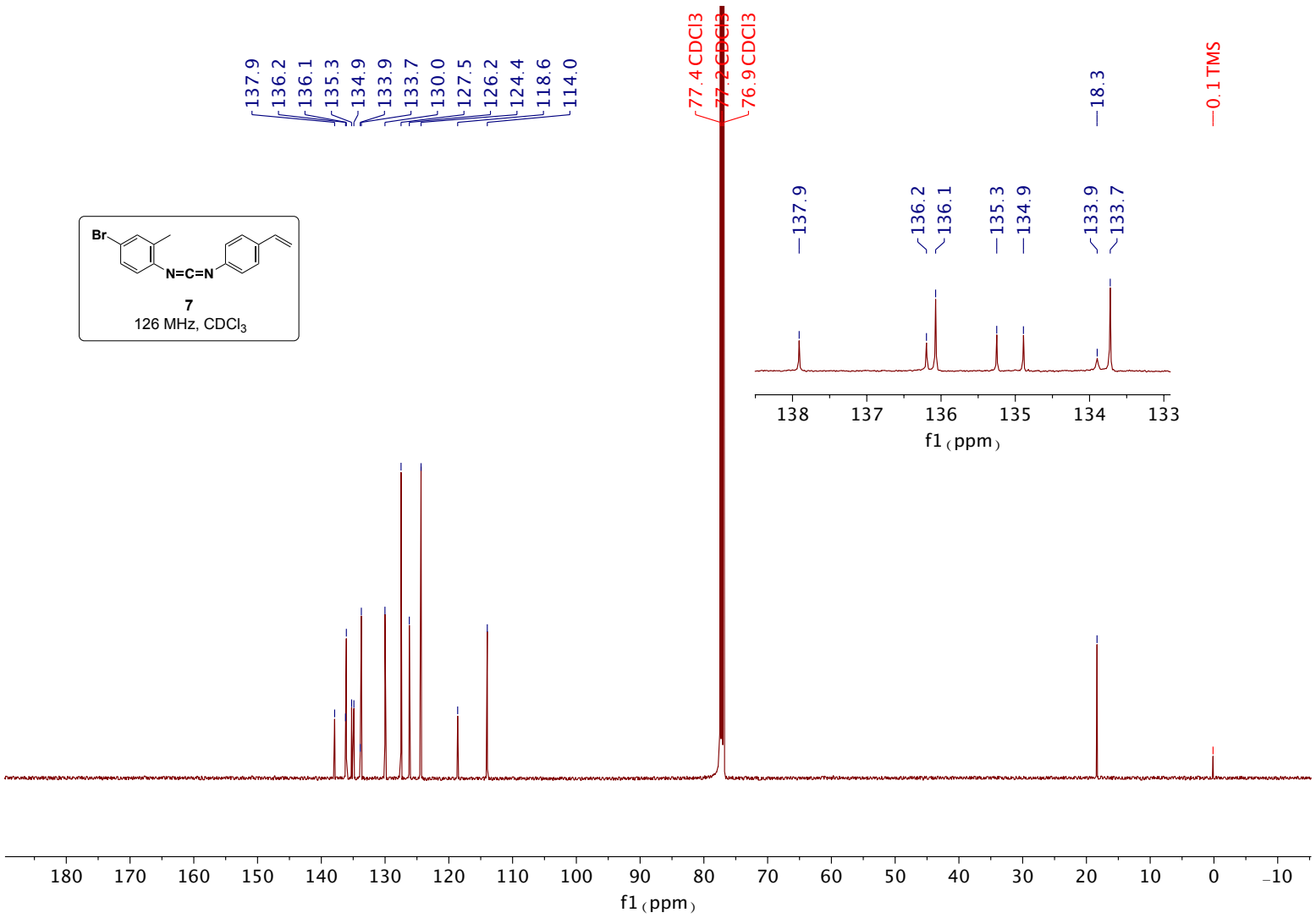
7.36
7.34
7.33
7.28
7.28
7.26
7.26 CDCl3
7.13
7.11
7.04
7.02
6.72
6.69
6.68
6.65
5.73
5.69
5.25
5.23
2.34
1.54 H2O
0.00 TMS
Br
N=C=N
7
400 MHz, CDCl3
1.98
0.97
0.80
1.95
0.98
0.97
1.00
0.99
3.03
f1 (ppm)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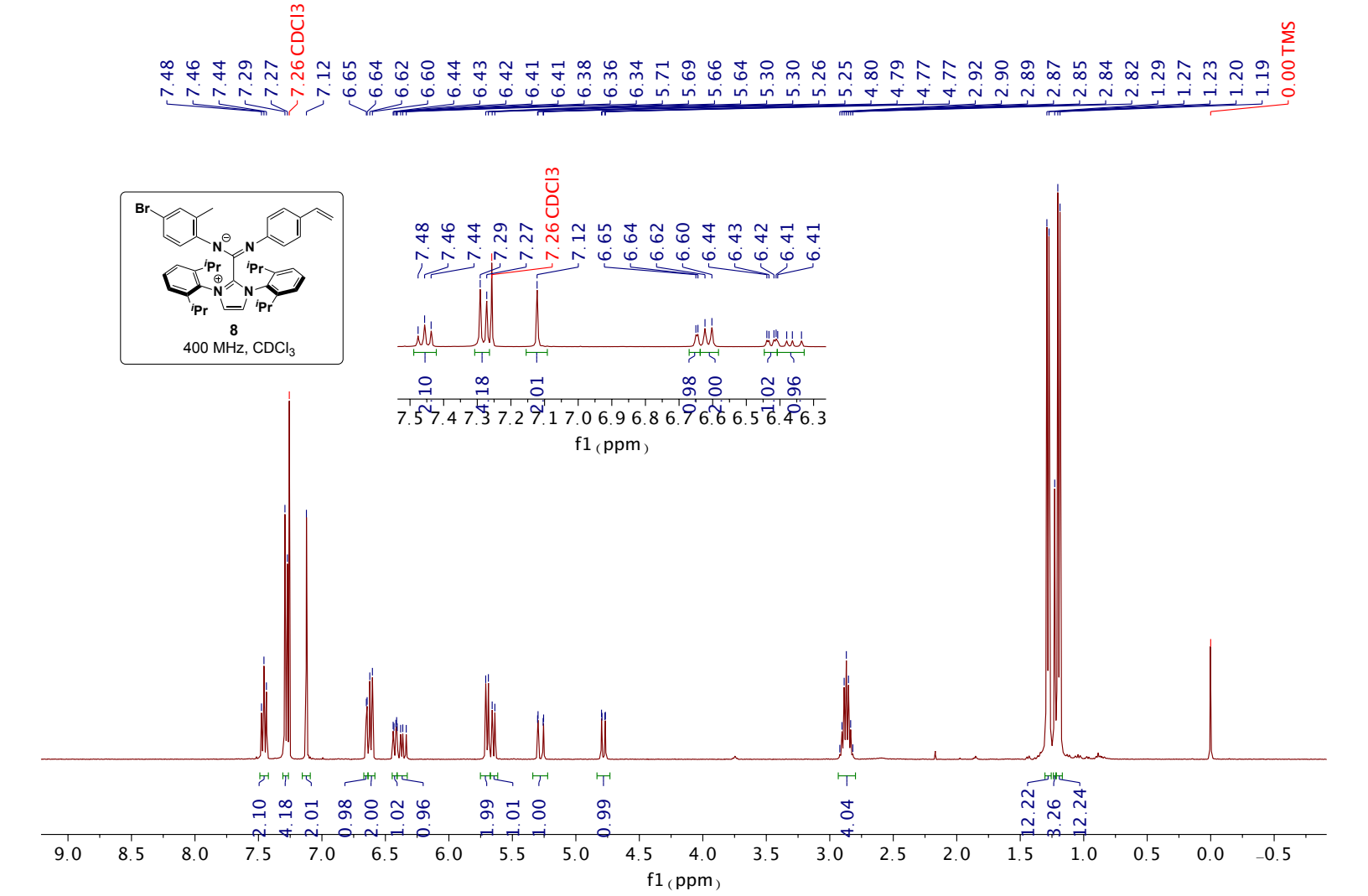
136.2
136.1
135.3
134.9
133.9
133.7
130.0
127.5
126.2
124.4
118.6
114.0
77.4 CDCl3
77.2 CDCl3
76.9 CDCl3
18.3
0.1 TMS
Br
N=C=N
7
126 MHz, CDCl3
