

Supporting Information

Synthesis, Structure–Activity Relationship Studies, and ADMET Properties of 3-Aminocyclohex-2-en-1-ones as Chemokine Receptor 2 (CXCR2) Antagonists

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Supplementary Table 1. Percentage inhibition of CXCR4 at 10 μ M of compounds **16-56**

Cpd	^a %Inhibition of CXCR4 at 10 μ M	Cpd	^a %Inhibition of CXCR4 at 10 μ M
16	37	37	-10
17	45	38	-20
18	23	39	-9
19	15	40	35
20	25	41	35
21	-4	42	20
22	16	43	10
23	21	44	11
24	16	45	11
25	11	46	4
26	2	47	22
27	6	48	11
28	36	49	18
29	-5	50	-5
30	20	51	1
31	6.5	52	7
32	1	53	-2
33	4	54	-2
34	-4	55	40
35	13	56	21
36	-9		

^aCXCR4 inhibition was determined using the CXCR4 Tango assay.

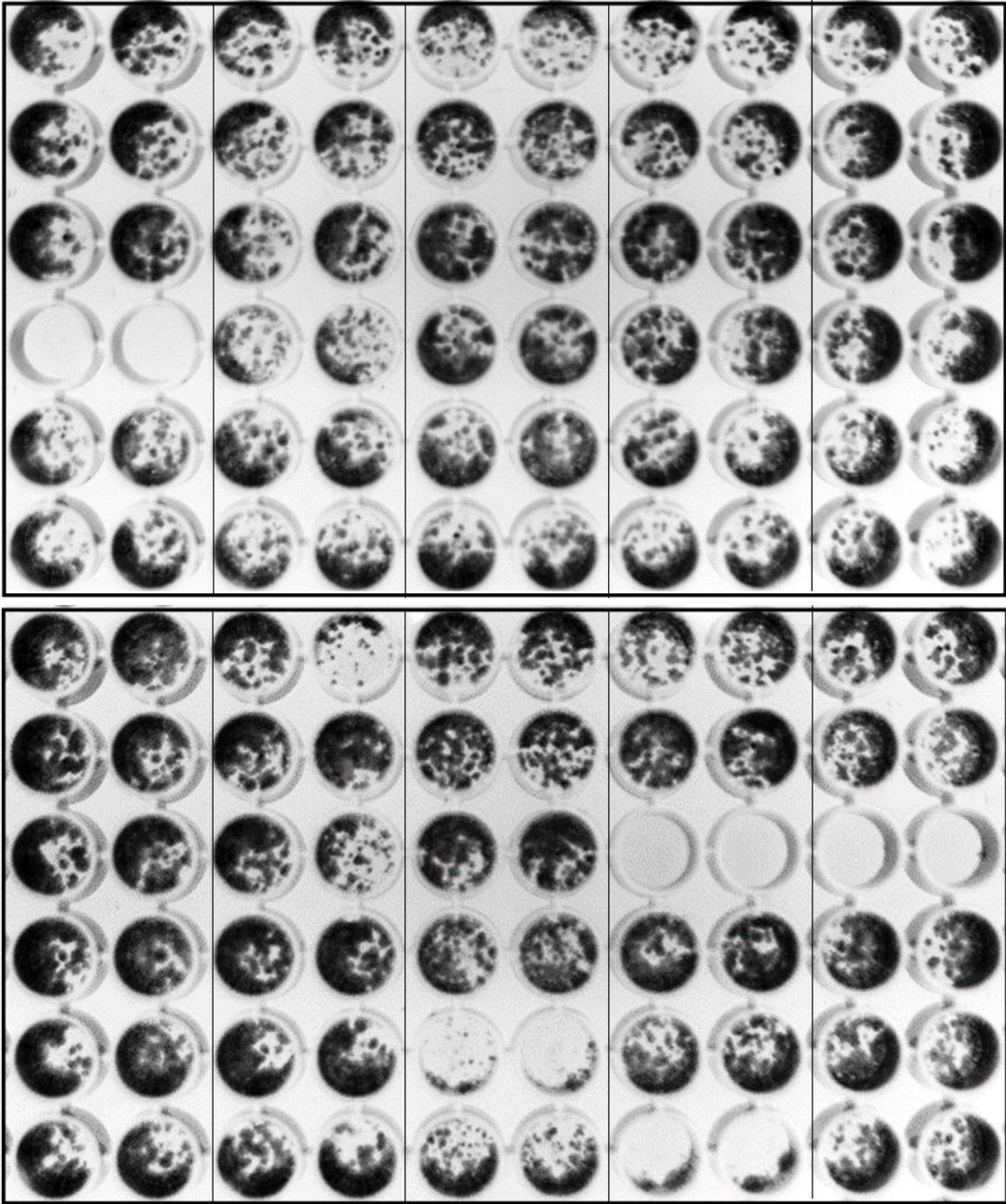
Supplementary Table 2. Cytotoxicity of compounds **16-56** in OVCAR8 cell

Cpd	IC₅₀ (μM)	Cpd	IC₅₀ (μM)
16	>50	37	>50
17	>50	38	>50
18	>50	39	>50
19	>50	40	>50
20	>50	41	>50
21	>50	42	>50
22	>50	43	>50
23	>50	44	>50
24	>50	45	>50
25	>50	46	>50
26	>50	47	>50
27	>50	48	>50
28	>50	49	>50
29	>50	50	>50
30	38.6	51	>50
31	>50	52	>50
32	>50	53	>50
33	>50	54	>50
34	>50	55	>50
35	>50	56	>50
36	>50		

Supplementary Table 3. Cytotoxicity of of compounds **16-56** at 30uM in CXCR2-U2OS cells

Cpd	%Inhibition in two independent		Cpd	%Inhibition in two independent	
	determinations			determinations	
	1st	2nd		1st	2nd
16	14.7	-8.3	37	13.7	-3.9
17	8.6	-0.7	38	18.4	-4.1
18	13.0	13.8	39	3.4	-5.4
19	58.0	44.7	40	-9.9	29.3
20	9.4	-2.0	41	15.0	7.3
21	15.1	12.1	42	16.3	0.9
22	-3.1	10.0	43	11.1	49.6
23	4.0	1.3	44	-5.7	-1.8
24	-0.6	1.8	45	-7.1	21.4
25	-15.2	19.0	46	10.5	11.4
26	35.9	41.0	47	21.5	0.7
27	9.0	1.8	48	15.7	29.5
28	7.1	5.3	49	19.7	-7.2
29	24.7	-1.1	50	17.9	9.6
30	37.2	32.6	51	3.7	-15.8
31	-2.3	3.0	52	15.7	-5.5
32	5.4	18.8	53	0.2	-5.7
33	-3.6	-8.7	54	1.4	4.4
34	-9.7	32.2	55	-14.2	24.8
35	20.5	8.3	56	7.2	22.2
36	8.6	-1.4			

Supplementary Figure 1. Inhibition of colony formation assay^a in CXCR2-U2OS cells by select compounds

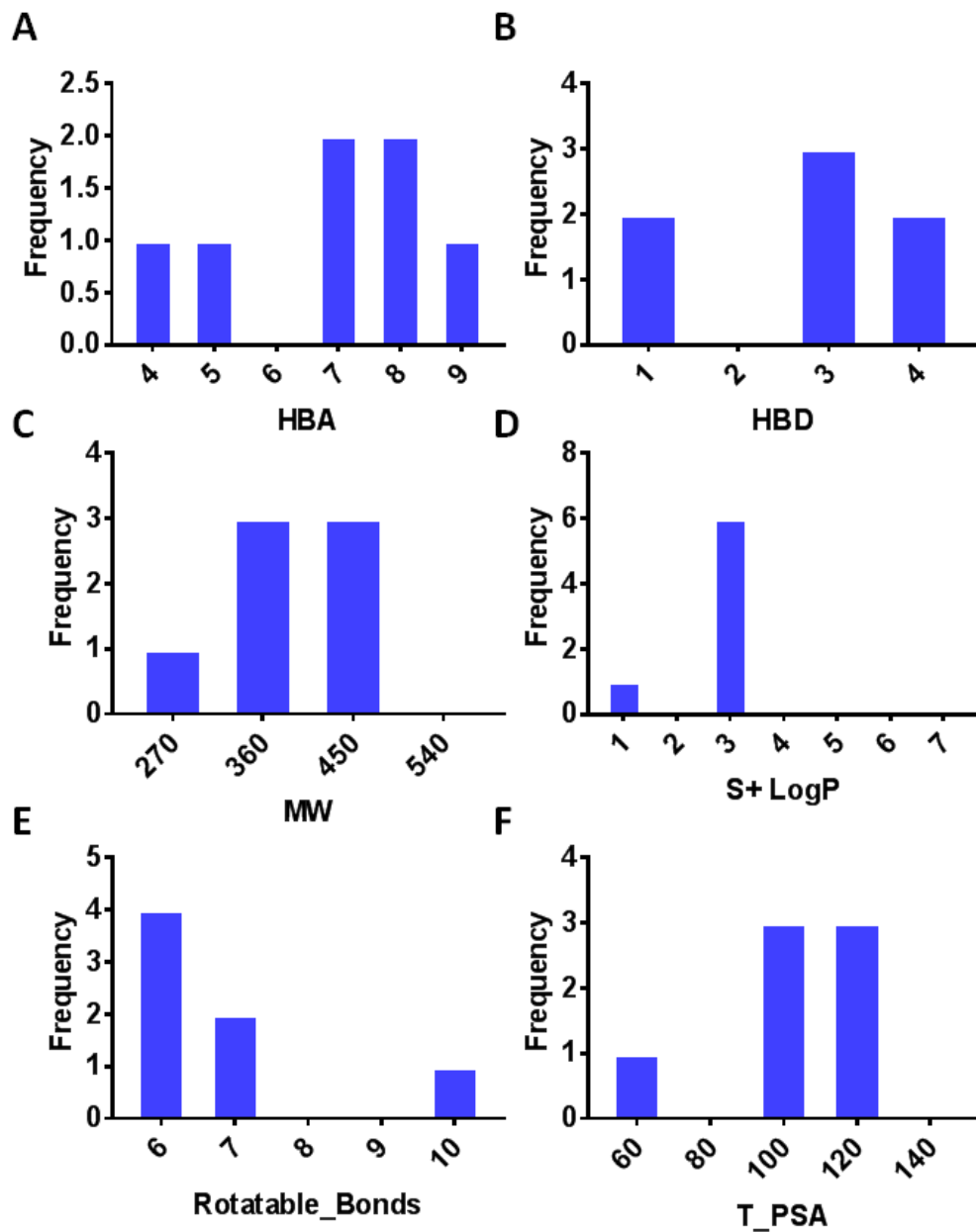


17	20	23	26	39
16	28	24	53	54
18	35	51	49	29
19	36	52	44	50
41	21	47	37	

42	22	27	38	
CTRL	2	3	25	
CTRL	31	55	48	
CTRL	32	56	43	1
CTRL	33	40		
CTRL	34	30	46	
CTRL		45		

^aCXCR2-U2OS cells were seeded at 300 cells per well in 96-well plates. The cells were continuously treated with select compounds at 30 uM for 7 days. Compounds were tested in duplicates

Supplementary Figure2. ADMET properties of CXCR2 clinical candidates. Frequency distribution plots for HBA (A), HBD (B), molecular weight (C), LogP (D), number of rotatable bonds (E) and topological polar surface area (F).



Compounds spectral information

4-Chloro-6,6-dimethyl-2-oxo-N-phenyl-1,2,5,6-tetrahydropyridine-3-carboxamide 6

^1H NMR (300 MHz, Chloroform-*d*) δ 11.73 (s, 1H), 7.63 – 7.51 (m, 3H), 7.37 (t, J = 7.9 Hz, 2H), 7.22 – 7.10 (m, 1H), 5.40 (s, 1H), 2.66 (s, 2H), 1.39 (s, 6H).

4-(Benzylamino)-6,6-dimethyl-2-oxo-N-phenyl-1,2,5,6-tetrahydropyridine-3-carboxamide 1

LC-MS m/z 350 [M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.30 (s, 1H), 12.03 (d, *J* = 8.9 Hz, 1H), 7.65 – 7.55 (m, 2H), 7.45 – 7.26 (m, 7H), 7.06 (t, *J* = 7.3 Hz, 1H), 5.29 (s, 1H), 4.57 (d, *J* = 6.3 Hz, 2H), 2.56 (s, 2H), 1.26 (s, 5H). Purity = 100%

Ethyl-4-hydroxy-2-oxo-1,2-dihydroquinoline-3-carboxylate 8

LC-MS m/z 234 [M + H]⁺, ¹H NMR (300 MHz, Chloroform-*d*) δ 11.24 (s, 1H), 8.04 (d, *J* = 8.3 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.30 – 7.05 (m, 2H), 4.56 (q, *J* = 7.1 Hz, 2H), 1.53 (t, *J* = 7.1 Hz, 3H).

4-Hydroxy-2-oxo-N-phenyl-1,2-dihydroquinoline-3-carboxamide 9

LC-MS m/z 281 [M + H]⁺, ¹H NMR (300 MHz, Chloroform-*d*) δ 12.20 (s, 1H), 9.12 – 8.94 (m, 2H), 8.20 (d, *J* = 8.2 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 3H), 7.39 (dt, *J* = 7.9, 15.2 Hz, 3H), 7.19 (d, *J* = 8.6 Hz, 2H).

4-Chloro-2-oxo-N-phenyl-1,2-dihydroquinoline-3-carboxamide 11

LC-MS m/z 299 [M + H]⁺ ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.72 (s, 1H), 11.50 (s, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.49 – 7.25 (m, 7H), 7.17 (t, *J* = 7.6 Hz, 1H).

4-(Benzylamino)-2-oxo-N-phenyl-1,2-dihydroquinoline-3-carboxamide 2

LC-MS m/z 370 [M + H]⁺. ¹H NMR (300 MHz, DMSO-*d*₆) δ 13.08 (s, 1H), 11.72 (s, 1H), 11.50 (s, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.71 – 7.52 (m, 3H), 7.49 – 7.25 (m, 8H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.05 (t, *J* = 7.4 Hz, 1H), 5.01 (d, *J* = 5.3 Hz, 2H). Purity = 95.30%

Ethyl-7-hydroxy-5-oxo-5H-thiazolo[3,2-*a*]pyrimidine-6-carboxylate 13

LC-MS m/z 241[M + H]⁺. ¹H NMR (300 MHz, Chloroform-d) δ 14.01 (s, 1H), 7.99 (d, J = 4.9 Hz, 1H), 6.98 (d, J = 4.9 Hz, 1H), 4.29 (q, J = 7.1 Hz, 2H), 1.47 (t, J = 7.1 Hz, 3H).

Ethyl-7-(benzylamino)-5-oxo-5H-thiazolo[3,2-a]pyrimidine-6-carboxylate 14

LC-MS m/z 330[M + H]⁺. ¹H NMR (300 MHz, Chloroform-d) δ 14.01 (s, 1H), 7.99 (d, J = 4.9 Hz, 1H), 6.98 (d, J = 4.9 Hz, 1H), 4.29 (q, J = 7.1 Hz, 2H), 1.32 (t, J = 7.1 Hz, 3H).

7-(Benzylamino)-5-oxo-5H-thiazolo[3,2-a]pyrimidine-6-carboxylic acid 15

LC-MS m/z 302[M + H]⁺. ¹H NMR (300 MHz, Chloroform-d) δ 13.72 (s, 1H), 7.83 (d, J = 4.9 Hz, 1H), 7.42 – 7.29 (m, 5H), 6.88 (d, J = 4.9 Hz, 1H), 4.81 (d, J = 6.0 Hz, 2H), 4.29 (q, J = 7.1 Hz, 2H), 1.32 (t, J = 7.1 Hz, 3H).

7-(Benzylamino)-5-oxo-N-phenyl-5H-thiazolo[3,2-a]pyrimidine-6-carboxamide 3

LC-MS m/z 377[M + H]⁺. ¹H NMR (300 MHz, Chloroform-d) δ 11.81 (s, 1H), 11.10 (s, 1H), 7.87 (s, 1H), 7.65 (d, J = 8.4 Hz, 2H), 7.36 (s, 7H), 7.11 (s, 1H), 6.80 (s, 1H), 4.82 (d, J = 5.8 Hz, 2H). Purity = 97.81%.

5-(Benzylimino)-3,3-dimethylcyclohexanone 58

LC-MS m/z 230[M + H]⁺. ¹H NMR (300 MHz, Methanol-d₄) δ 7.42 – 7.22 (m, 5H), 4.88 (s, 2H), 4.36 (s, 2H), 2.37 (s, 2H), 2.17 (s, 2H), 1.08 (s, 6H).

(R)-5,5-Dimethyl-3-((1-phenylethyl)amino)cyclohex-2-en-1-one 65

LC-MS m/z 244[M + H]⁺. ¹H NMR (300 MHz, DMSO-d₆) δ 7.43 – 7.16 (m, 6H), 4.58 (s, 1H), 4.46 (q, J = 6.7 Hz, 1H), 2.26 (s, 2H), 1.90 (d, J = 2.9 Hz, 2H), 1.39 (d, J = 6.8 Hz, 3H), 0.97 (s, 6H).

(S)-5,5-Dimethyl-3-((1-phenylethyl)amino)cyclohex-2-en-1-one 66

LC-MS m/z 244[M + H]⁺. ¹H NMR (300 MHz, DMSO-*d*₆) δ 7.43 – 7.16 (m, 7H), 4.58 (s, 1H), 4.47 (t, J = 6.8 Hz, 1H), 2.26 (s, 2H), 1.90 (d, J = 2.9 Hz, 2H), 1.39 (d, J = 6.8 Hz, 3H), 0.97 (s, 6H).

2-(Benzylamino)-N-(3-chlorophenyl)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 17

LC-MS m/z 383[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.72 (s, 1H), 12.51 (s, 1H), 7.73 (d, J = 2.6 Hz, 1H), 7.38 – 7.07 (m, 9H), 6.94 (d, J = 7.6 Hz, 1H), 4.53 (d, J = 5.9 Hz, 2H), 2.40 (s, 2H), 2.29 (s, 2H), 0.97 (s, 6H). Purity = 100%

2-(Benzylamino)-4,4-dimethyl-6-oxo-N-phenylcyclohex-1-enecarboxamide 16

LC-MS m/z 349[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.82 (s, 1H), 12.37 (s, 1H), 7.57 – 7.47 (m, 2H), 7.38 – 7.16 (m, 7H), 7.04 – 6.92 (m, 1H), 4.52 (d, J = 6.1 Hz, 2H), 2.39 (s, 2H), 2.29 (d, J = 1.0 Hz, 2H), 0.97 (s, 6H). Purity = 100%

2-(Benzylamino)-N-(4-chlorophenyl)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 18

LC-MS m/z 383[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.73 (s, 1H), 12.46 (s, 1H), 7.52 – 7.43 (m, 2H), 7.38 – 7.27 (m, 3H), 7.29 – 7.12 (m, 4H), 4.53 (d, J = 6.1 Hz, 2H), 2.40 (s, 2H), 2.28 (s, 2H), 0.97 (s, 6H). Purity = 100%

2-(Benzylamino)-N-(3,5-dichlorophenyl)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 19

LC-MS m/z 418[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.63 (s, 2H), 7.54 – 7.39 (m, 5H), 7.40 – 7.16 (m, 3H), 4.53 (d, J = 6.1 Hz, 2H), 2.40 (s, 2H), 2.28 (s, 2H), 0.97 (s, 6H). Purity = 95.50%

2-(Benzylamino)-4,4-dimethyl-6-oxo-N-(4-(trifluoromethyl)phenyl)cyclohex-1-enecarboxamide 40

LC-MS m/z 417[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.68 (s, 2H), 7.69 – 7.60 (m, 2H), 7.51 – 7.42 (m, 2H), 7.39 – 7.17 (m, 5H), 4.54 (d, $J = 6.1$ Hz, 2H), 2.41 (s, 2H), 2.30 (s, 2H), 0.98 (s, 6H). Purity = 100%

2-(Benzylamino)-N-(4-chloro-3-(trifluoromethyl)phenyl)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 42

LC-MS m/z 451[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.70 (s, 1H), 12.63 (s, 1H), 7.95 (d, $J = 2.6$ Hz, 1H), 7.63 (dd, $J = 2.6, 8.7$ Hz, 1H), 7.39 – 7.16 (m, 6H), 4.54 (d, $J = 6.1$ Hz, 2H), 2.41 (s, 2H), 2.29 (s, 2H), 0.97 (s, 6H). Purity = 100%

2-(Benzylamino)-N-(3,4-dichlorophenyl)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 20

LC-MS m/z 417[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.65 (s, 1H), 12.57 (s, 1H), 7.85 (dd, $J = 0.8, 2.0$ Hz, 1H), 7.39 – 7.16 (m, 7H), 4.53 (d, $J = 6.1$ Hz, 2H), 2.40 (s, 2H), 2.28 (s, 2H), 0.97 (s, 6H). Purity = 100%

2-(Benzylamino)-N-(2-fluorophenyl)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 28

LC-MS m/z 367[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.69 (s, 1H), 12.61 (s, 1H), 8.19 (td, $J = 2.0, 8.2$ Hz, 1H), 7.38 – 7.17 (m, 5H), 7.09 – 6.85 (m, 3H), 4.53 (d, $J = 6.0$ Hz, 2H), 2.40 (s, 2H), 2.31 (d, $J = 0.9$ Hz, 2H), 0.97 (s, 6H). Purity = 100%

2-(Benzylamino)-4,4-dimethyl-N-(4-nitrophenyl)-6-oxocyclohex-1-enecarboxamide 35

LC-MS m/z 394[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.97 (s, 1H), 12.59 (s, 1H), 8.16 – 8.05 (m, 2H), 7.75 – 7.65 (m, 2H), 7.41 – 7.18 (m, 5H), 4.56 (d, $J = 6.0$ Hz, 2H), 2.44 (s, 2H), 2.31 (s, 2H), 0.98 (s, 6H). Purity = 100%

N-(4-Aminophenyl)-2-(benzylamino)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 36

TLC-MS m/z 364[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.83 (s, 1H), 12.15 (s, 1H), 7.36 – 7.25 (m, 5H), 7.24 – 7.20 (m, 2H), 6.66 (d, J = 8.2 Hz, 2H), 4.50 (d, J = 6.2 Hz, 2H), 2.27 (s, 2H), 0.96 (s, 6H). Purity = 97.5%

2-(Benzylamino)-4,4-dimethyl-6-oxo-N-(p-tolyl)cyclohex-1-enecarboxamide 21

LC-MS m/z 363[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.85 (s, 1H), 12.28 (s, 1H), 7.39 (d, J = 7.9 Hz, 2H), 7.30 (d, J = 7.2 Hz, 2H), 7.24 (d, J = 12.2 Hz, 3H), 7.03 (d, J = 8.0 Hz, 2H), 4.52 (d, J = 6.0 Hz, 2H), 2.38 (s, 2H), 2.28 (s, 2H), 2.23 (s, 3H), 0.96 (s, 6H). Purity = 100%

2-(Benzylamino)-N-(4-methoxyphenyl)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 22

LC-MS m/z 379[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.84 (s, 1H), 12.20 (s, 1H), 7.41 (d, J = 8.6 Hz, 2H), 7.35 – 7.20 (m, 5H), 6.78 (d, J = 8.6 Hz, 2H), 4.51 (d, J = 6.0 Hz, 2H), 3.71 (s, 3H), 2.38 (s, 2H), 2.28 (s, 2H), 0.96 (s, 6H). Purity = 100%

2-(Benzylamino)-N-(4-(tert-butyl)phenyl)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 23

LC-MS m/z 405[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.85 (s, 1H), 12.26 (s, 1H), 7.41 (d, J = 8.4 Hz, 2H), 7.36 – 7.16 (m, 7H), 4.51 (d, J = 6.0 Hz, 2H), 2.38 (s, 2H), 2.28 (s, 2H), 1.23 (s, 9H), 0.96 (s, 6H). Purity = 100%

N-benzyl-2-(Benzylamino)-4,4-dimethyl-6-oxocyclohex-1-enecarboxamide 24

LC-MS m/z 363[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.79 (s, 1H), 10.58 (s, 1H), 7.36 – 7.03 (m, 9H), 4.52 – 4.42 (m, 4H), 2.34 (s, 2H), 2.23 (s, 2H), 0.94 (s, 6H). Purity = 98.13%

2-(Benzylamino)-N-(2-methoxyphenyl)-4,4-dimethyl-6-oxocyclohex-1-ene-1-carboxamide 27

Compound **27** was prepared from **58** and 4-methoxyphenyl isocyanate according to the general procedure I described above as a white solid (yield 51%). LC-MS m/z 379[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.96 (s, 1H), 12.66 (s, 1H), 8.41 (dd, $J = 1.7, 7.8$ Hz, 1H), 7.47 – 7.26 (m, 4H), 7.09 – 6.91 (m, 2H), 6.97 – 6.87 (m, 2H), 4.62 (d, $J = 6.1$ Hz, 2H), 3.97 (s, 3H), 2.48 (s, 2H), 2.40 (s, 2H), 1.05 (s, 6H). Purity = 97.20%

2-(Benzylamino)-N-(2-hydroxyphenyl)-4,4-dimethyl-6-oxocyclohex-1-ene-1-carboxamide 26

LC-MS m/z 365[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.87 (s, 1H), 12.28 (s, 1H), 7.45 – 7.30 (m, 4H), 7.18 – 7.03 (m, 2H), 7.08 – 6.98 (m, 2H), 6.88 (td, $J = 1.5, 7.5, 7.9$ Hz, 1H), 4.63 (d, $J = 5.9$ Hz, 2H), 2.53 (s, 2H), 2.41 (s, 2H), 1.08 (s, 6H). Purity = 100%

2-(Benzylamino)-N-(3-(N,N-dimethylsulfamoyl)phenyl)-4,4-dimethyl-6-oxocyclohex-1-ene-1-carboxamide 37

LC-MS m/z 456[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.78 (s, 2H), 8.12 (s, 1H), 7.88 – 7.77 (m, 1H), 7.53 – 7.30 (m, 6H), 4.64 (d, $J = 6.1$ Hz, 2H), 2.74 (s, 6H), 2.50 (s, 2H), 2.39 (s, 2H), 1.06 (s, 6H). Purity = 96.45%

3-(2-(Benzylamino)-4,4-dimethyl-6-oxocyclohex-1-ene-1-carboxamido)-N,N-dimethylbenzamide 38

LC-MS m/z 420[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.94 (s, 1H), 12.47 (s, 1H), 7.64 – 7.55 (m, 2H), 7.50 – 7.28 (m, 6H), 7.14 – 7.02 (m, 1H), 4.63 (d, $J = 6.1$ Hz, 2H), 3.12 (s, 3H), 3.02 (s, 3H), 2.47 (s, 2H), 2.38 (s, 2H), 1.07 (s, 6H). Purity = 100%

4-(2-(Benzylamino)-4,4-dimethyl-6-oxocyclohex-1-ene-1-carboxamido)-N,N-dimethylbenzamide 39

LC-MS m/z 420[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.83 (s, 1H), 12.66 (s, 1H), 7.65 (d, $J = 8.5$ Hz, 2H), 7.48 – 7.29 (m, 6H), 4.62 (d, $J = 6.0$ Hz, 2H), 3.07 (s, 6H), 2.49 (s, 2H), 2.38 (s, 2H), 1.06 (s, 5H). Purity = 97.58%

2-(Benzylamino)-4,4-dimethyl-N-(5-methylisoxazol-3-yl)-6-oxocyclohex-1-ene-1-carboxamide 29

LC-MS m/z 354[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.82 (s, 1H), 12.57 (s, 1H), 7.48 – 7.27 (m, 5H), 6.55 (d, $J = 1.0$ Hz, 1H), 4.62 (d, $J = 6.0$ Hz, 2H), 2.49 (s, 2H), 2.39 (s, 3H), 2.37 (s, 2H), 1.05 (s, 6H). Purity = 100%

N-(Benzo[d]thiazol-2-yl)-2-(benzylamino)-4,4-dimethyl-6-oxocyclohex-1-ene-1-carbothioamide 30

LC-MS m/z 406[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 14.30 (s, 1H), 12.21 (s, 1H), 7.90 (d, $J = 8.2$ Hz, 1H), 7.79 (d, $J = 7.9$ Hz, 1H), 7.53 – 7.28 (m, 7H), 4.68 (d, $J = 6.1$ Hz, 2H), 2.54 (s, 2H), 2.44 (s, 2H), 1.07 (s, 6H). Purity = 100%

2-(Benzylamino)-4,4-dimethyl-6-oxo-N-(4-(trifluoromethoxy)phenyl)cyclohex-1-ene-1-carboxamide 40

LC-MS m/z 433[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.81 (s, 1H), 12.59 (s, 1H), 7.62 (d, $J = 9.0$ Hz, 2H), 7.48 – 7.26 (m, 5H), 7.17 (d, $J = 8.4$ Hz, 2H), 4.62 (d, $J = 6.1$ Hz, 2H), 2.50 (s, 2H), 2.38 (s, 2H), 1.06 (s, 6H). Purity = 99.35%

(R)-N-(4-Chloro-3-(trifluoromethyl)phenyl)-4,4-dimethyl-6-oxo-2-((1-phenylethyl)amino)cyclohex-1-ene-1-carboxamide 55

LC-MS m/z 466[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.83 (s, 2H), 12.78 (s, 1H), 8.05 (d, $J = 2.5$ Hz, 1H), 7.76 (dd, $J = 2.6, 8.7$ Hz, 1H), 7.48 – 7.27 (m, 6H), 4.81 (p, $J = 6.8$ Hz, 1H), 2.49 (d, $J = 16.8$ Hz, 1H), 2.41 – 2.18 (m, 3H), 1.69 (d, $J = 6.8$ Hz, 3H), 1.04 (s, 3H), 0.84 (s, 3H). Purity = 99.50%

(S)-N-(4-Chloro-3-(trifluoromethyl)phenyl)-4,4-dimethyl-6-oxo-2-((1-phenylethyl)amino)cyclohex-1-ene-1-carboxamide 56

LC-MS m/z 466[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.83 (s, 2H), 12.78 (d, $J = 6.7$ Hz, 1H), 8.06 (d, $J = 2.5$ Hz, 1H), 7.77 (dd, $J = 2.5, 8.8$ Hz, 1H), 7.48 – 7.27 (m, 6H), 4.82 (t, $J = 6.9$ Hz, 1H), 2.49 (d, $J = 16.8$ Hz, 1H), 2.42 – 2.18 (m, 3H), 1.70 (d, $J = 6.8$ Hz, 3H), 1.04 (s, 3H), 0.84 (s, 3H). Purity = 99.09%

2-Hydroxy-4,4-dimethyl-6-oxo-N-(1-phenylethyl)cyclohex-1-ene-1-carboxamide 59

LC-MS m/z 354[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 11.70 (s, 1H), 7.55 – 7.45 (m, 2H), 7.29 (t, $J = 7.9$ Hz, 2H), 7.15 – 7.03 (m, 1H), 2.47 (s, 2H), 2.35 (s, 2H), 1.06 (s, 6H).

2-Chloro-4,4-dimethyl-6-oxo-N-phenylcyclohex-1-ene-1-carboxamide 62

LC-MS m/z 354[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 8.45 (s, 1H), 7.62 (d, $J = 8.0$ Hz, 2H), 7.36 (t, $J = 7.9$ Hz, 2H), 7.16 (t, $J = 7.4$ Hz, 1H), 2.79 (s, 2H), 2.47 (s, 2H), 1.16 (s, 6H).

2-Hydroxy-4,4-dimethyl-6-oxo-N-(1-phenylethyl)cyclohex-1-ene-1-carboxamide 60

LC-MS m/z 288[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 10.24 (d, $J = 7.9$ Hz, 1H), 7.43 – 7.22 (m, 6H), 5.16 (p, $J = 7.1$ Hz, 1H), 2.47 (s, 2H), 2.36 (s, 2H), 1.10 (d, $J = 5.0$ Hz, 6H).

2-(Benzylamino)-4,4-dimethyl-6-oxo-N-(1-phenylethyl)cyclohex-1-ene-1-carboxamide 25

LC-MS m/z 377[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.87 (s, 1H), 10.76 (s, 1H), 7.43 – 7.17 (m, 8H), 7.28 (s, 6H), 5.15 (q, $J = 6.9$ Hz, 1H), 4.53 (d, $J = 6.0$ Hz, 2H), 2.41 (s, 2H), 2.33 (s, 2H), 1.52 (d, $J = 7.0$ Hz, 3H), 1.03 (s, 6H). Purity = 96.89%

Methyl-(2-hydroxy-4,4-dimethyl-6-oxocyclohex-1-ene-1-carbonyl)glycinate 61

LC-MS m/z 256[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 10.62 (s, 1H), 4.10 (s, 2H), 3.77 (s, 3H), 2.43 (s, 2H), 2.34 (s, 2H), 1.03 (s, 6H).

Methyl-(2-(benzylamino)-4,4-dimethyl-6-oxocyclohex-1-ene-1-carbonyl)glycinate 31

LC-MS m/z 345[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.67 (s, 1H), 10.62 (s, 1H), 7.45 – 7.23 (m, 5H), 4.54 (dd, $J = 6.0, 10.7$ Hz, 2H), 4.10 (s, 2H), 3.77 (s, 3H), 2.43 (s, 2H), 1.03 (s, 6H). Purity = 96.27%.

(2-(Benzylamino)-4,4-dimethyl-6-oxocyclohex-1-ene-1-carbonyl)glycine 33

LC-MS m/z 331[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.46 (s, 1H), 7.47 – 7.23 (m, 7H), 4.59 (d, $J = 6.0$ Hz, 2H), 4.11 (s, 2H), 2.46 (s, 2H), 2.35 (s, 2H), 1.04 (s, 6H). Purity = 98.99%.

2-(Benzylamino)-4,4-dimethyl-6-oxo-N-(2-oxo-2-(phenylamino)ethyl)cyclohex-1-ene-1-carboxamide 32

LC-MS m/z 406[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.59 (s, 1H), 8.54 (s, 1H), 7.51 (d, $J = 8.0$ Hz, 2H), 7.41 (q, $J = 5.3, 6.1$ Hz, 2H), 7.30 (d, $J = 9.8$ Hz, 8H), 7.10 (t, $J = 7.4$ Hz, 1H), 4.61 (d, $J = 5.7$ Hz, 2H), 4.12 (s, 2H), 2.48 (s, 2H), 2.37 (s, 2H), 1.06 (s, 6H). Purity = 98.49%.

2-(Benzylamino)-4,4-dimethyl-N-(2-(methylamino)-2-oxoethyl)-6-oxocyclohex-1-ene-1-carboxamide 34

LC-MS m/z 344[M + H]⁺. $\delta^1\text{H}$ NMR (300 MHz, Chloroform-*d*) δ 12.60 (s, 1H), 10.62 (s, 1H), 7.41 (s, 1H), 7.42 – 7.24 (m, 5H), 6.42 (s, 1H), 4.55 (dd, $J = 6.0, 18.9$ Hz, 2H), 4.02 (s, 2H), 2.83 (d, $J = 4.3$ Hz, 3H), 2.46 (s, 2H), 2.34 (s, 2H), 1.04 (s, 6H). Purity = 98.81%.

2-(Benzylthio)-4,4-dimethyl-6-oxo-N-phenylcyclohex-1-ene-1-carboxamide 43

LC-MS m/z 366[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 11.38 (s, 1H), 7.71 – 7.61 (m, 2H), 7.48 – 7.21 (m, 7H), 7.08 (t, $J = 7.4$ Hz, 1H), 4.14 (s, 2H), 4.20 – 4.00 (m, 1H), 2.86 (s, 2H), 2.45 (s, 2H), 1.09 (s, 6H). Purity = 100%

2-((2-Hydroxyphenyl)amino)-4,4-dimethyl-6-oxo-N-phenylcyclohex-1-ene-1-carboxamide 45

LC-MS m/z 351[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 13.61 (s, 1H), 12.46 (s, 1H), 7.69 – 7.59 (m, 2H), 7.35 (t, $J = 7.9$ Hz, 2H), 7.17 – 7.03 (m, 2H), 7.03 – 6.92 (m, 2H), 2.38 (d, $J = 8.7$ Hz, 4H), 1.03 (s, 6H). Purity = 100.00%

2-((1-Hydroxypropan-2-yl)amino)-4,4-dimethyl-6-oxo-N-phenylcyclohex-1-ene-1-carboxamide 46

LC-MS m/z 317[M + H]⁺. δ 12.59 (d, $J = 18.9$ Hz, 2H), 7.64 – 7.54 (m, 2H), 7.38 – 7.25 (m, 3H), 7.07 (t, $J = 7.5$ Hz, 1H), 3.81 – 3.59 (m, 2H), 2.64 (d, $J = 16.5$ Hz, 1H), 2.43 (d, $J = 36.1$ Hz, 3H), 1.31 (d, $J = 6.6$ Hz, 3H), 1.10 (d, $J = 4.0$ Hz, 6H). Purity = 90.04%

2-(((5,5-Dimethyl-3-oxo-2-(phenylcarbamoyl)cyclohex-1-en-1-yl)amino)methyl)benzoate 48

LC-MS m/z 407[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.88 (s, 1H), 12.51 (s, 1H), 8.09 (dd, $J = 1.4, 8.1$ Hz, 1H), 7.66 – 7.53 (m, 3H), 7.43 (dt, $J = 3.4, 7.4$ Hz, 2H), 7.32 (t, $J = 7.8$ Hz, 2H), 7.07 (t, $J = 7.4$ Hz, 1H), 5.04 (d, $J = 6.3$ Hz, 2H), 3.97 (s, 3H), 2.48 (s, 2H), 2.38 (s, 2H), 1.06 (s, 6H). Purity = 100%

2-((2-Hydroxy-1-phenylethyl)amino)-4,4-dimethyl-6-oxo-N-phenylcyclohex-1-ene-1-carboxamide 50

LC-MS m/z 379[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 13.20 (d, $J = 7.3$ Hz, 1H), 12.52 (s, 1H), 7.69 – 7.59 (m, 2H), 7.47 – 7.28 (m, 7H), 7.09 (t, $J = 7.4$ Hz, 1H),

4.82 (q, $J = 6.9$ Hz, 1H), 3.97 (dd, $J = 3.7, 5.7$ Hz, 2H), 2.53 (d, $J = 16.7$ Hz, 1H), 2.40 – 2.05 (m, 3H), 1.03 (s, 3H), 0.85 (s, 3H). Purity = 97.57%

2-((2-Methoxybenzyl)amino)-4,4-dimethyl-6-oxo-N-phenylcyclohex-1-ene-1-carb oxamide 47

LC-MS m/z 379[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.80 (s, 1H), 12.50 (s, 1H), 7.66 – 7.56 (m, 2H), 7.38 – 7.27 (m, 2H), 7.26 – 7.20 (m, 1H), 7.12 – 6.86 (m, 4H), 4.58 (d, $J = 6.2$ Hz, 2H), 3.91 (s, 3H), 2.52 (s, 2H), 2.38 (s, 2H), 1.08 (s, 6H). Purity = 98.90%

2-((2-Hydroxybenzyl)amino)-4,4-dimethyl-6-oxo-N-phenylcyclohex-1-ene-1-carb oxamide 44

C-MS m/z 364[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.72 (s, 1H), 12.52 (s, 1H), 7.73 (dd, $J = 3.3, 5.7$ Hz, 2H), 7.56 (td, $J = 2.3, 5.6$ Hz, 5H), 7.29 (d, $J = 2.5$ Hz, 2H), 6.78 (d, $J = 8.0$ Hz, 1H), 6.09 (s, 1H), 4.58 (d, $J = 6.0$ Hz, 2H), 2.56 (s, 2H), 2.38 (s, 2H), 1.08 (s, 6H). Purity = 95.32%

4,4-Dimethyl-6-oxo-N-phenyl-2-((pyridin-2-ylmethyl)amino)cyclohex-1-ene-1-car boxamide 51

LC-MS m/z 350[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 13.04 (s, 1H), 12.48 (s, 1H), 8.68 – 8.59 (m, 1H), 7.78 (td, $J = 1.7, 7.7$ Hz, 1H), 7.67 – 7.57 (m, 2H), 7.33 (td, $J = 4.4, 7.8$ Hz, 4H), 7.07 (t, $J = 7.4$ Hz, 1H), 4.77 (d, $J = 6.1$ Hz, 2H), 2.54 (s, 2H), 2.38 (s, 2H), 1.07 (s, 6H). Purity = 100%.

4,4-Dimethyl-6-oxo-N-phenyl-2-((pyridin-3-ylmethyl)amino)cyclohex-1-ene-1-car boxamide 52

LC-MS m/z 350[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 13.01 (s, 1H), 12.42 (s, 1H), 8.64 (s, 2H), 7.75 (d, $J = 7.9$ Hz, 1H), 7.59 (d, $J = 8.0$ Hz, 2H), 7.48 – 7.29 (m, 3H), 7.08 (t, $J = 7.4$ Hz, 1H), 4.66 (d, $J = 6.1$ Hz, 2H), 2.48 (s, 2H), 2.39 (s, 2H), 1.08 (s, 6H). Purity = 99.00%

**3-(((5,5-Dimethyl-3-oxo-2-(phenylcarbamoyl)cyclohex-1-en-1-yl)amino)methyl)-
N,N-dimethylbenzamide 53**

LC-MS m/z 354[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.94 (s, 1H), 12.47 (s, 1H), 7.64 – 7.55 (m, 2H), 7.50 – 7.28 (m, 6H), 7.14 – 7.02 (m, 1H), 4.63 (d, J = 6.1 Hz, 2H), 3.12 (s, 3H), 3.02 (s, 3H), 2.47 (s, 2H), 2.38 (s, 2H), 1.07 (s, 6H). Purity = 96.00%

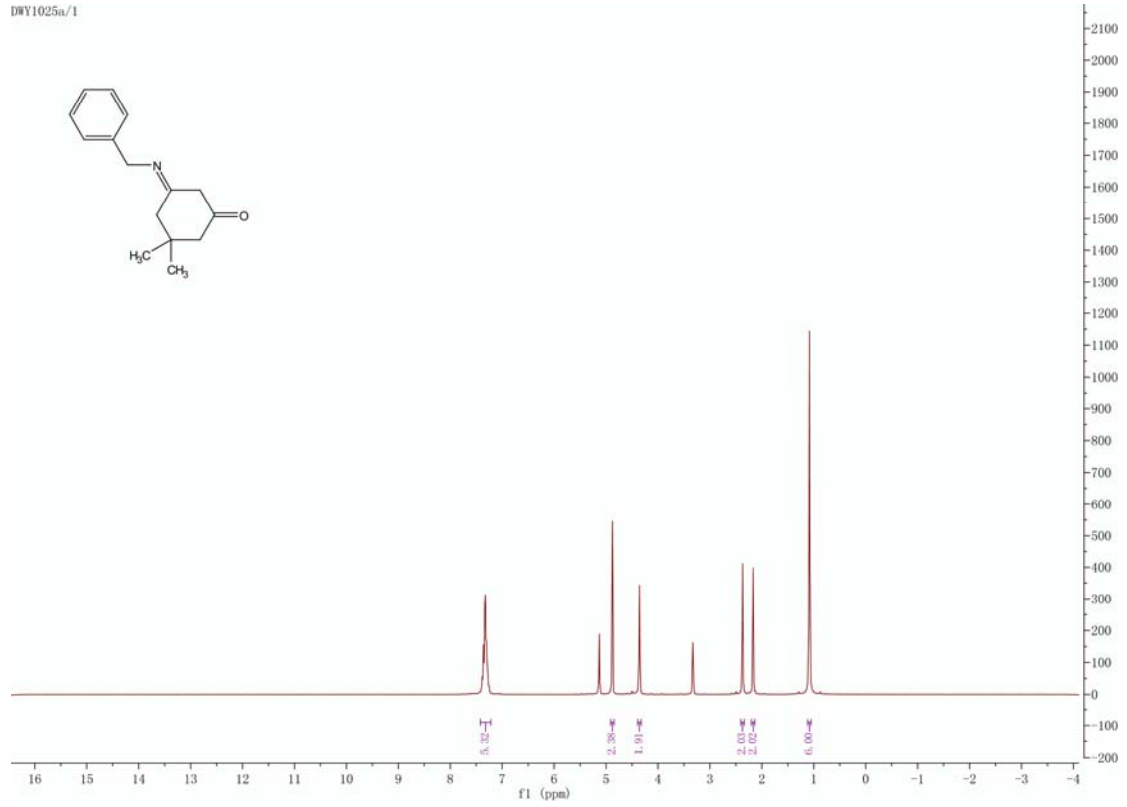
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LC-MS m/z 363[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 13.03 – 12.93 (m, 0H), 12.51 (s, 1H), 7.68 – 7.58 (m, 2H), 7.45 – 7.26 (m, 8H), 7.09 (t, J = 7.4 Hz, 1H), 4.80 (p, J = 6.8 Hz, 1H), 2.47 (d, J = 16.6 Hz, 1H), 2.32 (d, J = 4.5 Hz, 2H), 2.22 (d, J = 16.8 Hz, 1H), 1.67 (d, J = 6.8 Hz, 3H), 1.03 (s, 3H), 0.84 (s, 3H). Purity = 100%

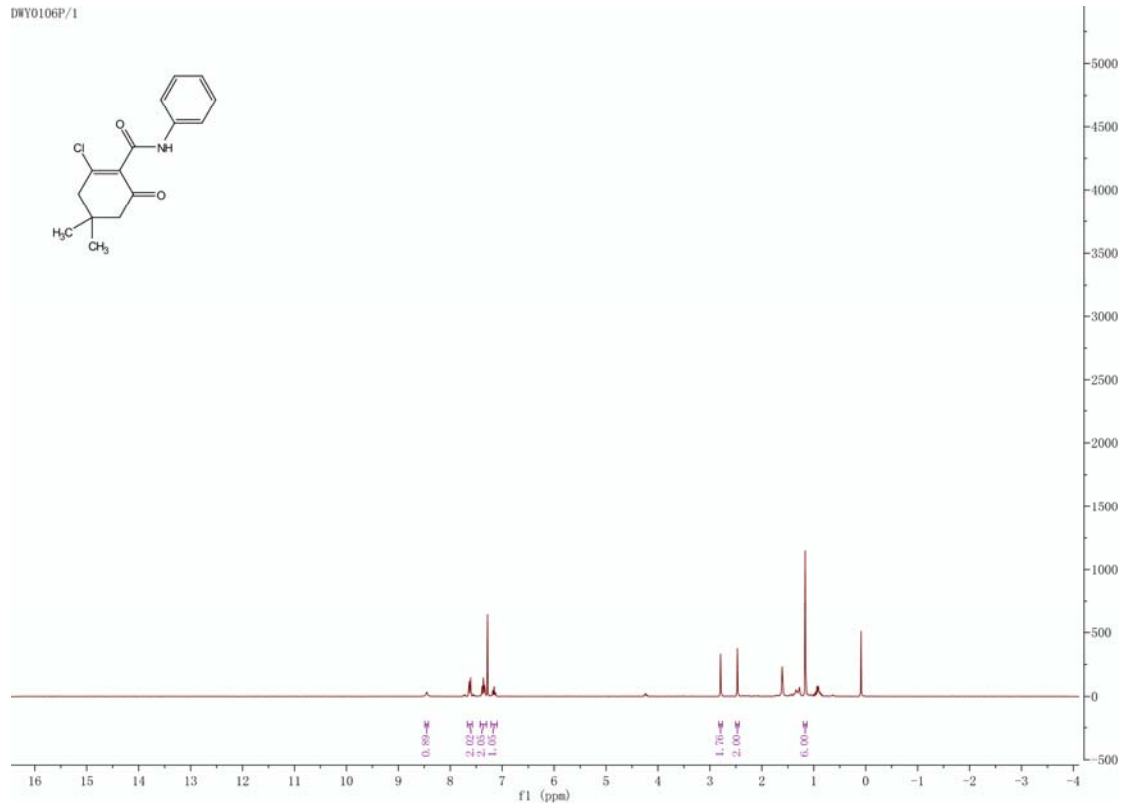
4,4-Dimethyl-2-(((3-methylisoxazol-5-yl)methyl)amino)-6-oxo-N-phenylcyclohex-1-ene-1-carboxamide 54

LC-MS m/z 354[M + H]⁺. ¹H NMR (300 MHz, Chloroform-*d*) δ 12.94 (s, 1H), 12.41 (s, 1H), 7.64 – 7.54 (m, 2H), 7.33 (t, J = 7.9 Hz, 2H), 7.08 (t, J = 7.4 Hz, 1H), 6.06 (s, 1H), 4.61 (d, J = 6.2 Hz, 2H), 2.54 (s, 2H), 2.46 (s, 3H), 2.38 (s, 2H), 1.09 (s, 6H). Purity = 100%

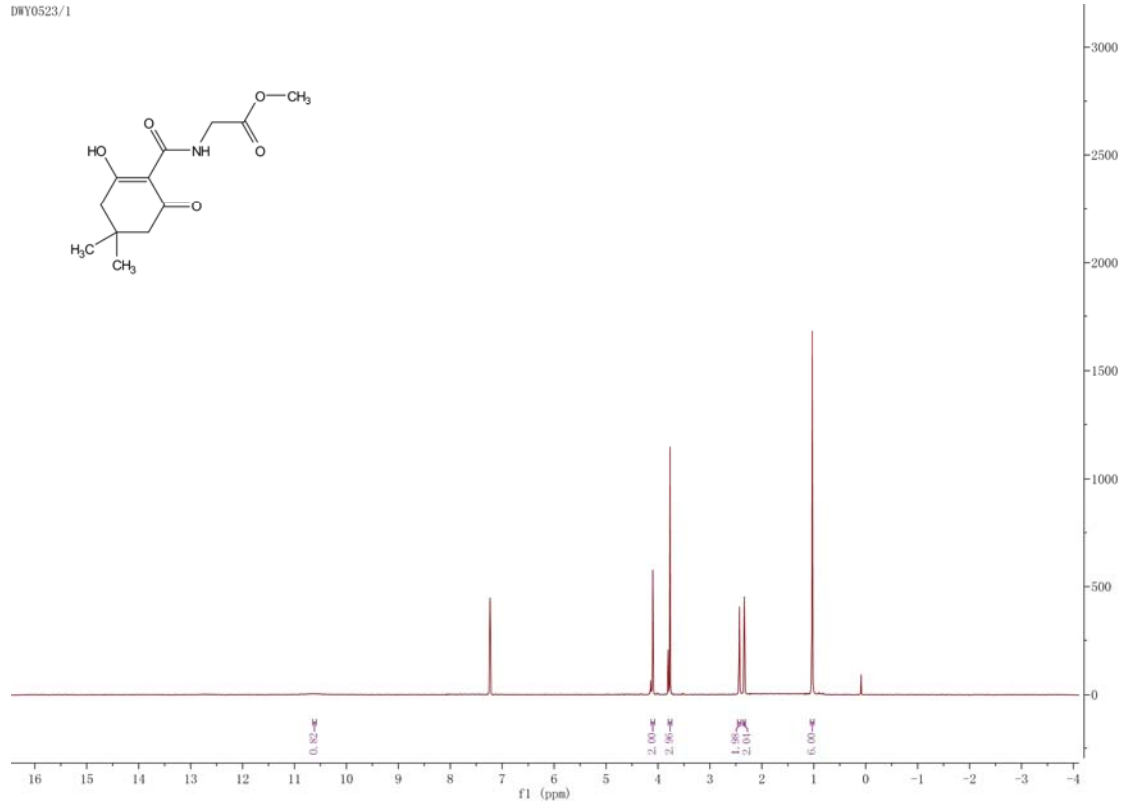
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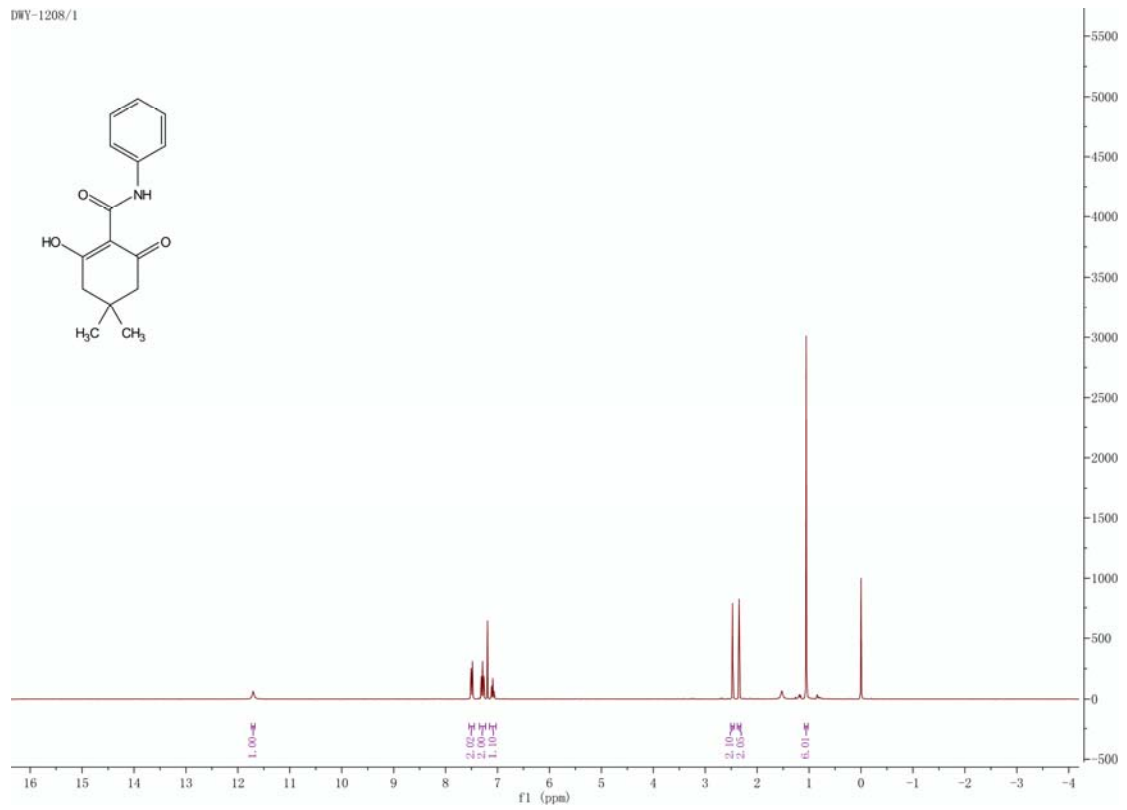
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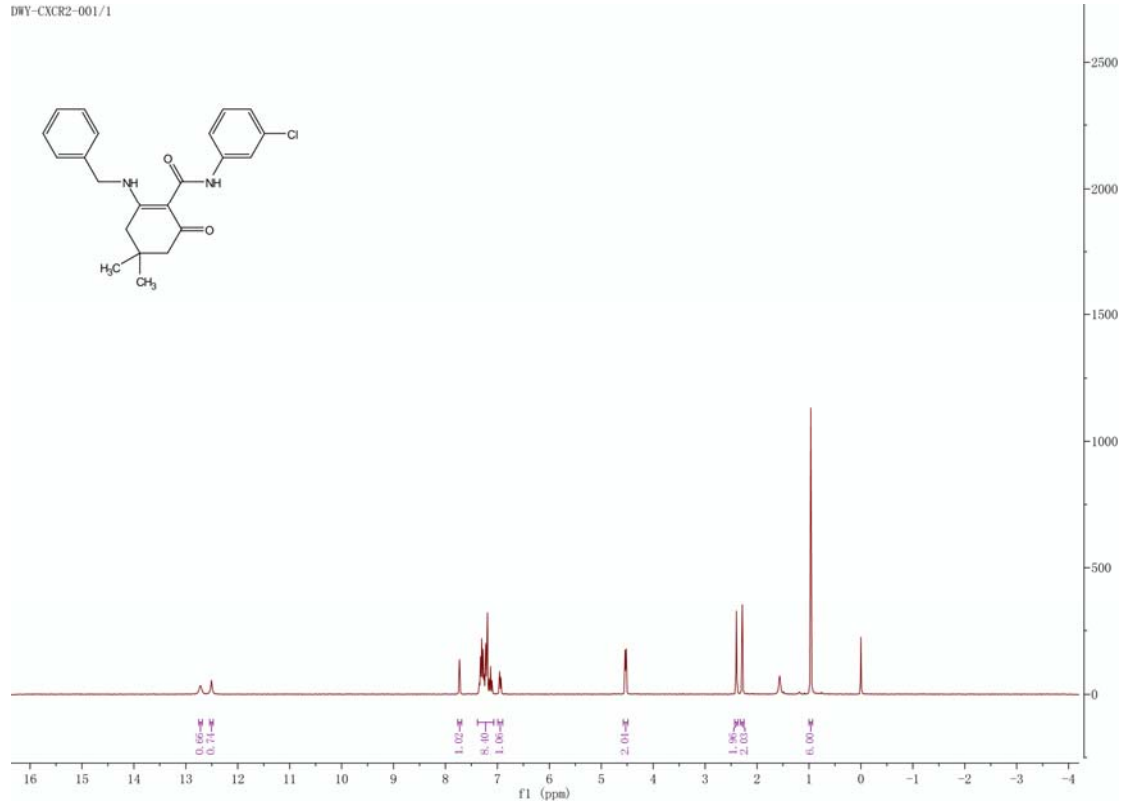
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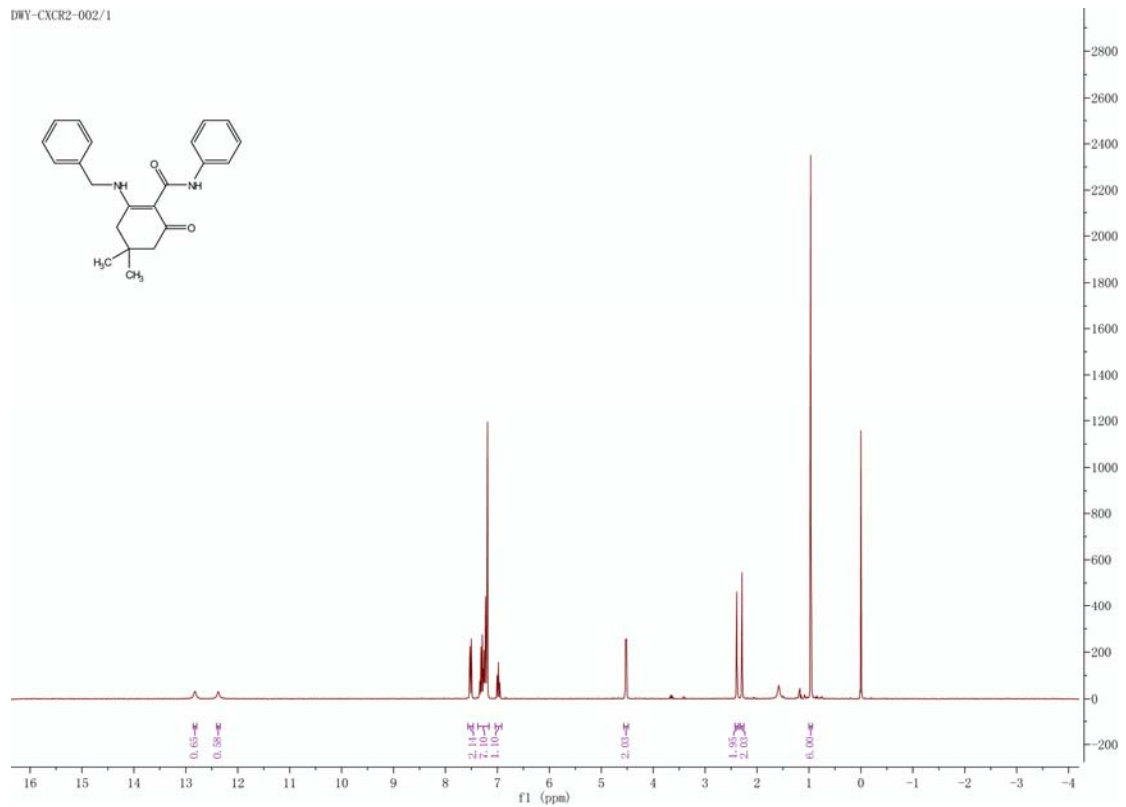
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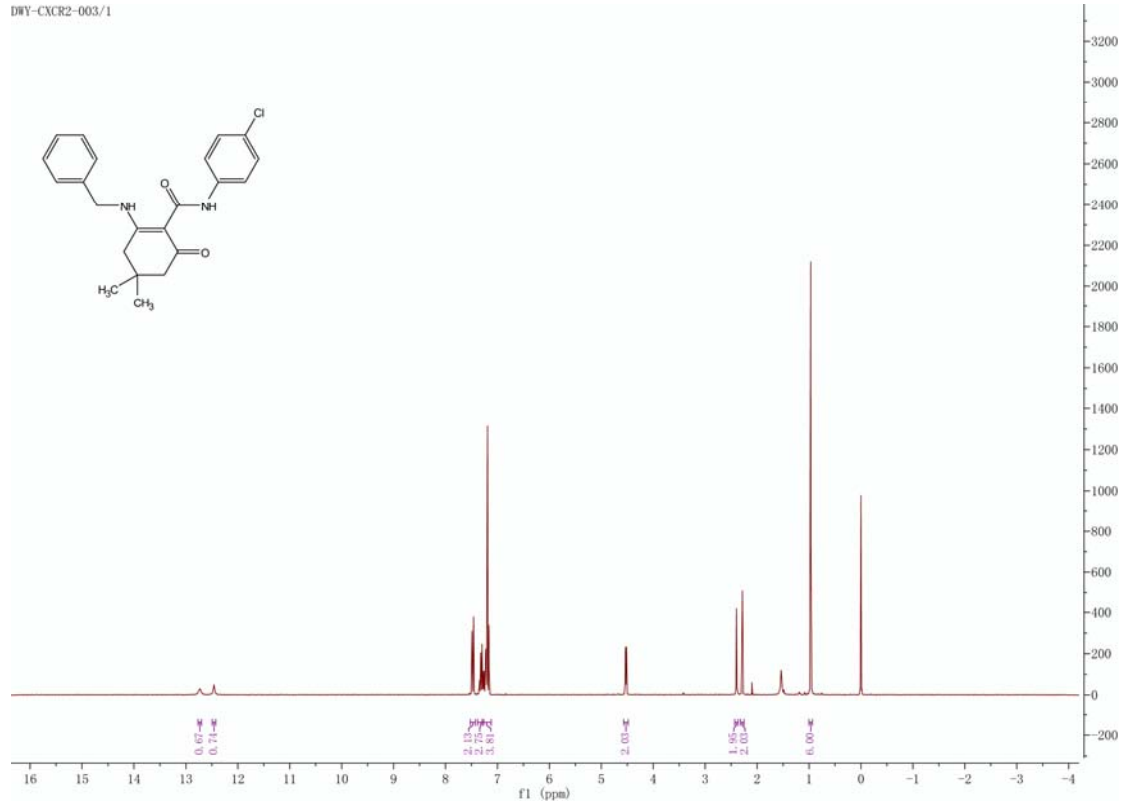
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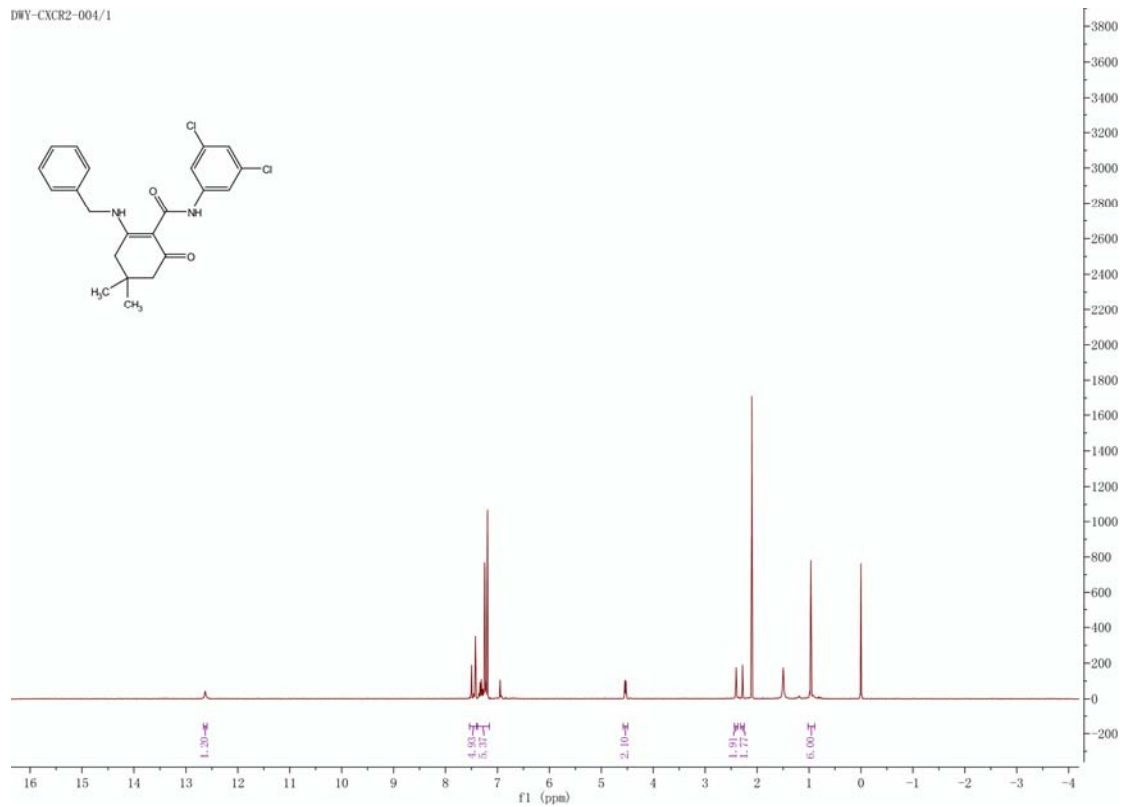
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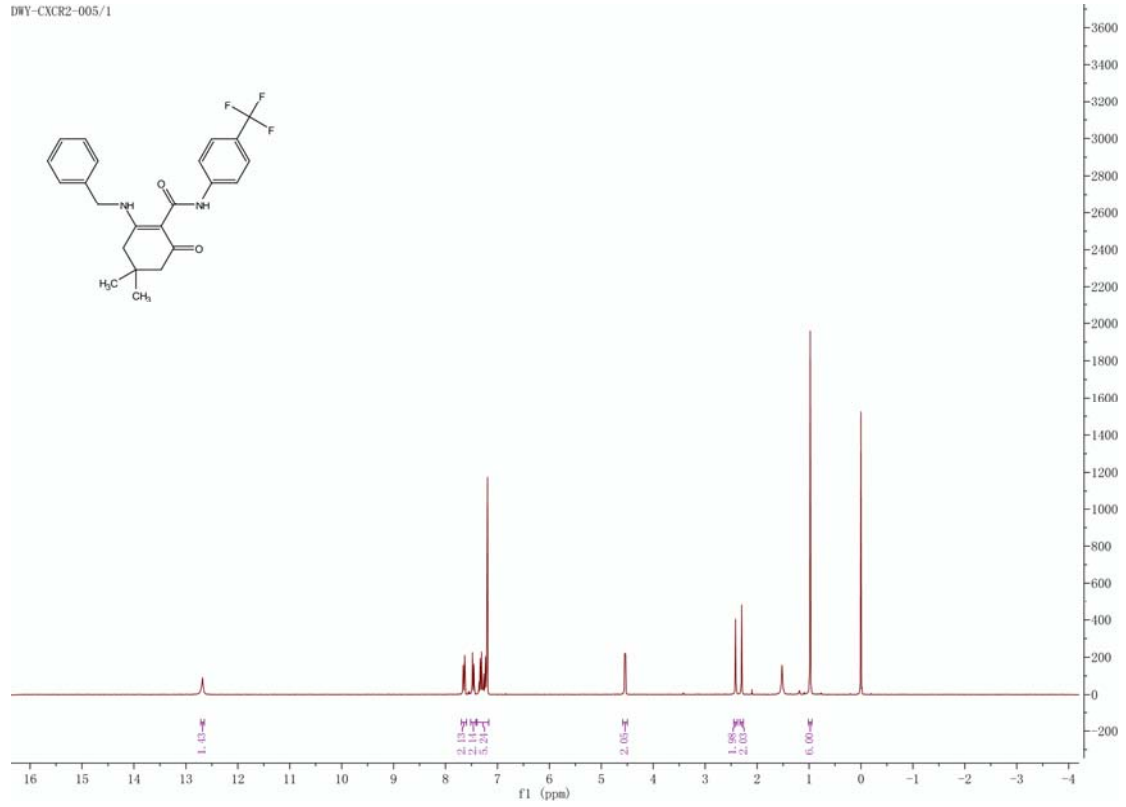
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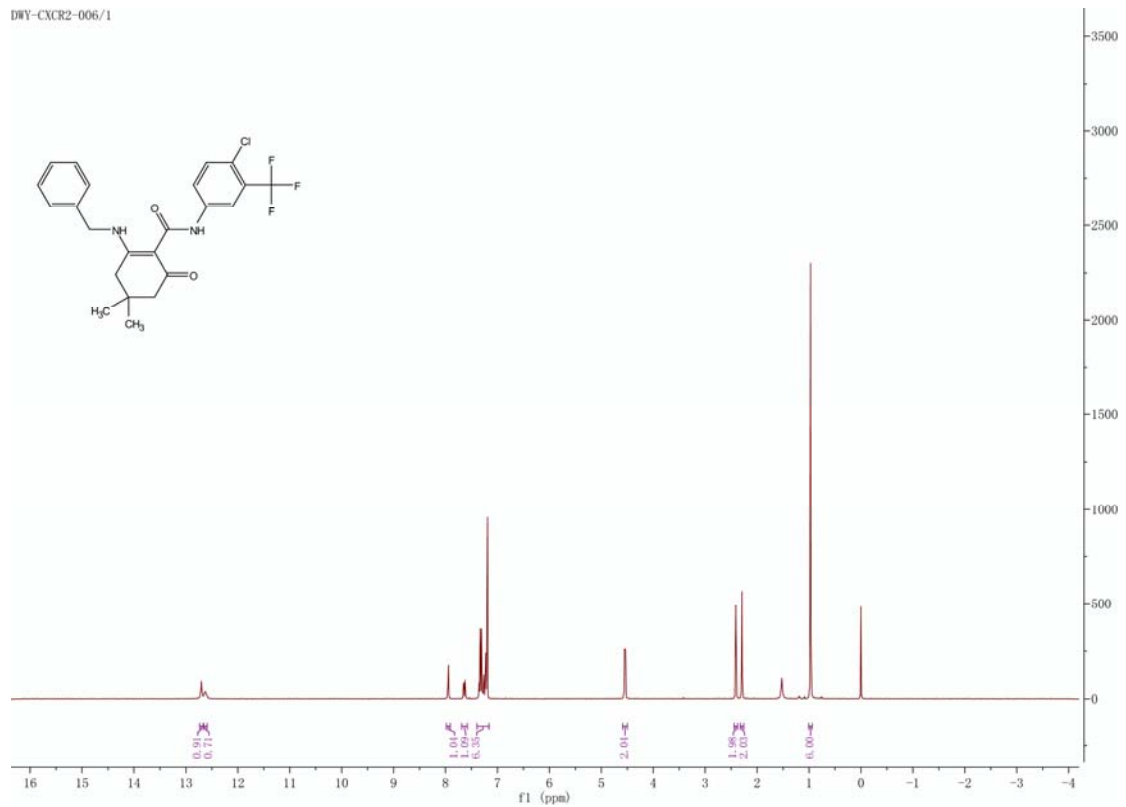
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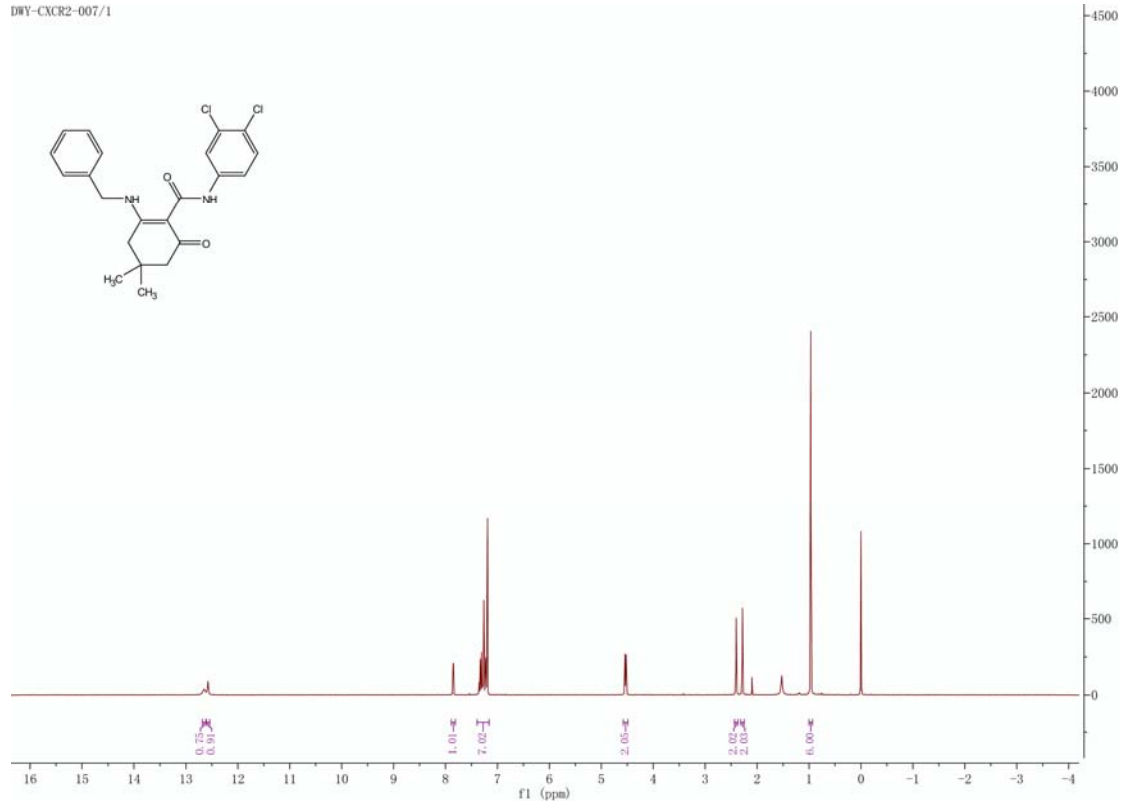
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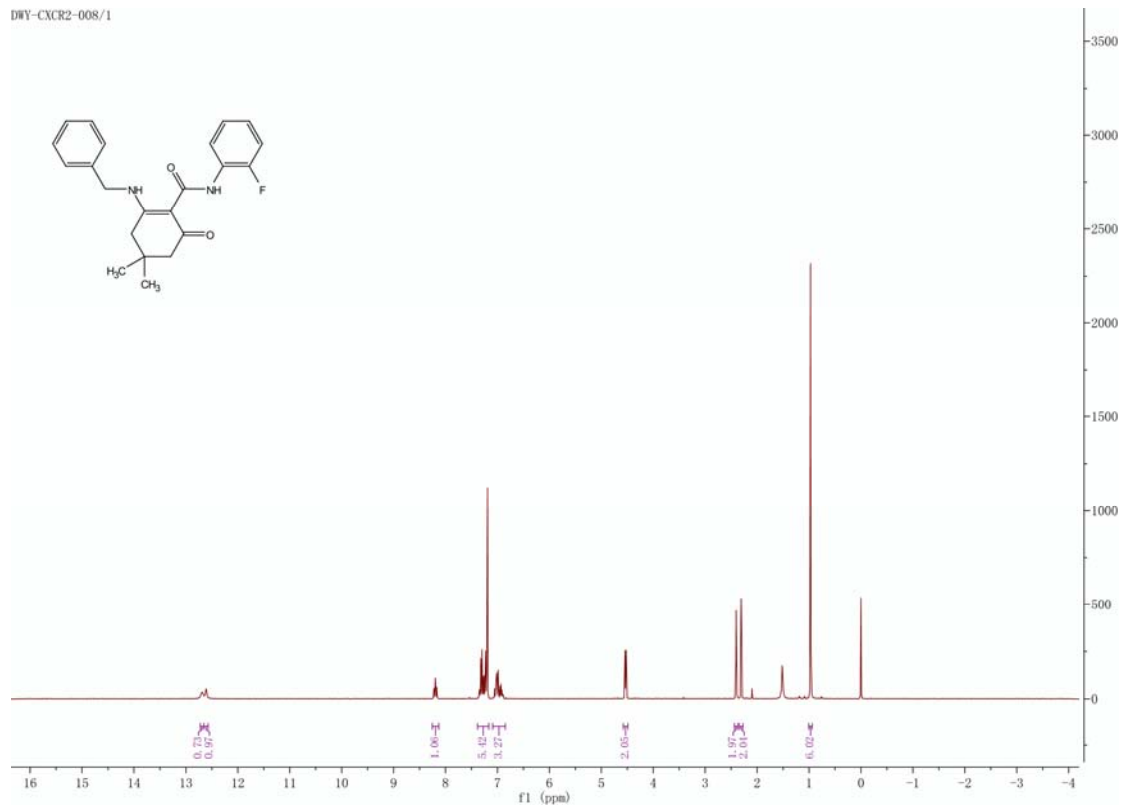
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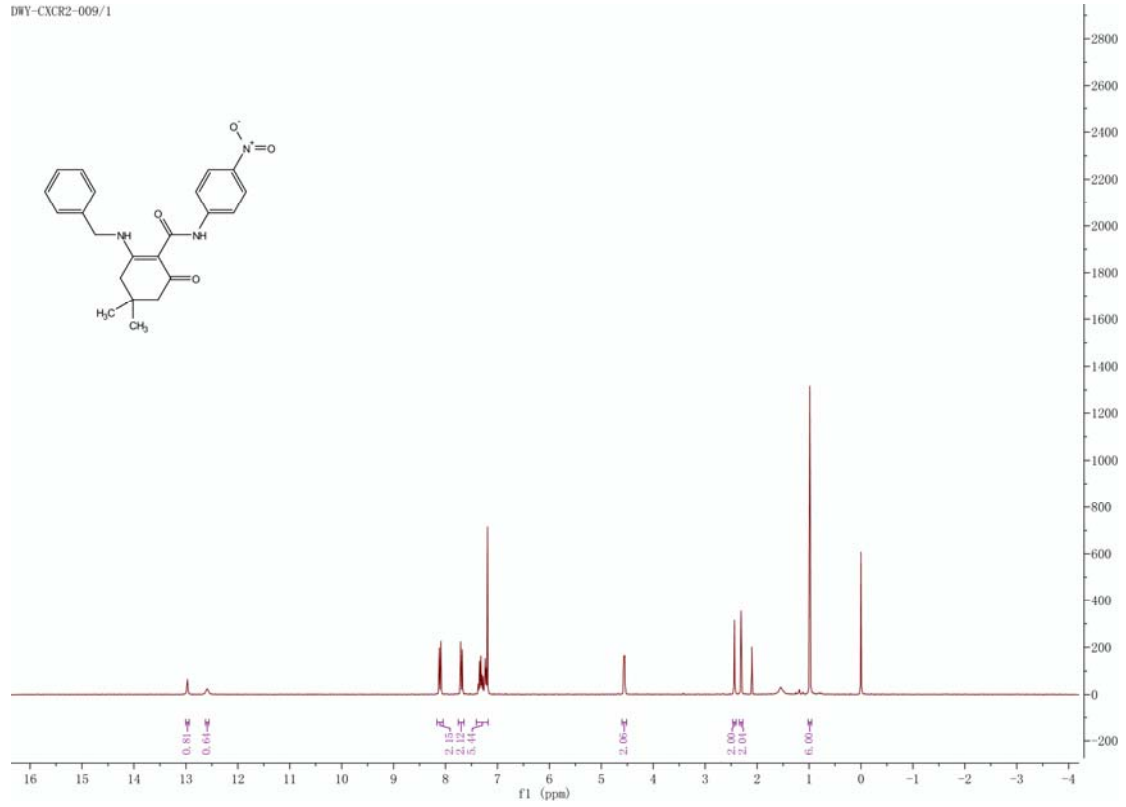
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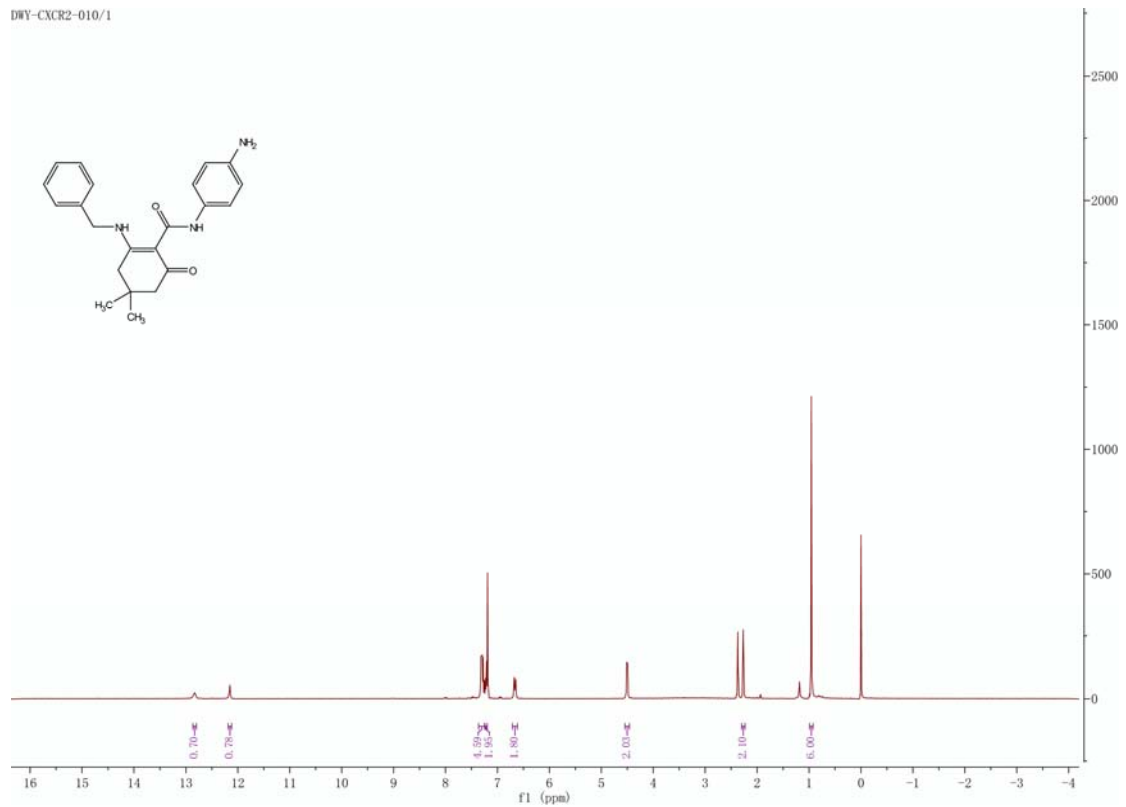
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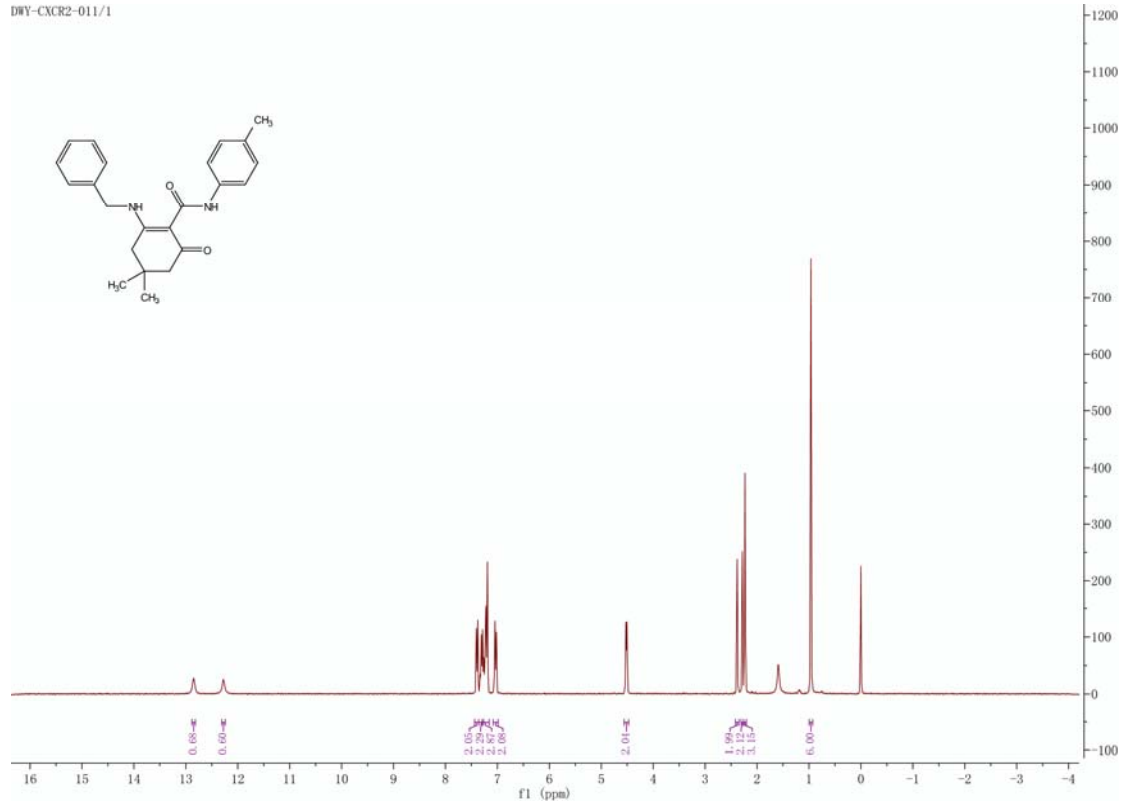
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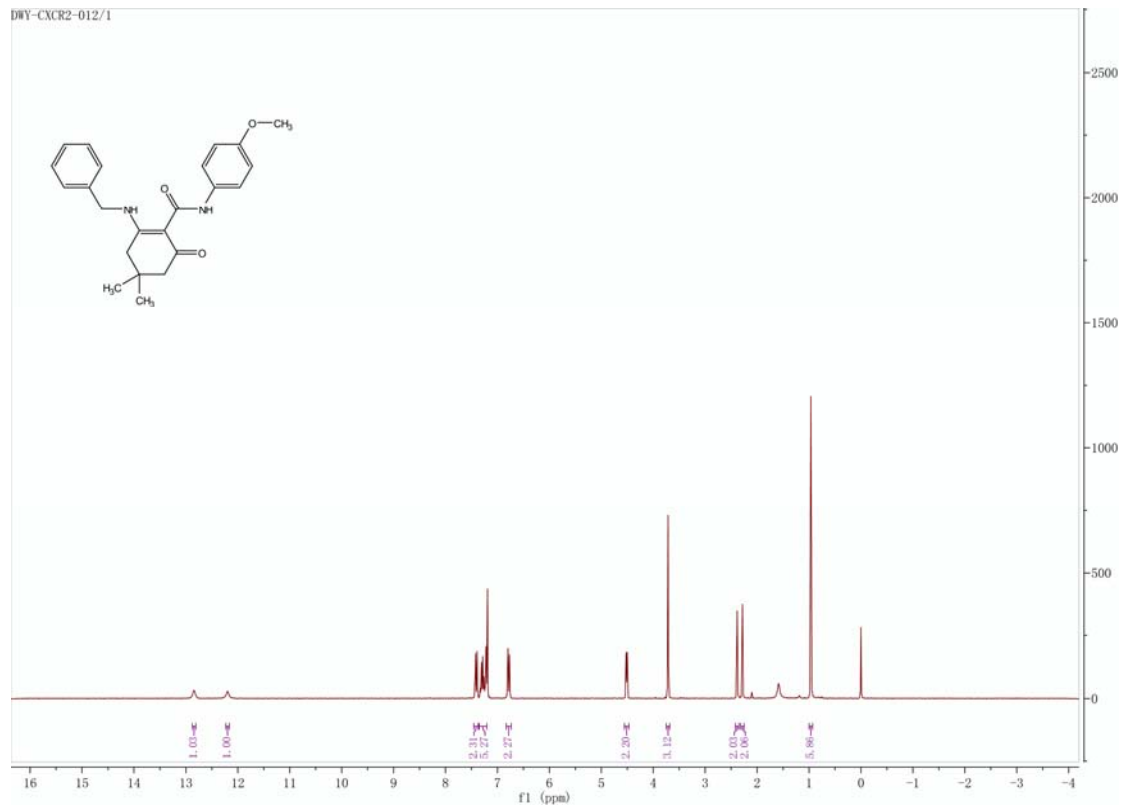
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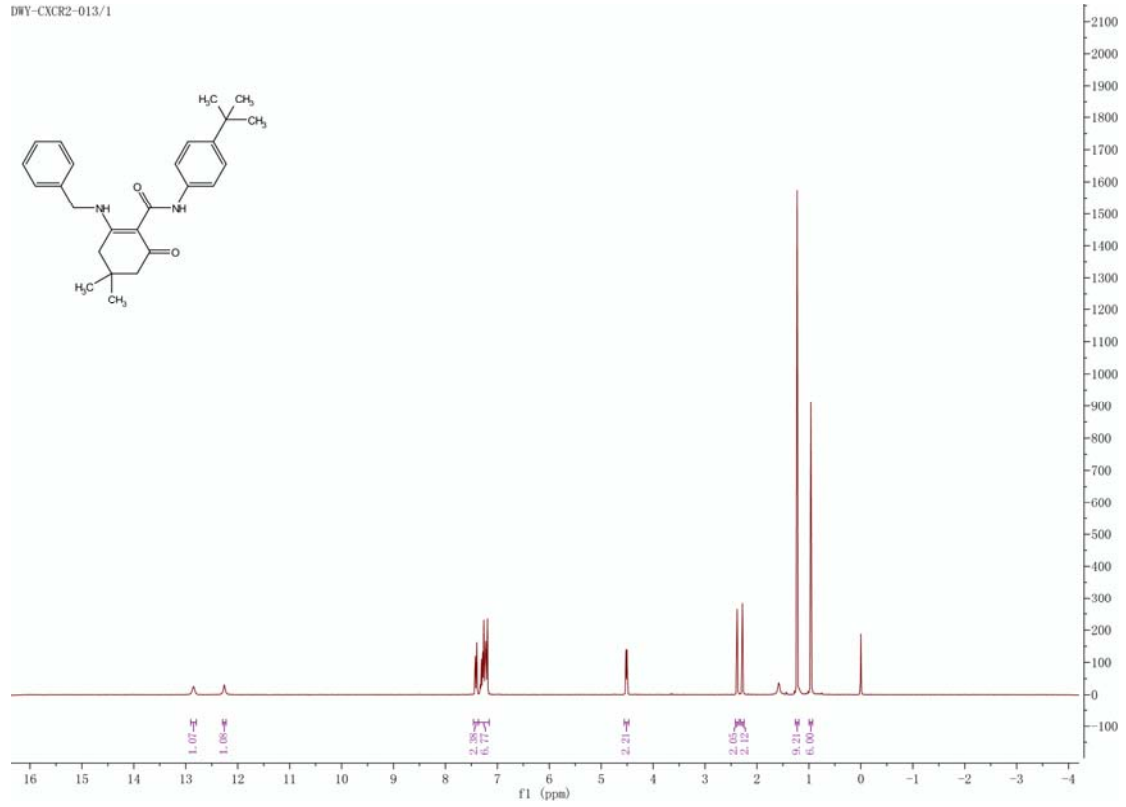
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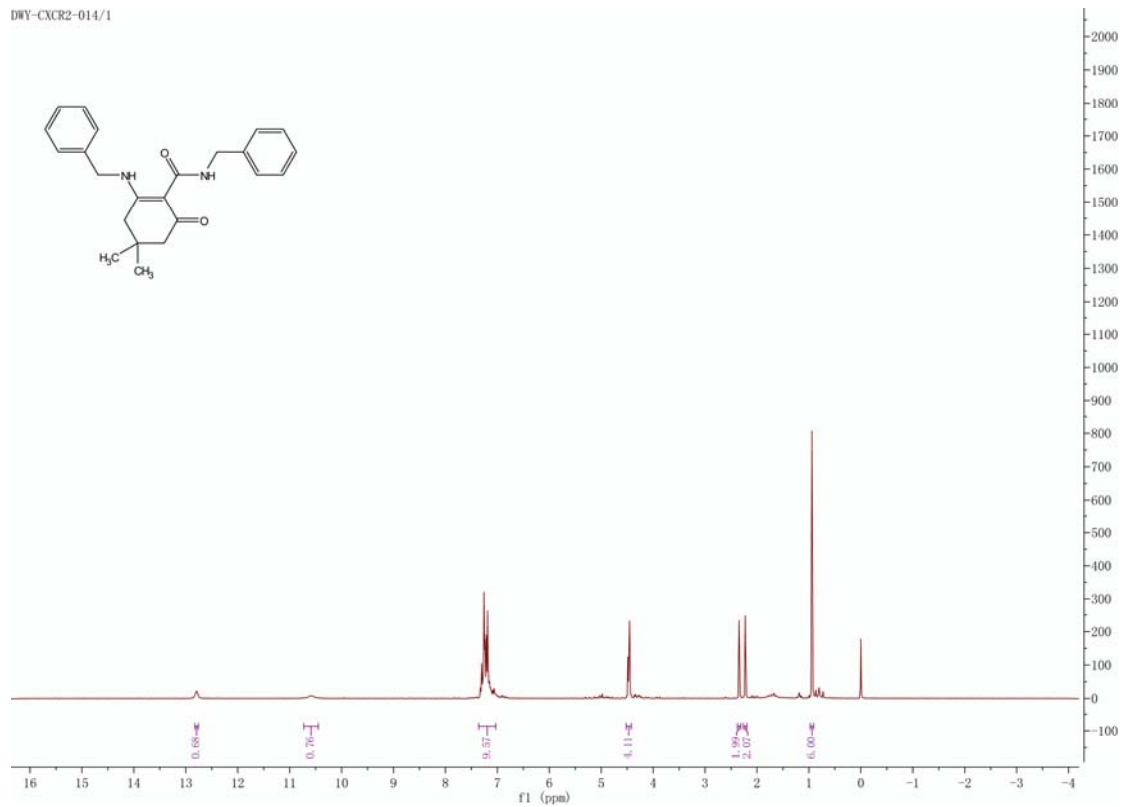
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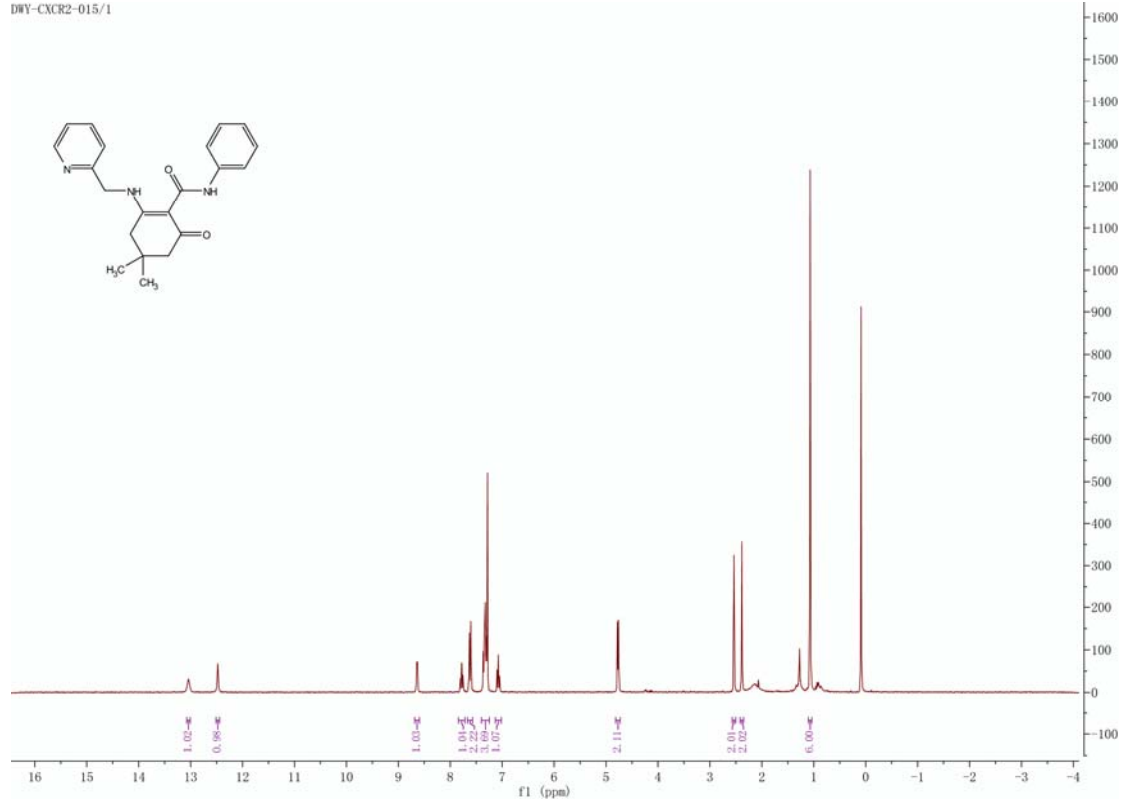
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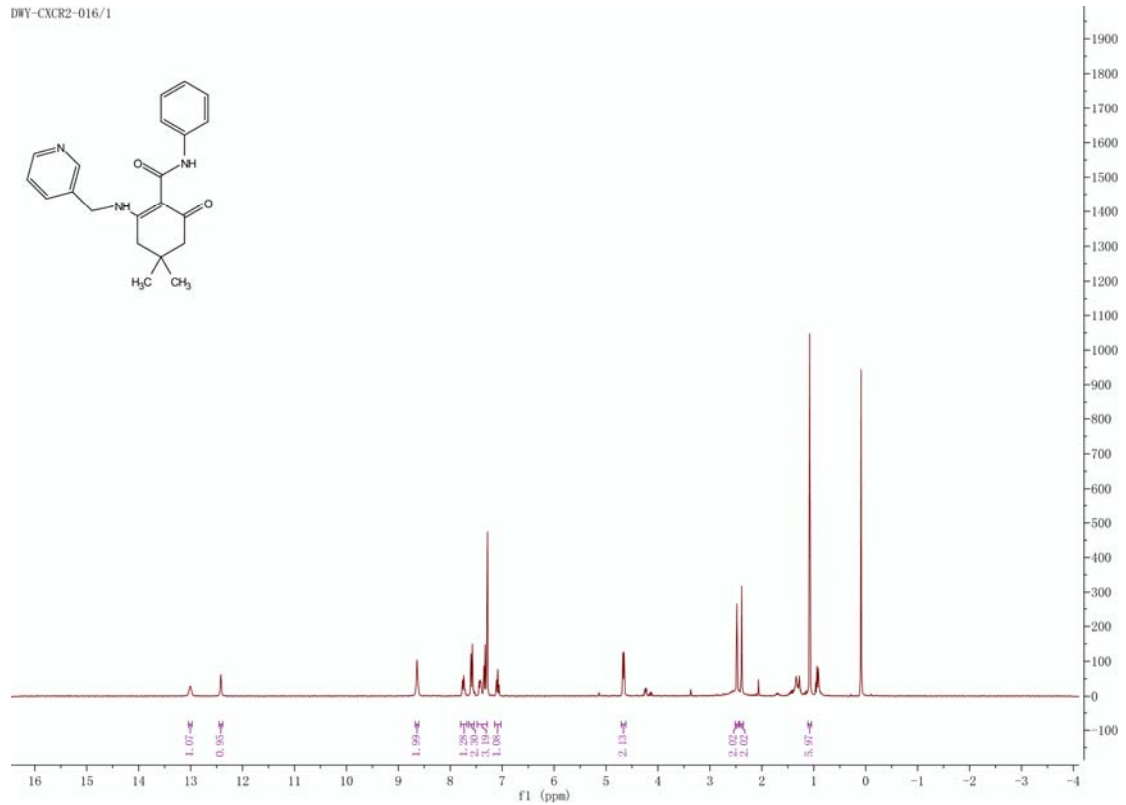