f1 (ppm)
f1 (ppm)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Br
8
400 MHz, CDCl3
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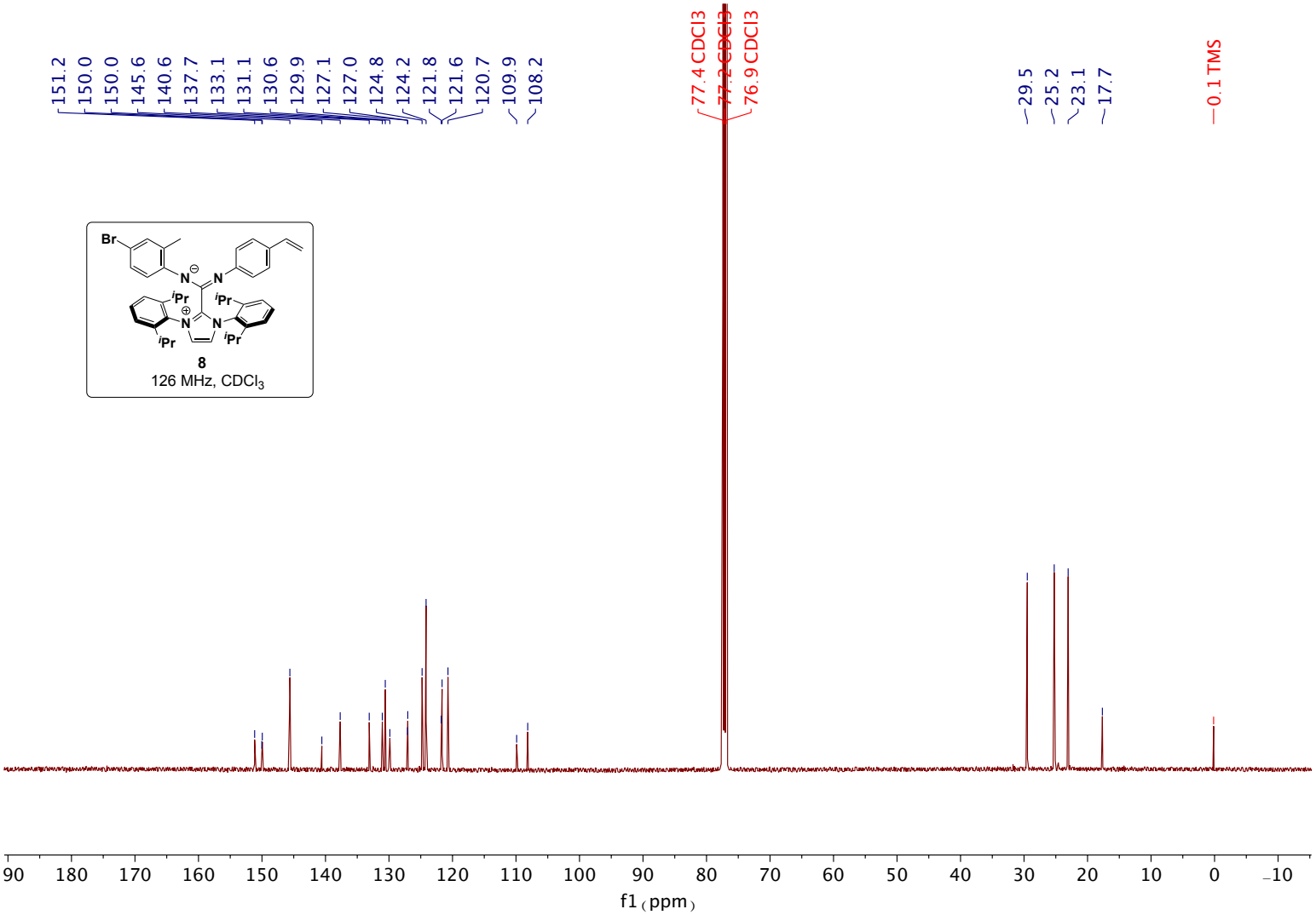
f1 (ppm)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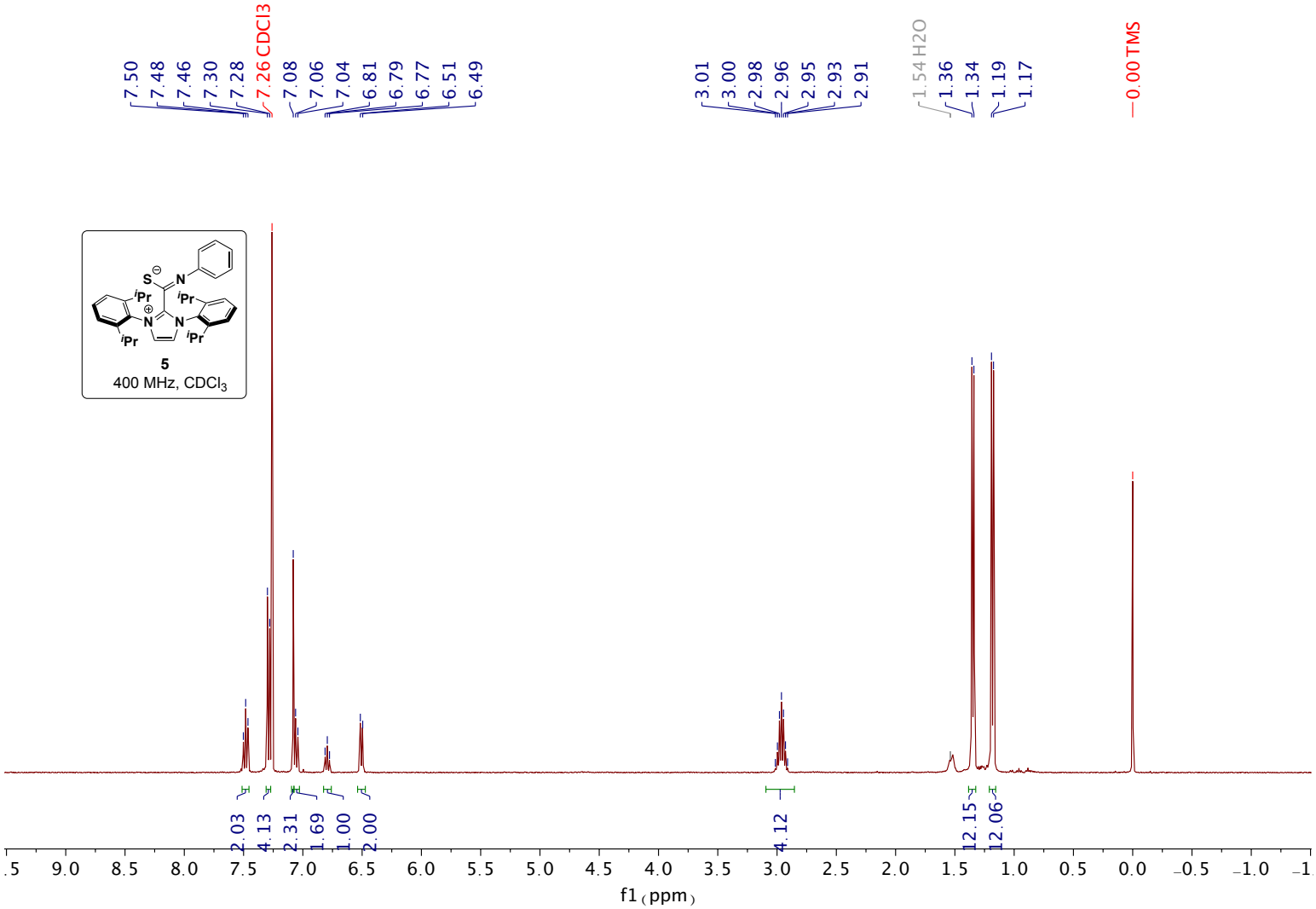
150.0
150.0
145.6
140.6
137.7
133.1
131.1
130.6
129.9
127.1
127.0
124.8
124.2
121.8
121.6
120.7
109.9
108.2
77.4 CDCl3
77.2 CDCl3
76.9 CDCl3
29.5
25.2
23.1
17.7
0.1 TMS
Br
N
N
iPr
iPr
N
N
iPr
iPr
8