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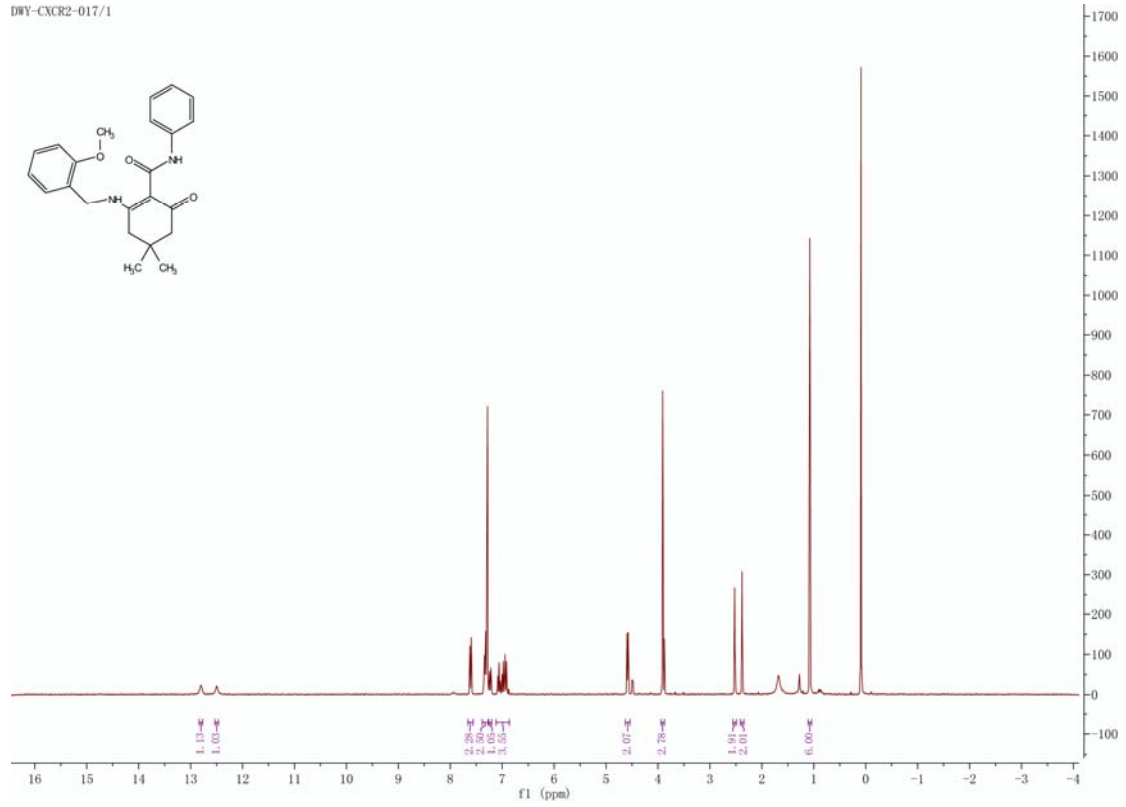
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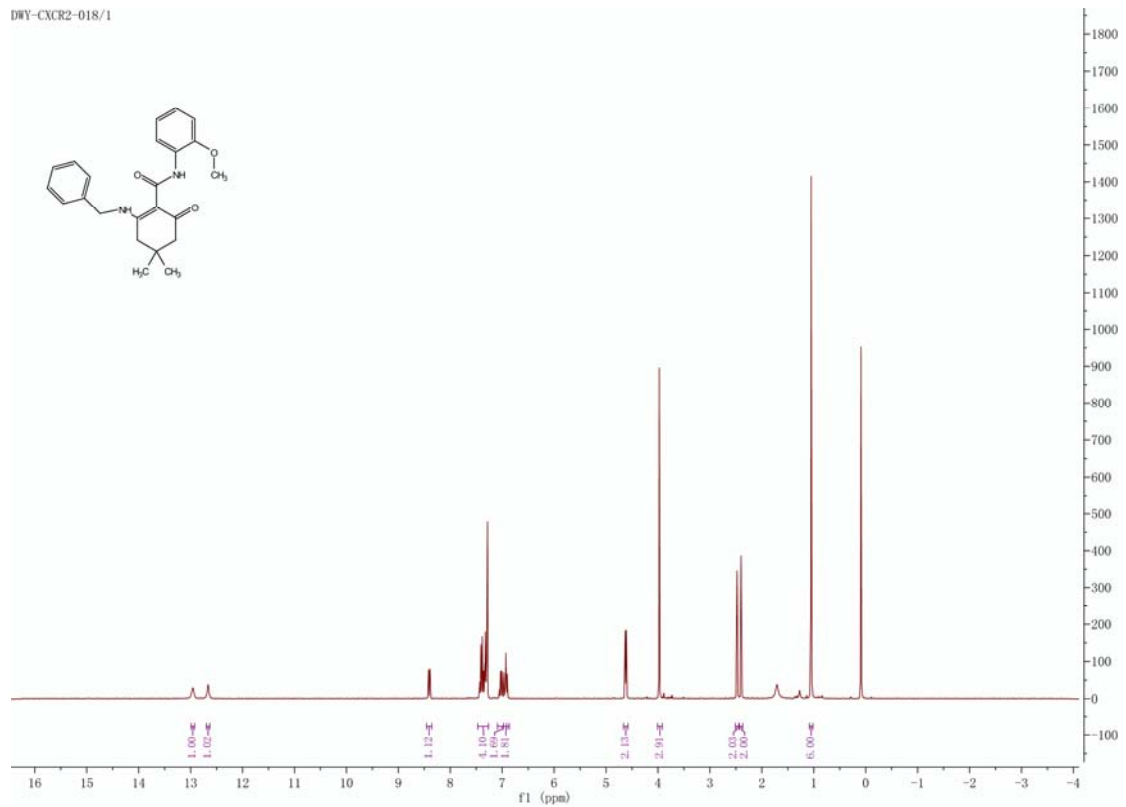
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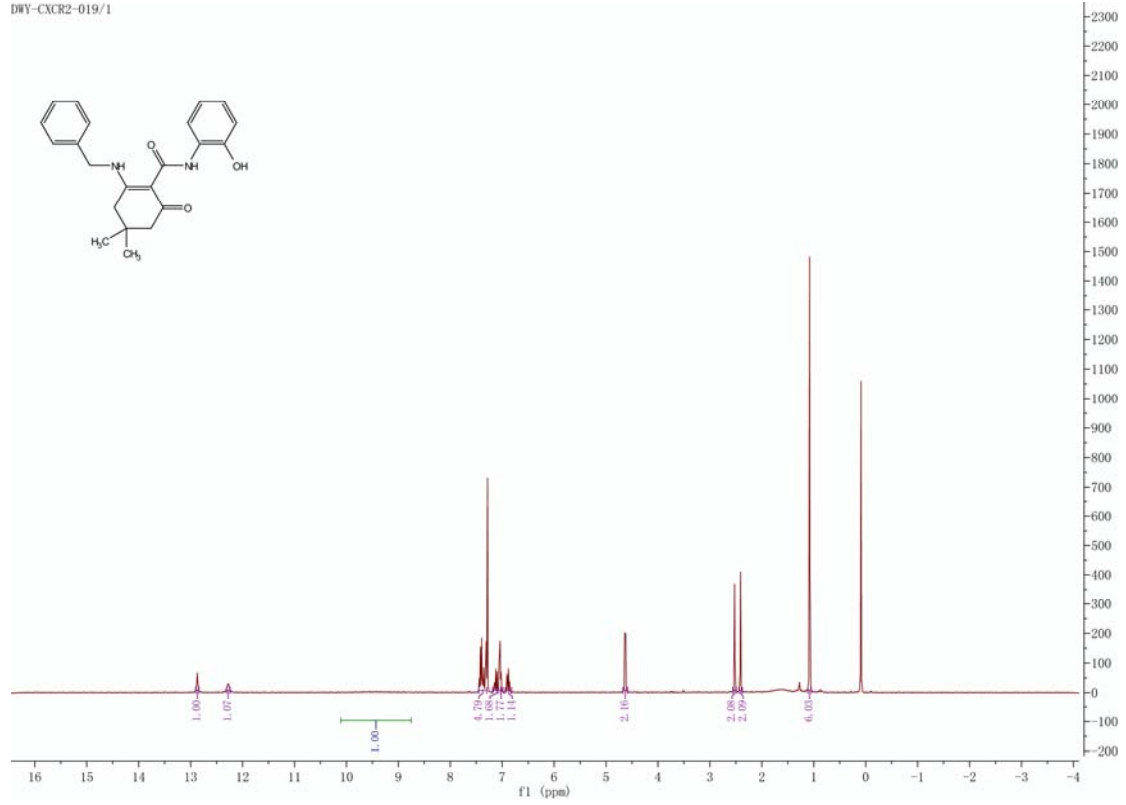
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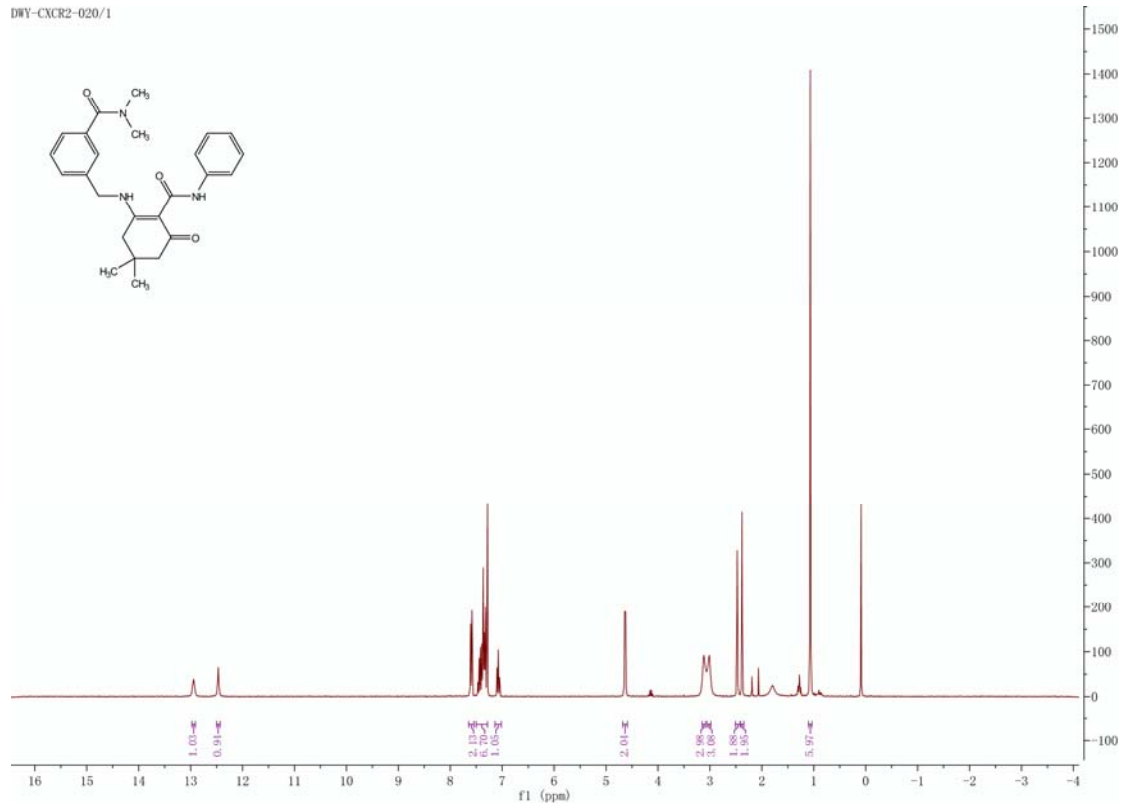
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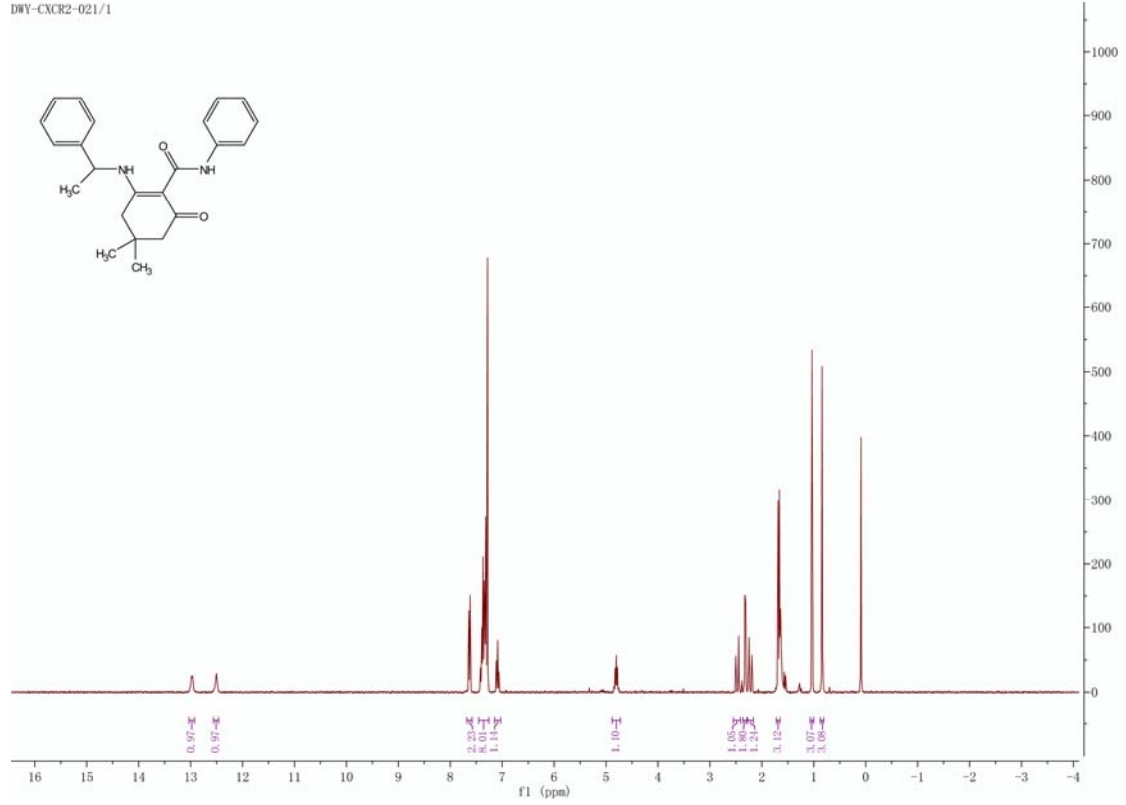
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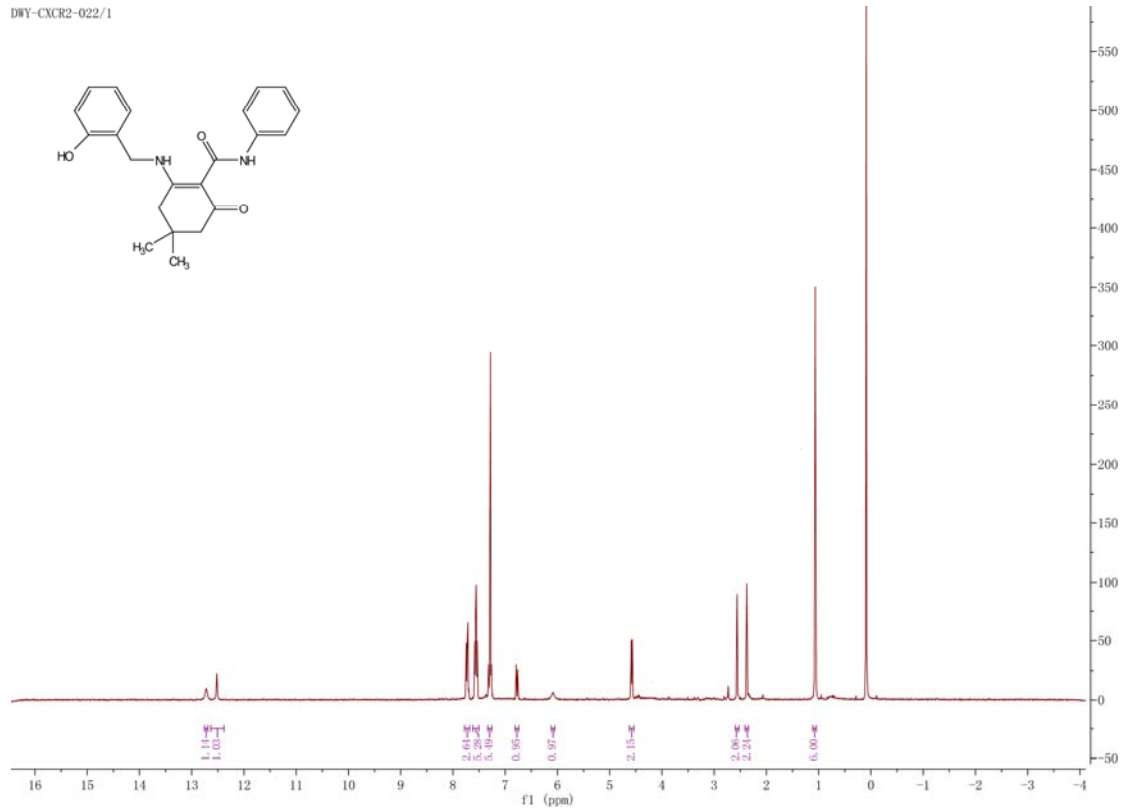
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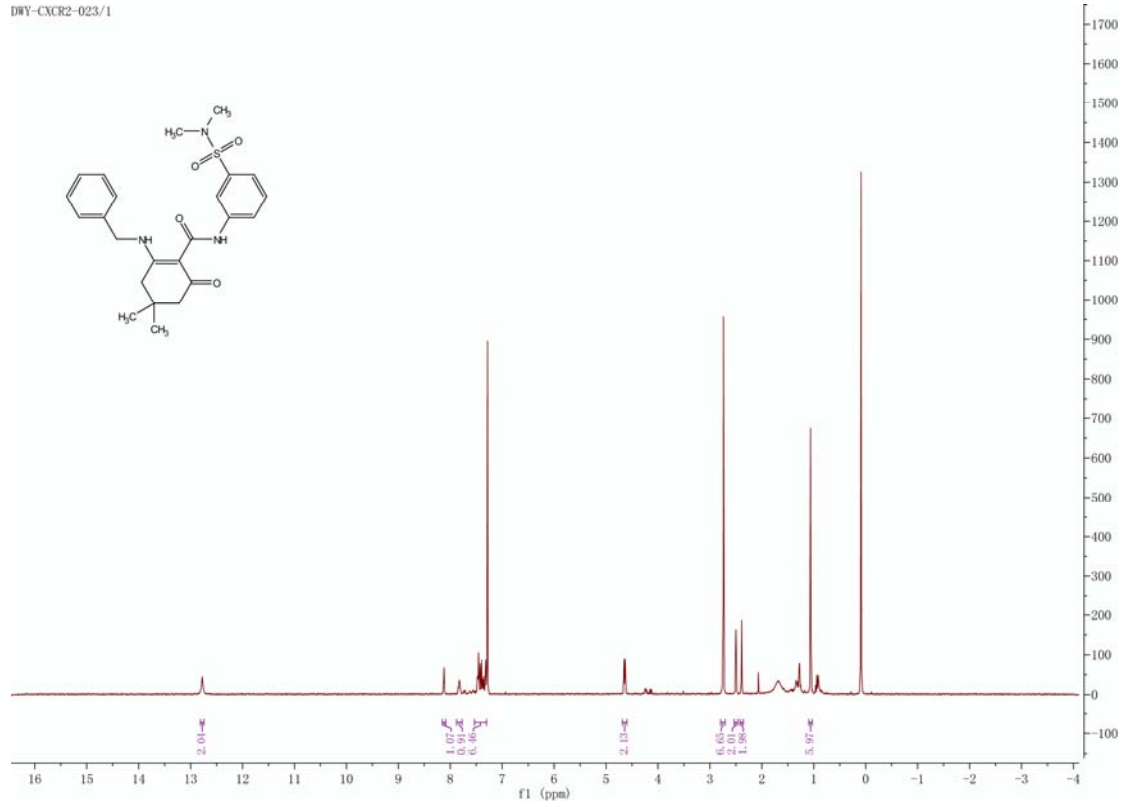
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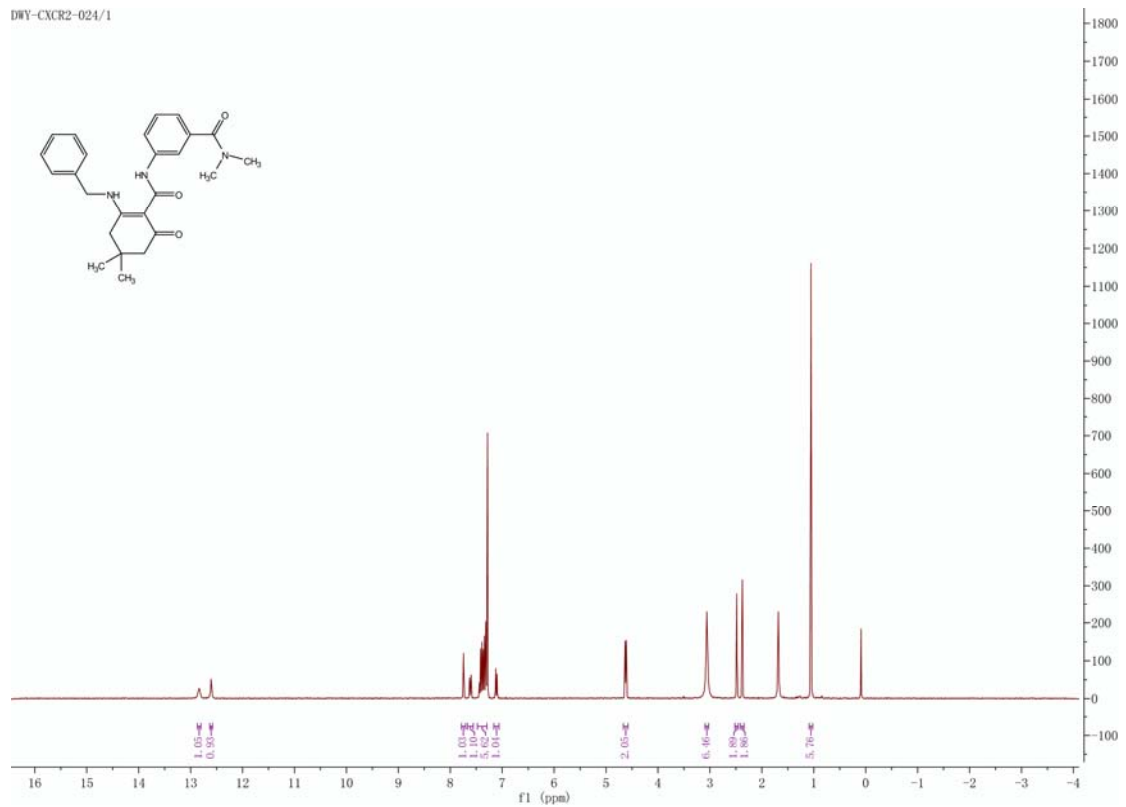
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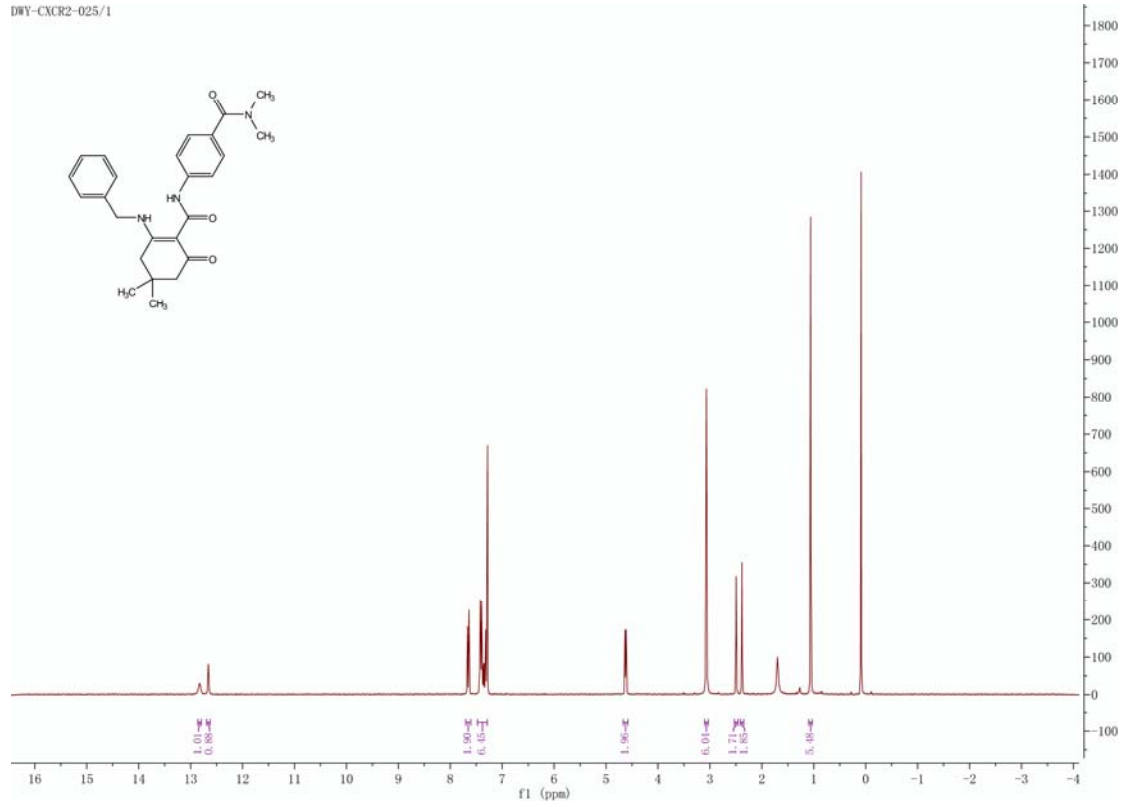
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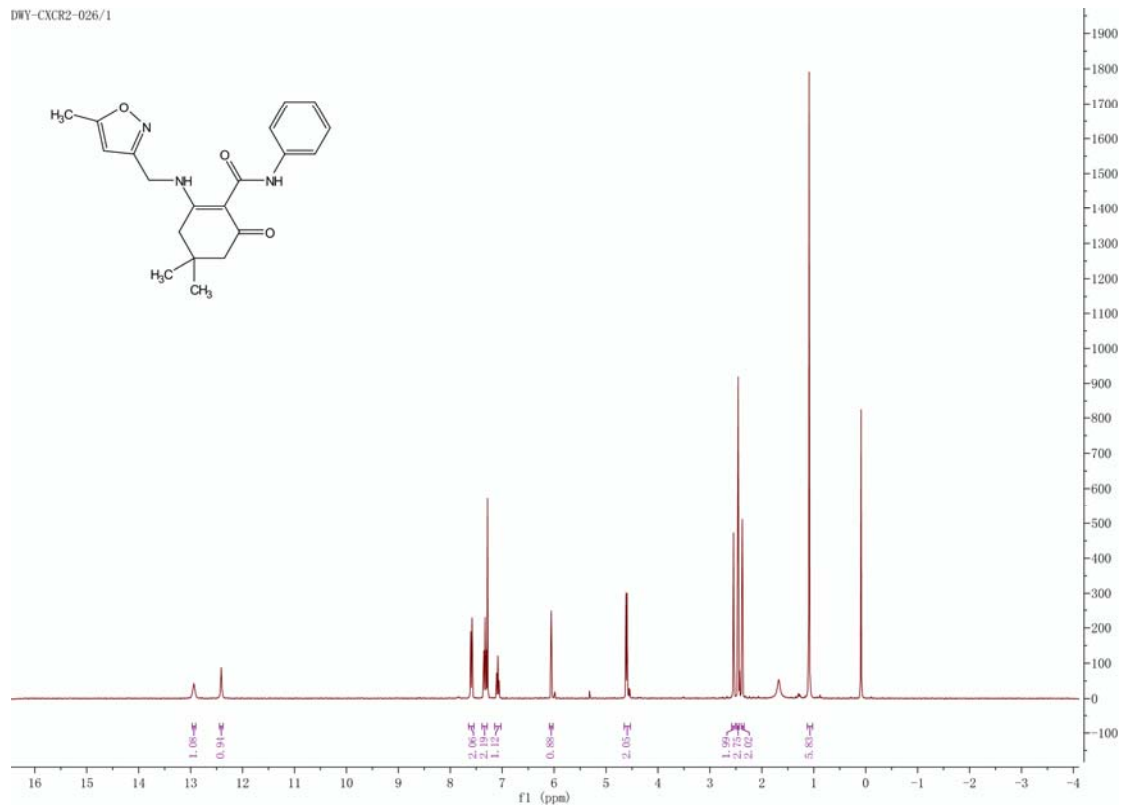
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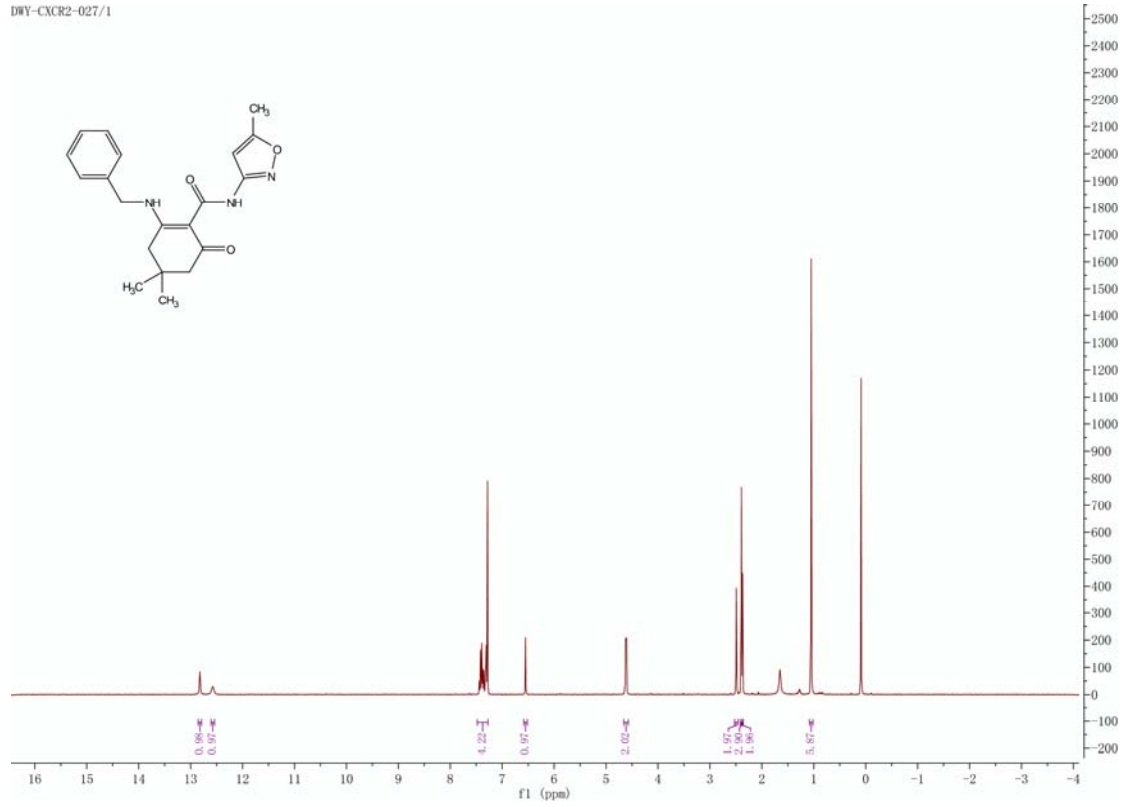
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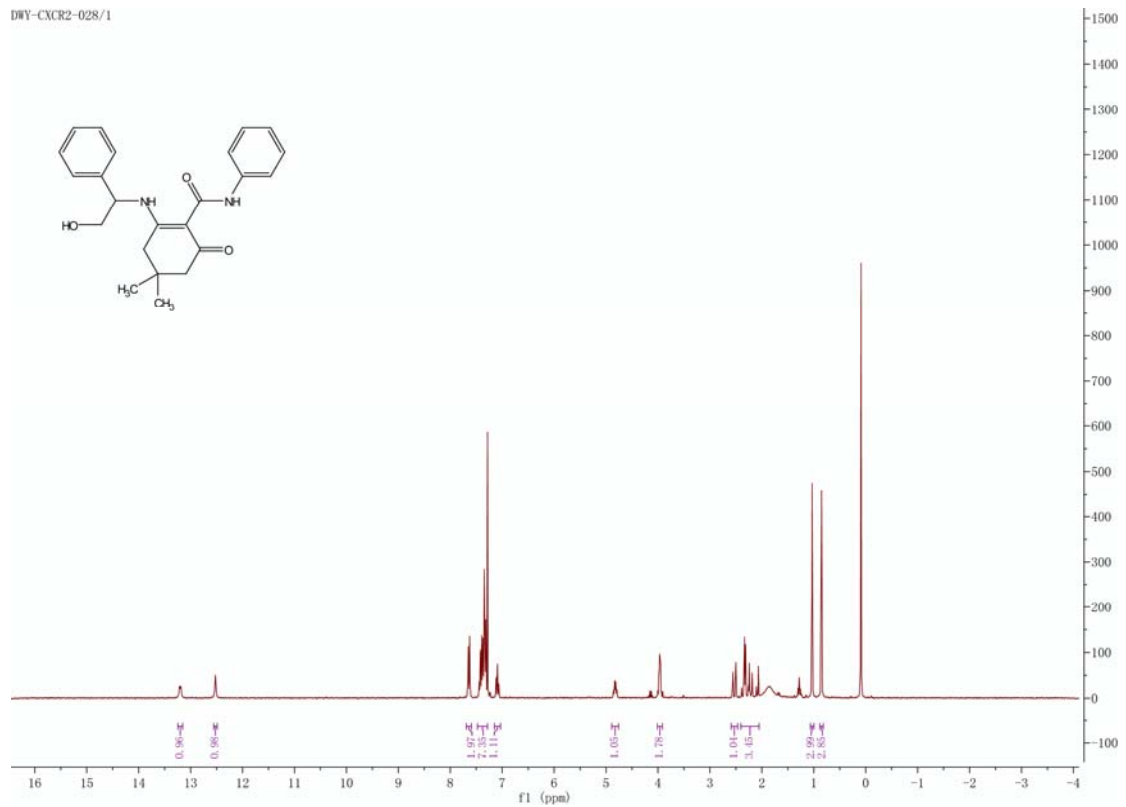
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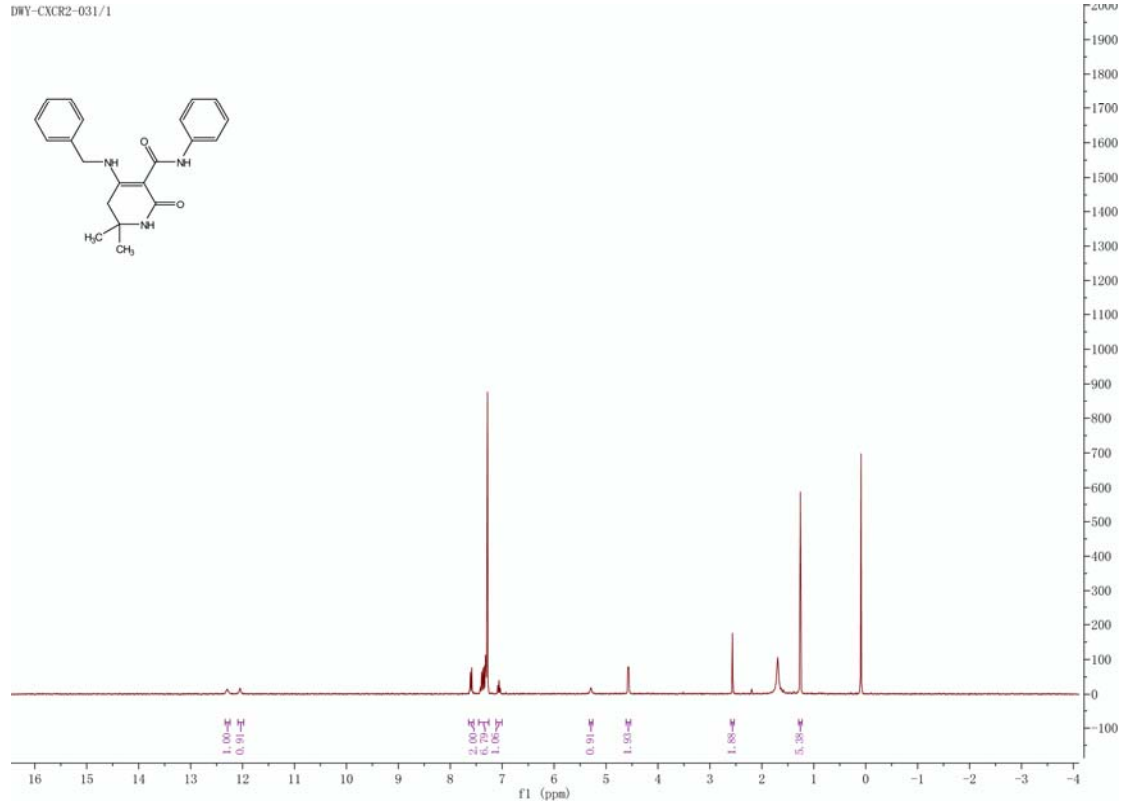
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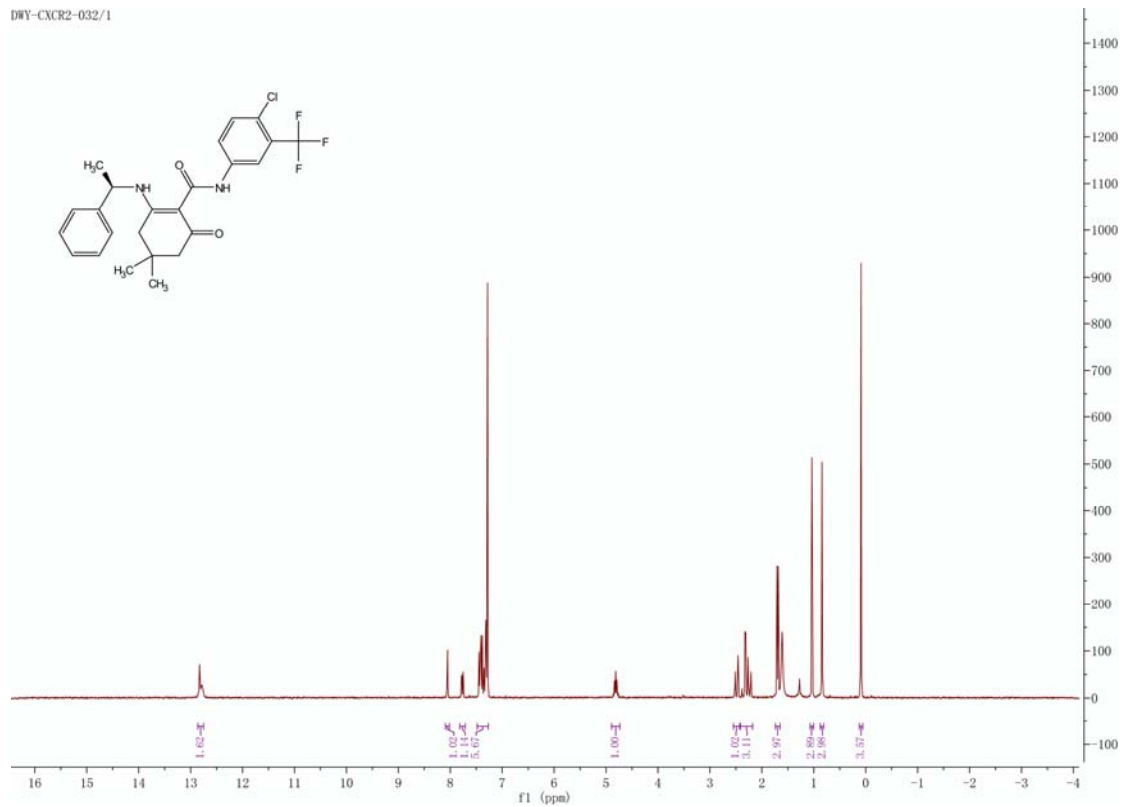
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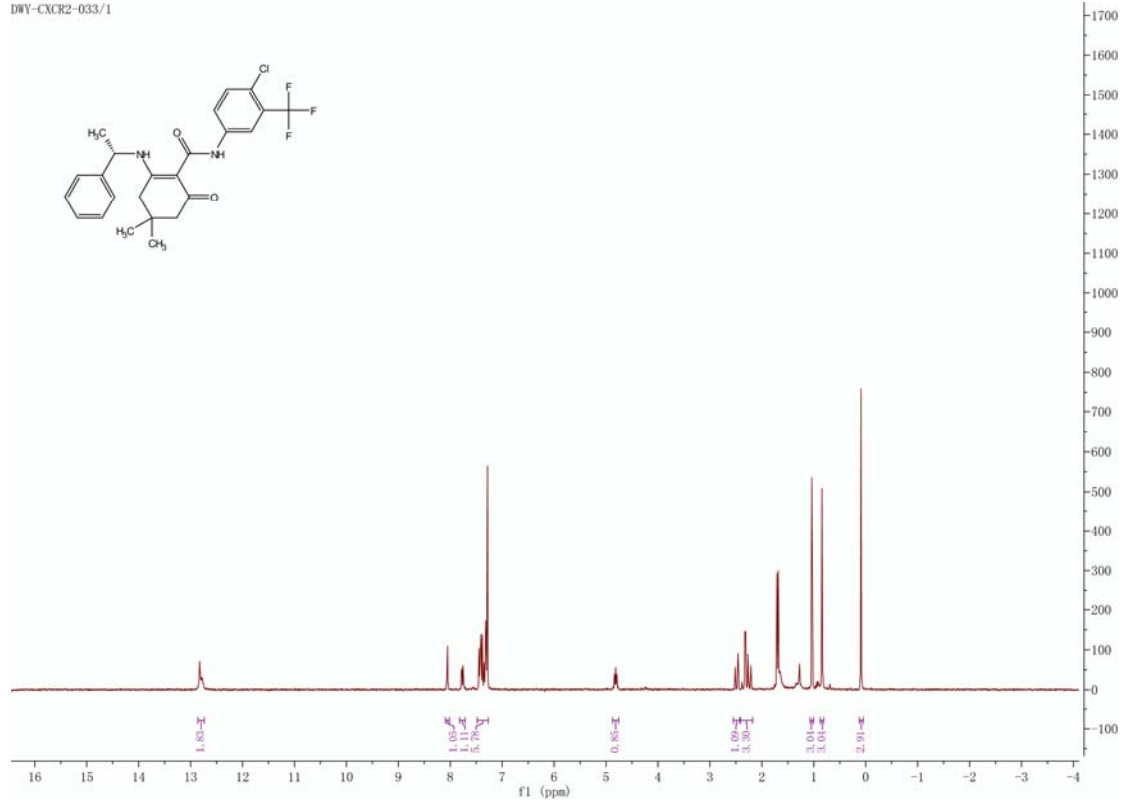
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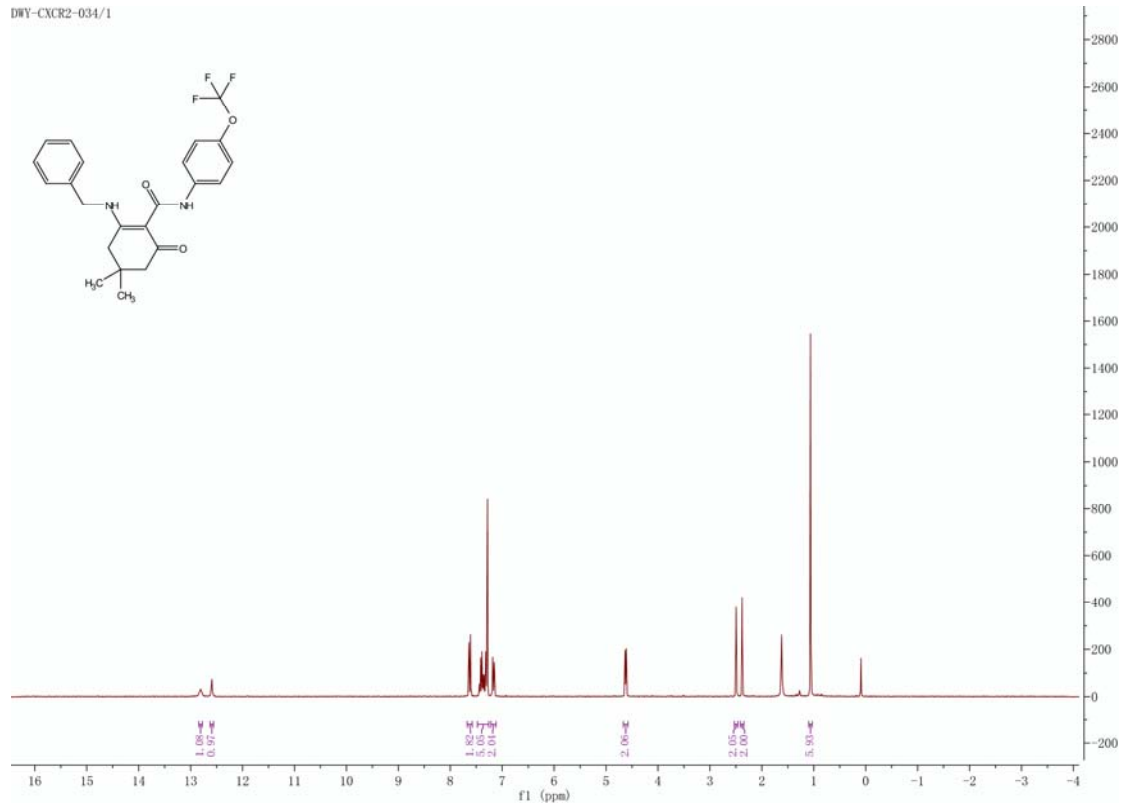
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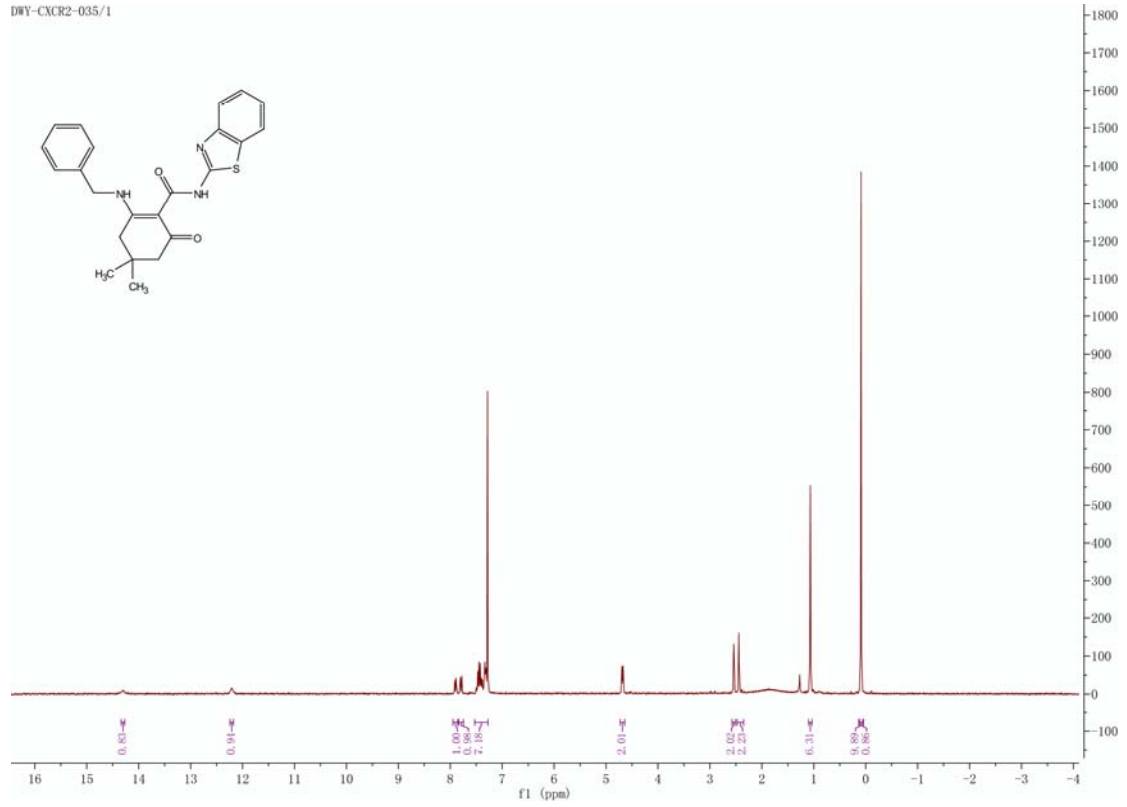
DIY-CXCR2-033/1



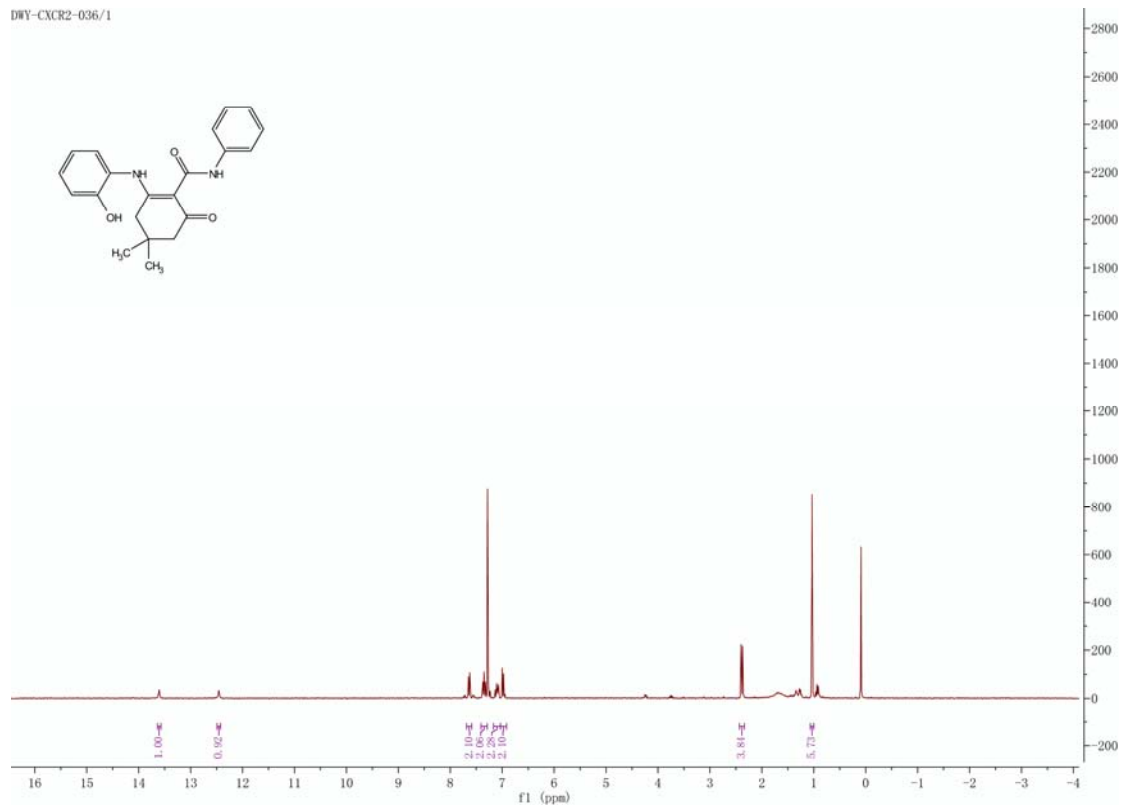
DIY-CXCR2-034/1



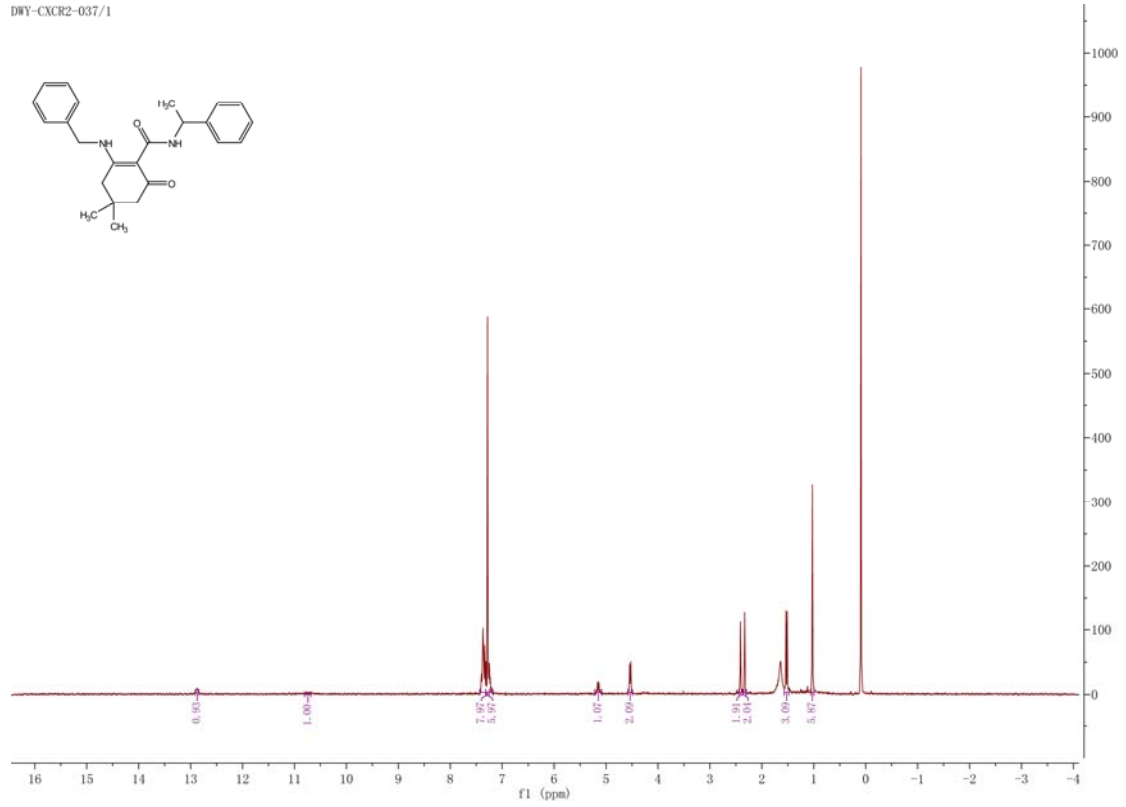
DIY-CXCR2-035/1



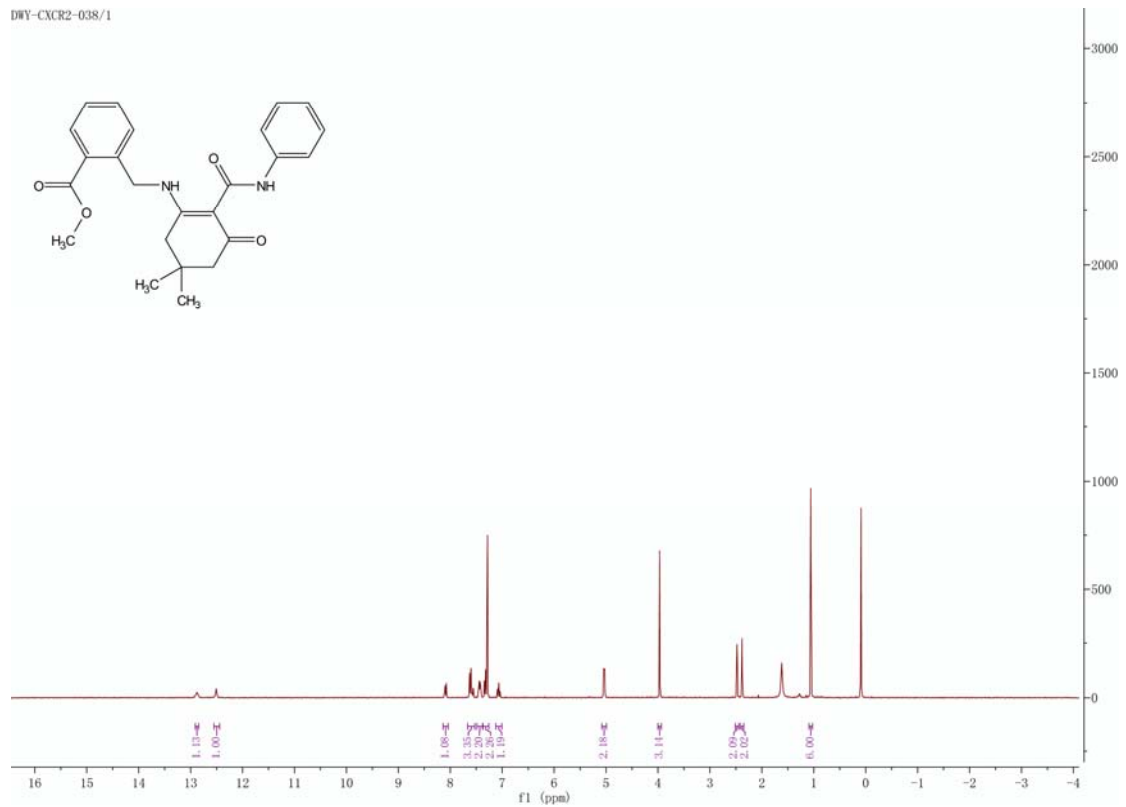
DIY-CXCR2-036/1



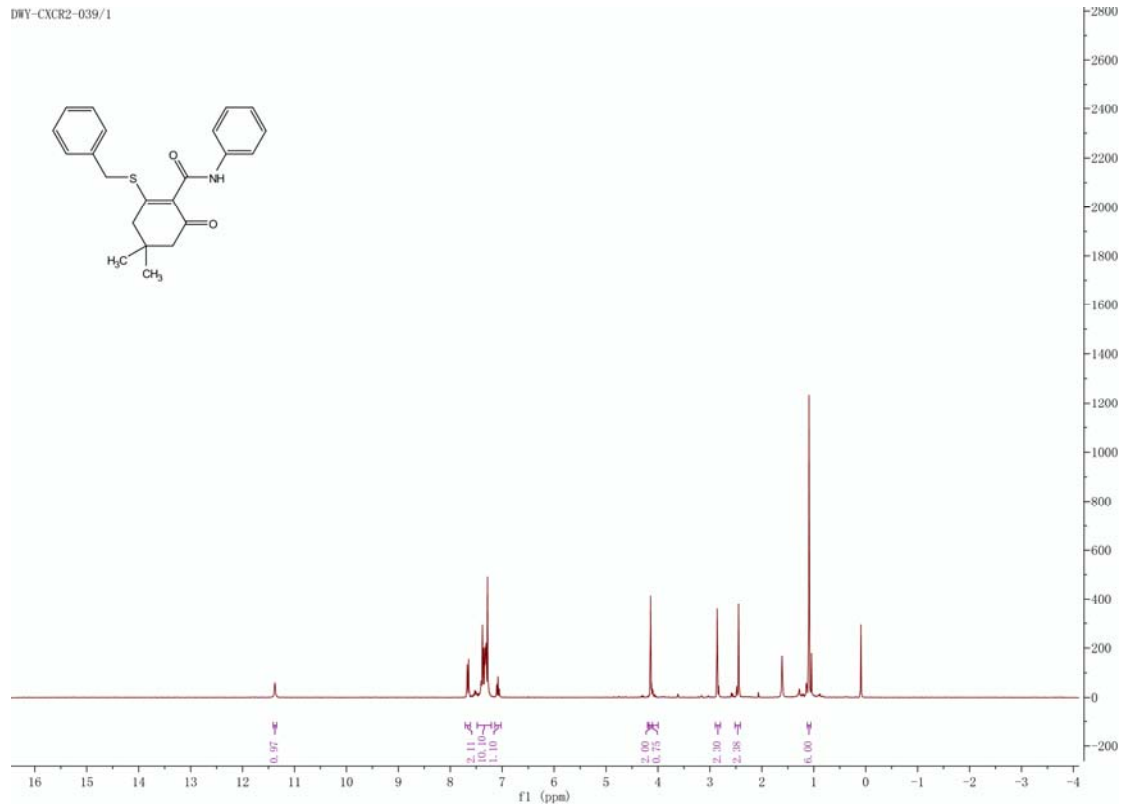
DIY-CXCR2-037/1



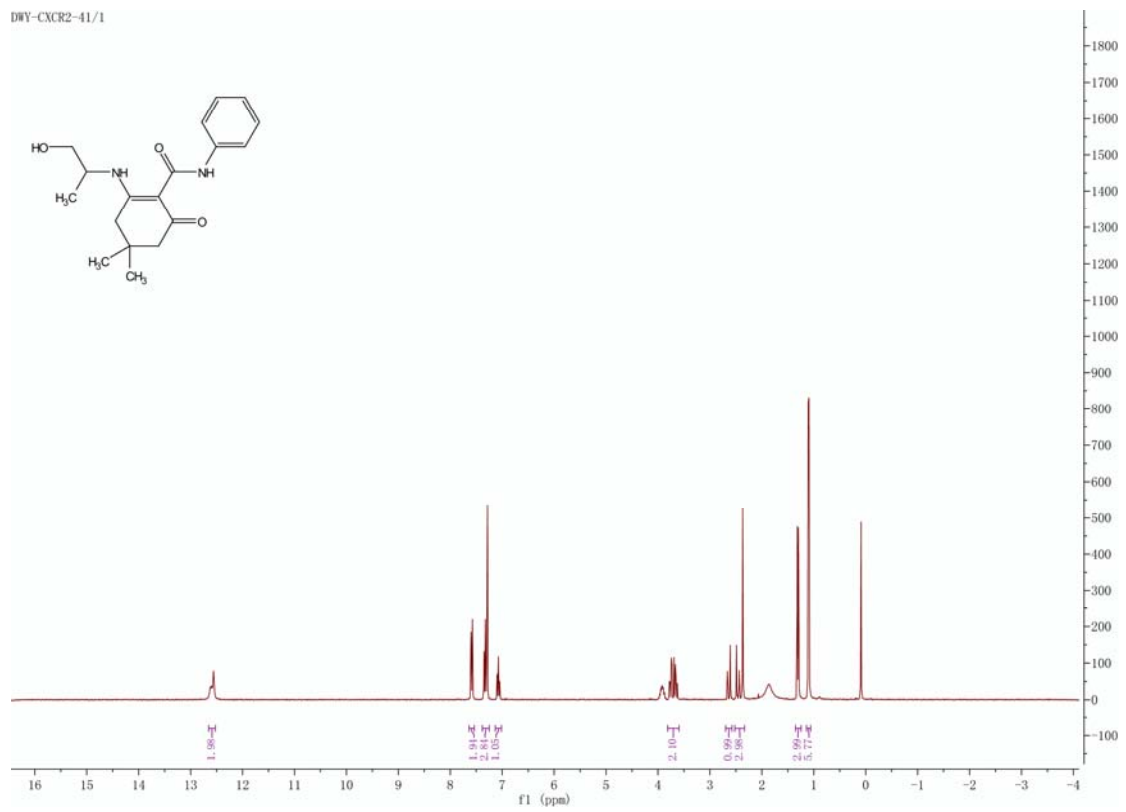
DIY-CXCR2-038/1



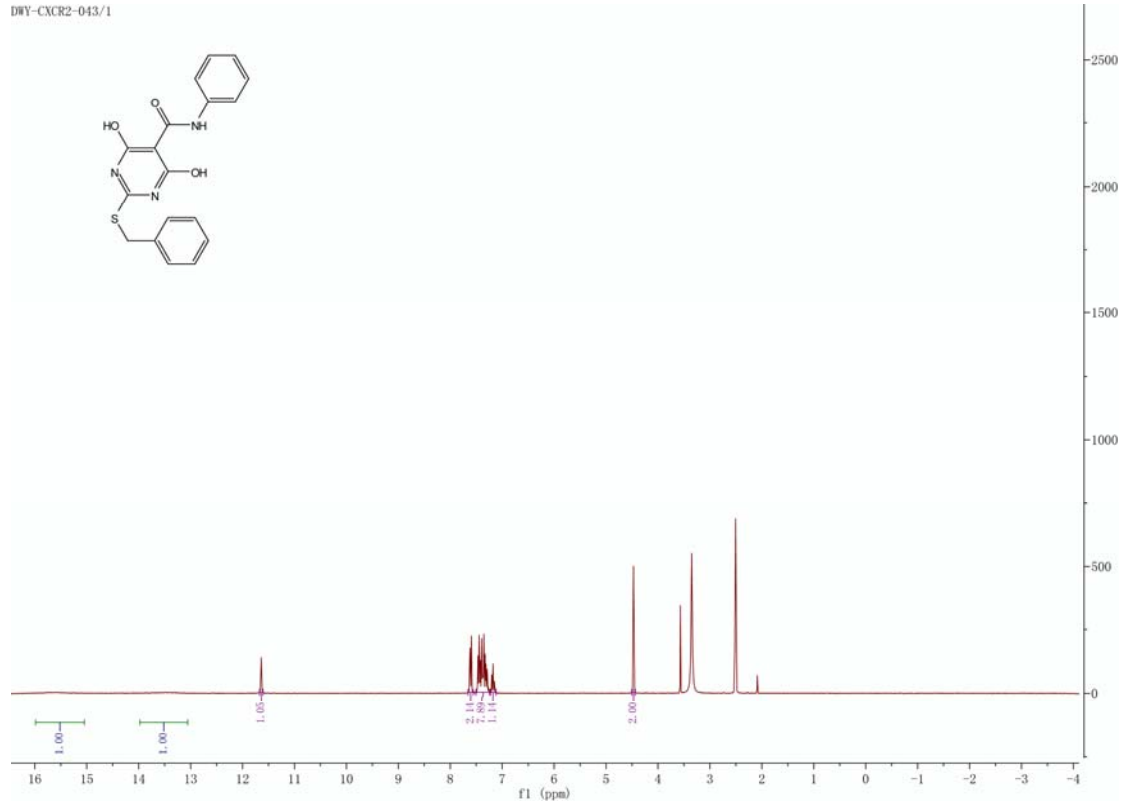
DIY-CXCR2-039/1



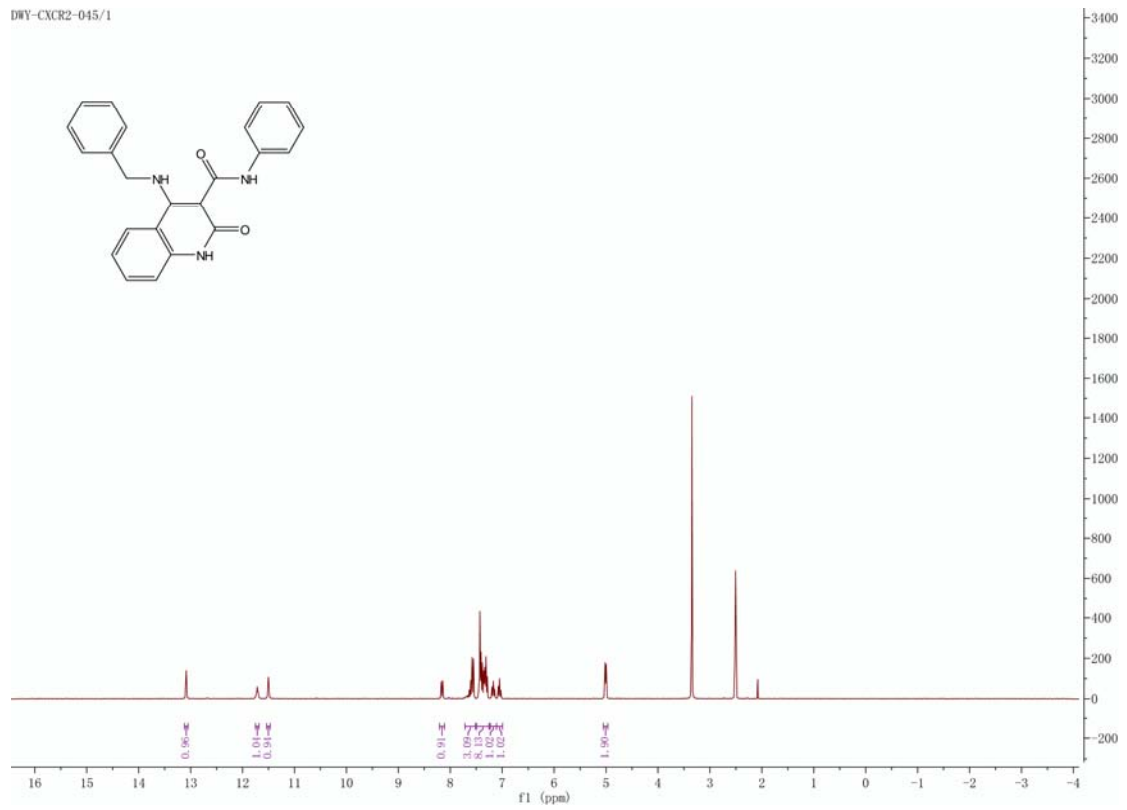
DIY-CXCR2-41/1



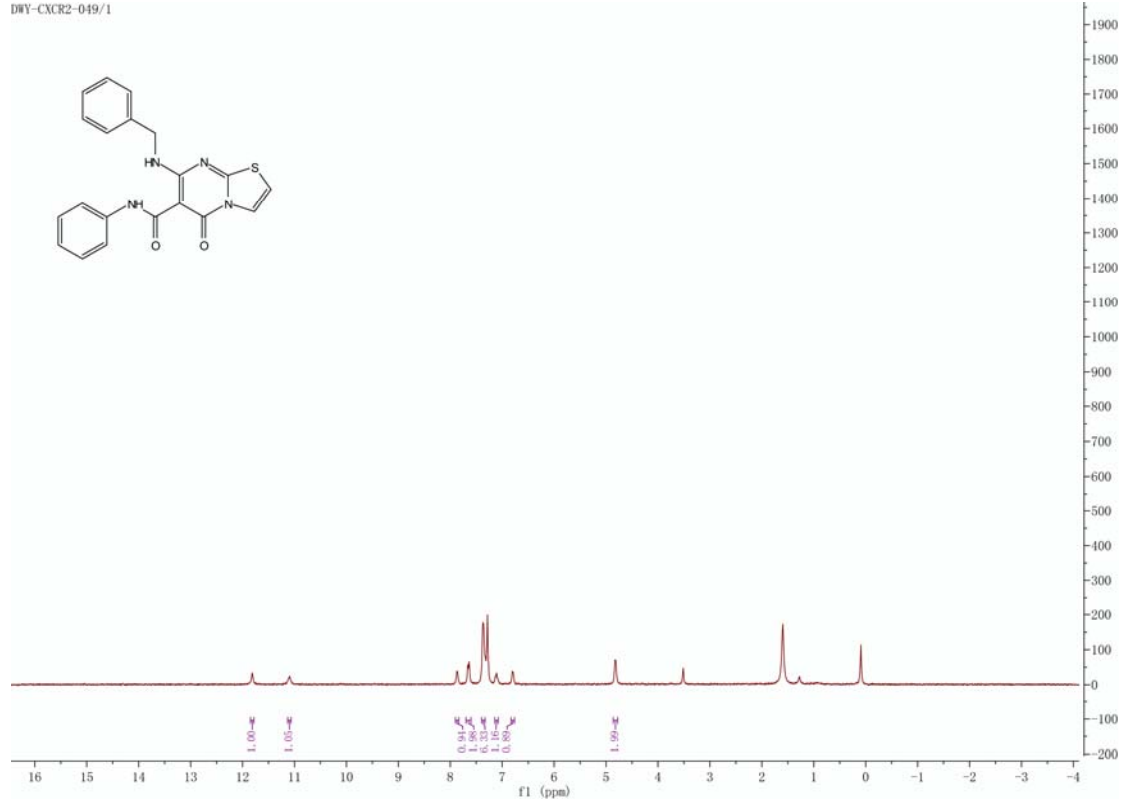
DIY-CXCR2-043/1



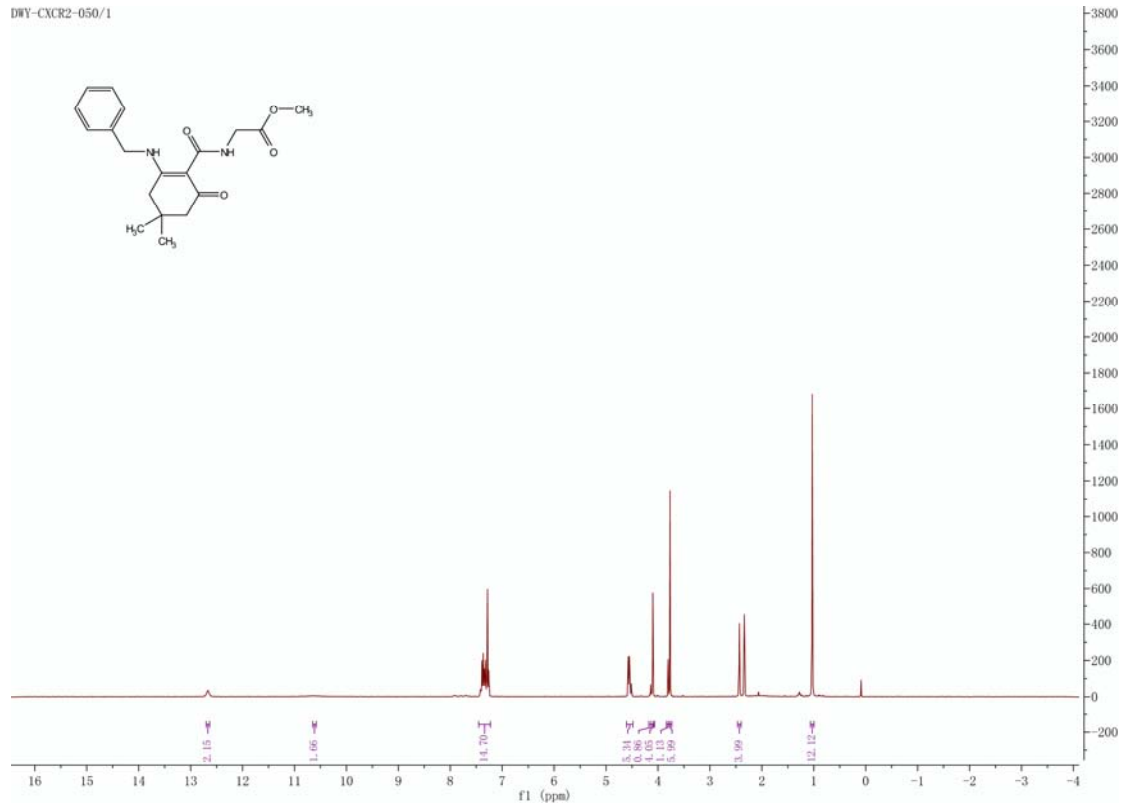
DIY-CXCR2-045/1



DIY-CXCR2-049/1



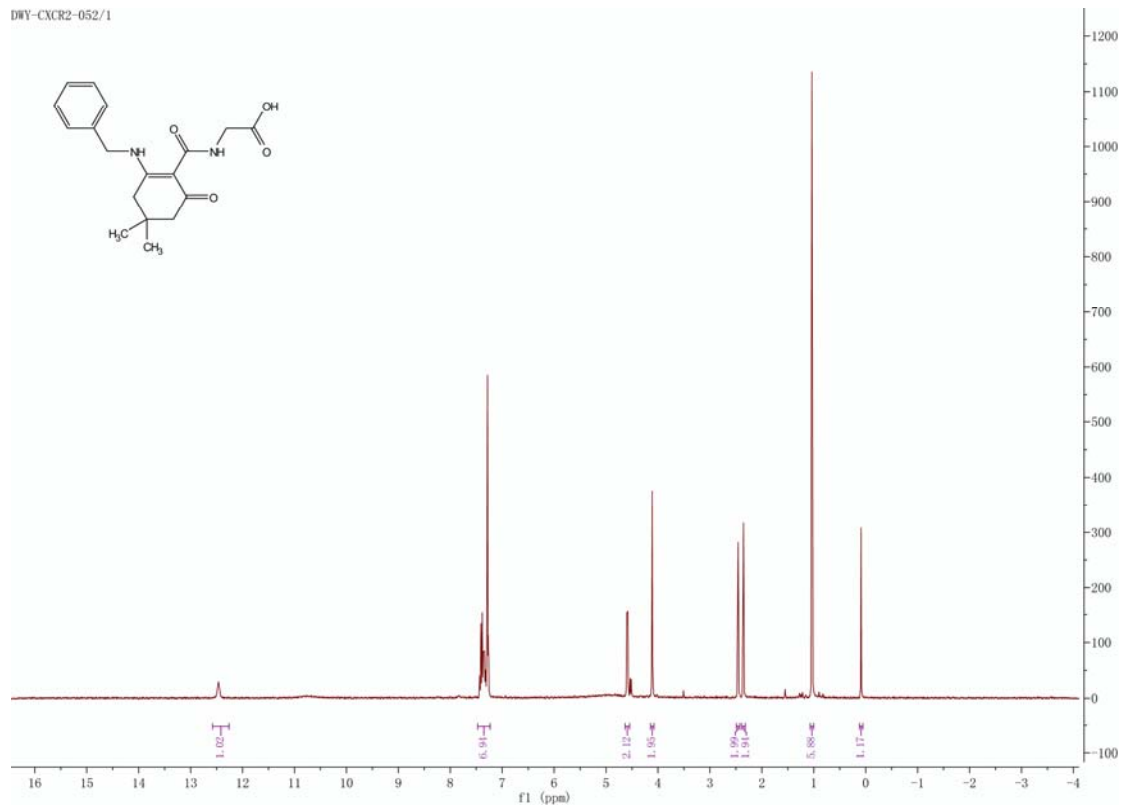
DIY-CXCR2-050/1



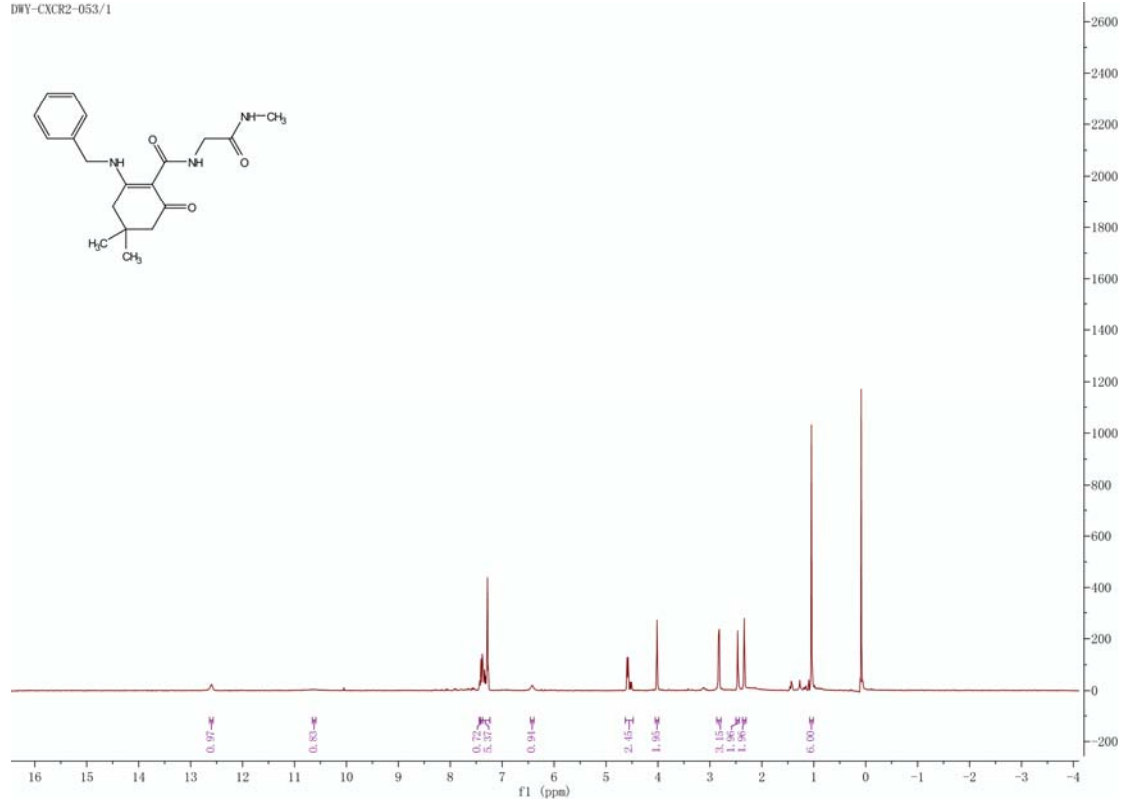
DWY-CXCR2-051 (1/1)