126 MHz, CDCl3
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.28
7.26 CDCl3
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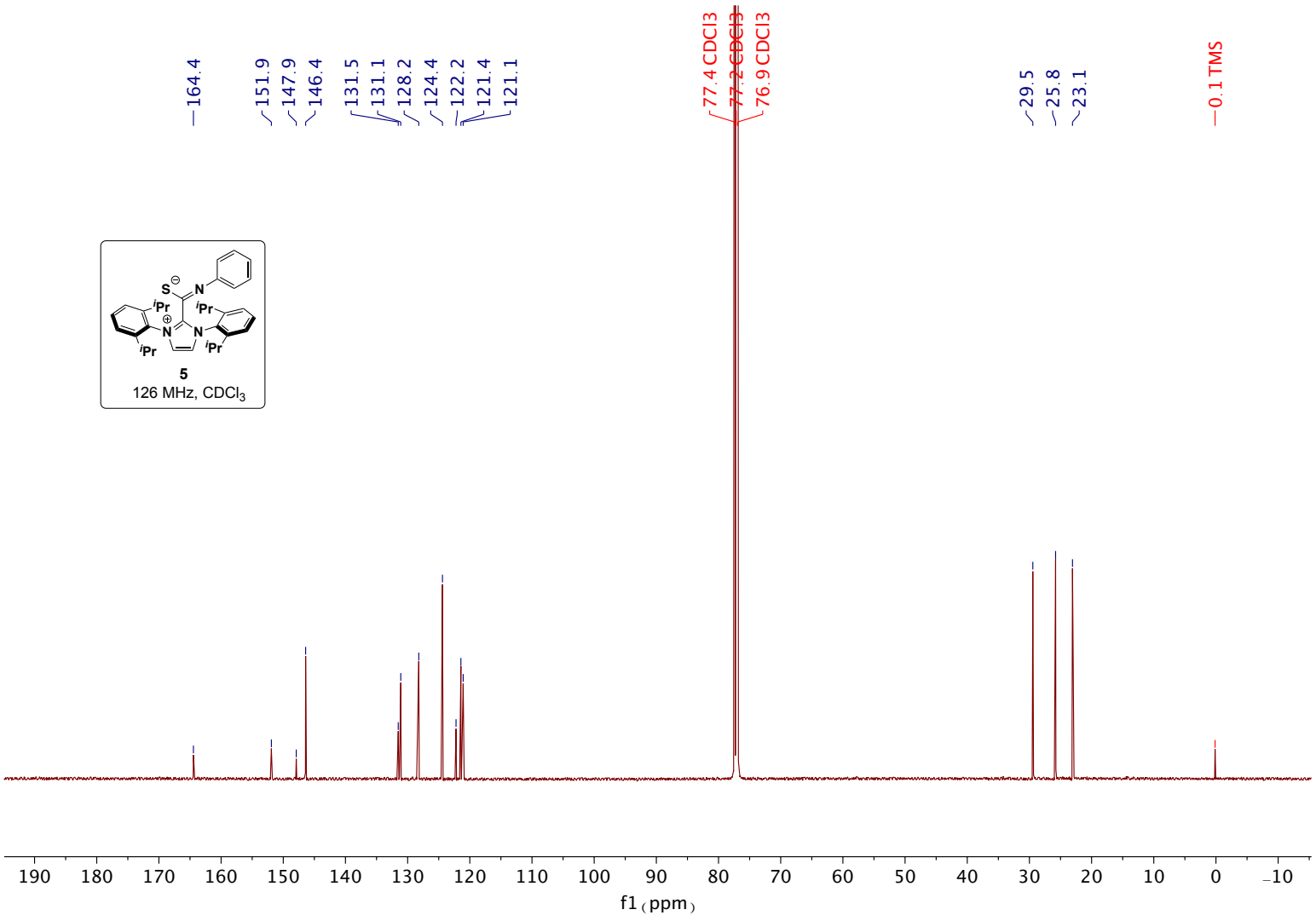
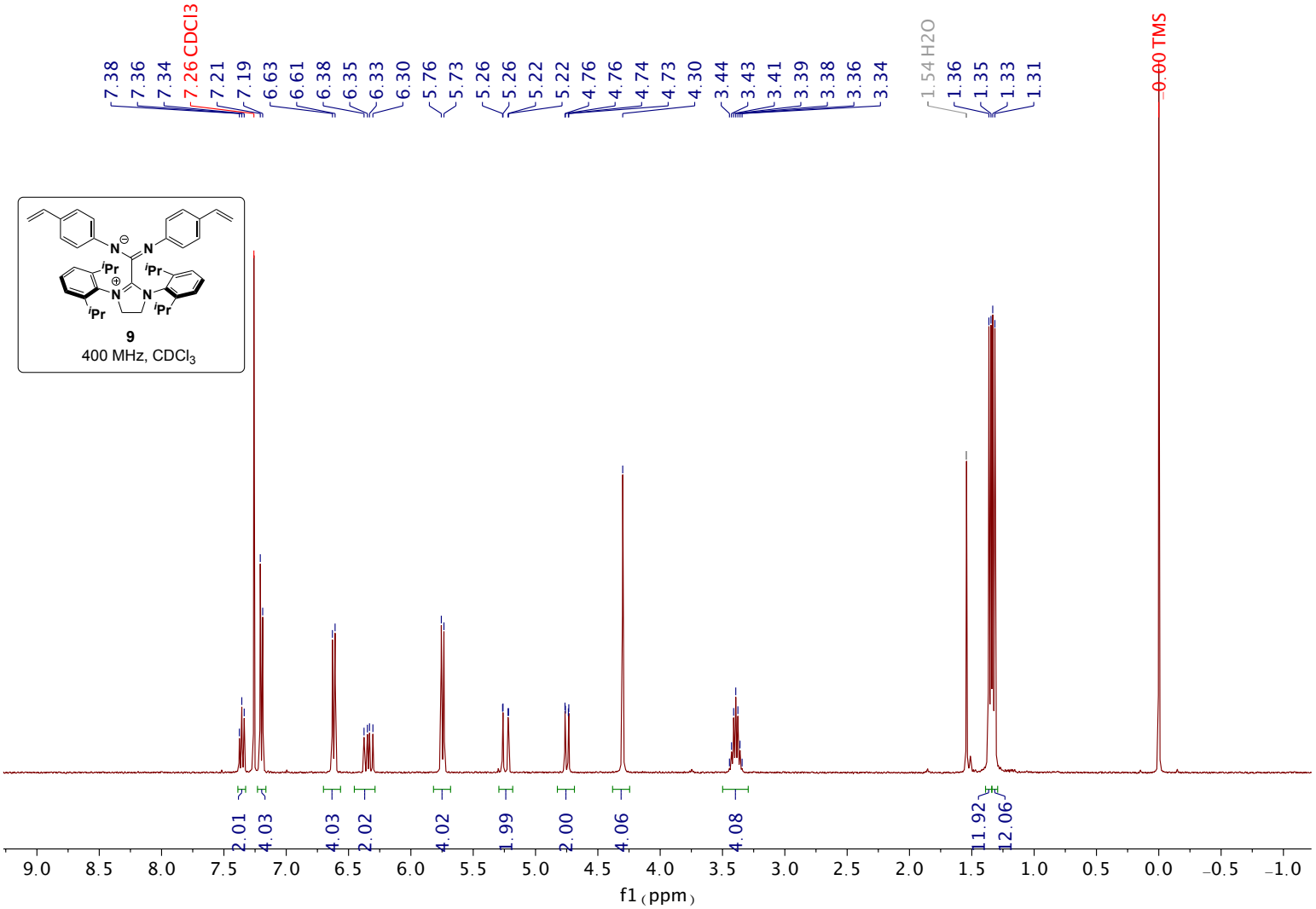
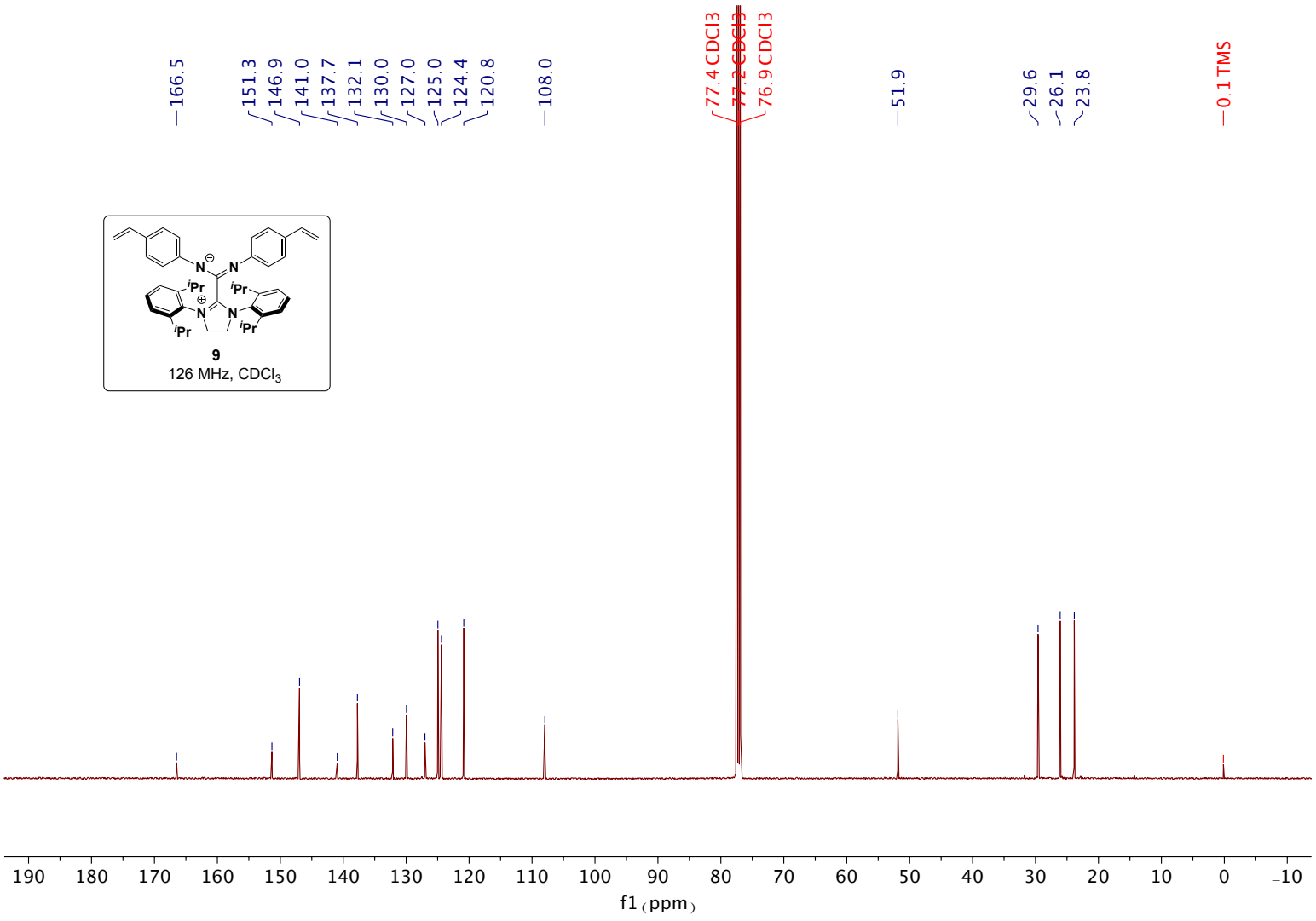
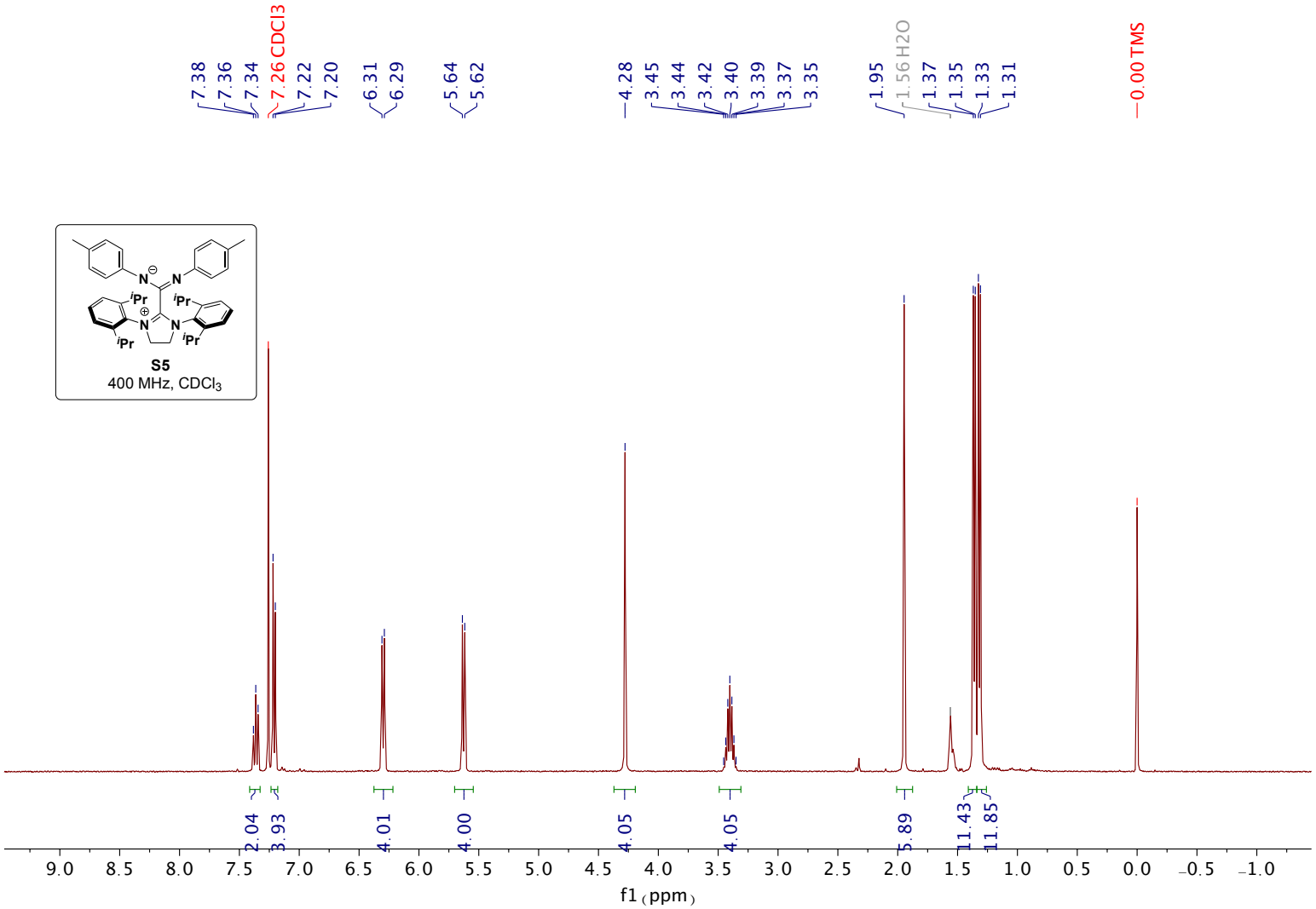
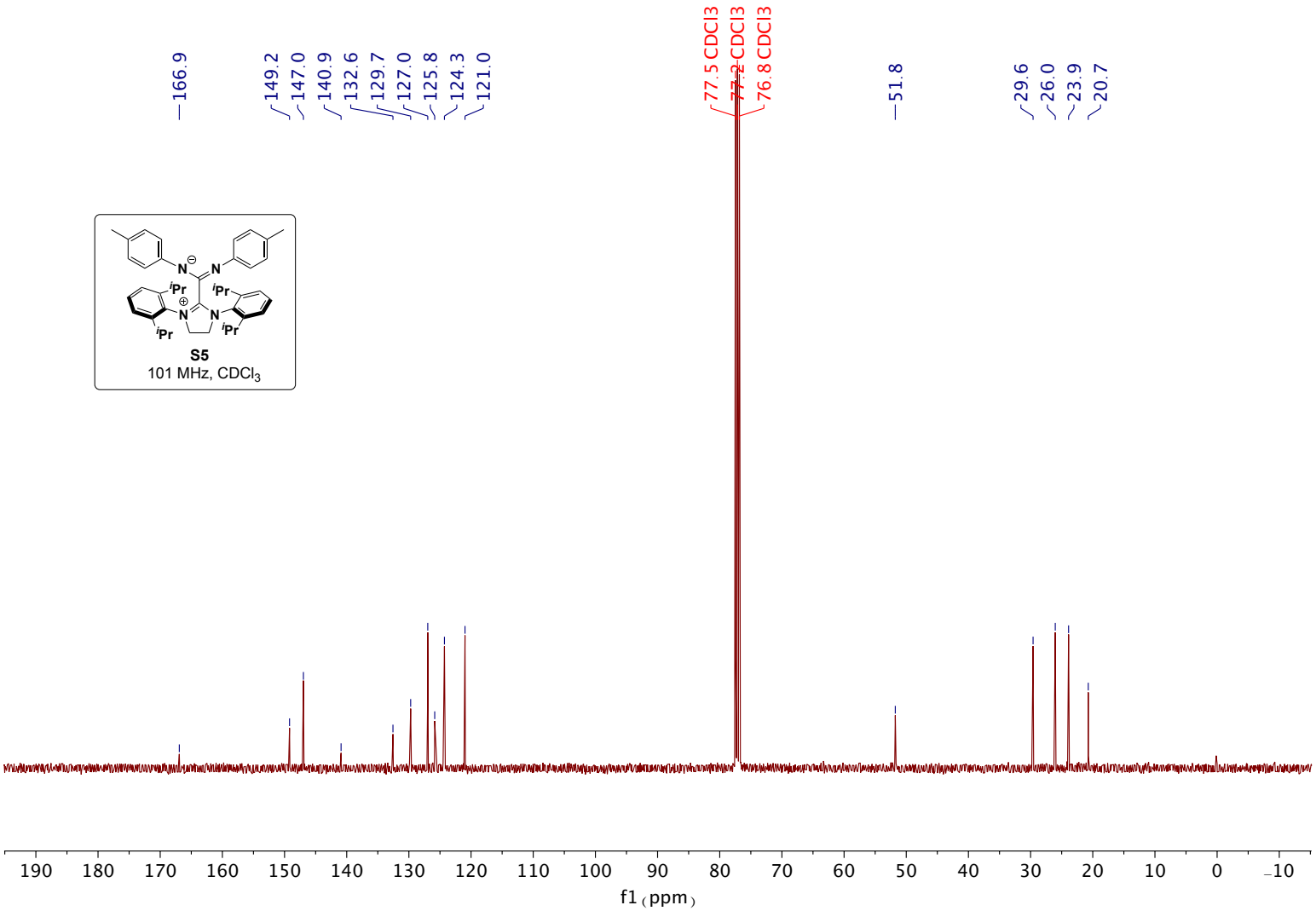
7.06
7.04
6.81
6.79
6.77
6.51
6.49
3.01
3.00
2.98
2.96
2.95
2.93
2.91
1.54 H2O
1.36
1.34
1.19
1.17
0.00 TMS
5
400 MHz, CDCl3
2.03
4.13
2.31
1.69
1.00
2.00
4.12
12.15
12.06
f1 (ppm)

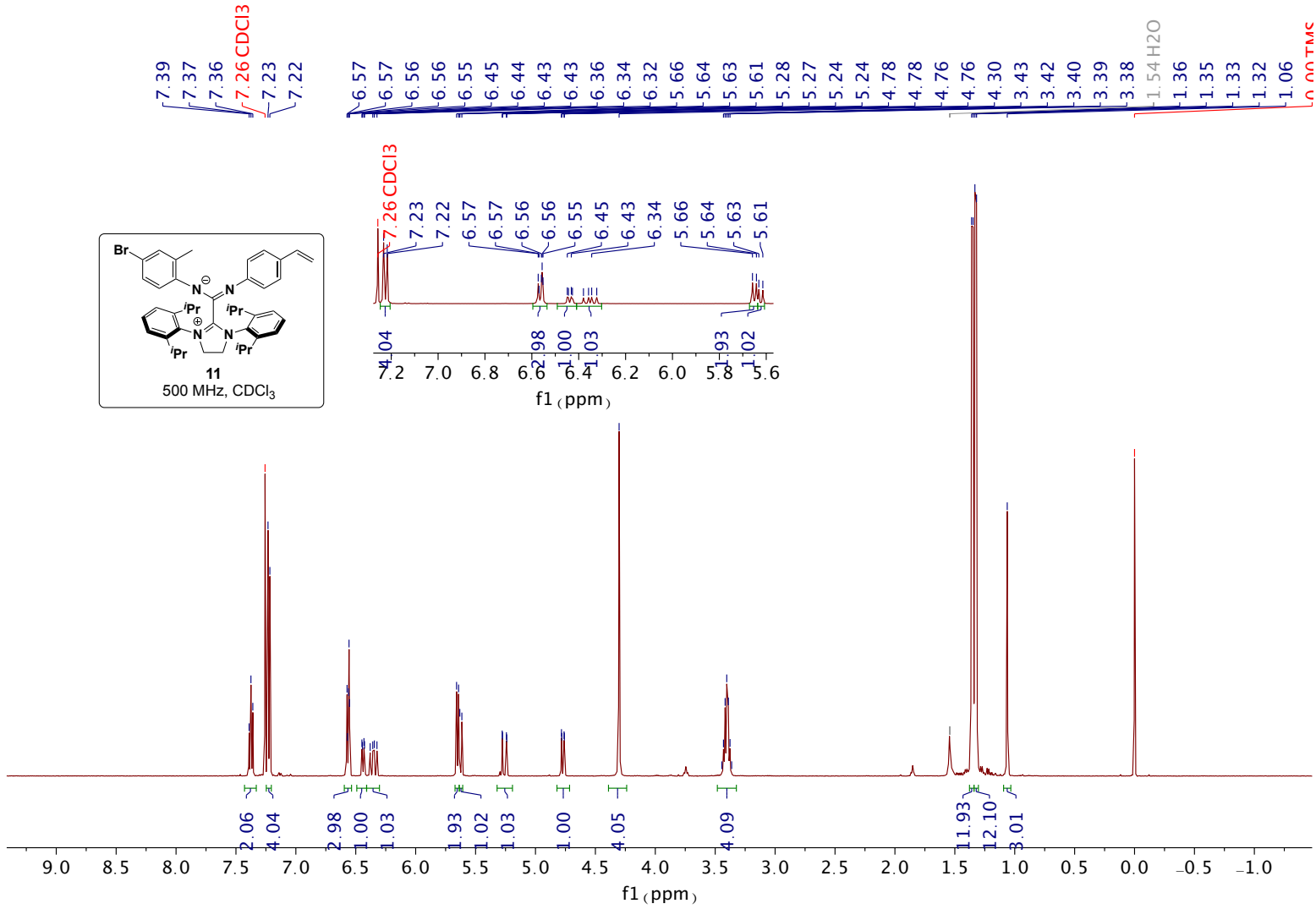

164.4
151.9
147.9
146.4
131.5
131.1
128.2
124.4
122.2
121.4
121.1
77.4 CDCl3
77.2 CDCl3
76.9 CDCl3
29.5
25.8
23.1
0.1 TMS
5
126 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

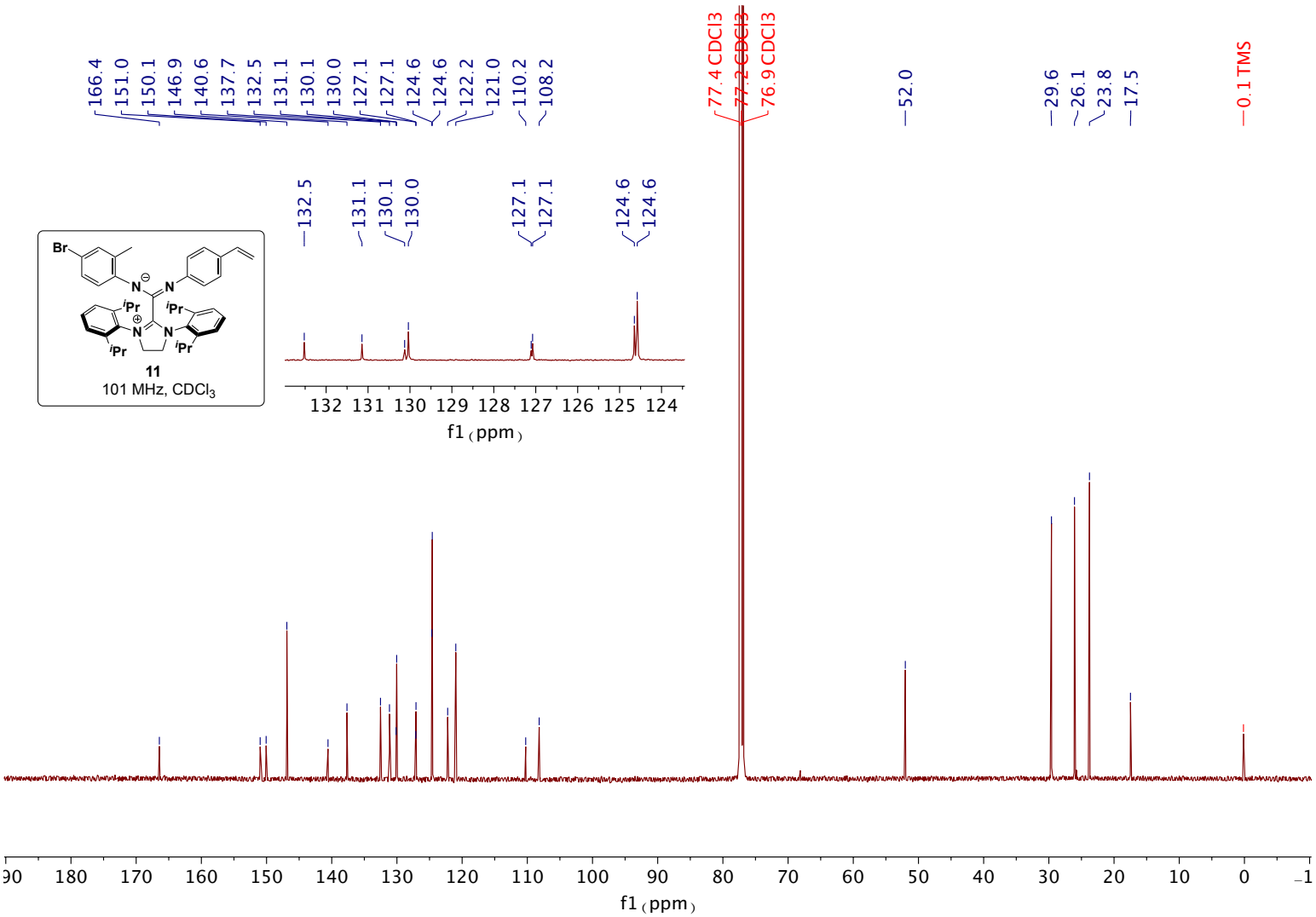

7.38
7.36
7.34
7.26 CDCl3
7.21
7.19
6.63
6.61
6.38
6.35
6.33
6.30
5.76
5.73
5.26
5.26
5.22
5.22
4.76
4.76
4.74
4.73
4.30
3.44
3.43
3.41
3.39
3.38
3.36
3.34
1.54 H2O
1.36
1.35
1.33