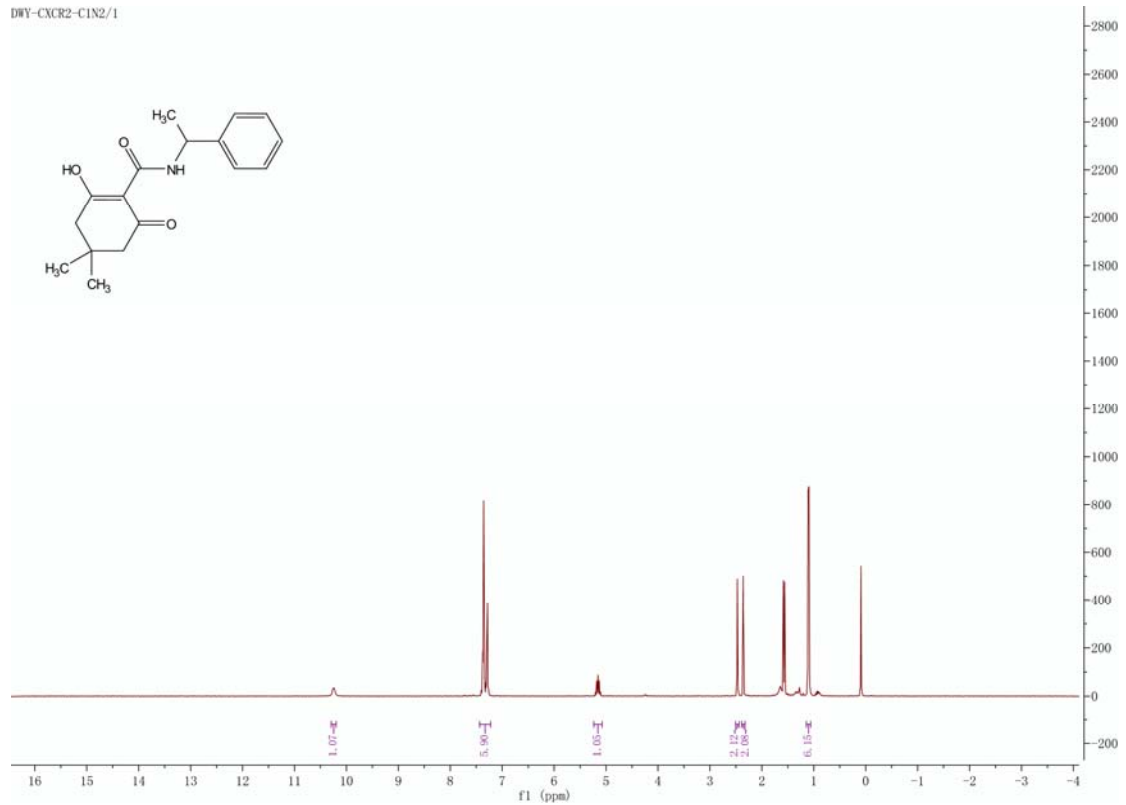
DWY-CXCR2-052/1



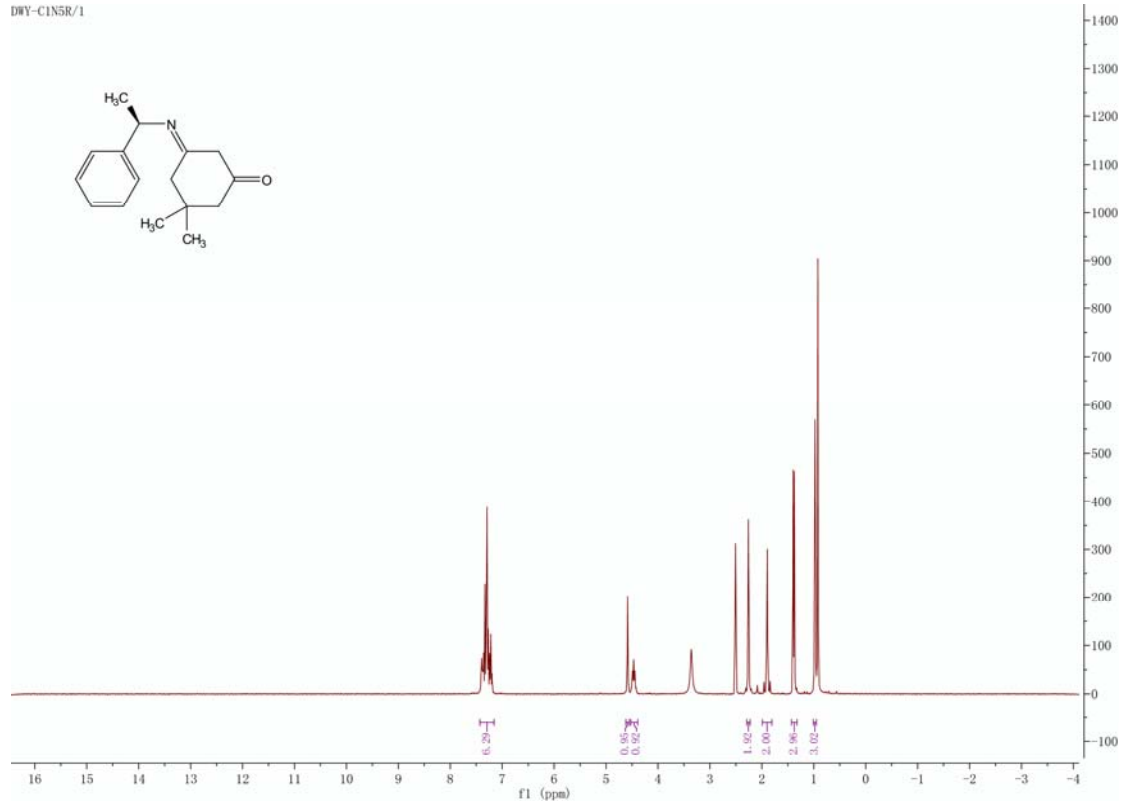
DIY-CXCR2-053/1



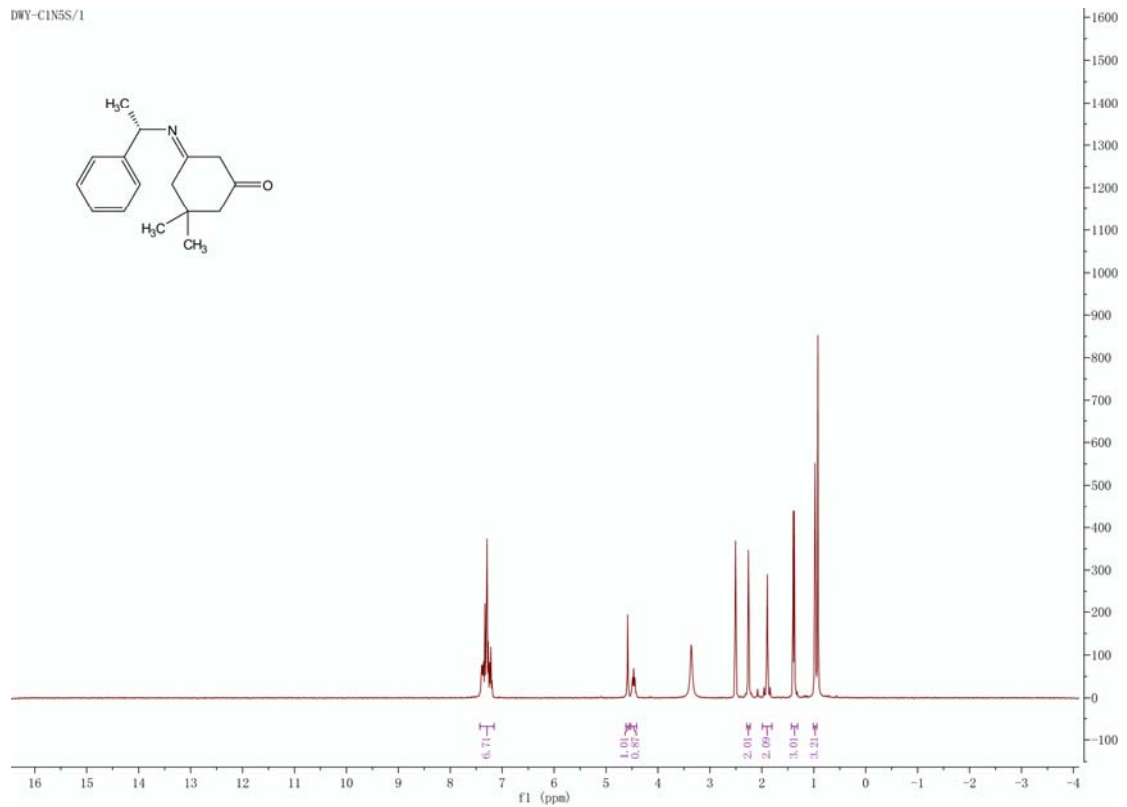
DIY-CXCR2-C1N2/1



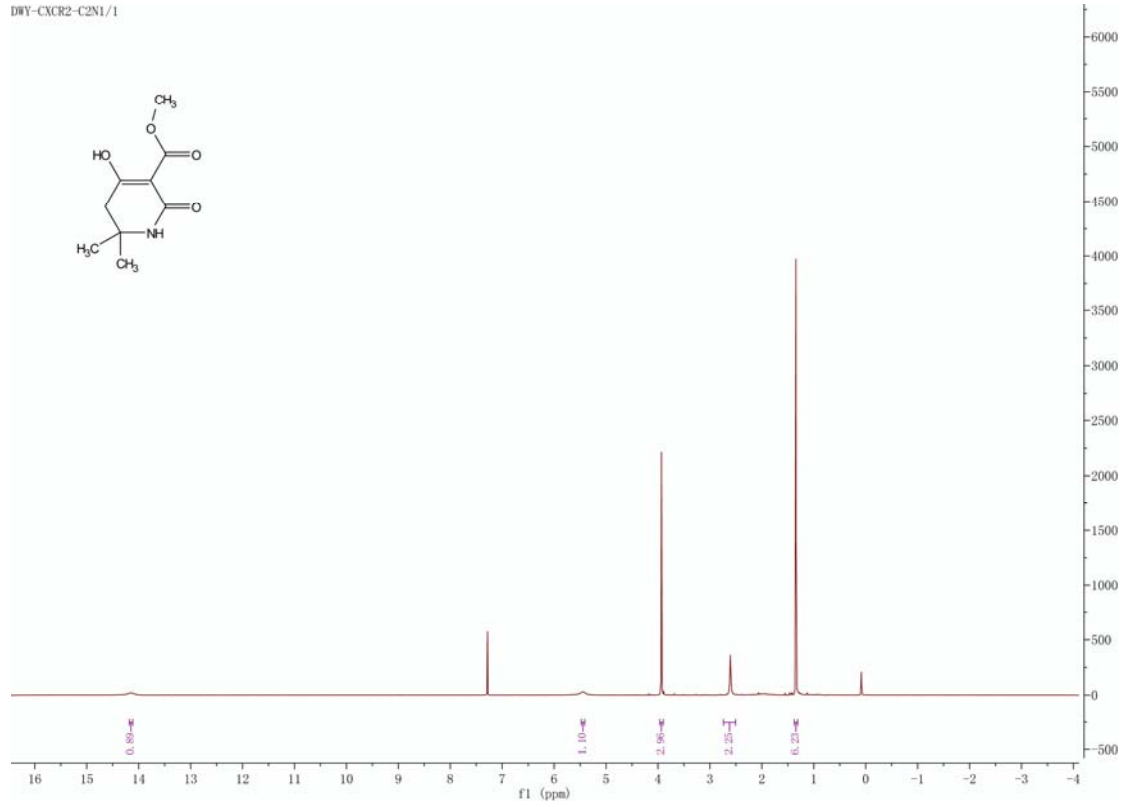
DIY-C1N5R/1



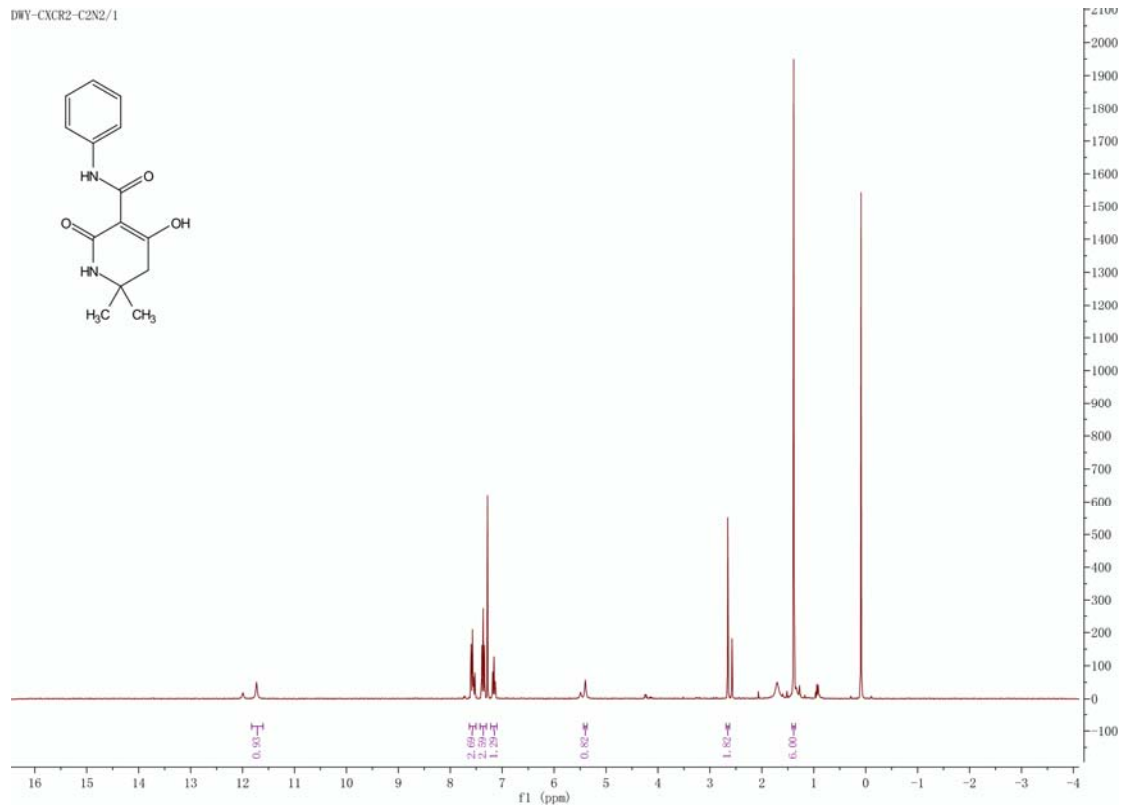
DIY-C1N5S/1



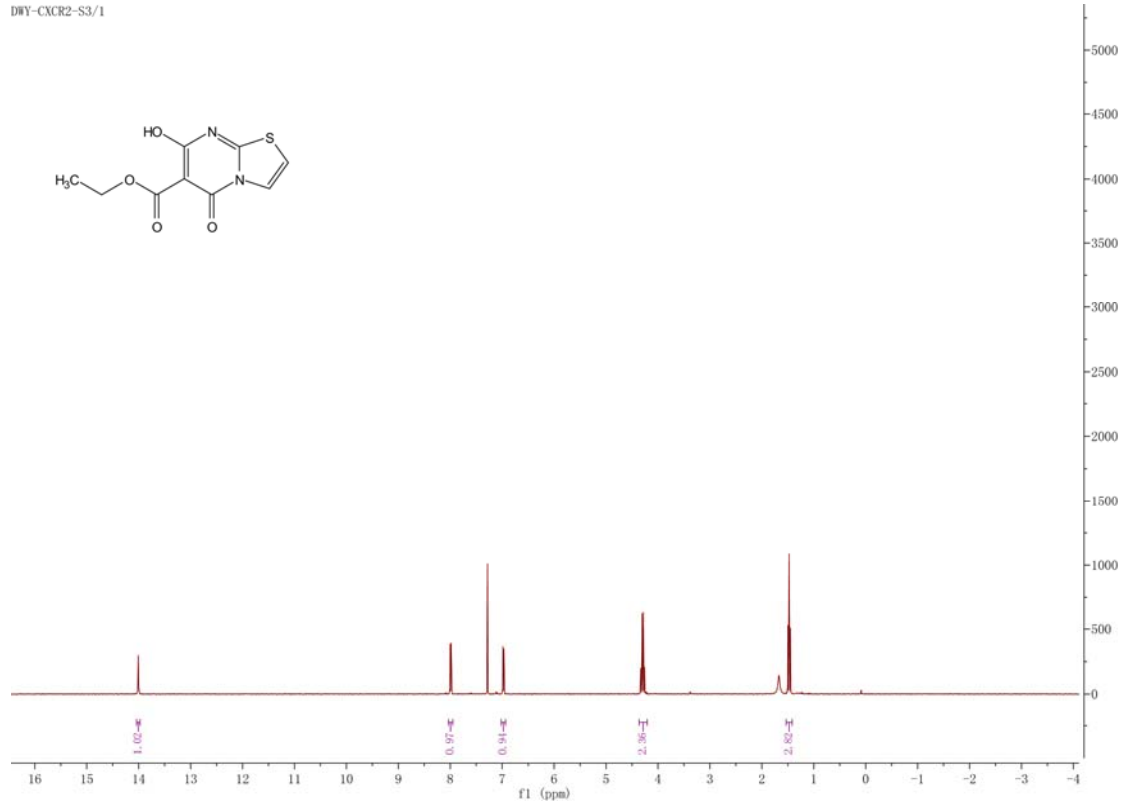
DIY-CXCR2-C2N1/1



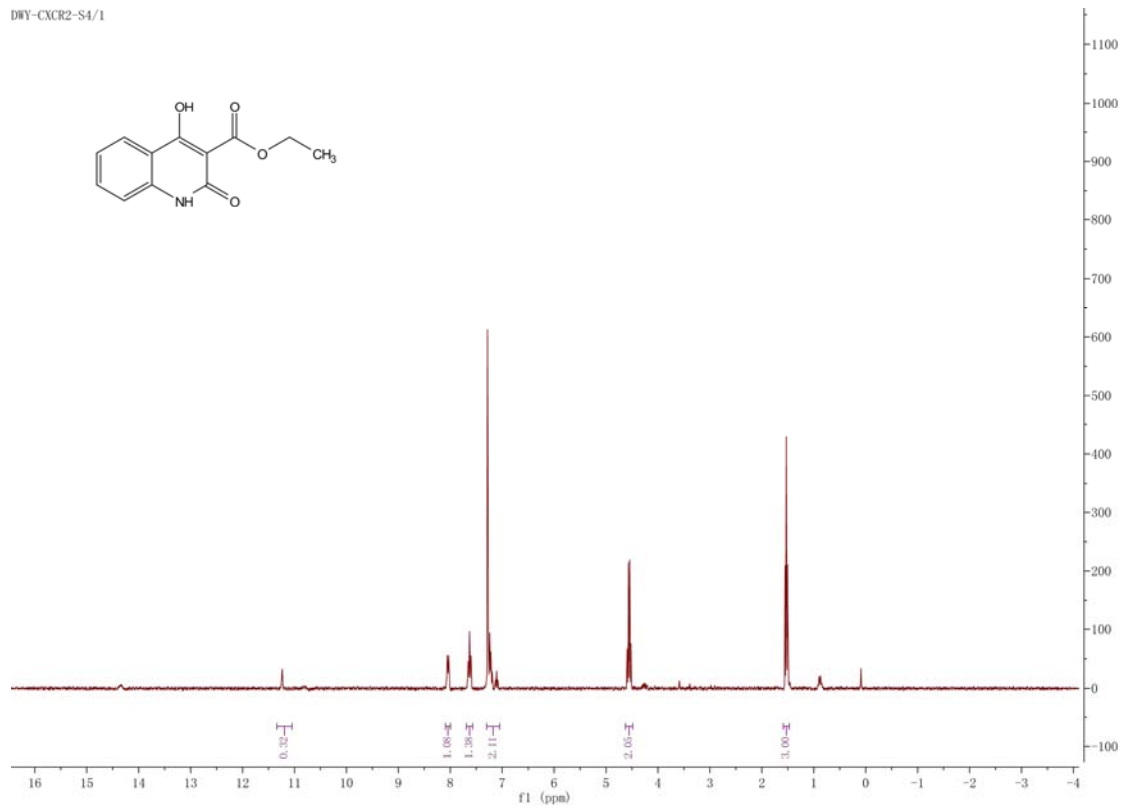
DIY-CXCR2-C2N2/1



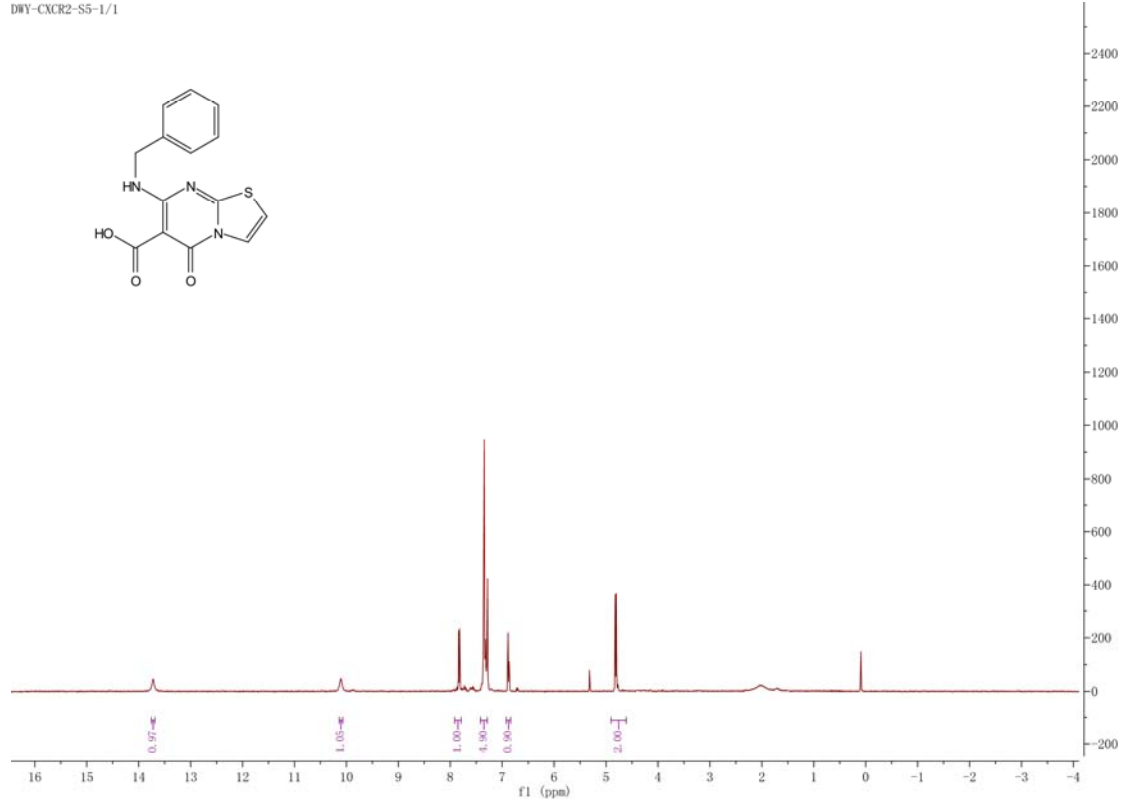
DIY-CXCR2-S3/1



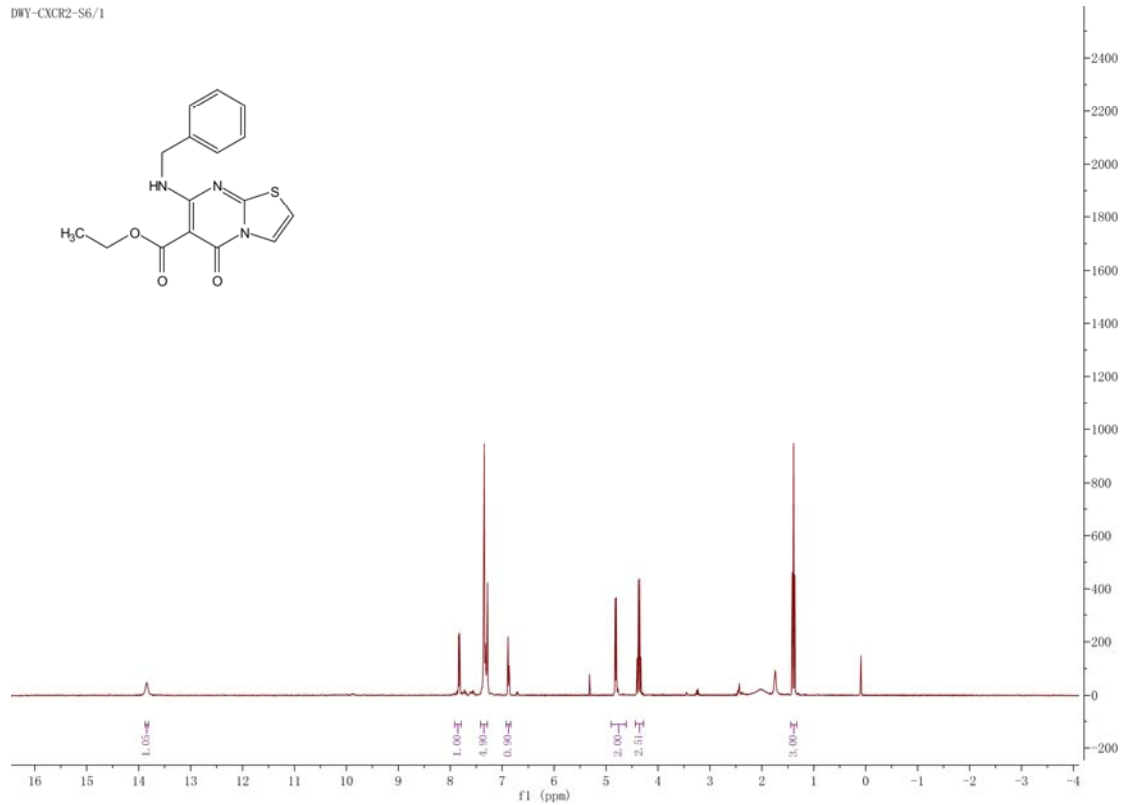
DIY-CXCR2-S4/1



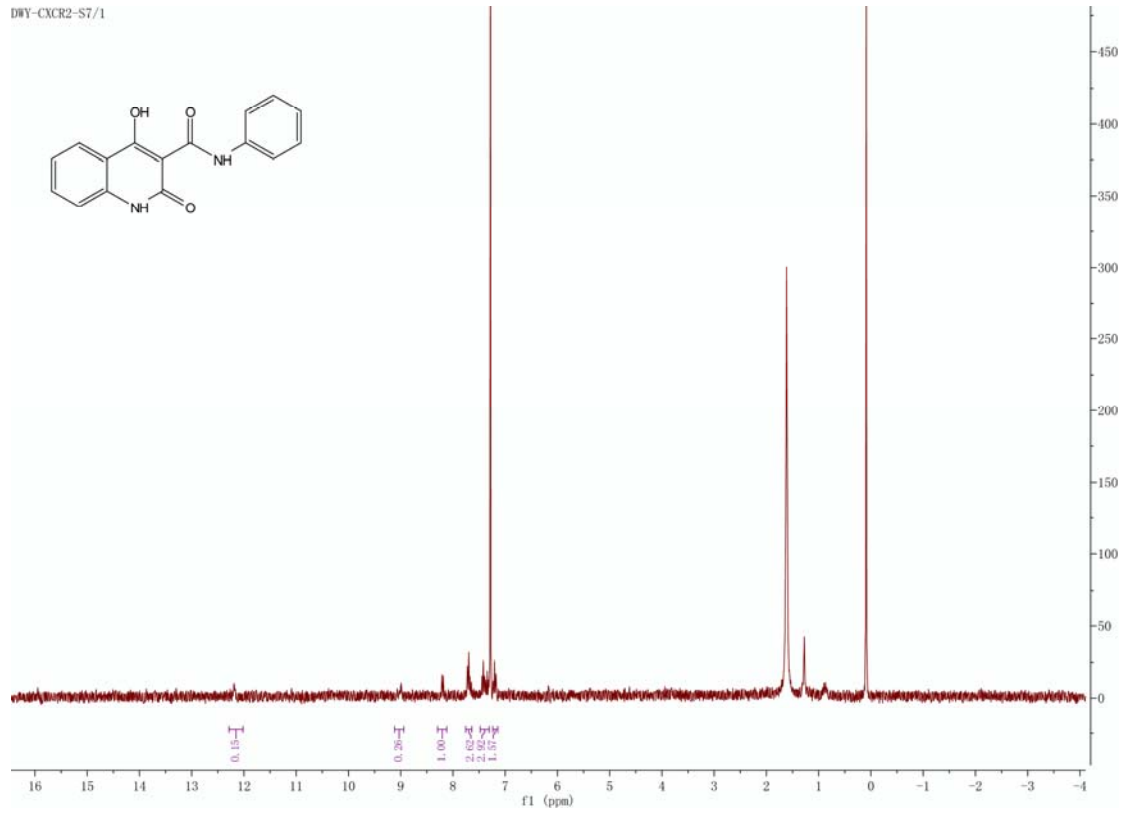
DIY-CXCR2-S5-1/1



DIY-CXCR2-S6/1



DIY-CXCR2-S7/1



DIY-CXCR2-S8/1



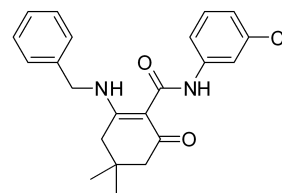
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<Sample Information>

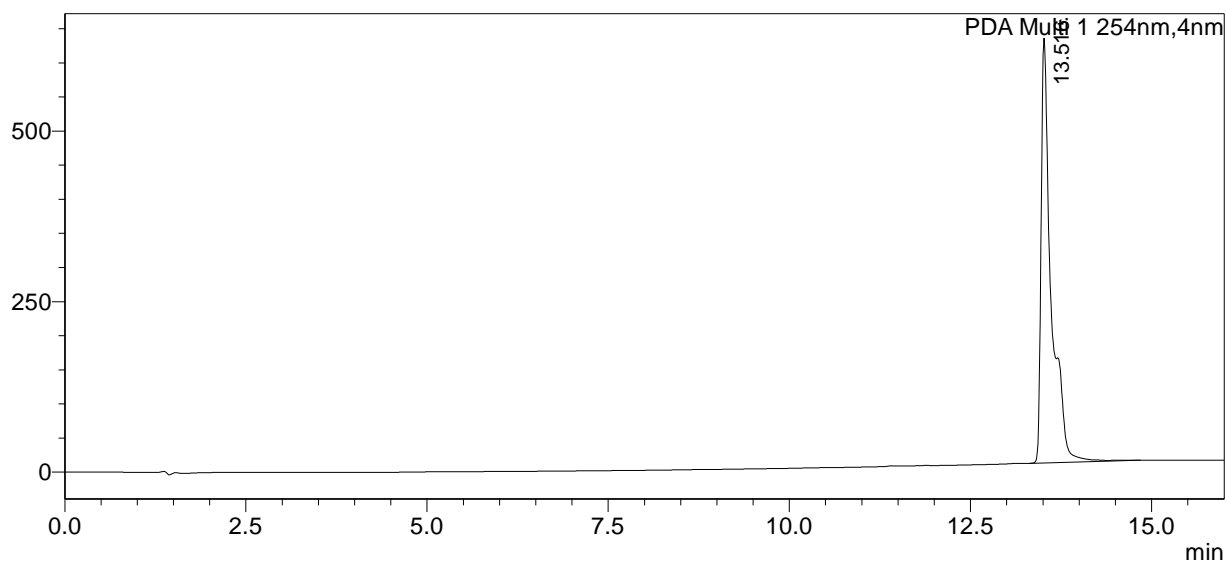
Sample Name : DWY-CXCR2-001
 Sample ID : DWY-CXCR2-001
 Data Filename : DWY-CXCR2-001.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm
 Batch Filename :
 Vial # : 3-11
 Injection Volume : 10 uL
 Date Acquired : 10/28/2016 4:23:23 PM
 Date Processed : 10/28/2016 4:39:24 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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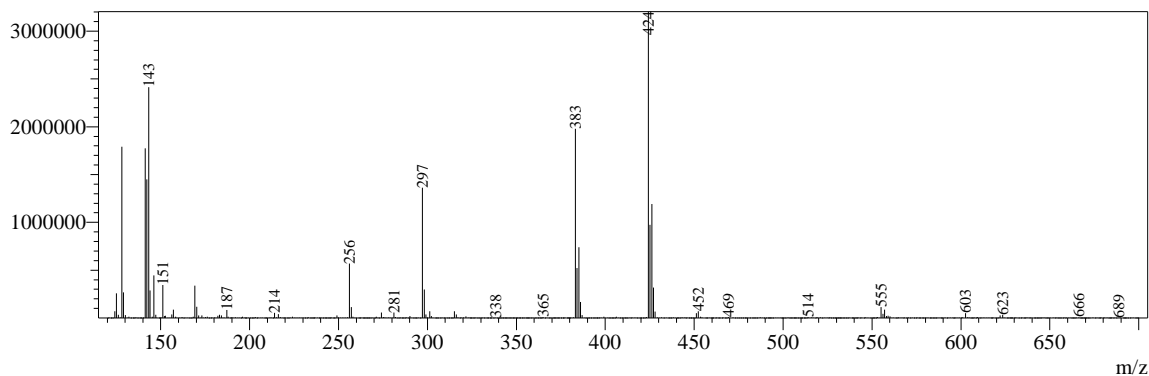


Peak Table

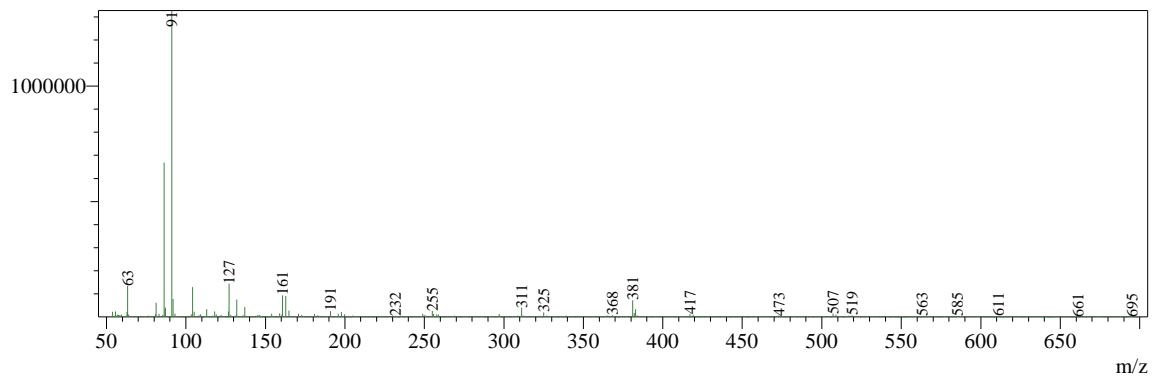
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	13.516	6040284	100.000
Total		6040284	100.000

MS Spectrum

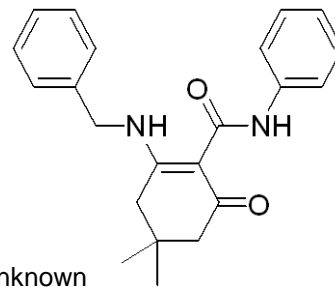
R.Time:13.513(Scan#:8109)
 MassPeaks:634
 Segment 1 - Event 1



R.Time:13.515(Scan#:8110)
MassPeaks:1046
Segment 1 - Event 2



Analysis Report



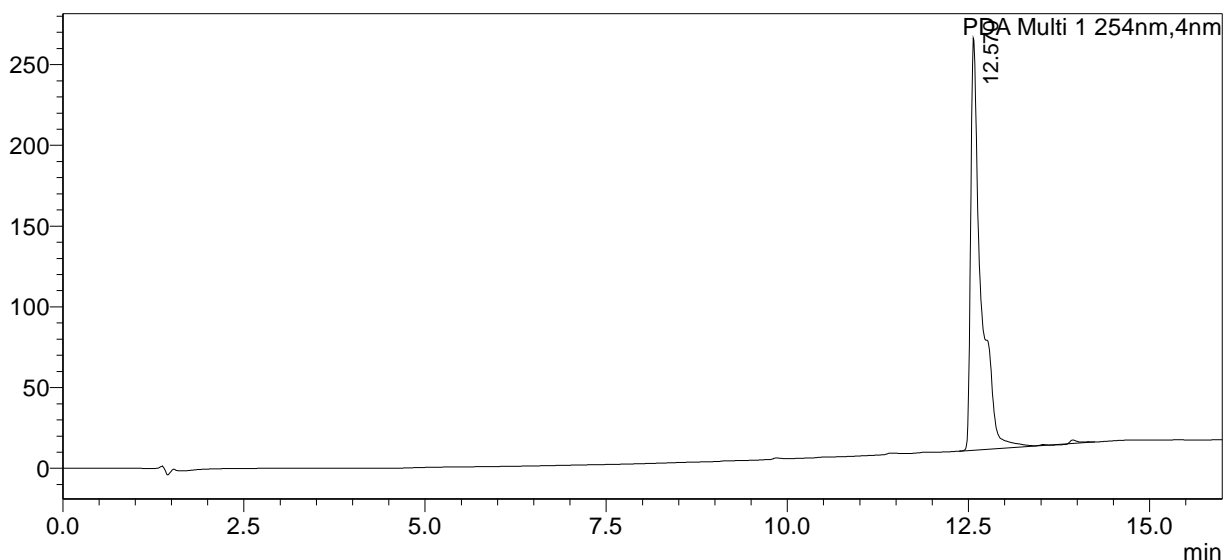
<Sample Information>

Sample Name : DWY-CXCR2-002
 Sample ID : DWY-CXCR2-002
 Data Filename : DWY-CXCR2-002.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm
 Batch Filename :
 Vial # : 3-12
 Injection Volume : 10 uL
 Date Acquired : 10/28/2016 5:13:42 PM
 Date Processed : 10/28/2016 5:29:43 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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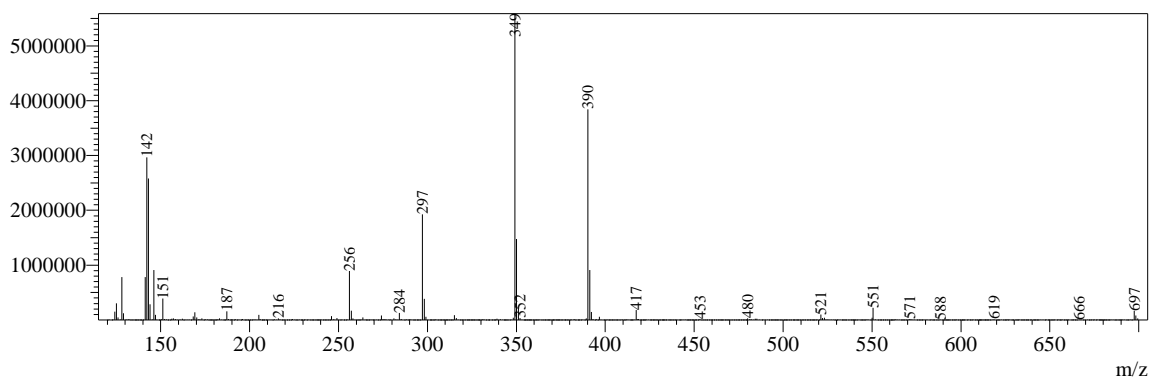


Peak Table

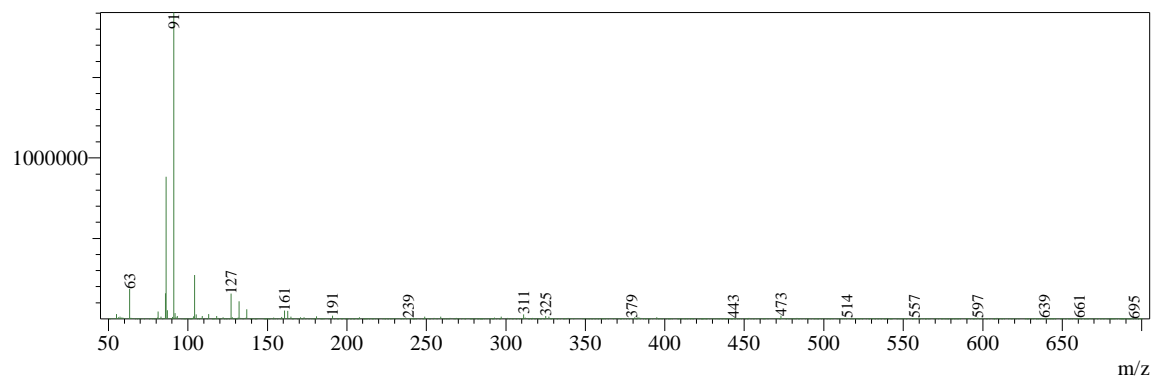
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	12.570	2521313	100.000
Total		2521313	100.000

MS Spectrum

R.Time:12.570(Scan#:7543)
 MassPeaks:638
 Segment 1 - Event 1

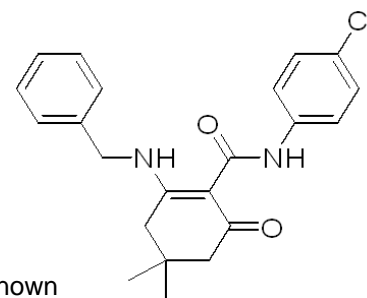


R. Time: 12.572 (Scan#: 7544)
Mass Peaks: 1022
Segment 1 - Event 2



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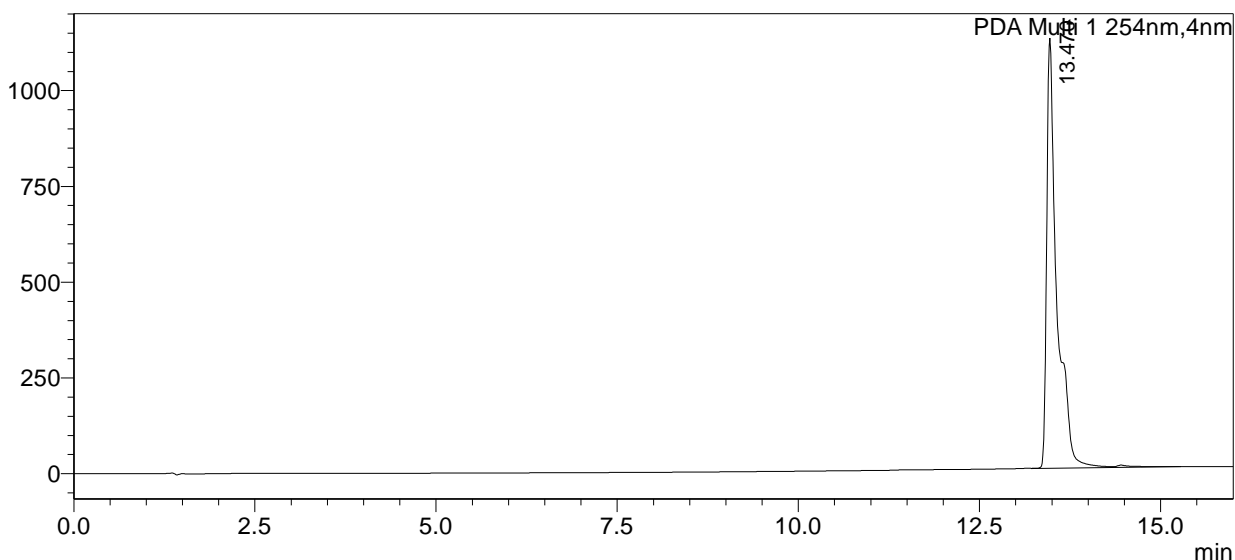
<Sample Information>

Sample Name : DWY-CXCR2-003
 Sample ID : DWY-CXCR2-003
 Data Filename : DWY-CXCR2-003.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm
 Batch Filename :
 Vial # : 3-13
 Injection Volume : 10 uL
 Date Acquired : 10/28/2016 7:45:16 PM
 Date Processed : 10/28/2016 8:09:06 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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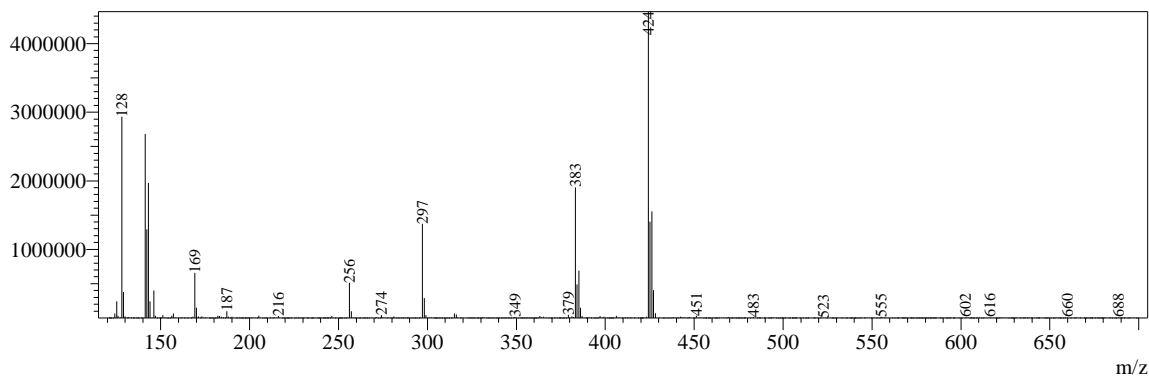


Peak Table

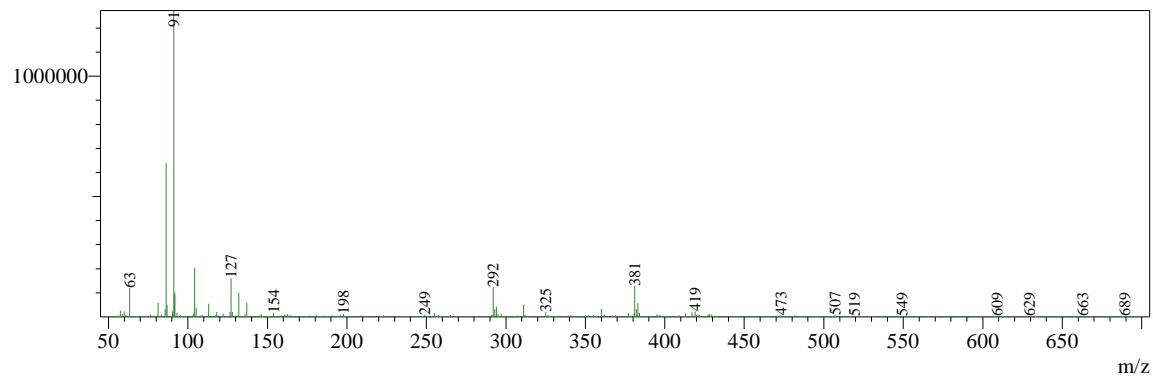
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	13.470	11040001	100.000
Total		11040001	100.000

MS Spectrum

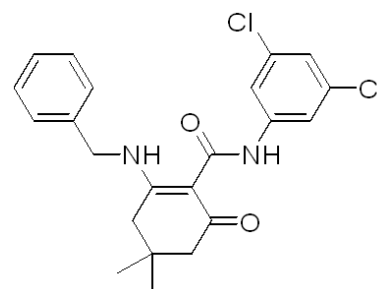
R.Time:13.470(Scan#:8083)
 MassPeaks:640
 Segment 1 - Event 1



R. Time:13.472(Scan#:8084)
MassPeaks:1035
Segment 1 - Event 2



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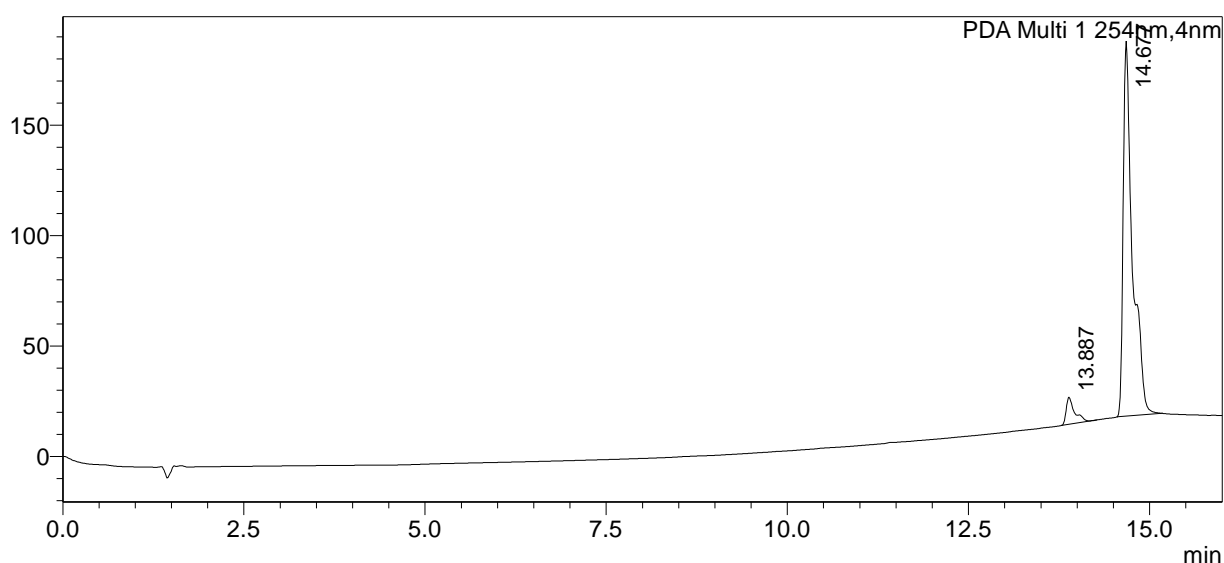


<Sample Information>

Sample Name	: DWY-CXCR2-004	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-004	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-004_2.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm		
Batch Filename	:		
Vial #	: 3-16		
Injection Volume	: 10 uL		
Date Acquired	: 11/7/2016 7:40:15 PM		
Date Processed	: 11/7/2016 8:05:00 PM		

<Chromatogram>

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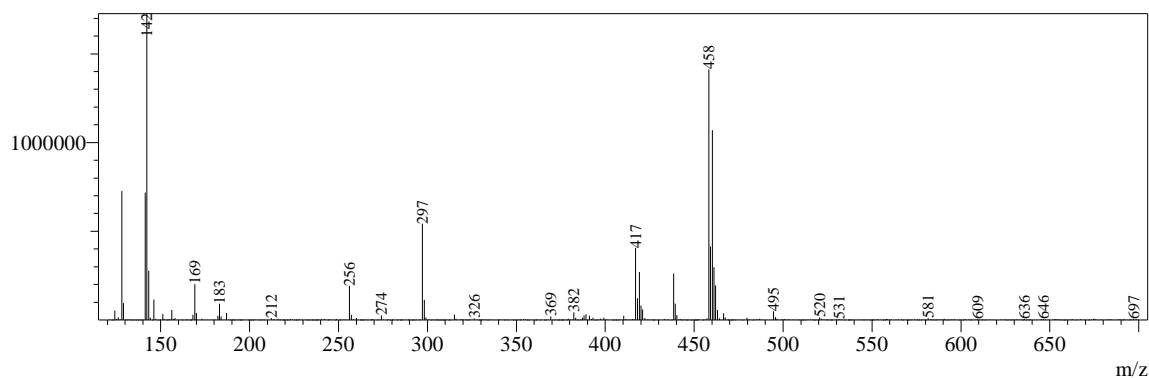


Peak Table

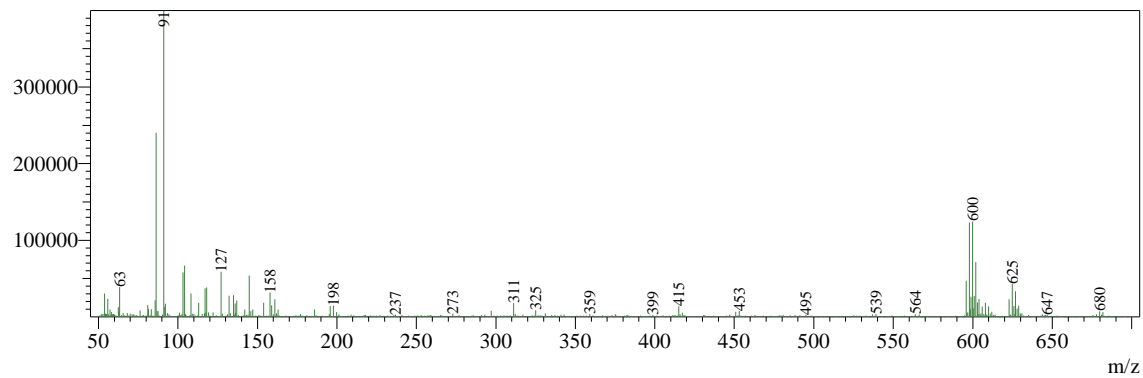
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	13.887	100283	6.225
2	14.677	1510814	93.775
Total		1611096	100.000

MS Spectrum

R.Time:14.677(Scan#:8807)
MassPeaks:630
Segment 1 - Event 1



R.Time:14.678(Scan#:8808)
MassPeaks:1036
Segment 1 - Event 2

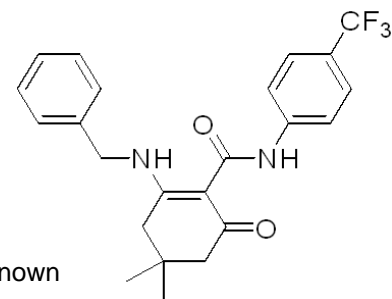




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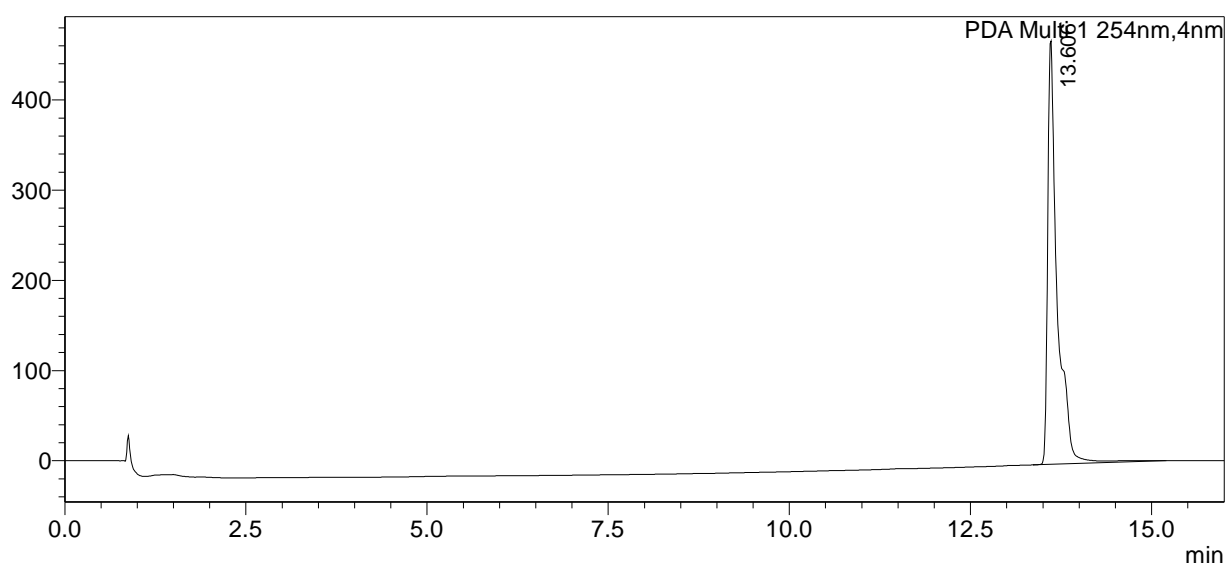
<Sample Information>

Sample Name : DWY-CXCR2-005
 Sample ID : DWY-CXCR2-005
 Data Filename : DWY-CXCR2-005_2.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm
 Batch Filename : DWY-CXCR2-004~006.lcb
 Vial # : 3-21
 Injection Volume : 10 uL
 Date Acquired : 10/31/2016 6:04:13 PM
 Date Processed : 10/31/2016 6:20:14 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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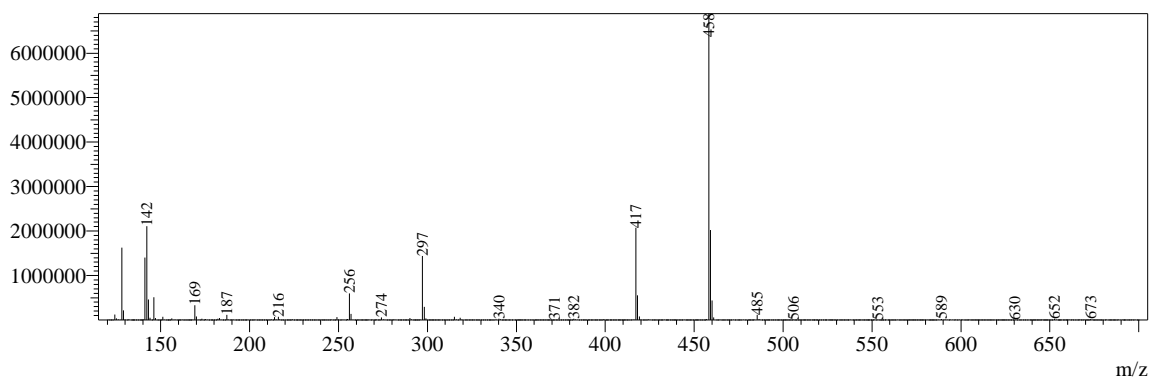
Peak Table

PDA Ch1 254nm

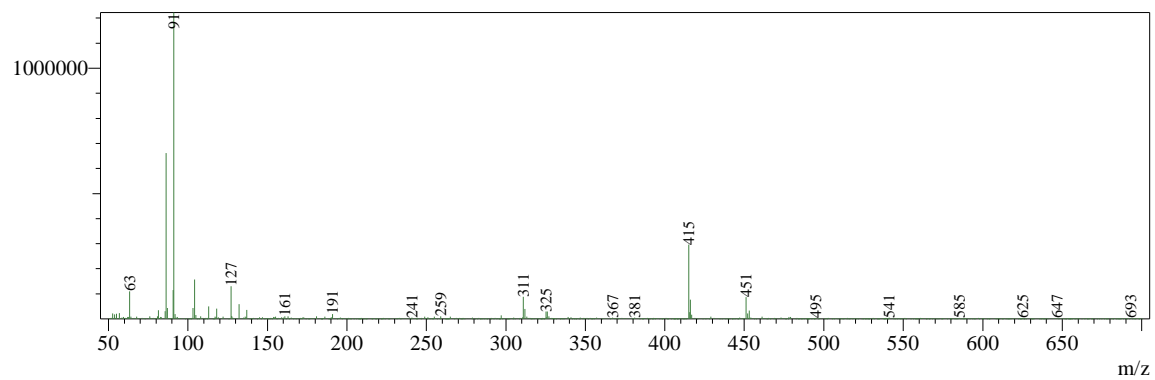
Peak#	Ret. Time	Area	Area%
1	13.606	4317279	100.000
Total		4317279	100.000

MS Spectrum

R.Time:13.603(Scan#:8163)
 MassPeaks:644
 Segment 1 - Event 1



R.Time:13.605(Scan#:8164)
MassPeaks:1050
Segment 1 - Event 2



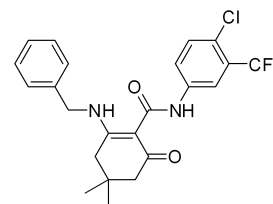
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<Sample Information>

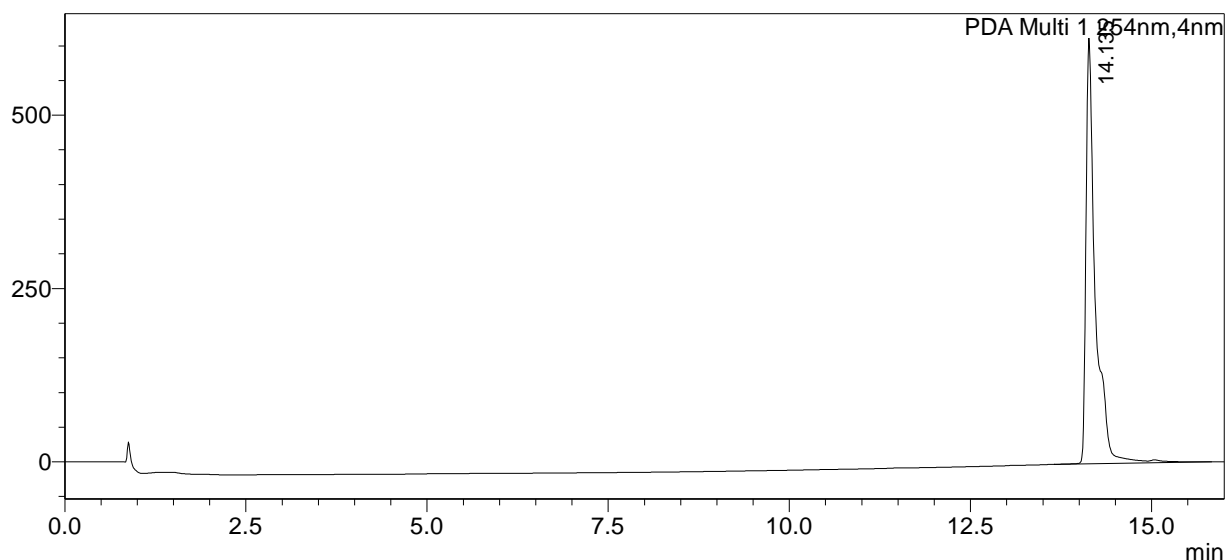
Sample Name : DWY-CXCR2-006
 Sample ID : DWY-CXCR2-006
 Data Filename : DWY-CXCR2-006_3.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm
 Batch Filename : DWY-CXCR2-004~006.lcb
 Vial # : 3-22
 Injection Volume : 10 uL
 Date Acquired : 10/31/2016 6:20:38 PM
 Date Processed : 10/31/2016 6:36:39 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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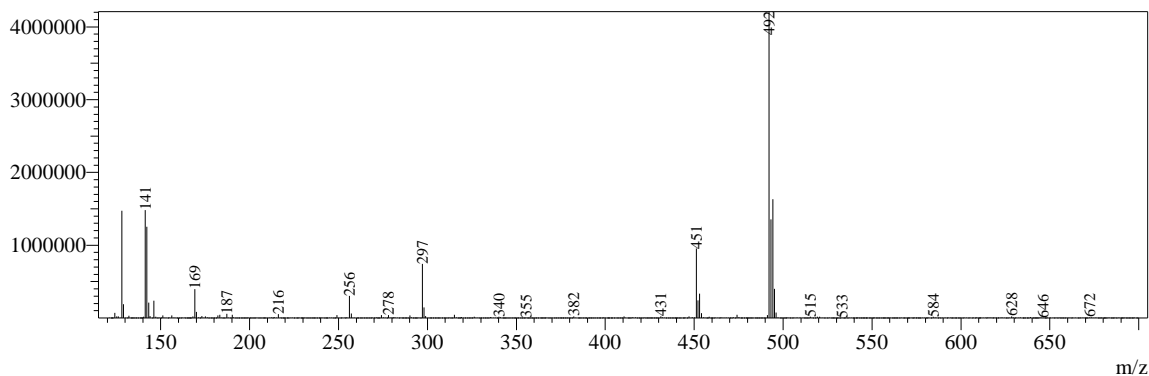


Peak Table

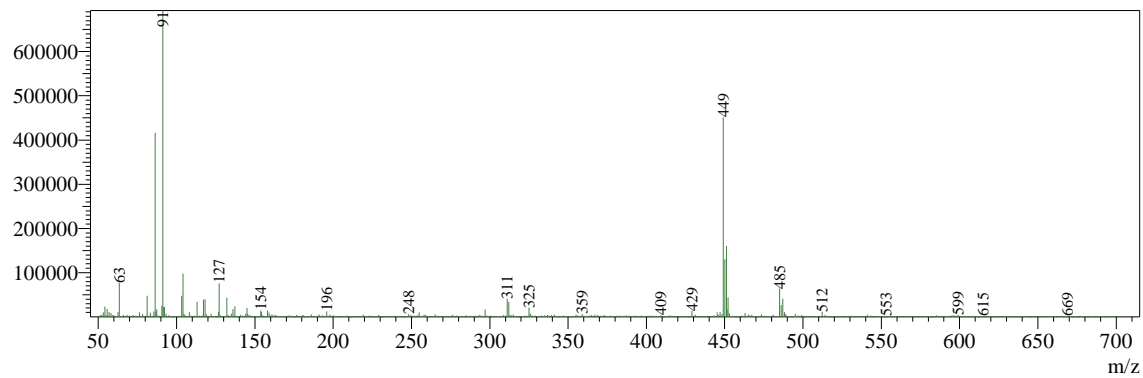
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	14.135	5573001	100.000
Total		5573001	100.000