1.31
0.00 TMS
9
400 MHz, CDCl3
2.01
4.03
4.03
2.02
4.02
1.99
2.00
4.06
4.08
11.92
12.06
f1 (ppm)

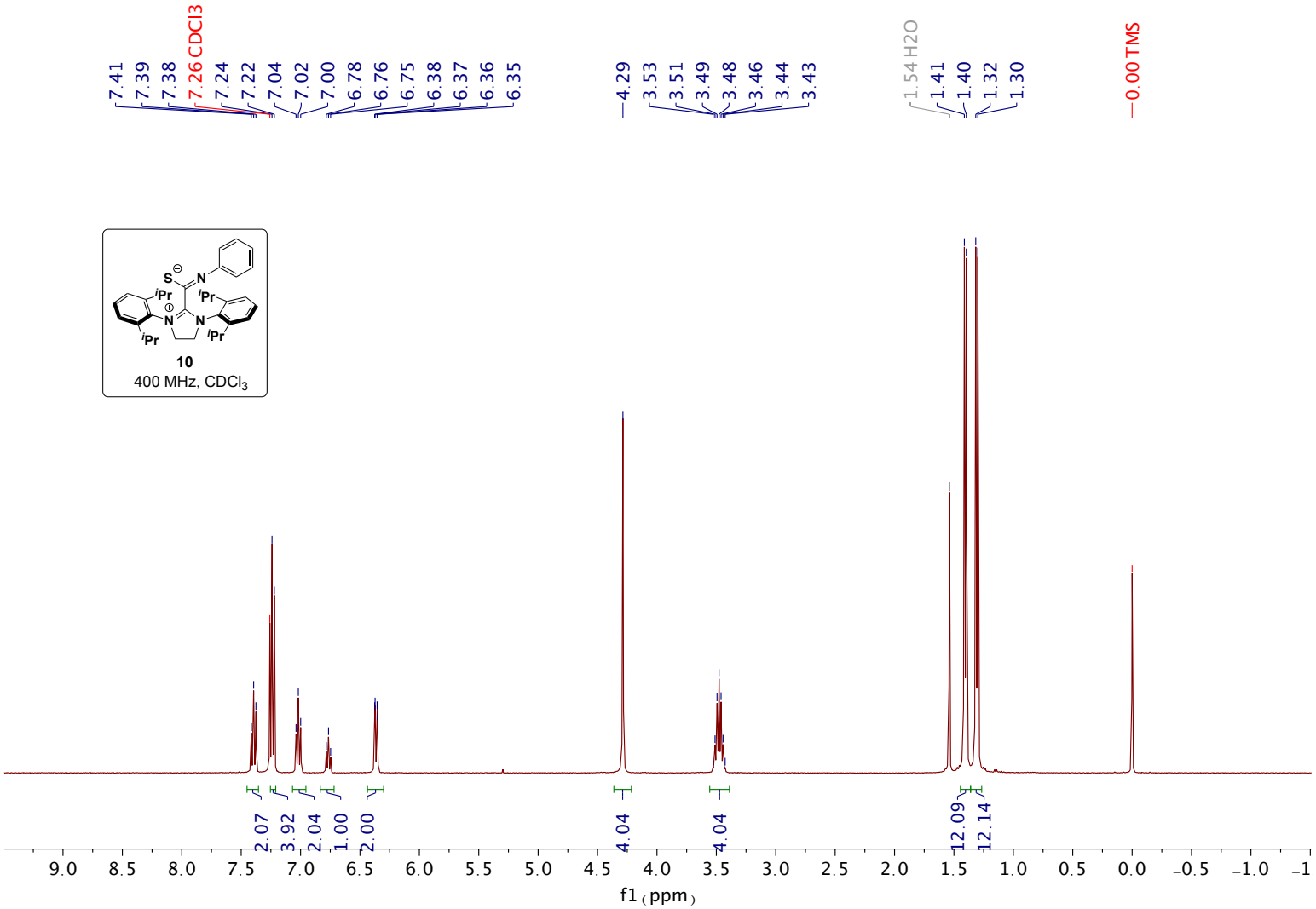

166.5
151.3
146.9
141.0
137.7
132.1
130.0
127.0
125.0
124.4
120.8
108.0
77.4 CDCl3
77.2 CDCl3
76.9 CDCl3
51.9
29.6
26.1
23.8
0.1 TMS
9
126 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

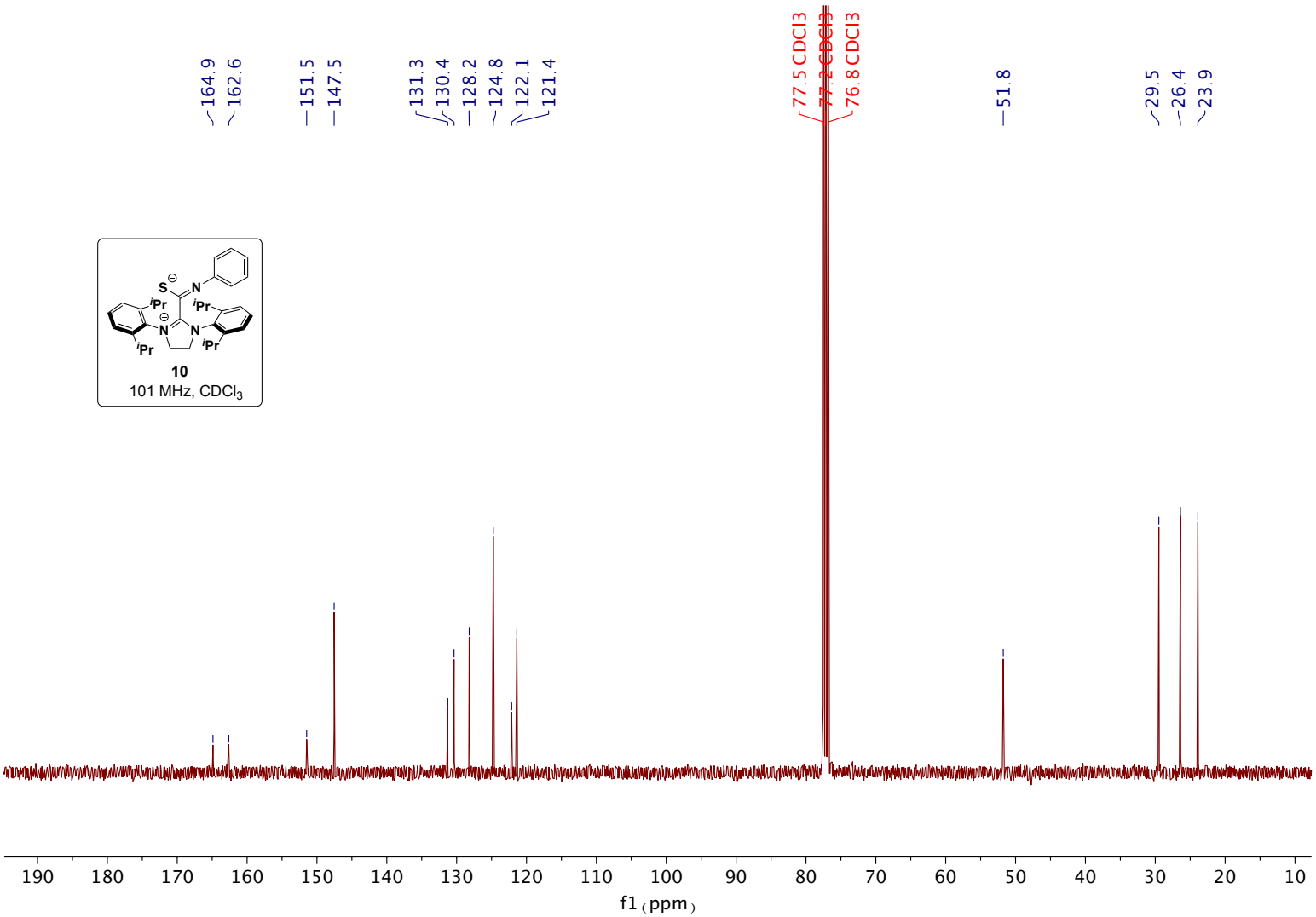

7.38
7.36
7.34
7.26 CDCl3
7.22
7.20
6.31
6.29
5.64
5.62
4.28
3.45
3.44
3.42
3.40
3.39
3.37
3.35
1.95
1.56 H2O
1.37
1.35
1.33
1.31
0.00 TMS
S5
400 MHz, CDCl3
2.04
3.93
4.01
4.00
4.05
4.05
5.89
11.43
11.85
f1 (ppm)


166.9
149.2
147.0
140.9
132.6
129.7
127.0
125.8
124.3
121.0
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
51.8
29.6
26.0
23.9
20.7
S5
101 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.39
7.37
7.36
7.26 CDCl3
7.23
7.22
6.57
6.57
6.56
6.56
6.55
6.45
6.44
6.43
6.43
6.36
6.34
6.32
5.66
5.64
5.63
5.61
5.28
5.27
5.24
5.24
4.78
4.78
4.76
4.76
4.30
3.43
3.42
3.40
3.39
3.38
1.54 H2O
1.36
1.35
1.33
1.32
1.06
0.00 TMS
Br
N
N
iPr
iPr
iPr
N
N
iPr
11
500 MHz, CDCl3
2.06
4.04
2.98
1.00
1.03
1.93
1.02
1.03
1.00
4.05
4.09
11.93
12.10
3.01
f1 (ppm)


166.4
151.0
150.1
146.9
140.6
137.7
132.5
131.1
130.1
130.0
127.1
127.1
124.6
124.6
122.2
121.0
110.2
108.2
77.4 CDCl3
77.2 CDCl3
76.9 CDCl3
52.0
29.6
26.1
23.8
17.5
0.1 TMS
132.5
131.1
130.1
130.0
127.1
127.1
124.6
124.6
Br
iPr
iPr
iPr
iPr
11
101 MHz, CDCl3
132 131 130 129 128 127 126 125 124
f1 (ppm)
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


7.41
7.39
7.38
7.26 CDCl3
7.24
7.22
7.04
7.02
7.00
6.78
6.76
6.75
6.38
6.37
6.36
6.35
4.29
3.53
3.51
3.49
3.48
3.46
3.44
3.43
1.54 H2O
1.41
1.40
1.32
1.30
0.00 TMS
10
400 MHz, CDCl3
2.07
3.92
2.04
1.00
2.00
4.04
4.04
12.09
12.14
f1 (ppm)


164.9
162.6
151.5
147.5
131.3
130.4
128.2
124.8
122.1
121.4
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
51.8
29.5
26.4
23.9
10
101 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)