MS Spectrum

R.Time:14.133(Scan#:8481)
 MassPeaks:637
 Segment 1 - Event 1

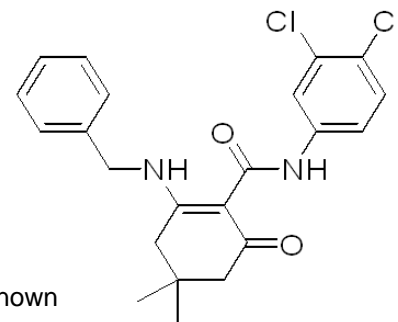


R. Time: 14.135(Scan#:8482)
MassPeaks:1040
Segment 1 - Event 2



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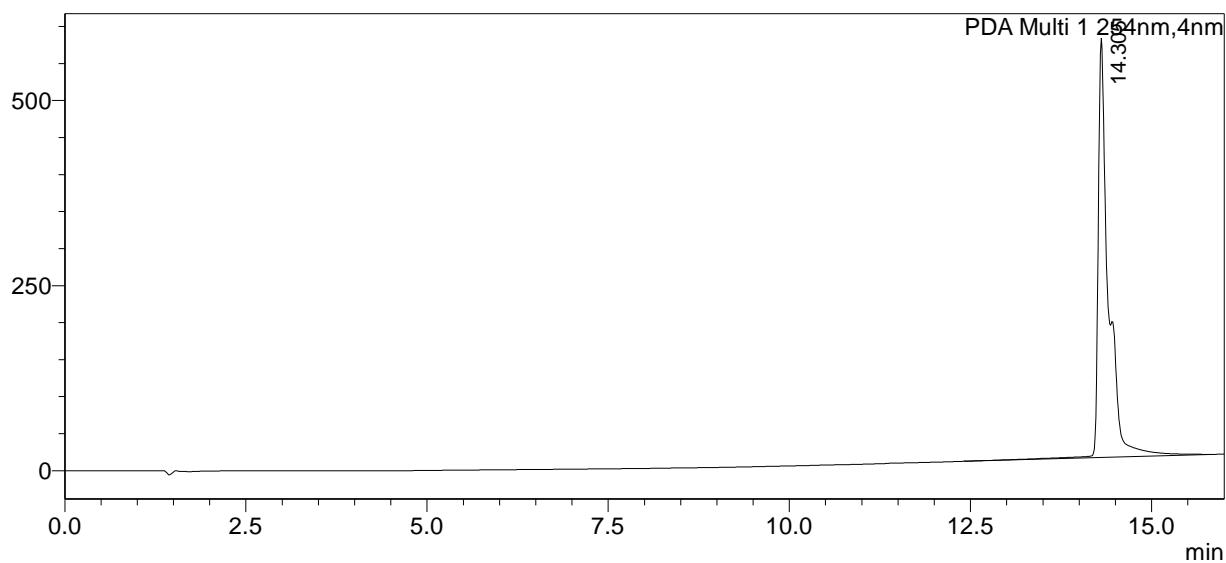
<Sample Information>

Sample Name : DWY-CXCR2-007
 Sample ID : DWY-CXCR2-007
 Data Filename : DWY-CXCR2-007(1).lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm
 Batch Filename :
 Vial # : 3-15
 Injection Volume : 10 uL
 Date Acquired : 11/7/2016 7:22:40 PM
 Date Processed : 11/7/2016 7:38:43 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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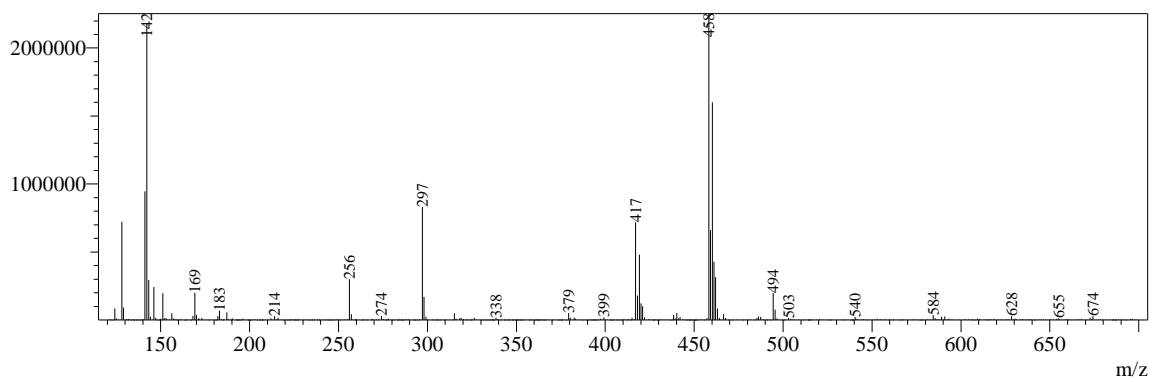
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	14.305	5591318	100.000
Total		5591318	100.000

MS Spectrum

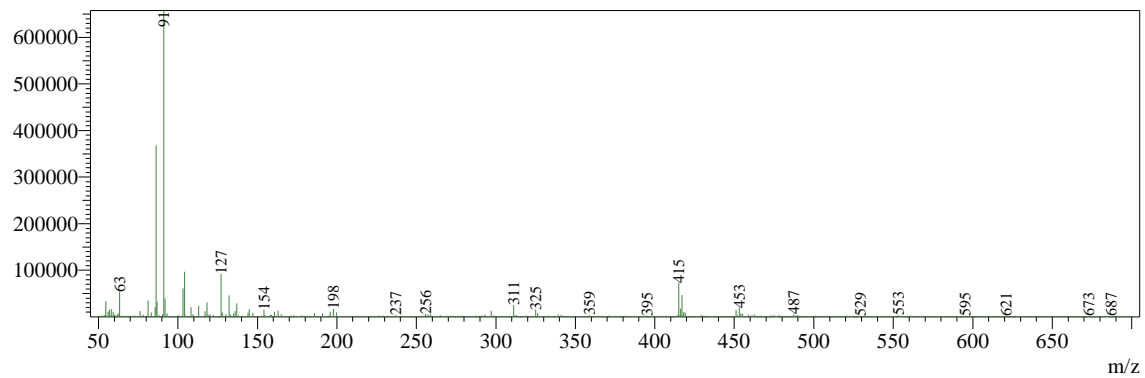
R.Time:14.303(Scan#:8583)
 MassPeaks:458
 Segment 1 - Event 1

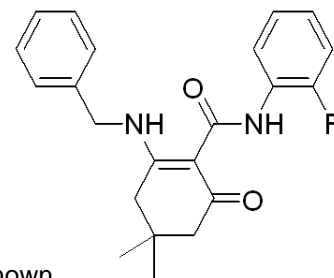


R. Time: 14.305(Scan#: 8584)

MassPeaks: 91

Segment 1 - Event 2



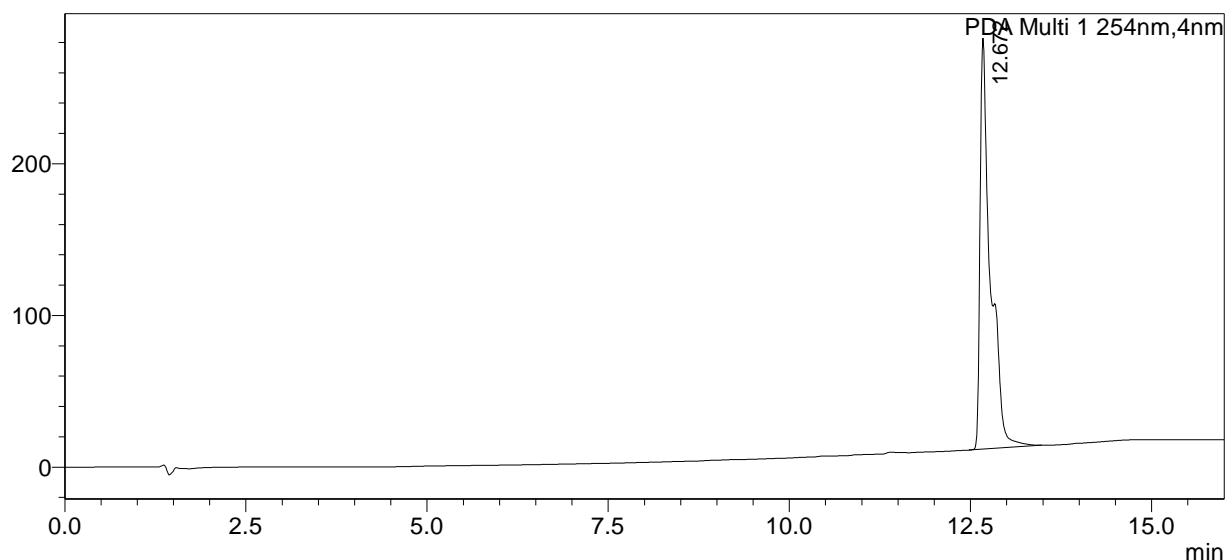


<Sample Information>

Sample Name	: DWY-CXCR2-008	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-008	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-008.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm		
Batch Filename	:		
Vial #	: 1-25		
Injection Volume	: 10 uL		
Date Acquired	: 11/1/2016 8:14:36 PM		
Date Processed	: 11/1/2016 8:30:38 PM		

<Chromatogram>

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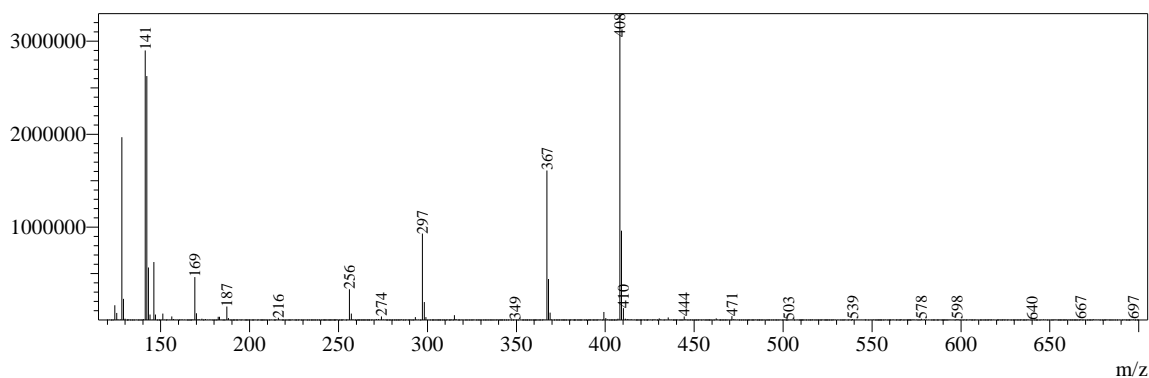


Peak Table

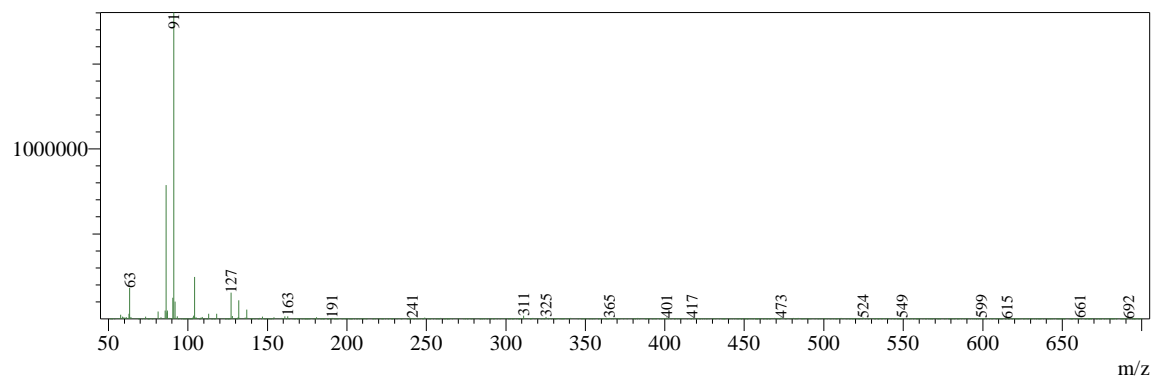
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	12.672	2708959	100.000
Total		2708959	100.000

MS Spectrum

R.Time:12.670(Scan#:7603)
MassPeaks:408
Segment 1 - Event 1

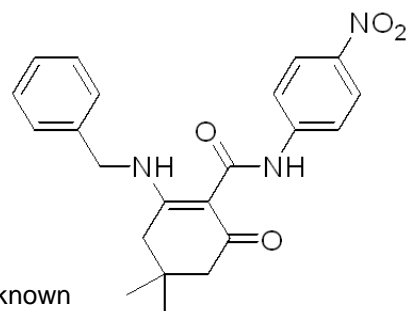


R. Time:12.672(Scan#:7604)
MassPeaks:91
Segment 1 - Event 2



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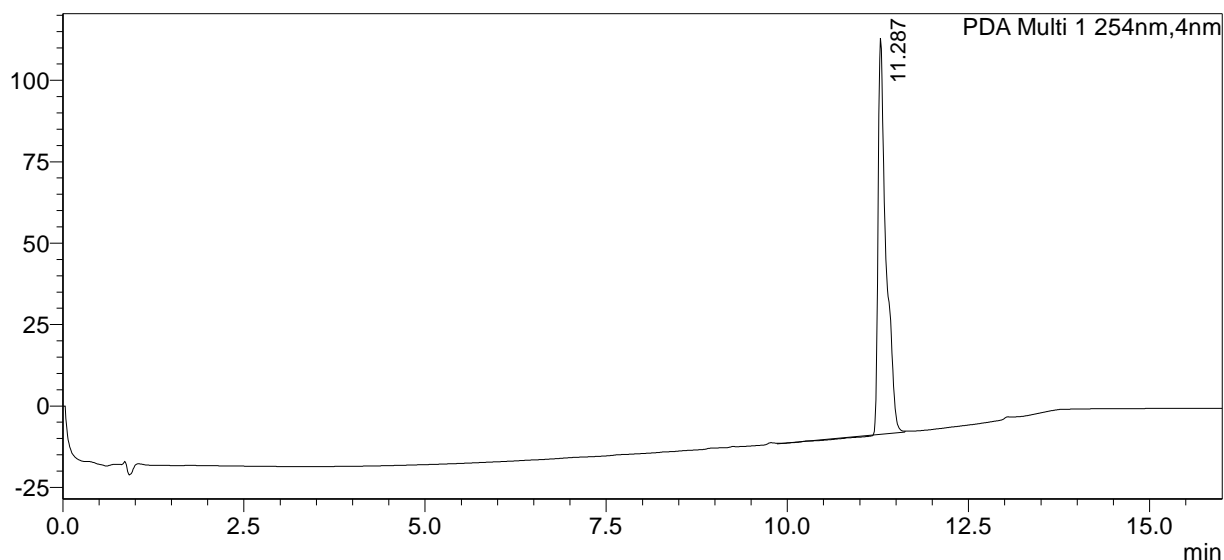
<Sample Information>

Sample Name : DWY-CXCR2-009
 Sample ID : DWY-CXCR2-009
 Data Filename : DWY-CXCR2-009_2.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm
 Batch Filename : DWY-CXCR2-009.lcb
 Vial # : 2-22
 Injection Volume : 10 uL
 Date Acquired : 11/3/2016 1:47:18 PM
 Date Processed : 11/3/2016 2:03:20 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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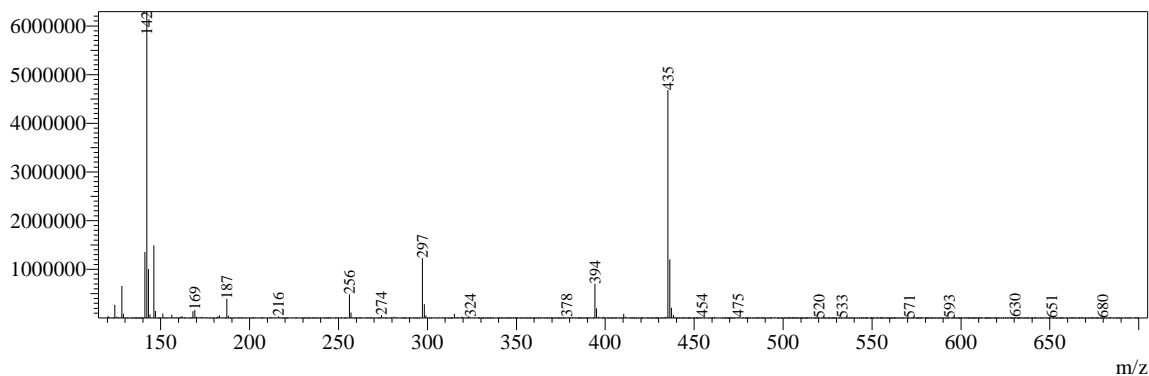
Peak Table

PDA Ch1 254nm

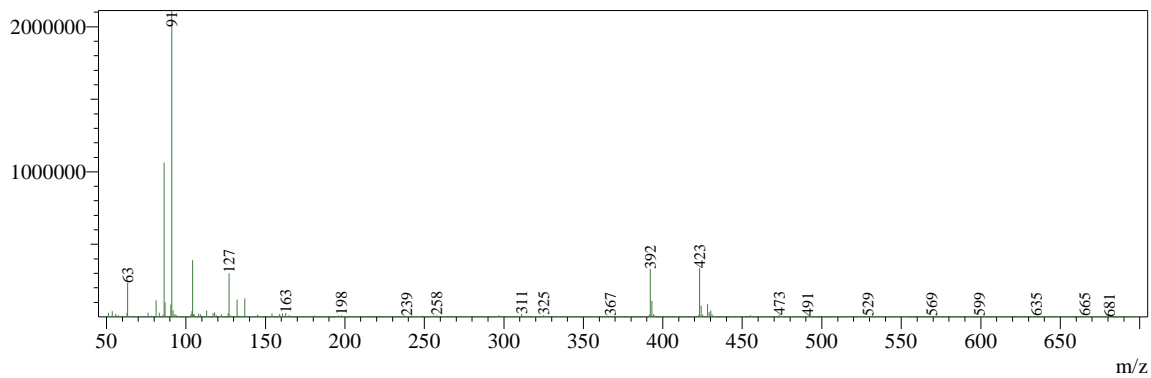
Peak#	Ret. Time	Area	Area%
1	11.287	921910	100.000
Total		921910	100.000

MS Spectrum

R.Time:11.287(Scan#:6773)
 MassPeaks:142
 Segment 1 - Event 1

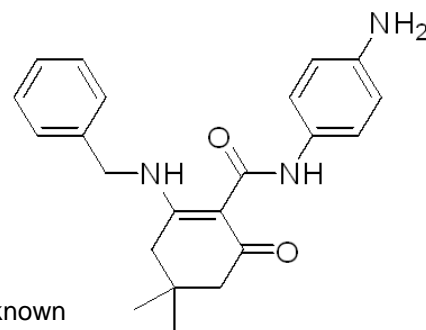


R. Time: 11.288(Scan#: 6774)
MassPeaks: 91
Segment 1 - Event 2



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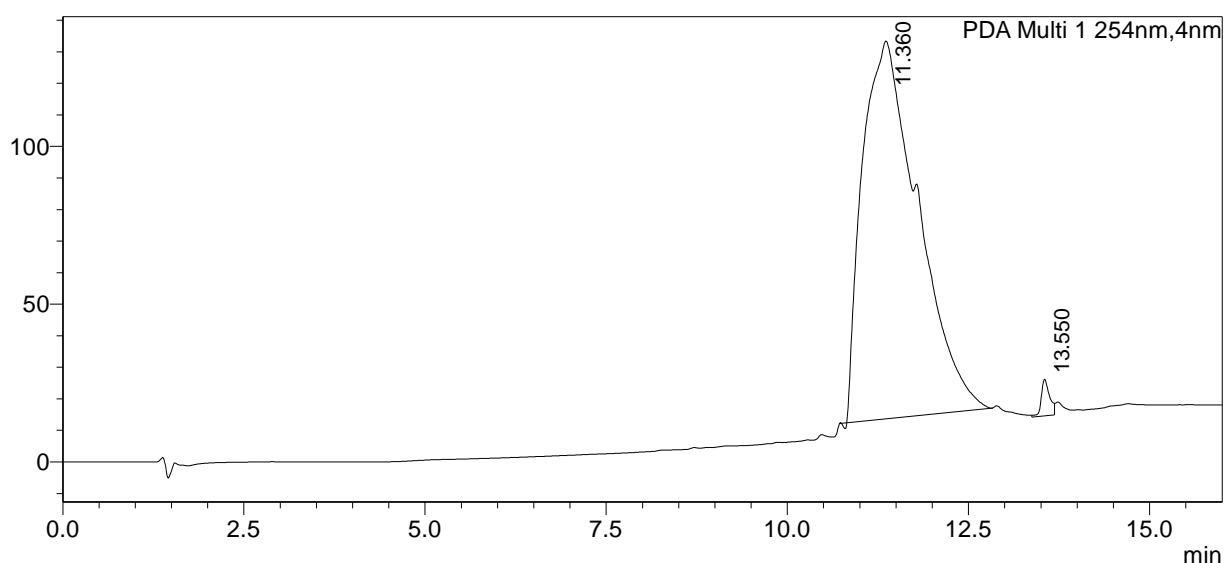
<Sample Information>

Sample Name : DWY-CXCR2-010
 Sample ID : DWY-CXCR2-010
 Data Filename : DWY-CXCR2-010.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm
 Batch Filename :
 Vial # : 3-32
 Injection Volume : 10 uL
 Date Acquired : 11/3/2016 8:54:22 PM
 Date Processed : 11/3/2016 9:10:22 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

mAU

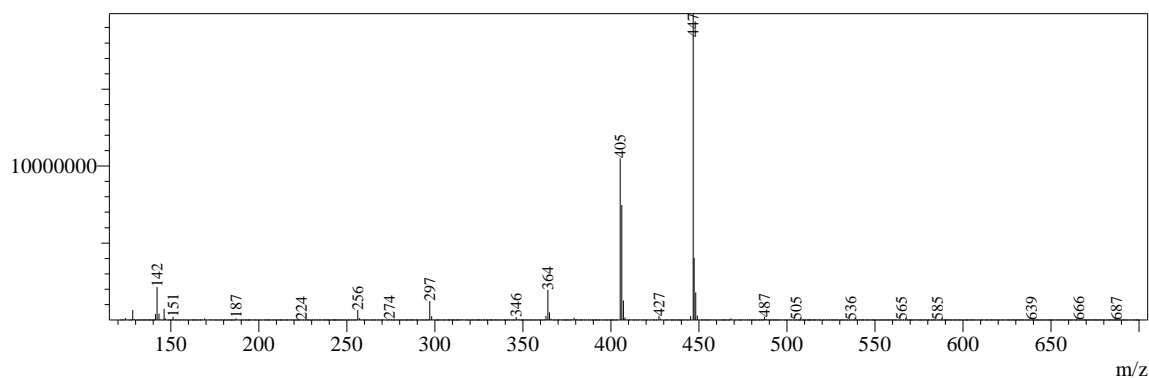


Peak Table

Peak#	Ret. Time	Area	Area%
1	11.360	6394469	98.559
2	13.550	93519	1.441
Total		6487988	100.000

MS Spectrum

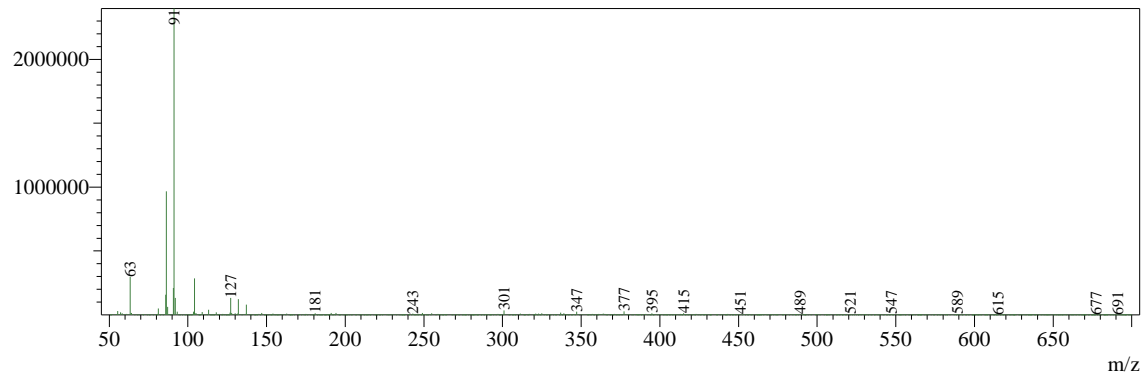
R.Time:11.360(Scan#:6817)
 MassPeaks:447
 Segment 1 - Event 1

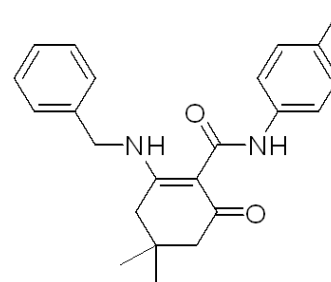


R. Time: 11.362 (Scan#: 6818)

Mass Peaks: 91

Segment 1 - Event 2



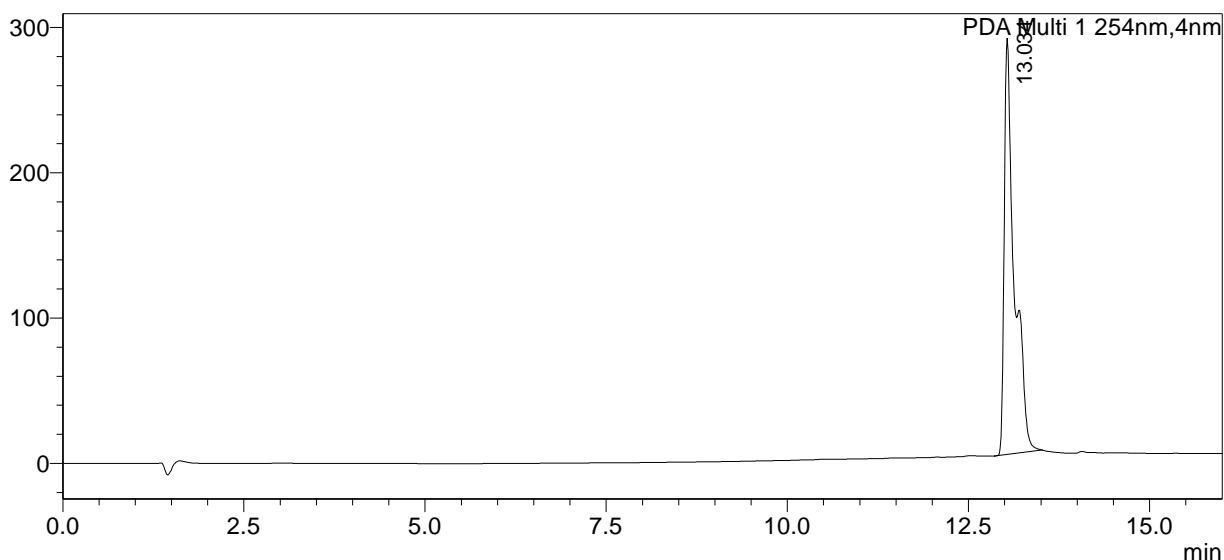


<Sample Information>

Sample Name	: DWY-CXCR2-011	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-011	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-011_1.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm		
Batch Filename	: DWY-CXCR2-011~12.lcb		
Vial #	: 3-35		
Injection Volume	: 10 uL		
Date Acquired	: 11/11/2016 2:26:30 PM		
Date Processed	: 11/11/2016 3:07:49 PM		

<Chromatogram>

mAU

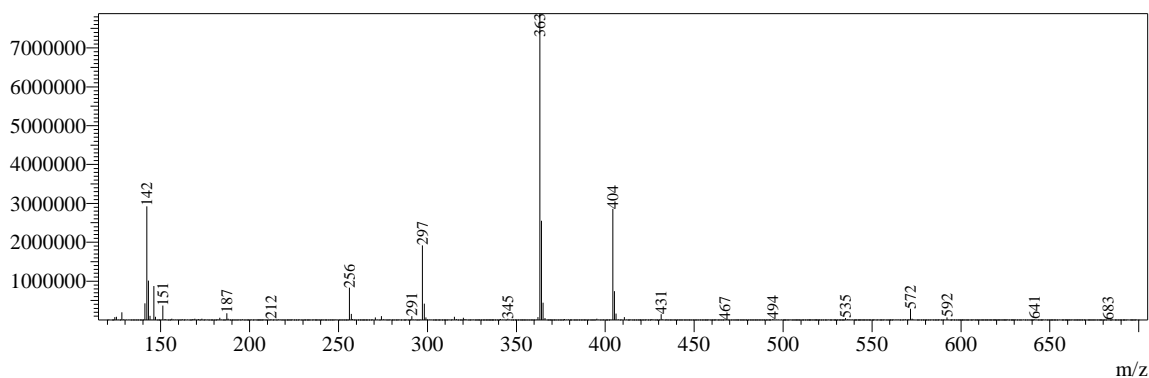


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	13.034	2767372	100.000
Total		2767372	100.000

MS Spectrum

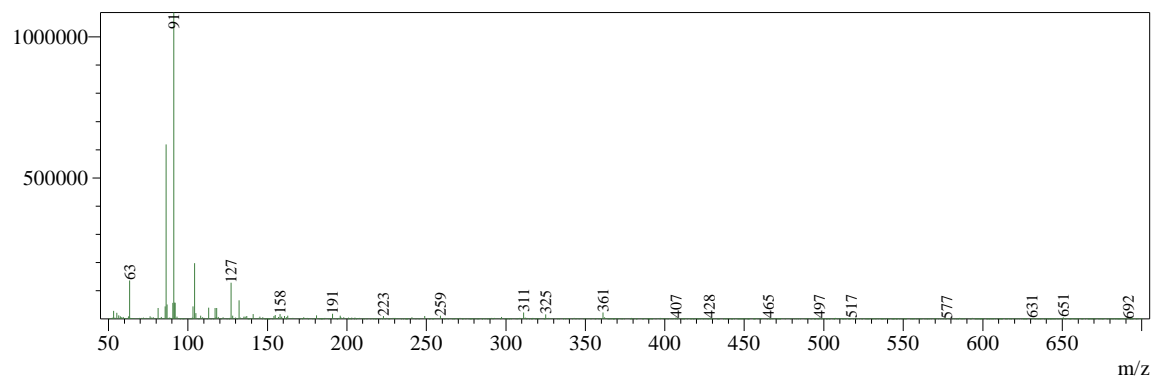
R.Time:13.033(Scan#:7821)
MassPeaks:363
Segment 1 - Event 1

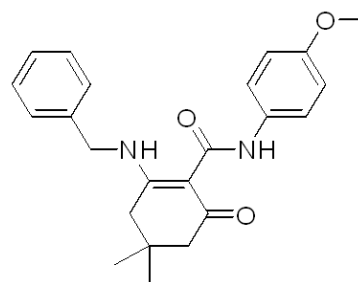


R. Time:13.035(Scan#:7822)

MassPeaks:91

Segment 1 - Event 2



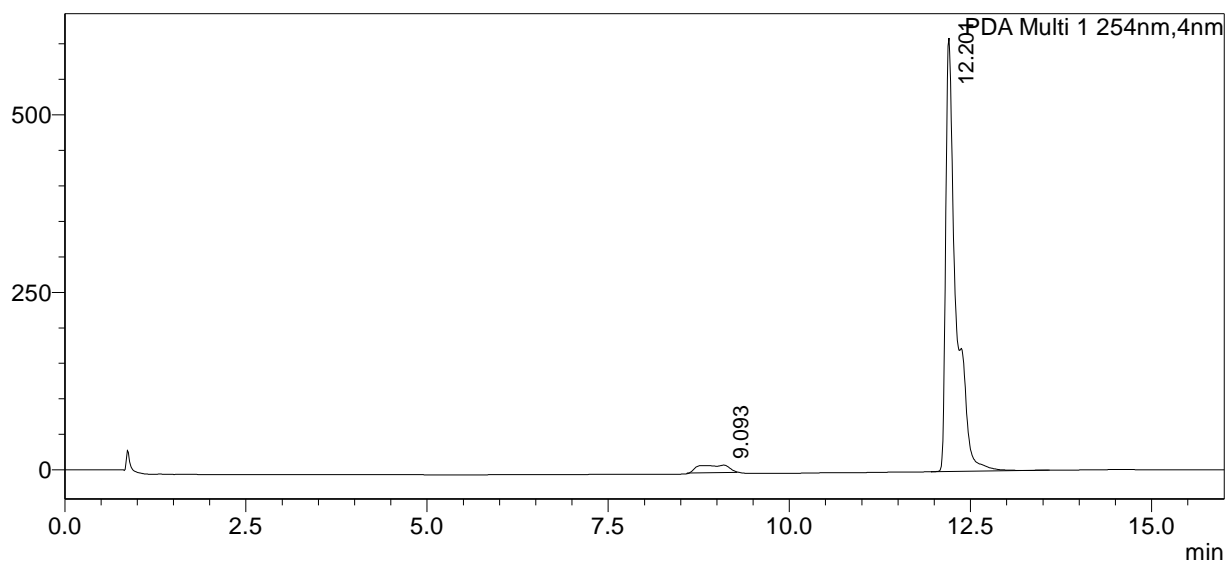


<Sample Information>

Sample Name	: DWY-CXCR2-012	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-012	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-012_2.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm		
Batch Filename	: DWY-CXCR2-011~12.lcb		
Vial #	: 3-36		
Injection Volume	: 10 uL		
Date Acquired	: 11/11/2016 2:42:56 PM		
Date Processed	: 11/11/2016 3:10:47 PM		

<Chromatogram>

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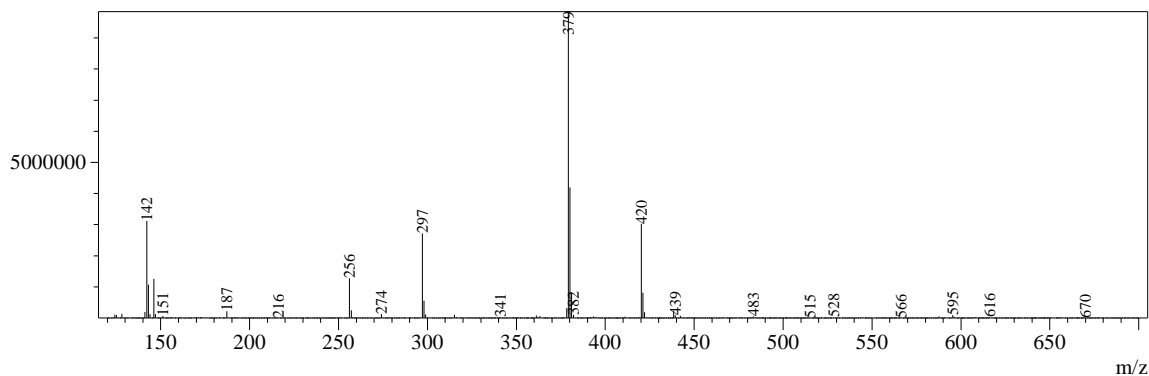


Peak Table

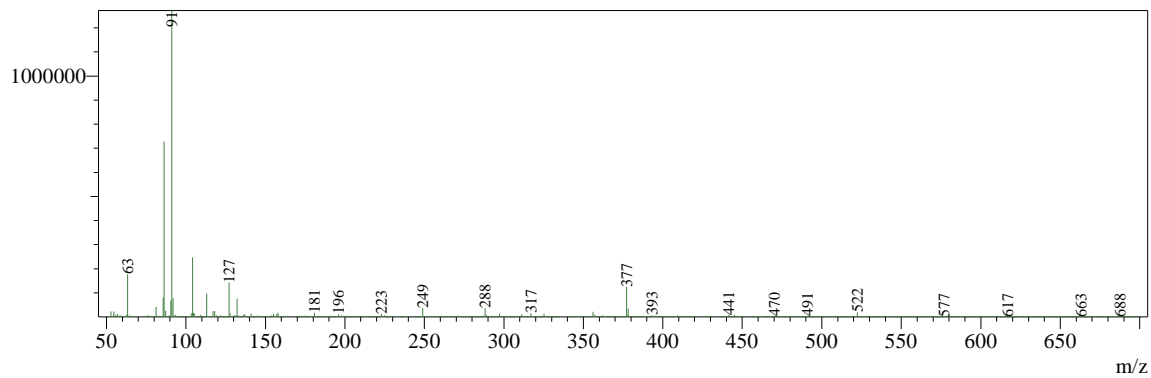
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	9.093	306079	4.817
2	12.201	6048664	95.183
Total		6354743	100.000

MS Spectrum

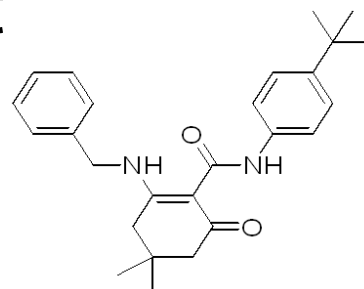
R. Time: 12.200 (Scan#: 7321)
 Mass Peaks: 379
 Segment 1 - Event 1



R. Time:12.202(Scan#:7322)
MassPeaks:91
Segment 1 - Event 2



Analysis Report



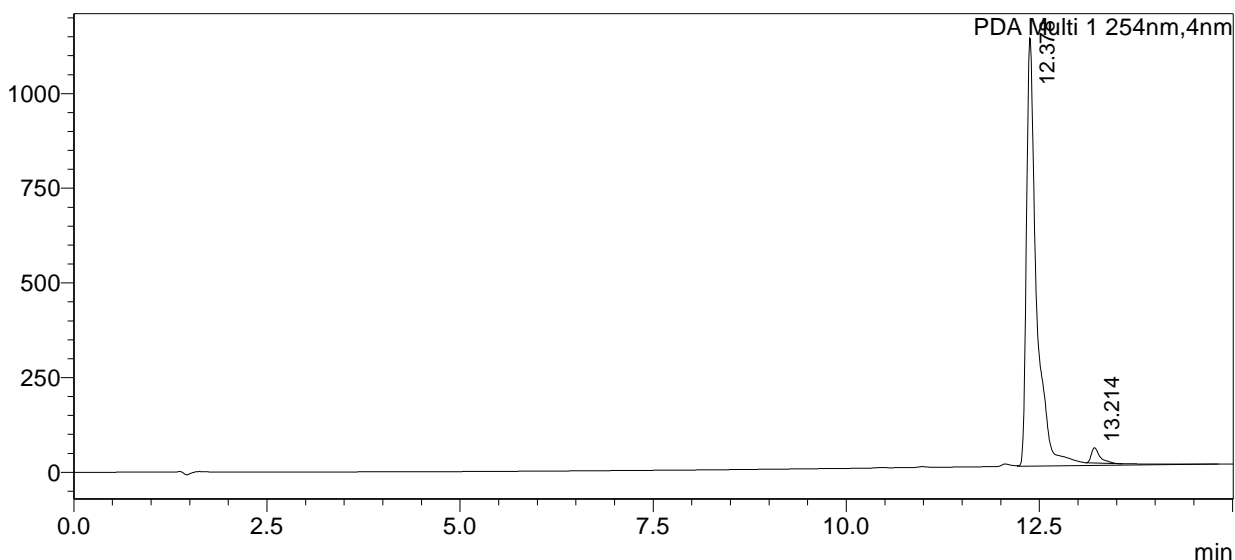
<Sample Information>

Sample Name : DWY-CXCR2-013
 Sample ID : DWY-CXCR2-013
 Data Filename : DWY-CXCR2-013_1.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename : DWY-CXCR2-013.lcb
 Vial # : 3-2
 Injection Volume : 10 uL
 Date Acquired : 11/14/2016 5:28:27 PM
 Date Processed : 11/14/2016 5:43:30 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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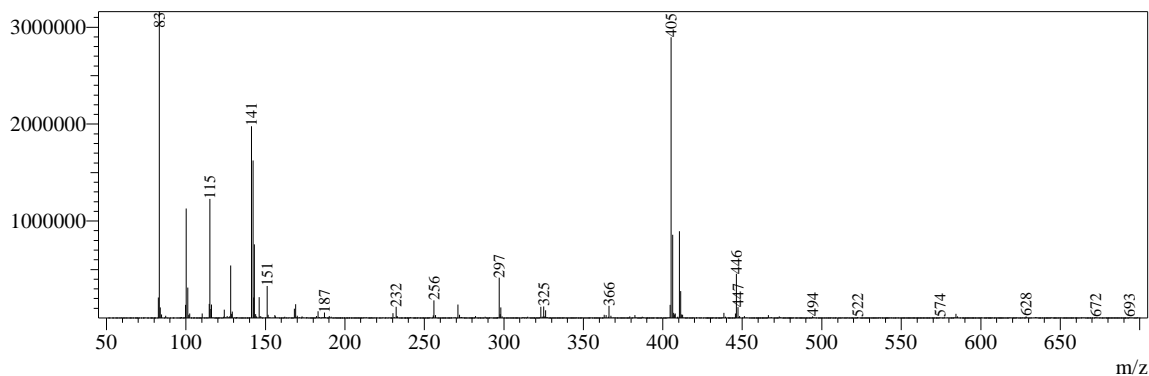


Peak Table

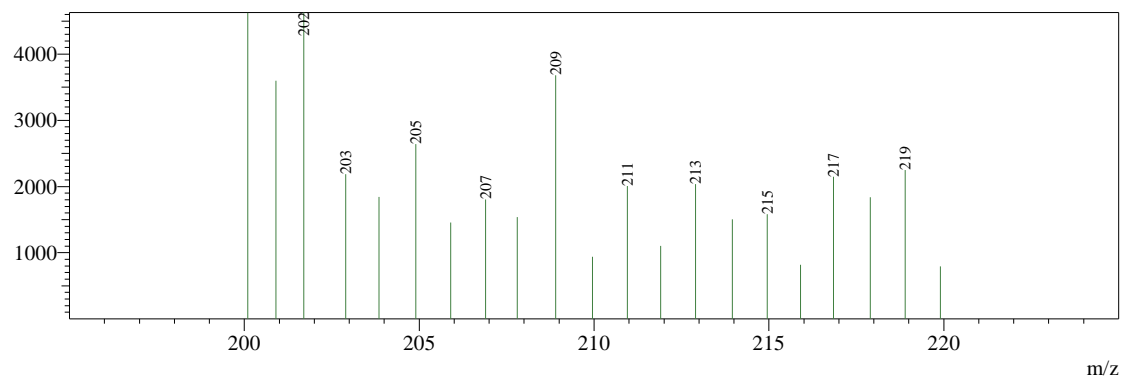
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	12.378	10643628	97.148
2	13.214	312488	2.852
Total		10956116	100.000

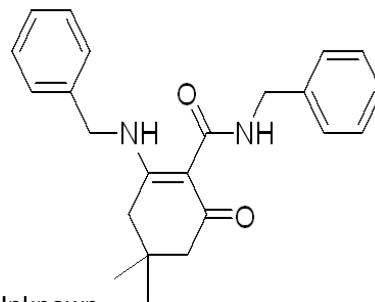
MS Spectrum

R.Time:13.213(Scan#:7929)
 MassPeaks:83
 Segment 1 - Event 1



R. Time:13.215(Scan#:7930)
MassPeaks:202
Segment 1 - Event 2



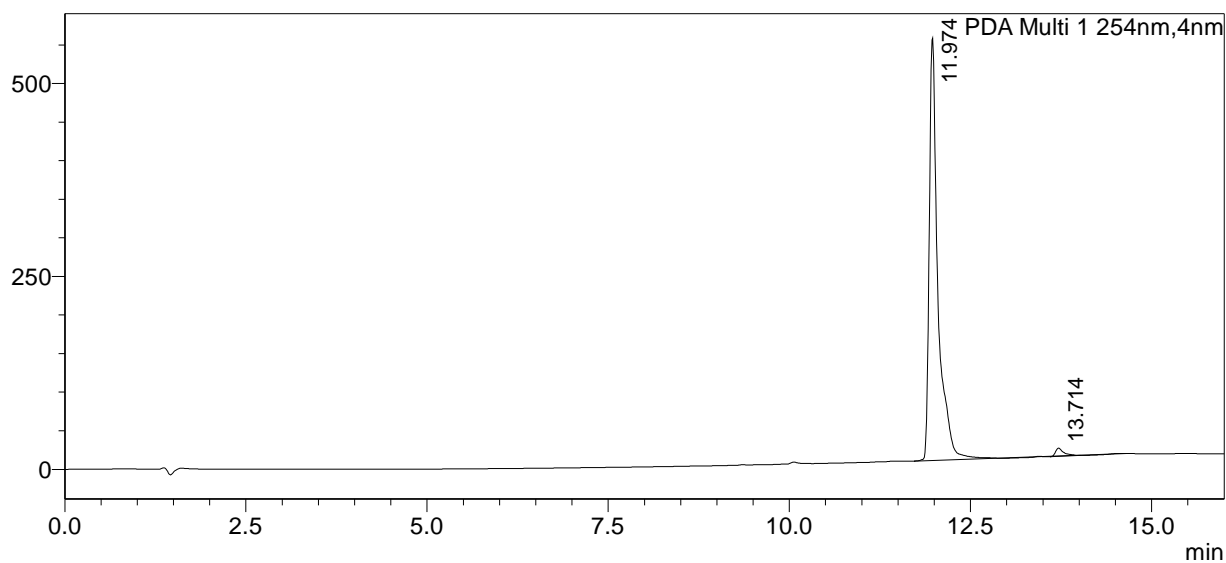


<Sample Information>

Sample Name	: DWY-CXCR2-014	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-014	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-014.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_DING.lcm		
Batch Filename	:		
Vial #	: 3-4		
Injection Volume	: 10 uL		
Date Acquired	: 11/14/2016 8:36:56 PM		
Date Processed	: 11/18/2016 4:26:54 PM		

<Chromatogram>

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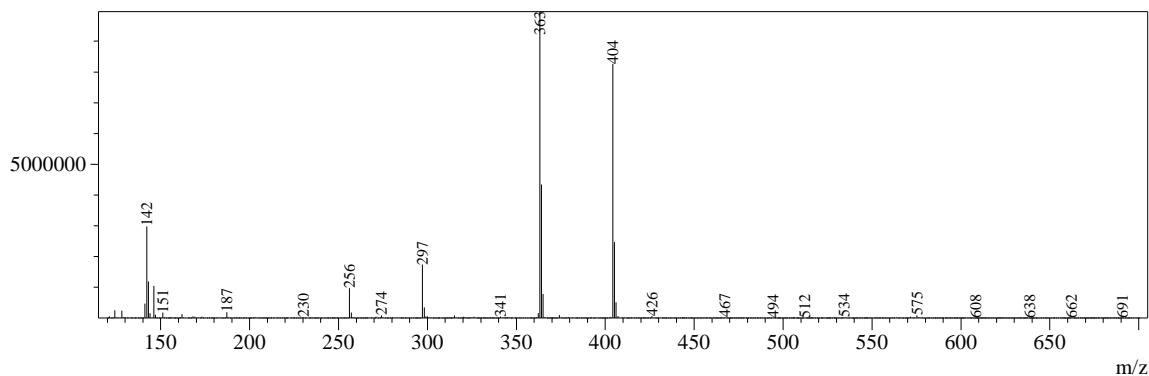


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	11.974	4551954	98.135
2	13.714	86495	1.865
Total		4638450	100.000

MS Spectrum

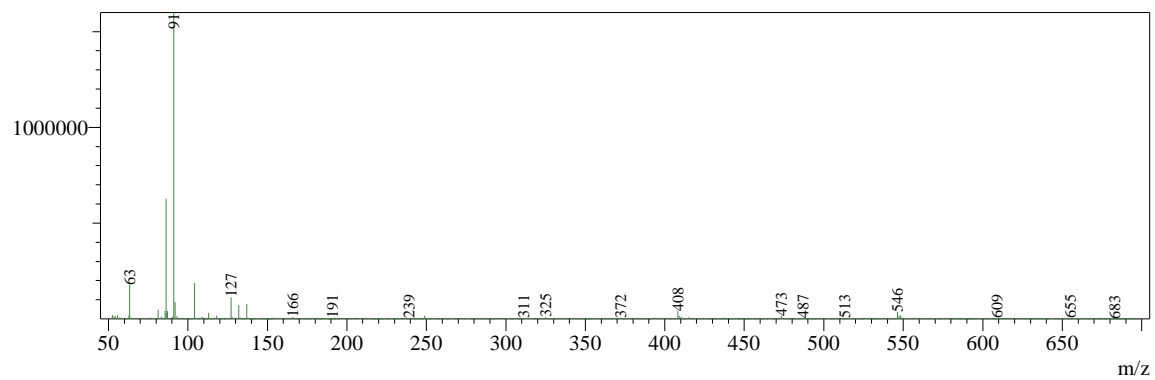
R.Time:11.973(Scan#:7185)
MassPeaks:363
Segment 1 - Event 1



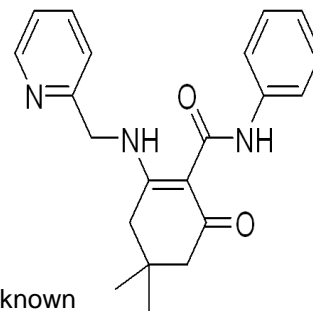
R. Time: 11.975 (Scan#: 7186)

Mass Peaks: 91

Segment 1 - Event 2



Analysis Report

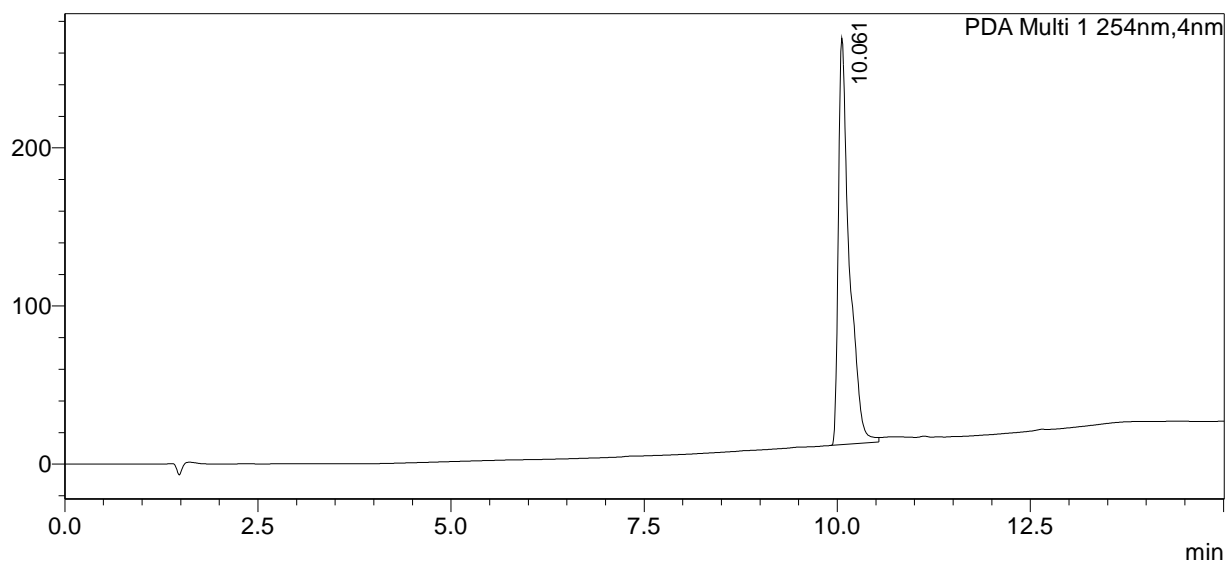


<Sample Information>

Sample Name	: DWY-CXCR2-015	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-015	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-015r.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 1-1		
Injection Volume	: 5 uL		
Date Acquired	: 12/14/2016 12:44:30 PM		
Date Processed	: 12/14/2016 12:59:32 PM		

<Chromatogram>

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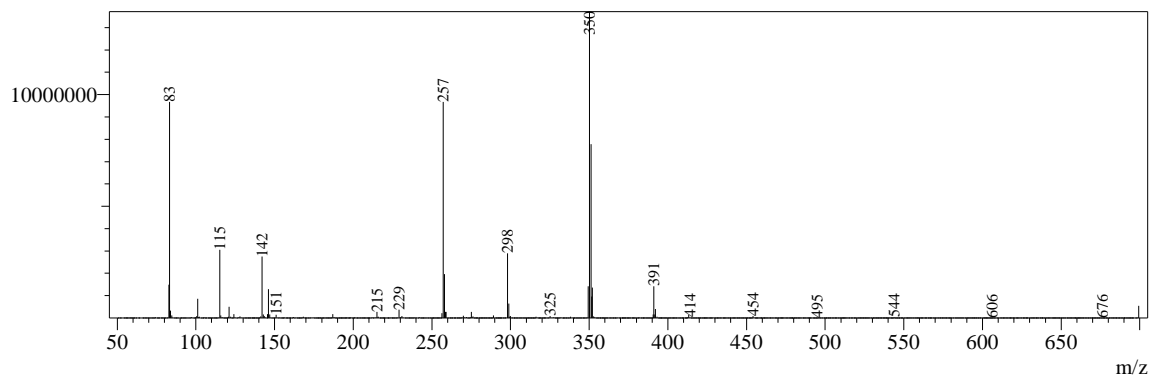


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	10.061	2537978	100.000
Total		2537978	100.000

MS Spectrum

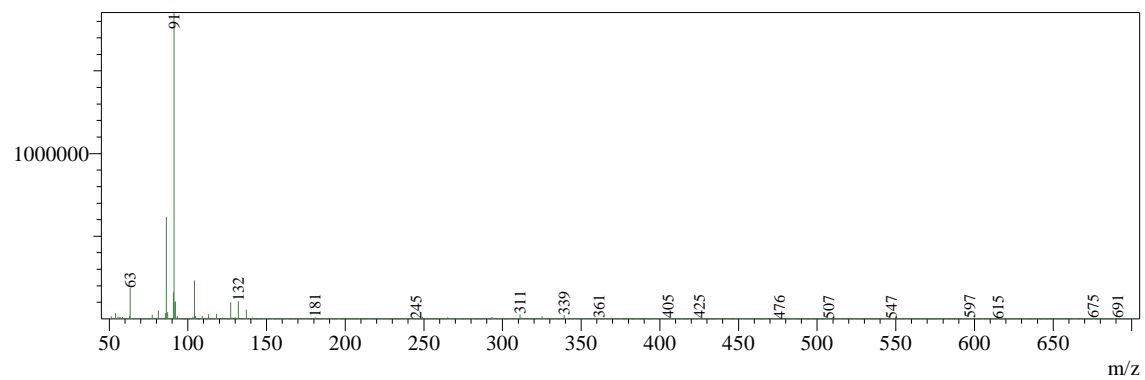
R.Time:10.060(Scan#:6037)
MassPeaks:350
Segment 1 - Event 1



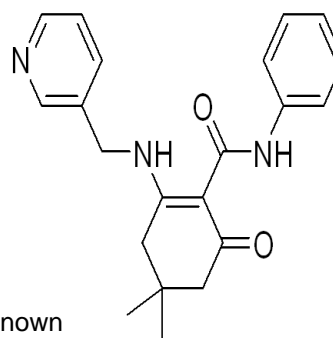
R. Time:10.061(Scan#:6038)

MassPeaks:91

Segment 1 - Event 2



Analysis Report

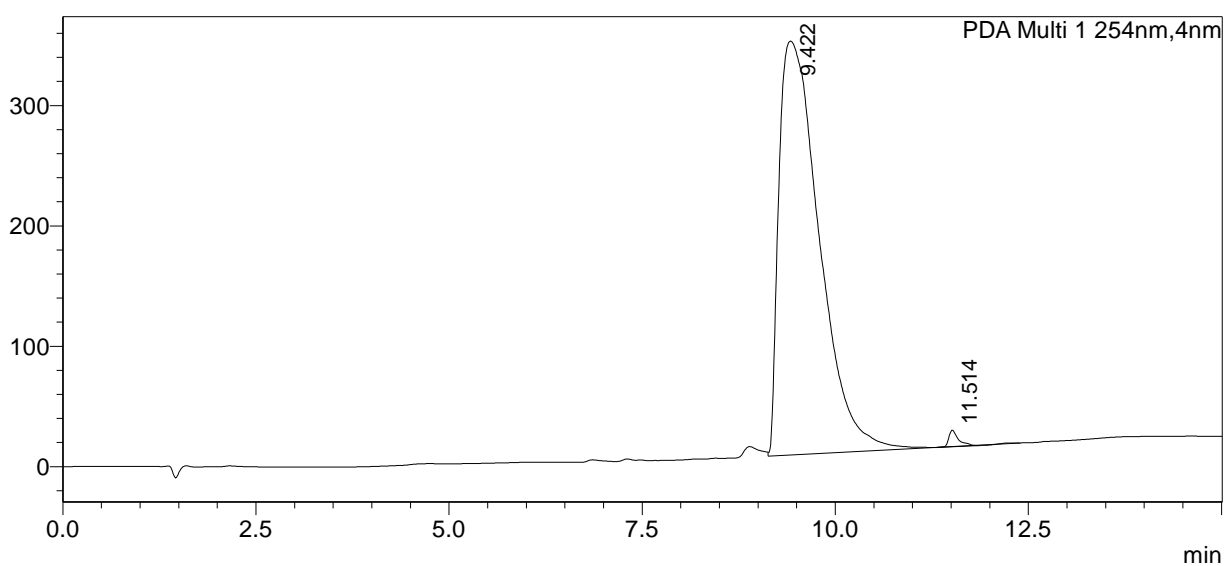


<Sample Information>

Sample Name	: DWY-CXCR2-016	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-016	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-016.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 3-5		
Injection Volume	: 10 uL		
Date Acquired	: 12/19/2016 4:45:41 PM		
Date Processed	: 12/19/2016 5:00:42 PM		

<Chromatogram>

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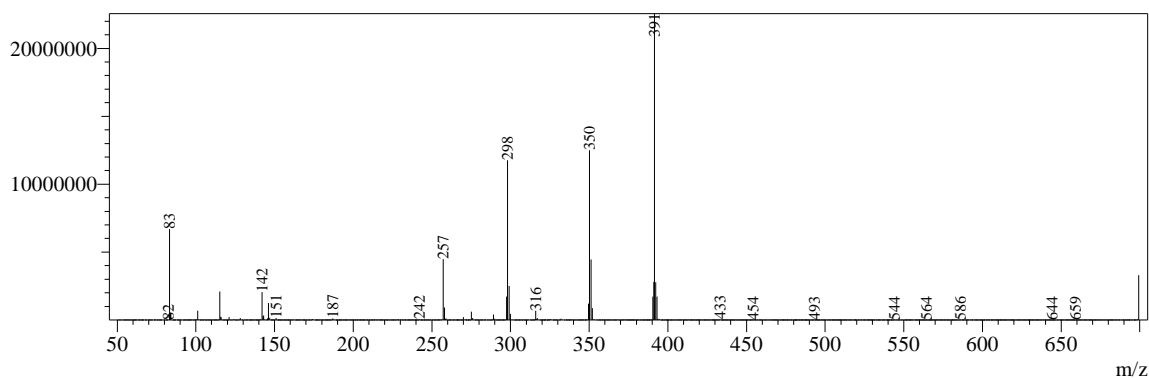


Peak Table

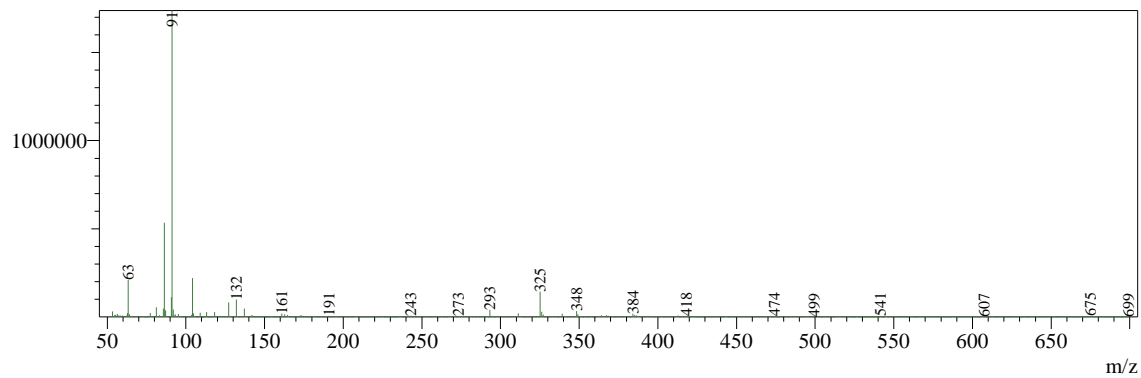
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	9.422	12480826	99.036
2	11.514	121540	0.964
Total		12602366	100.000

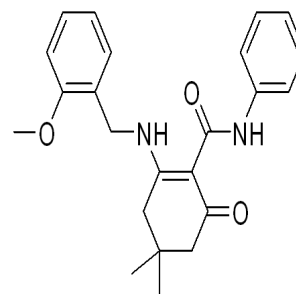
MS Spectrum

R.Time:9.420(Scan#:5653)
MassPeaks:391
Segment 1 - Event 1



R.Time:9.421(Scan#:5654)
MassPeaks:91
Segment 1 - Event 2



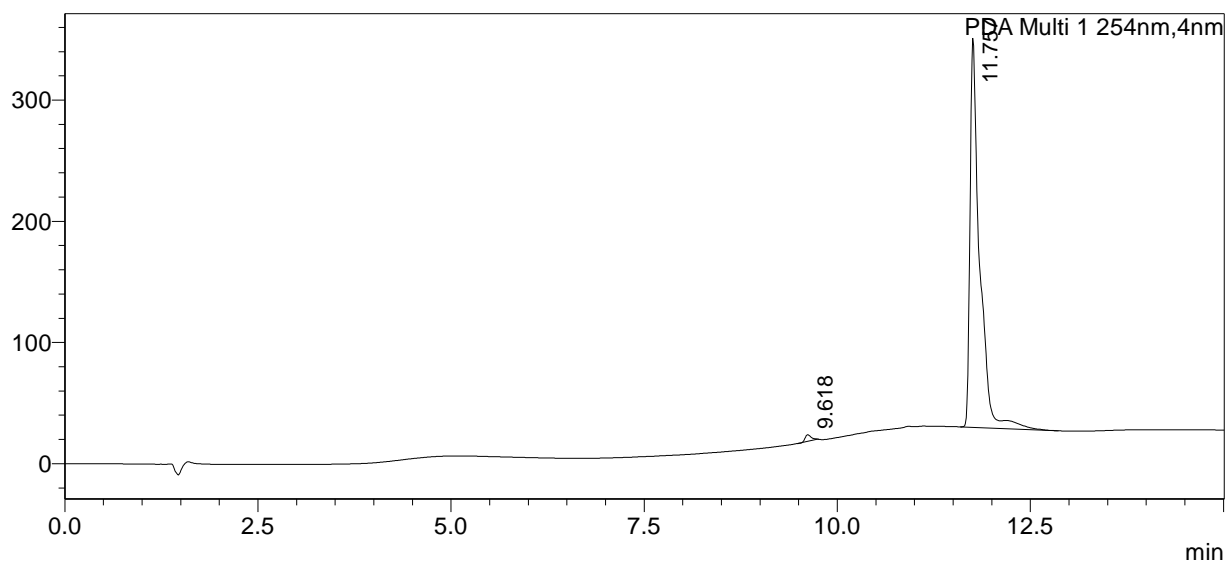


<Sample Information>

Sample Name	: DWY-CXCR2-017	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-017	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-017-1.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 3-11		
Injection Volume	: 10 uL		
Date Acquired	: 12/21/2016 10:29:01 AM		
Date Processed	: 12/21/2016 10:51:40 AM		

<Chromatogram>

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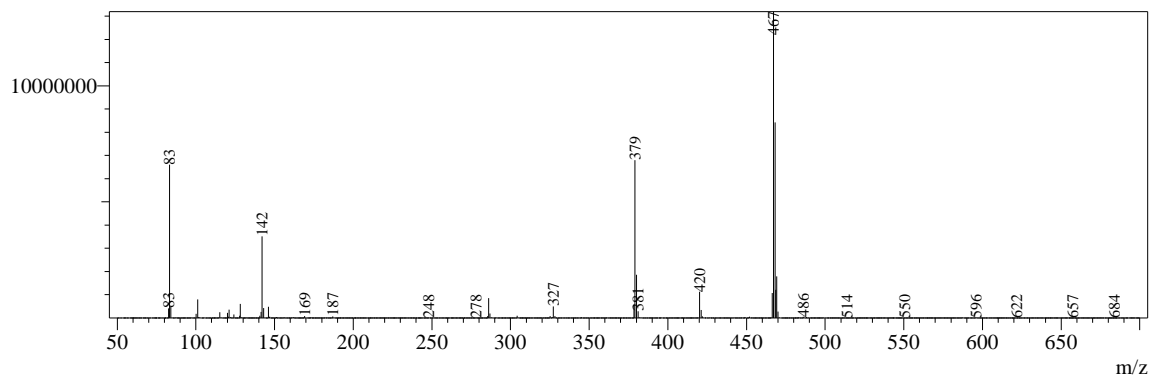


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	9.618	30216	1.079
2	11.757	2770264	98.921
Total		2800480	100.000

MS Spectrum

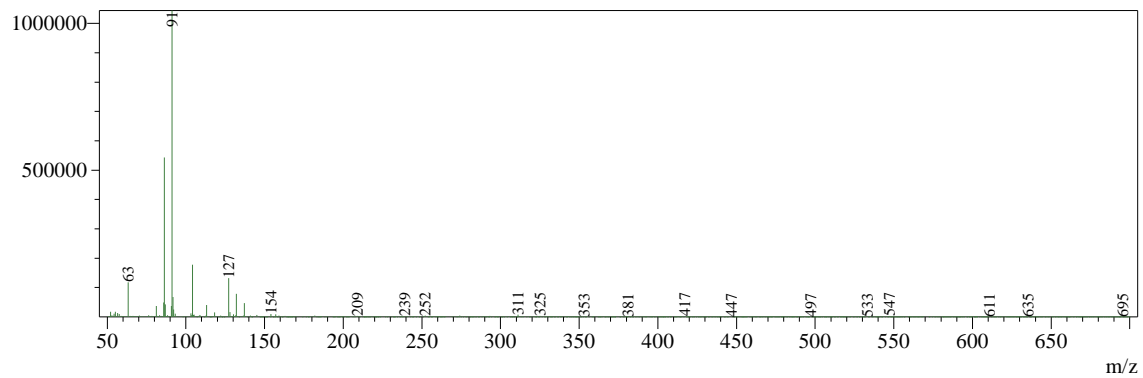
R.Time:11.757(Scan#:7055)
MassPeaks:467
Segment 1 - Event 1



R.Time:11.758(Scan#:7056)

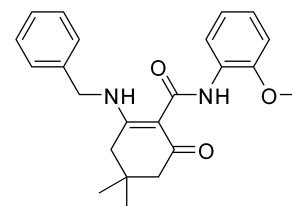
MassPeaks:91

Segment 1 - Event 2



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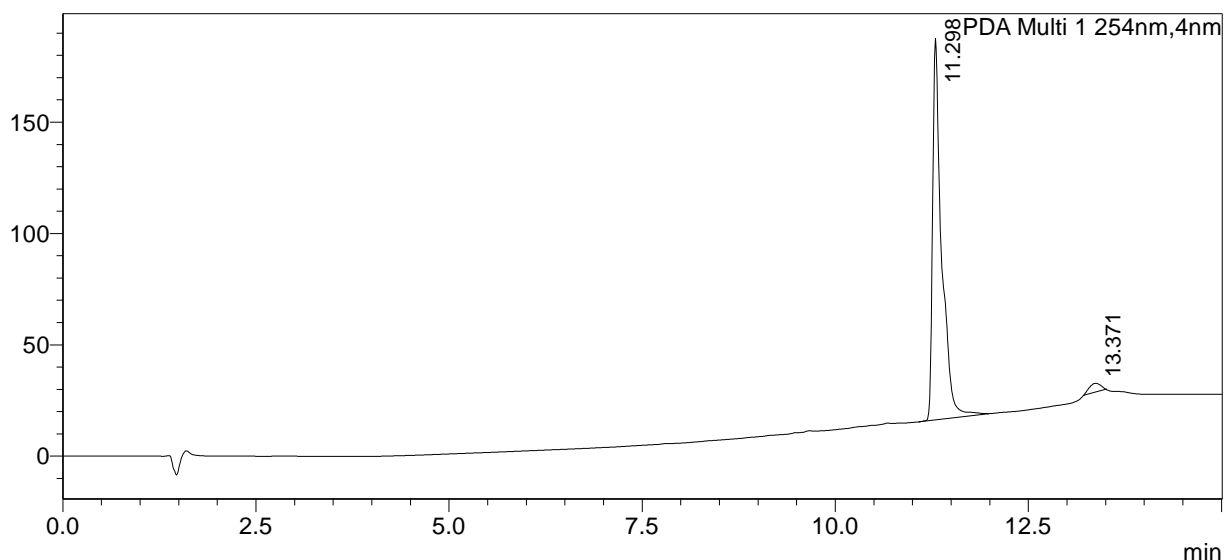
<Sample Information>

Sample Name : DWY-CXCR2-018
 Sample ID : DWY-CXCR2-018
 Data Filename : DWY-CXCR2-018.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 1-4
 Injection Volume : 10 uL
 Date Acquired : 12/21/2016 4:47:25 PM
 Date Processed : 12/22/2016 1:34:14 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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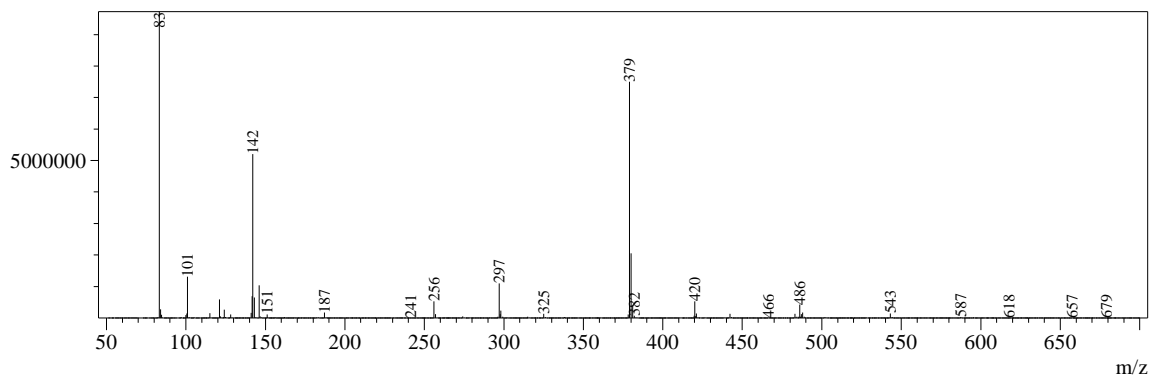


Peak Table

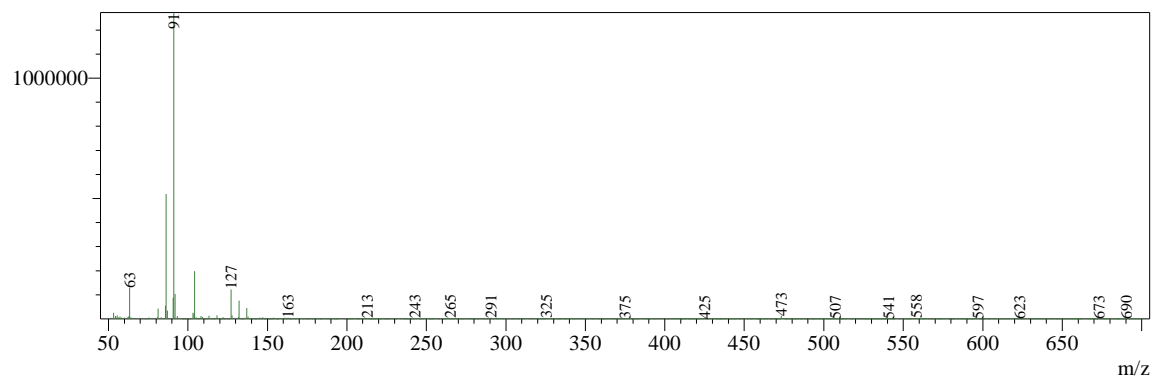
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	11.298	1394711	97.096
2	13.371	41713	2.904
Total		1436424	100.000

MS Spectrum

R.Time:11.297(Scan#:6779)
 MassPeaks:83
 Segment 1 - Event 1

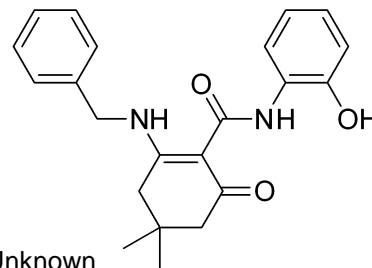


R.Time:11.298(Scan#:6780)
MassPeaks:91
Segment 1 - Event 2



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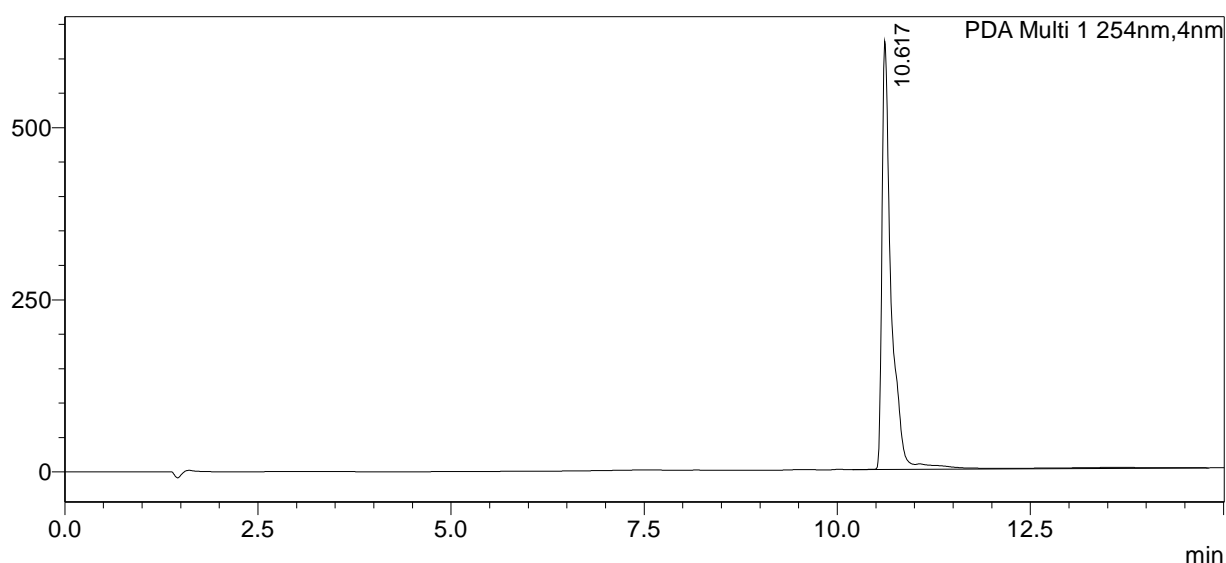
<Sample Information>

Sample Name : DWY-CXCR2-019
 Sample ID : DWY-CXCR2-019
 Data Filename : DWY-CXCR2-019.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 3-8
 Injection Volume : 10 uL
 Date Acquired : 1/6/2017 5:02:49 PM
 Date Processed : 1/6/2017 5:17:51 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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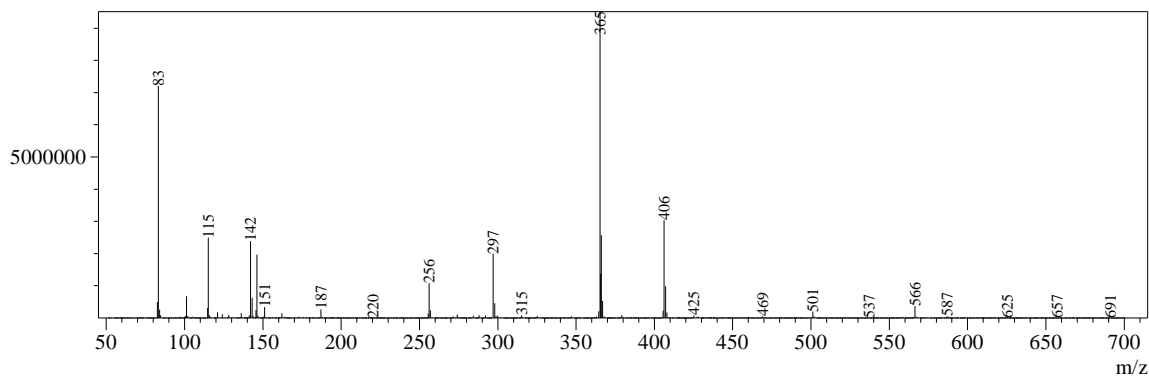
Peak Table

PDA Ch1 254nm

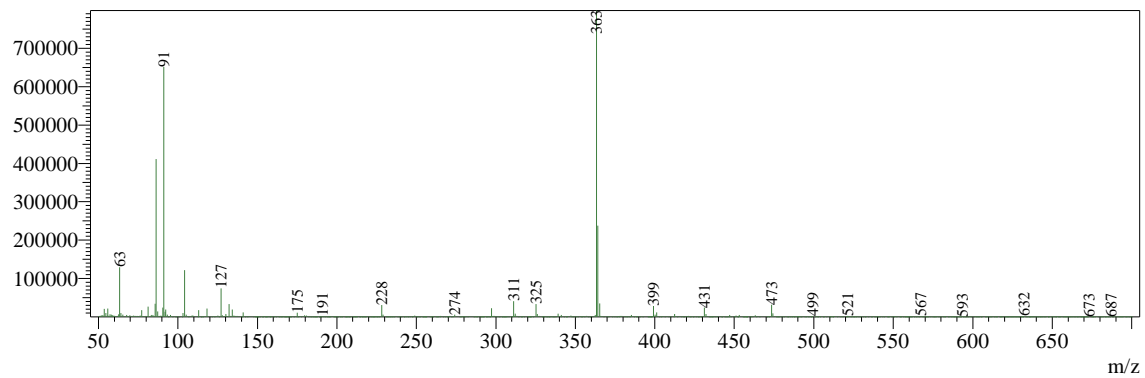
Peak#	Ret. Time	Area	Area%
1	10.617	5330931	100.000
Total		5330931	100.000

MS Spectrum

R.Time:10.617(Scan#:6371)
 MassPeaks:365
 Segment 1 - Event 1



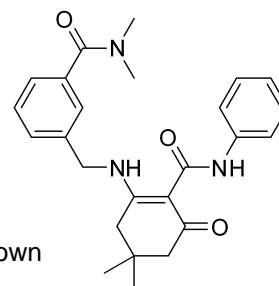
R.Time:10.618(Scan#:6372)
MassPeaks:363
Segment 1 - Event 2



<Sample Information>

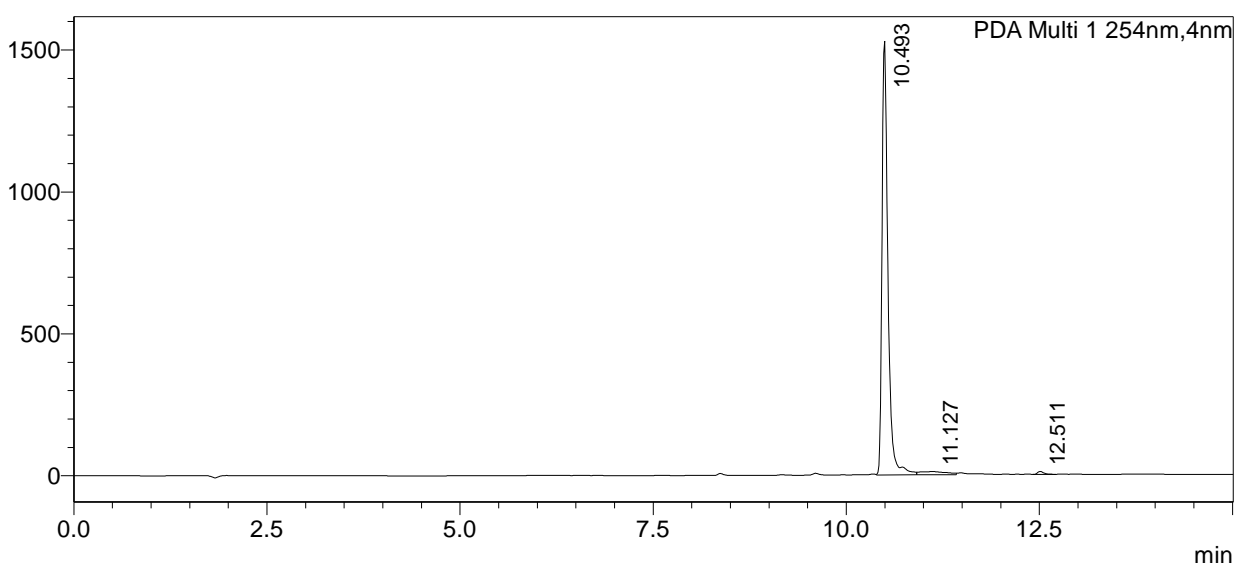
Sample Name : DWY-CXCR2-021
 Sample ID : DWY-CXCR2-021
 Data Filename : DWY-CXCR2-020(RE.lcd)
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 3-30
 Injection Volume : 10 uL
 Date Acquired : 1/10/2017 10:15:00 AM
 Date Processed : 1/10/2017 10:30:02 AM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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Peak Table

PDA Ch1 254nm

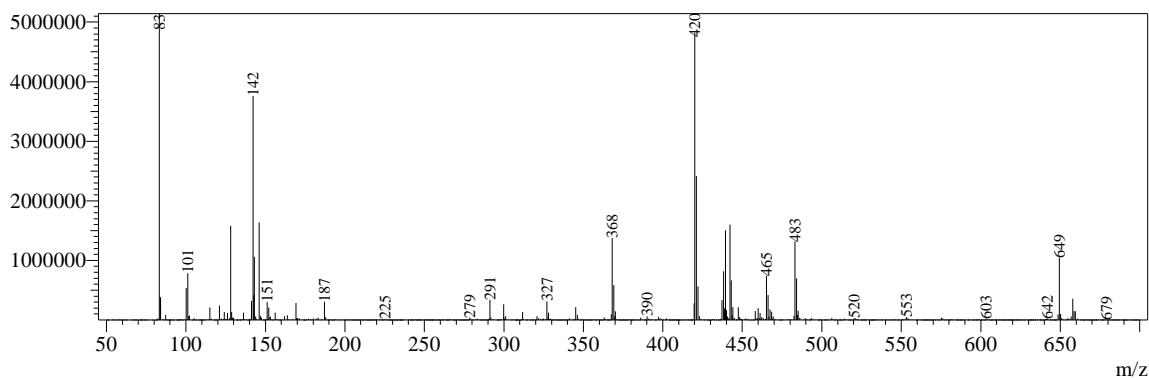
Peak#	Ret. Time	Area	Area%
1	10.493	8169157	95.940
2	11.127	281832	3.310
3	12.511	63884	0.750
Total		8514873	100.000

MS Spectrum

R.Time:10.490(Scan#:6295)

MassPeaks:83

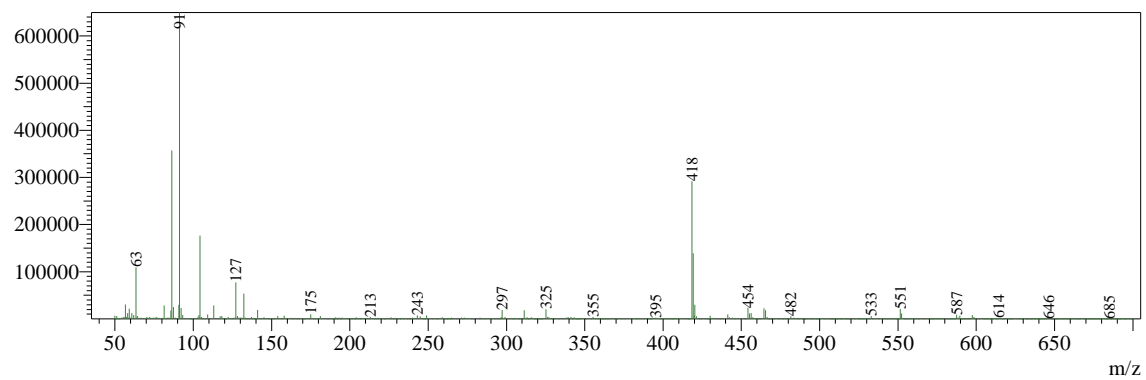
Segment 1 - Event 1



R. Time:10.491(Scan#:6296)

MassPeaks:91

Segment 1 - Event 2



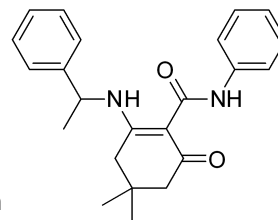
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<Sample Information>

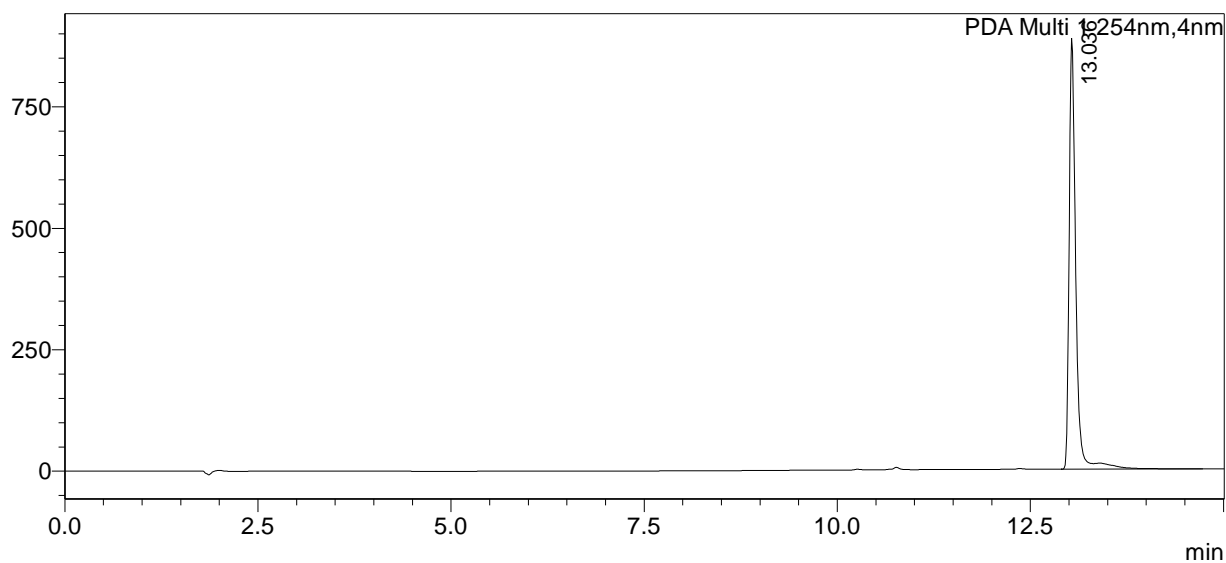
Sample Name : DWY-CXCR2-021
 Sample ID : DWY-CXCR2-021
 Data Filename : DWY-CXCR2-021.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 3-37
 Injection Volume : 10 uL
 Date Acquired : 1/9/2017 6:25:05 PM
 Date Processed : 1/9/2017 6:40:07 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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Peak Table

PDA Ch1 254nm

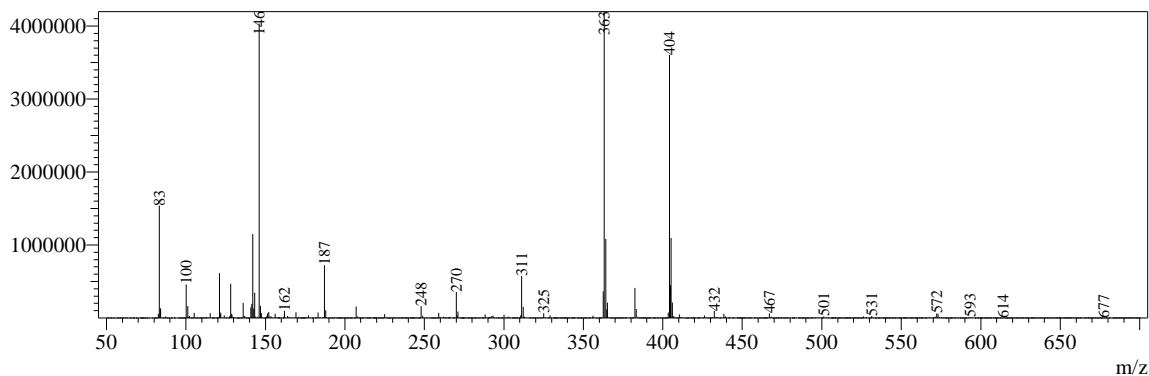
Peak#	Ret. Time	Area	Area%
1	13.036	5323136	100.000
Total		5323136	100.000

MS Spectrum

R.Time:13.033(Scan#:7821)

MassPeaks:363

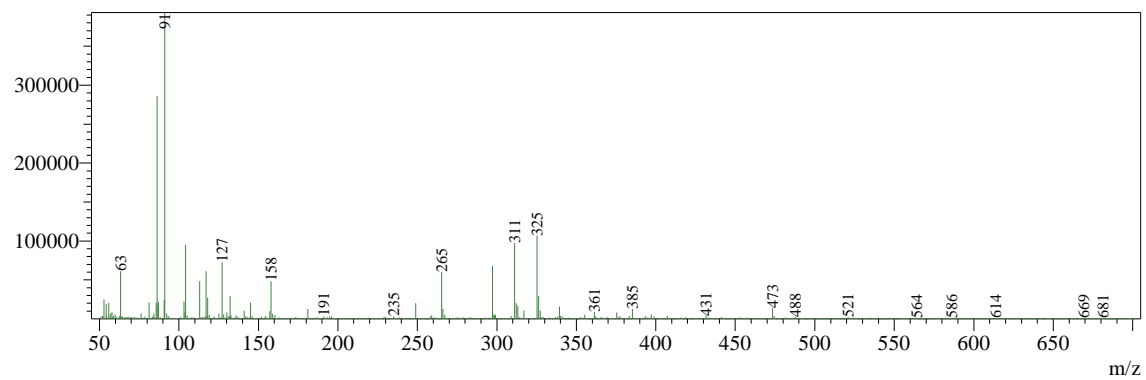
Segment 1 - Event 1

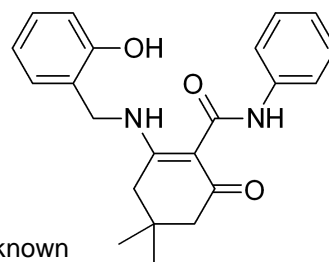


R. Time:13.035(Scan#:7822)

MassPeaks:91

Segment 1 - Event 2



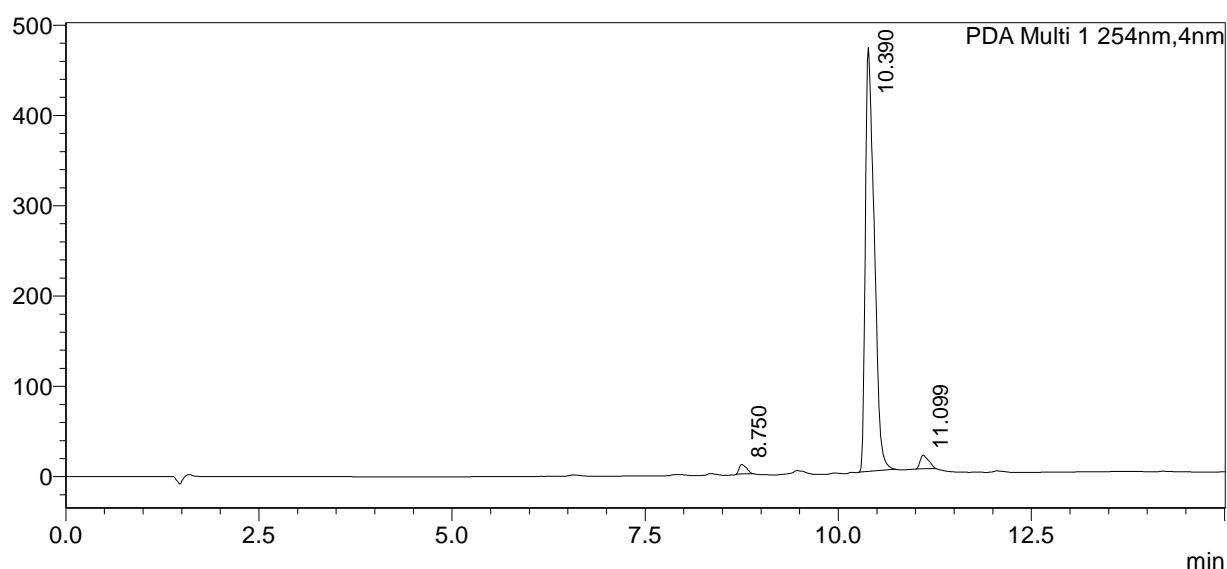


<Sample Information>

Sample Name	: DWY-CXCR2-022	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-022	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-022(RE2.lcd)	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 3-53		
Injection Volume	: 10 uL		
Date Acquired	: 1/13/2017 3:16:20 PM		
Date Processed	: 1/13/2017 3:32:57 PM		

<Chromatogram>

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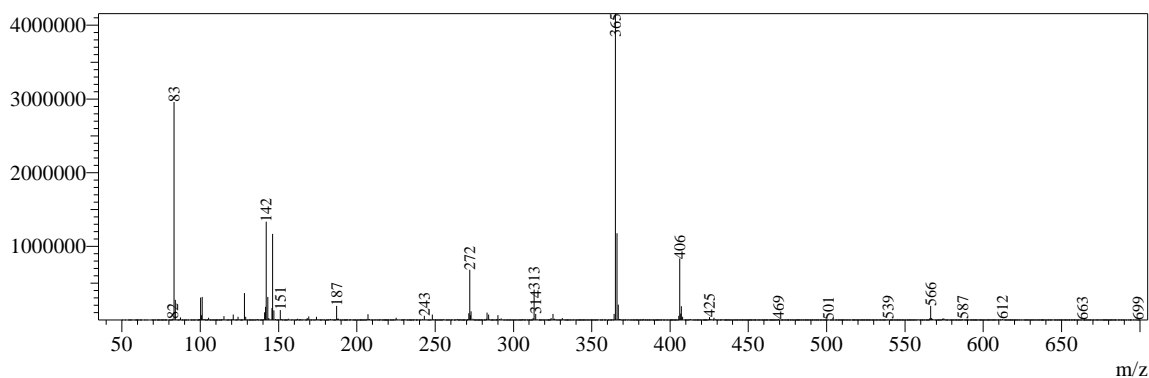


Peak Table

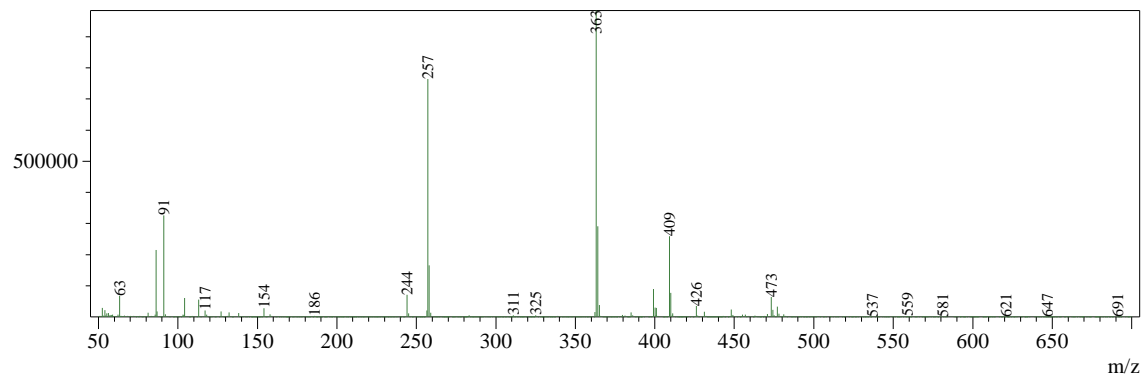
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	8.750	69399	1.757
2	10.390	3764738	95.325
3	11.099	115248	2.918
Total		3949385	100.000

MS Spectrum

R.Time:10.390(Scan#:6235)
MassPeaks:365
Segment 1 - Event 1



R.Time:10.391(Scan#:6236)
MassPeaks:363
Segment 1 - Event 2

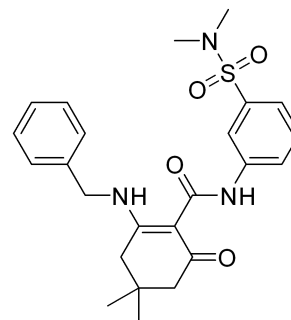


Analysis Report

<Sample Information>

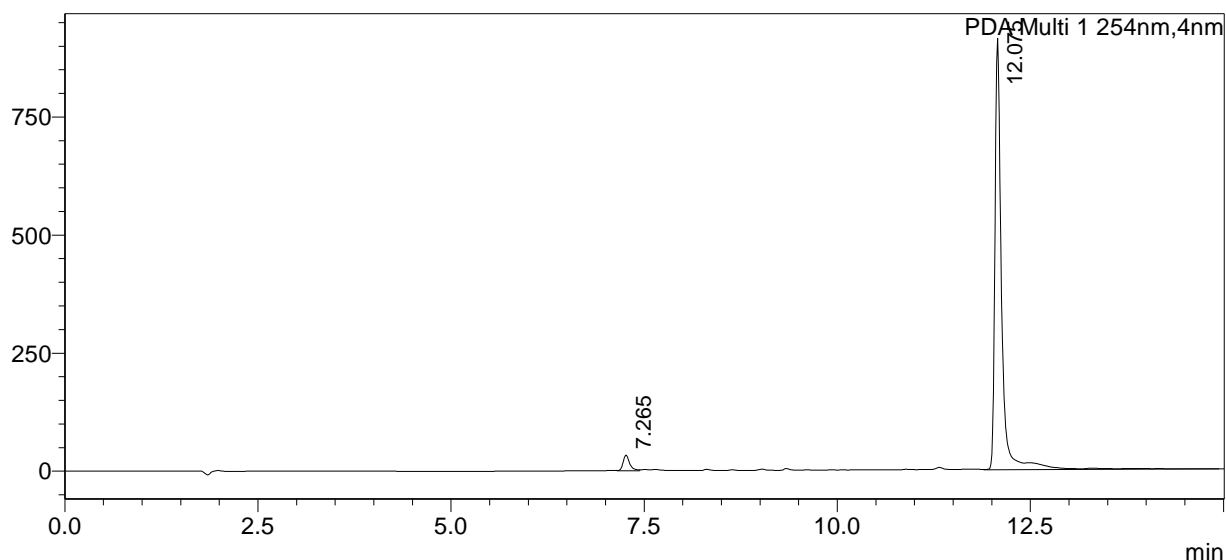
Sample Name : DWY-CXCR2-023
 Sample ID : DWY-CXCR2-023
 Data Filename : DWY-CXCR2-023.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 3-27
 Injection Volume : 10 uL
 Date Acquired : 1/13/2017 9:07:43 PM
 Date Processed : 1/13/2017 9:22:45 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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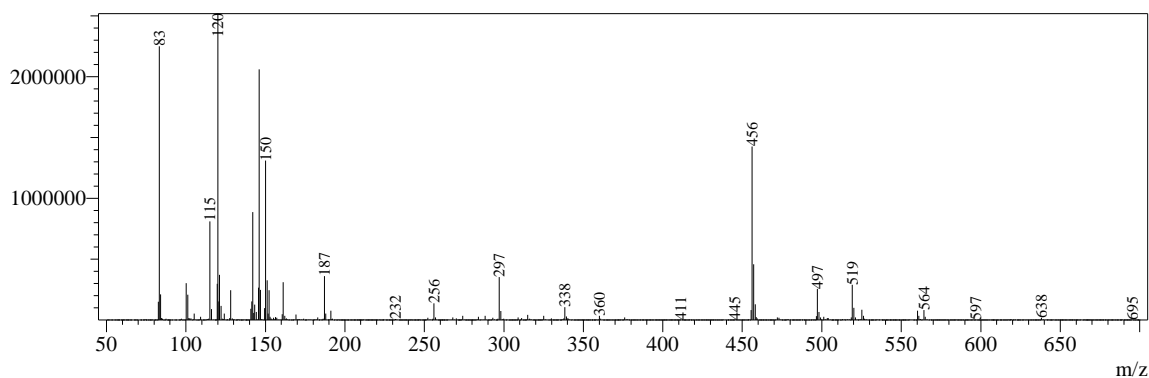


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	7.265	202358	3.544
2	12.075	5507414	96.456
Total		5709771	100.000

MS Spectrum

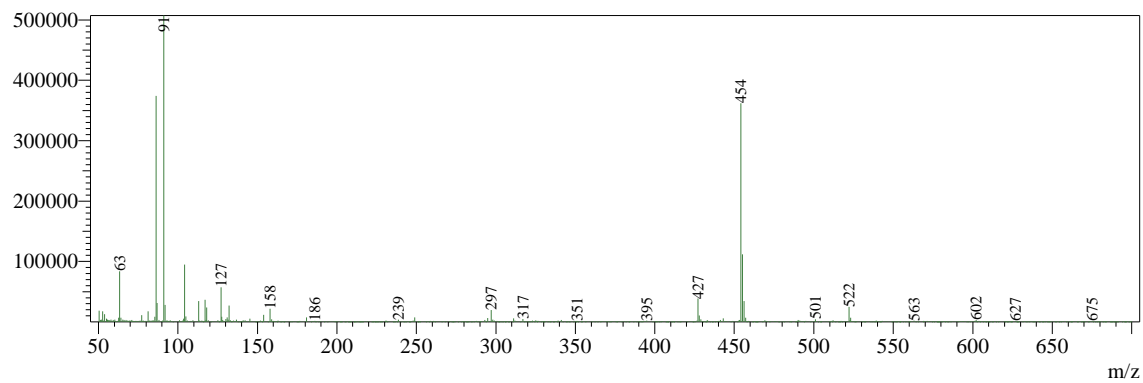
R.Time:12.073(Scan#:7245)
 MassPeaks:120
 Segment 1 - Event 1



R. Time: 12.075 (Scan#: 7246)

Mass Peaks: 91

Segment 1 - Event 2



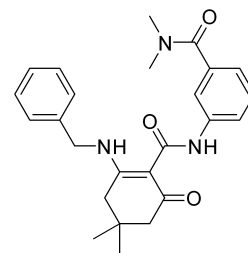
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Analysis Report

<Sample Information>

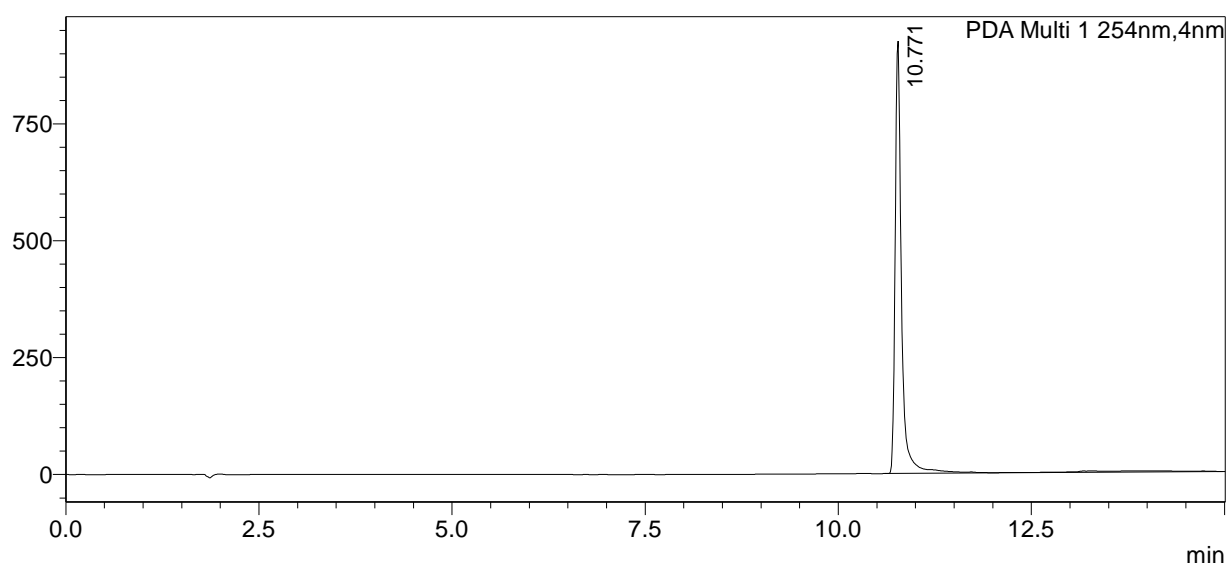
Sample Name : DWY-CXCR2-024
 Sample ID : DWY-CXCR2-024
 Data Filename : DWY-CXCR2-024(re.lcd)
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 1-36
 Injection Volume : 10 uL
 Date Acquired : 1/17/2017 10:36:59 AM
 Date Processed : 1/17/2017 10:52:00 AM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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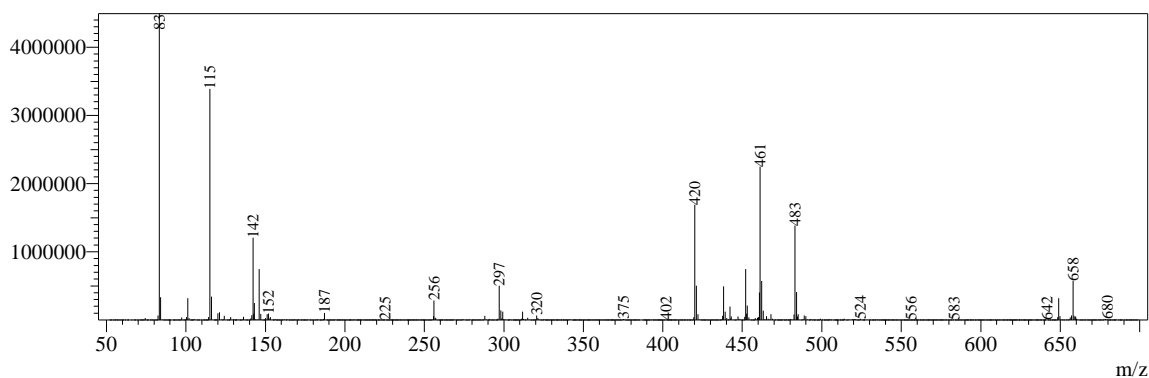
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	10.771	5335178	100.000
Total		5335178	100.000

MS Spectrum

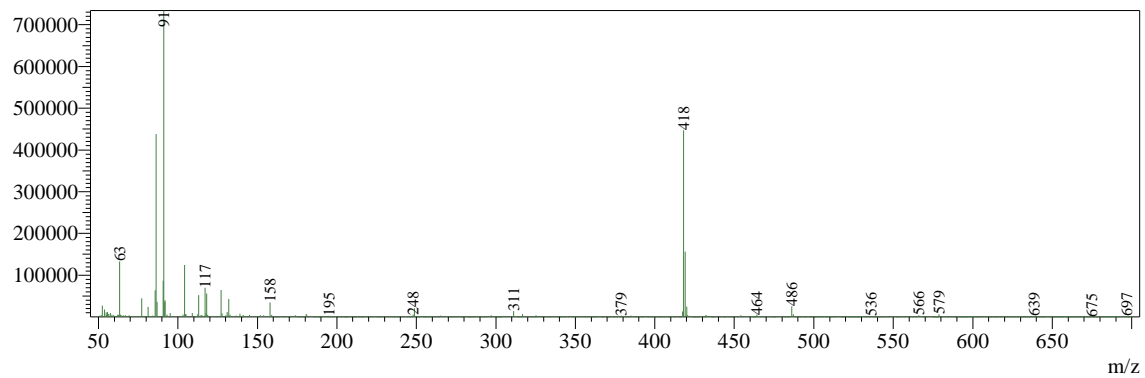
R.Time:10.770(Scan#:6463)
 MassPeaks:83
 Segment 1 - Event 1



R. Time: 10.771 (Scan#: 6464)

Mass Peaks: 91

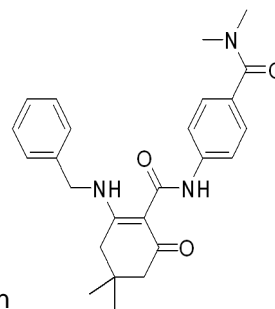
Segment 1 - Event 2



<Sample Information>

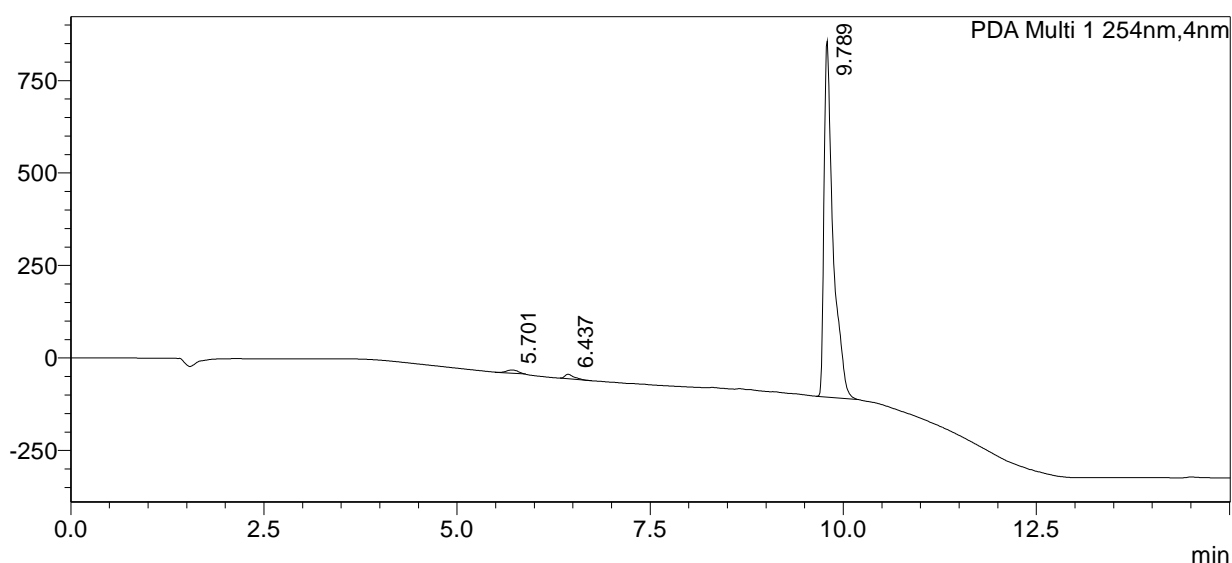
Sample Name : DWY-CXCR2-025
 Sample ID : DWY-CXCR2-025
 Data Filename : DWY-CXCR2-025.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 3-26
 Injection Volume : 10 uL
 Date Acquired : 1/17/2017 3:27:22 PM
 Date Processed : 1/18/2017 1:42:48 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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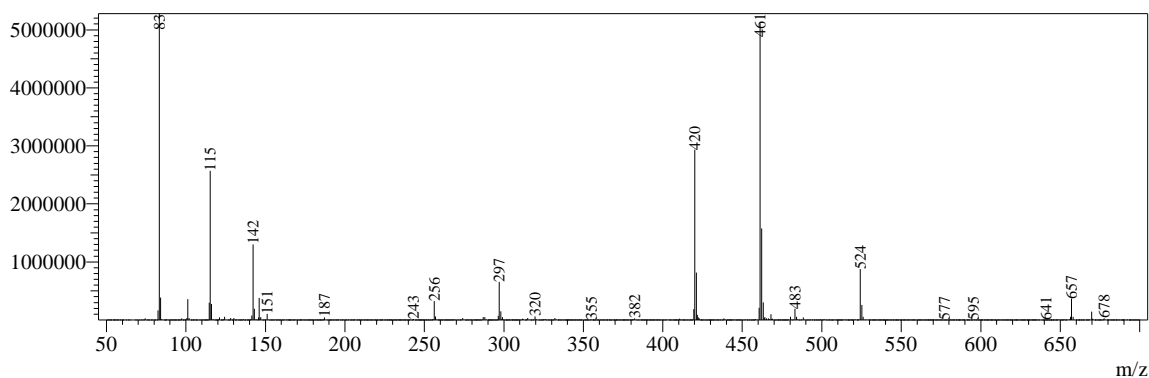


Peak Table

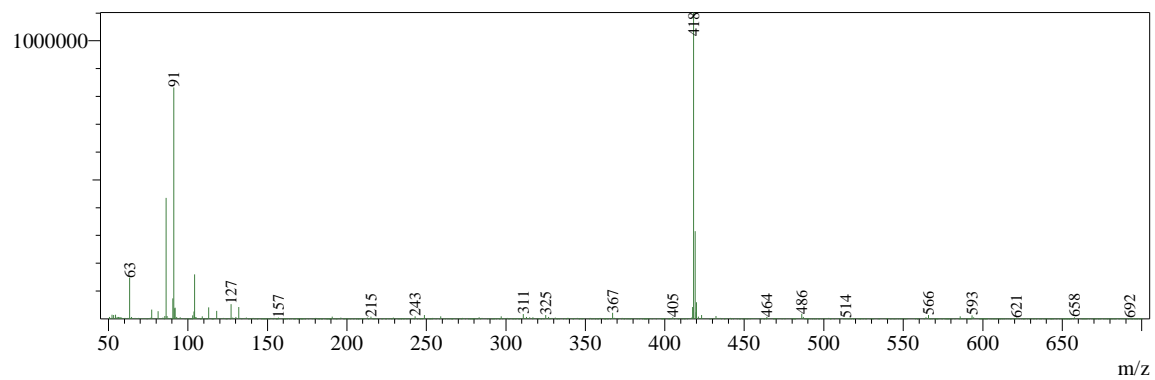
Peak#	Ret. Time	Area	Area%
1	5.701	89412	1.114
2	6.437	104147	1.298
3	9.789	7833153	97.589
Total		8026712	100.000

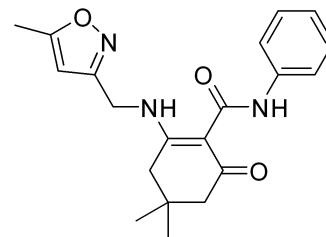
MS Spectrum

R.Time:9.787(Scan#:5873)
 MassPeaks:83
 Segment 1 - Event 1



R.Time:9.788(Scan#:5874)
MassPeaks:418
Segment 1 - Event 2



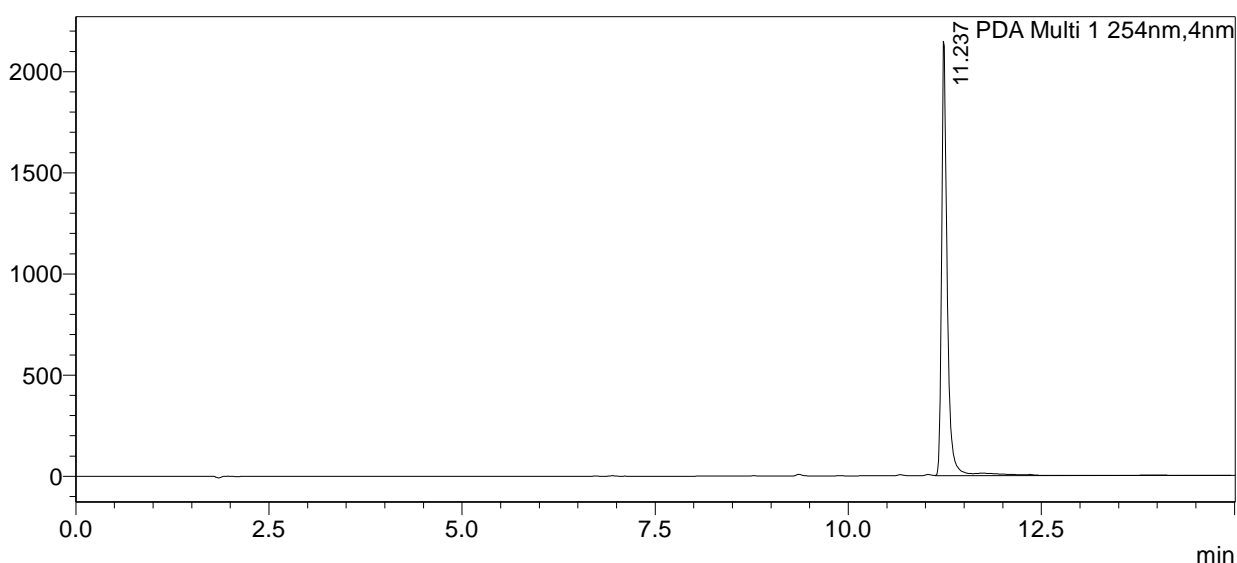


<Sample Information>

Sample Name	: DWY-CXCR2-025	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-025	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-026.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 4-46		
Injection Volume	: 10 uL		
Date Acquired	: 1/18/2017 11:01:52 AM		
Date Processed	: 1/18/2017 11:16:55 AM		

<Chromatogram>

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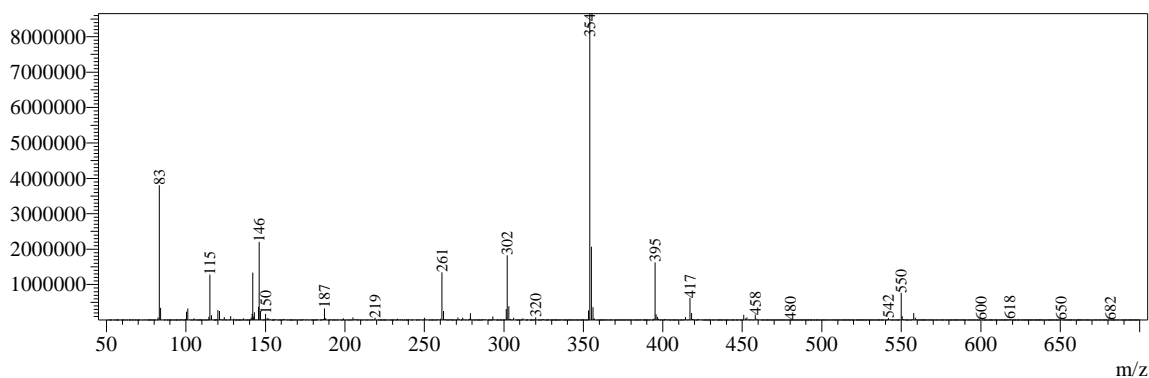


Peak Table

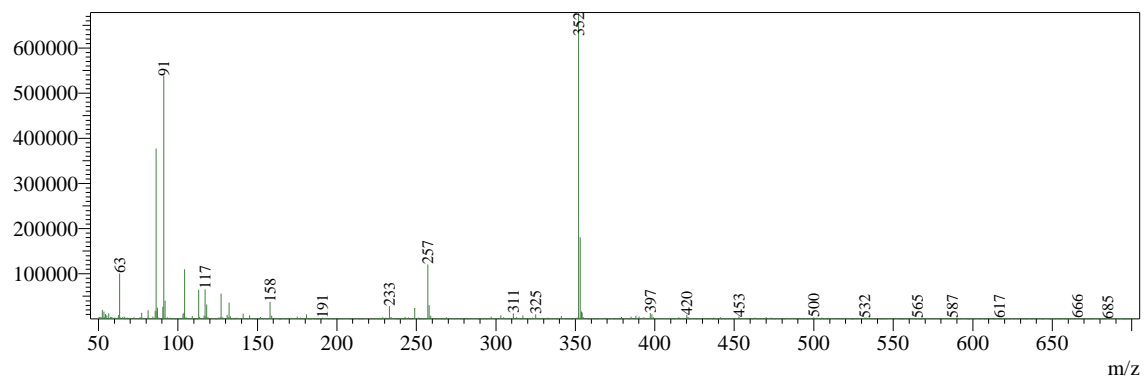
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	11.237	11000909	100.000
Total		11000909	100.000

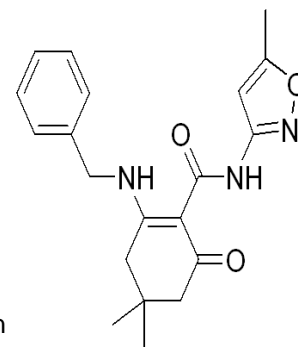
MS Spectrum

R.Time:11.237(Scan#:6743)
MassPeaks:354
Segment 1 - Event 1



R.Time:11.238(Scan#:6744)
MassPeaks:352
Segment 1 - Event 2





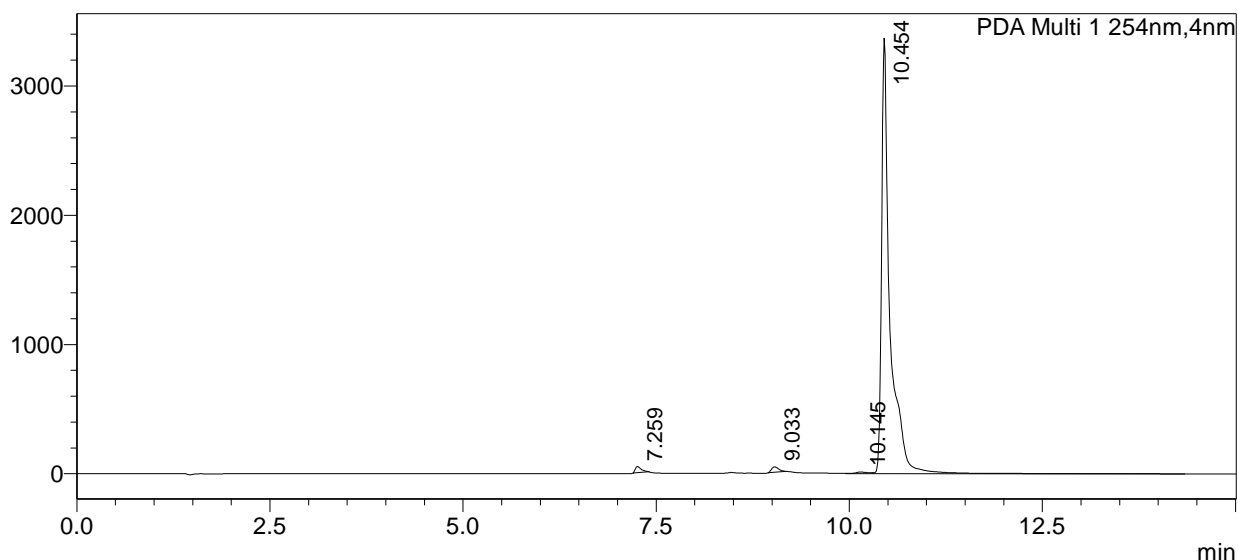
<Sample Information>

Sample Name : DWY-CXCR2-027
 Sample ID : DWY-CXCR2-027
 Data Filename : DWY-CXCR2-027(re2.lcd)
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 4-2
 Injection Volume : 10 uL
 Date Acquired : 1/19/2017 2:38:10 PM
 Date Processed : 1/19/2017 2:54:45 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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Peak Table

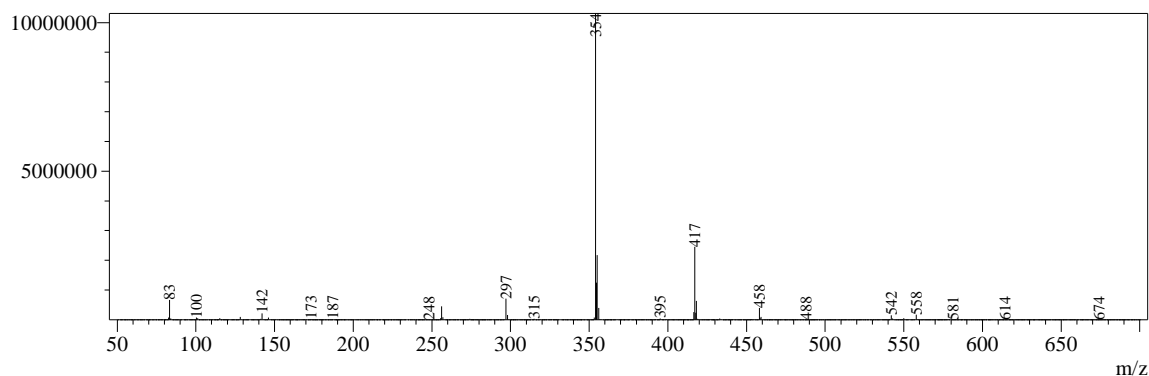
Peak#	Ret. Time	Area	Area%
1	7.259	262516	0.993
2	9.033	267003	1.010
3	10.145	184161	0.696
4	10.454	25733721	97.302
Total		26447401	100.000

MS Spectrum

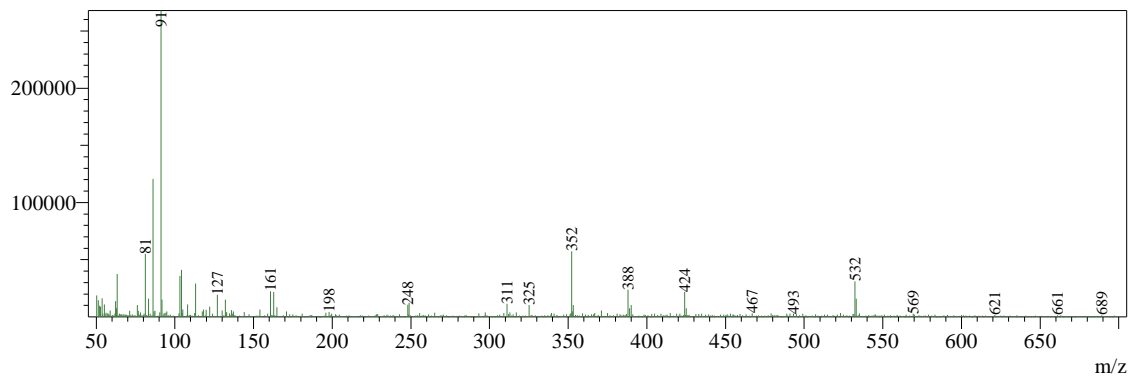
R. Time: 10.453 (Scan#: 6273)

MassPeaks: 354

Segment 1 - Event 1



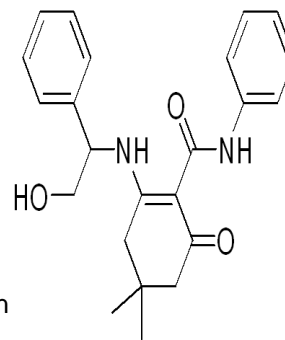
R.Time:10.455(Scan#:6274)
MassPeaks:91
Segment 1 - Event 2



<Sample Information>

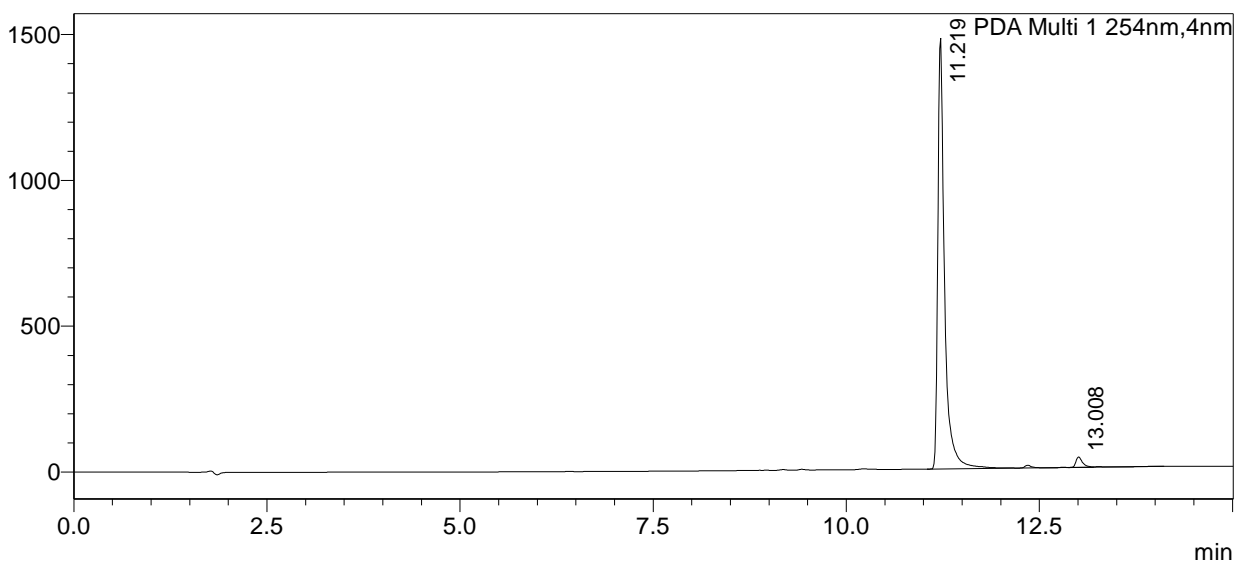
Sample Name : DWY-CXCR2-028
 Sample ID : DWY-CXCR2-028
 Data Filename : DWY-CXCR2-028.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 2-5
 Injection Volume : 10 uL
 Date Acquired : 2/1/2017 12:35:39 PM
 Date Processed : 2/1/2017 5:30:24 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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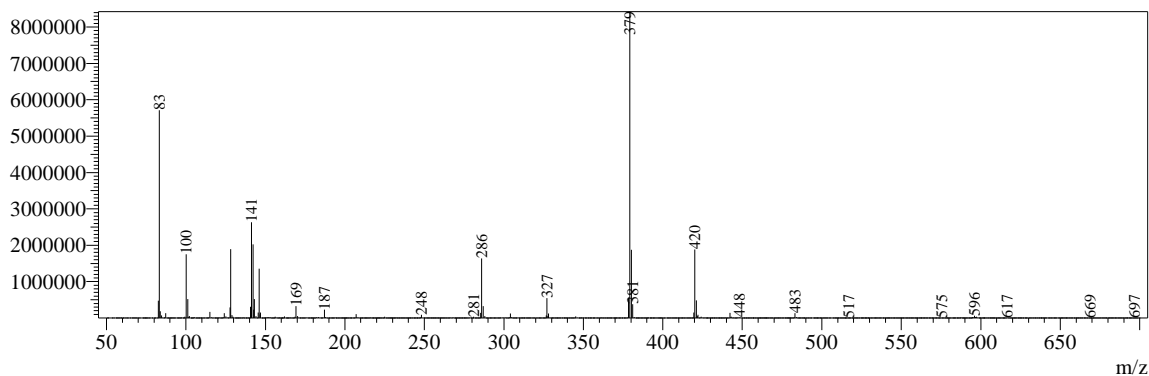
Peak Table

PDA Ch1 254nm

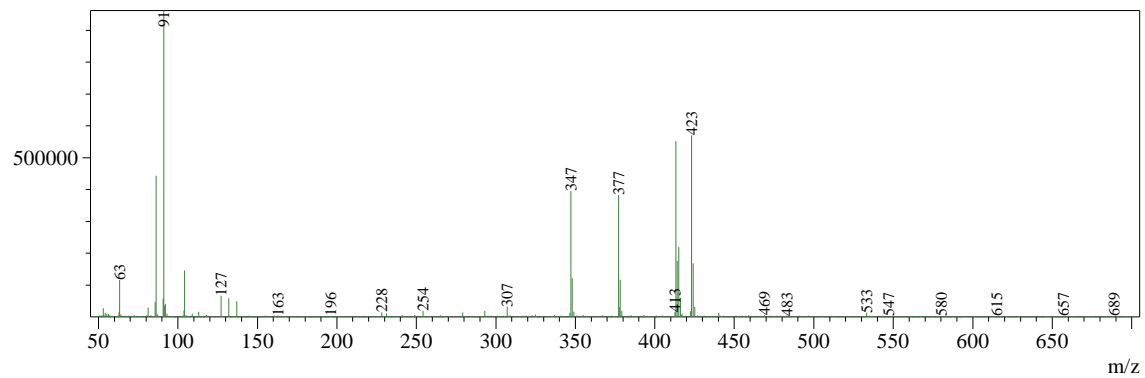
Peak#	Ret. Time	Area	Area%
1	11.219	8915028	97.577
2	13.008	221359	2.423
Total		9136387	100.000

MS Spectrum

R.Time:11.217(Scan#:6731)
 MassPeaks:379
 Segment 1 - Event 1



R.Time:11.218(Scan#:6732)
MassPeaks:91
Segment 1 - Event 2



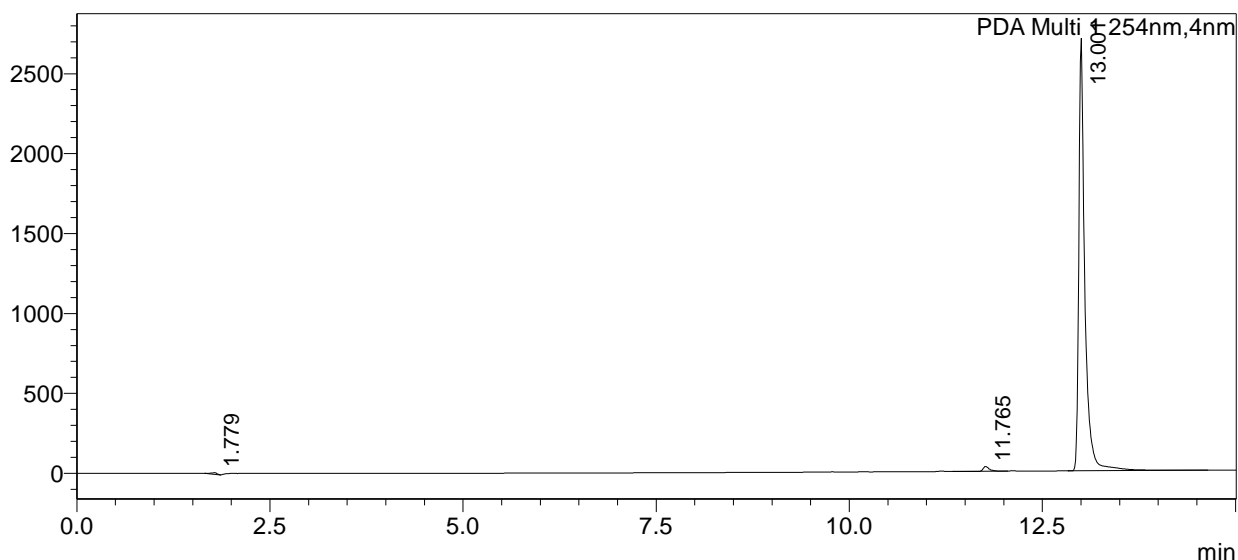
<Sample Information>

Sample Name : DWY-CXCR2-029R
 Sample ID : DWY-CXCR2-029
 Data Filename : DWY-CXCR2-029(RE1.lcd)
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 2-7
 Injection Volume : 10 uL
 Date Acquired : 2/1/2017 2:18:59 PM
 Date Processed : 2/1/2017 2:34:01 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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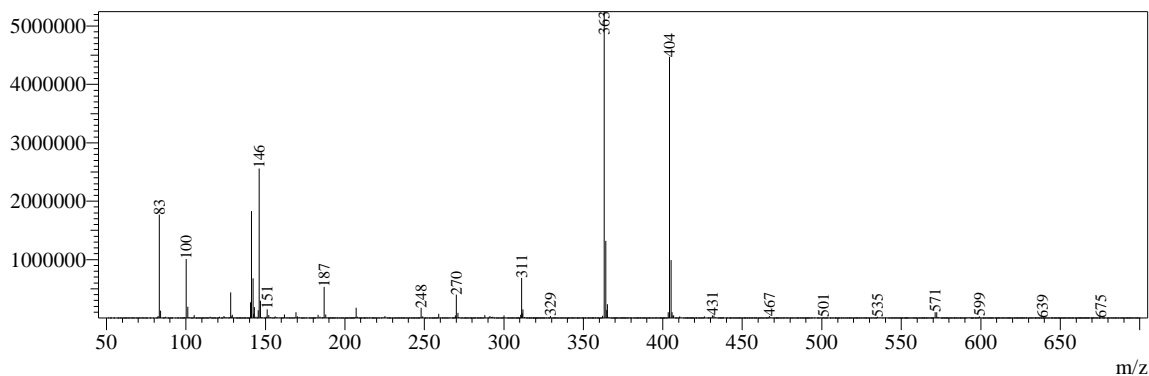


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	1.779	50901	0.339
2	11.765	176884	1.179
3	13.001	14774534	98.482
Total		15002319	100.000

MS Spectrum

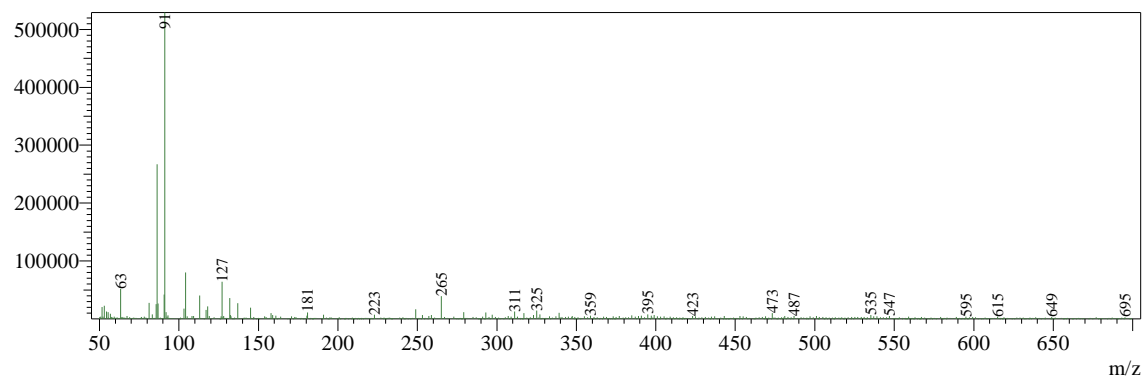
R.Time:13.000(Scan#:7801)
 MassPeaks:363
 Segment 1 - Event 1



R. Time:13.001(Scan#:7802)

MassPeaks:91

Segment 1 - Event 2





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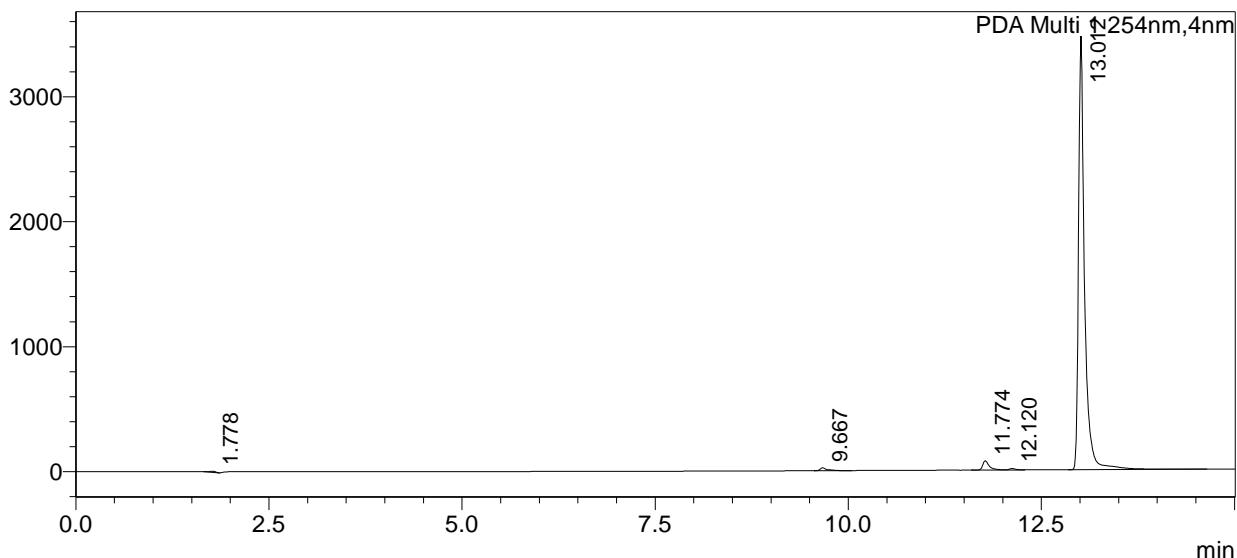
Analysis Report

<Sample Information>

Sample Name : DWY-CXCR2-030(S)
 Sample ID : DWY-CXCR2-030
 Data Filename : DWY-CXCR2-030(S).lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 2-14 Sample Type : Unknown
 Injection Volume : 10 uL
 Date Acquired : 2/1/2017 5:03:51 PM Acquired by : System Administrator
 Date Processed : 2/1/2017 5:18:54 PM Processed by : System Administrator

<Chromatogram>

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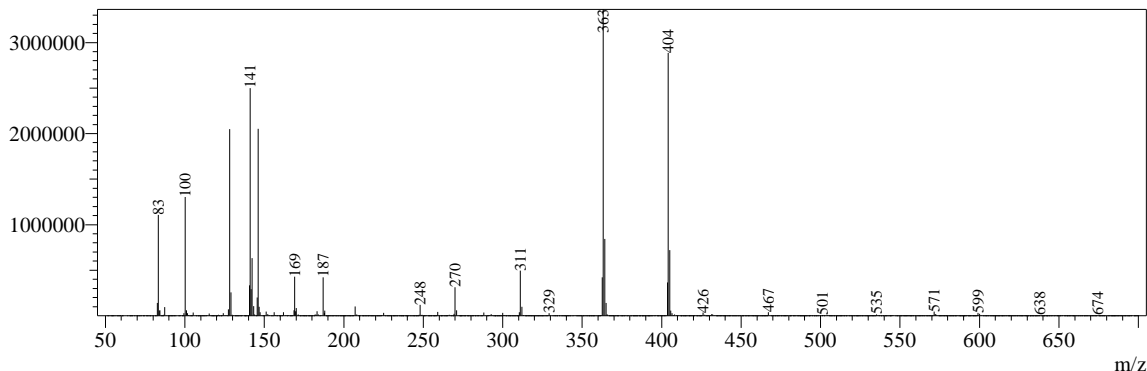


Peak Table

Peak#	Ret. Time	Area	Area%
1	1.778	50727	0.257
2	9.667	154667	0.785
3	11.774	460565	2.336
4	12.120	77563	0.393
5	13.012	18969144	96.228
Total		19712665	100.000

R. Time: 13.010 (Scan#: 7807)
 MassPeaks: 363
 Segment 1 - Event 1

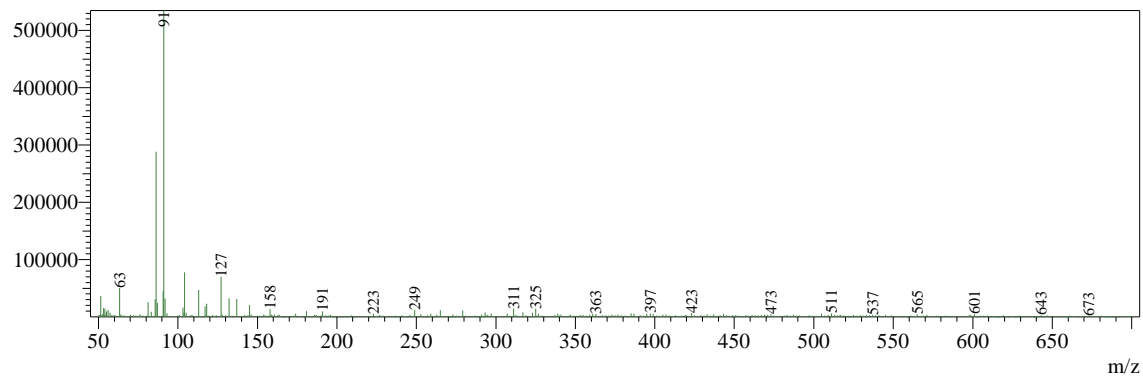
MS Spectrum

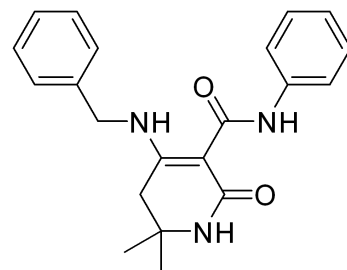


R. Time:13.011(Scan#:7808)

MassPeaks:91

Segment 1 - Event 2



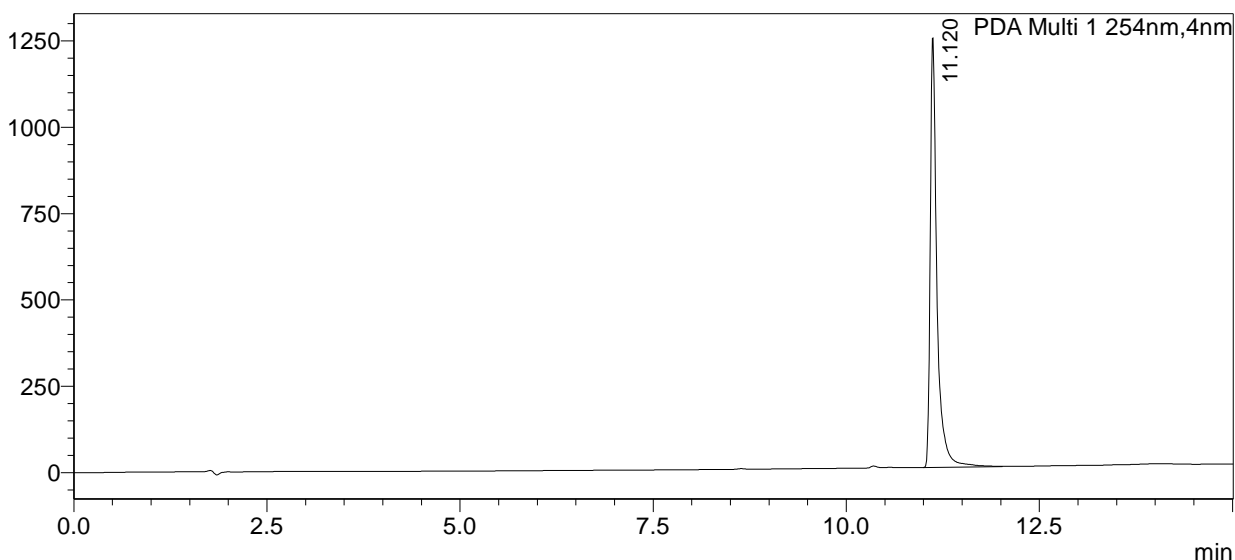


<Sample Information>

Sample Name	: DWY-CXCR2-031	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-031	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-031.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 2-9		
Injection Volume	: 10 uL		
Date Acquired	: 2/1/2017 4:37:41 PM		
Date Processed	: 2/1/2017 5:30:33 PM		

<Chromatogram>

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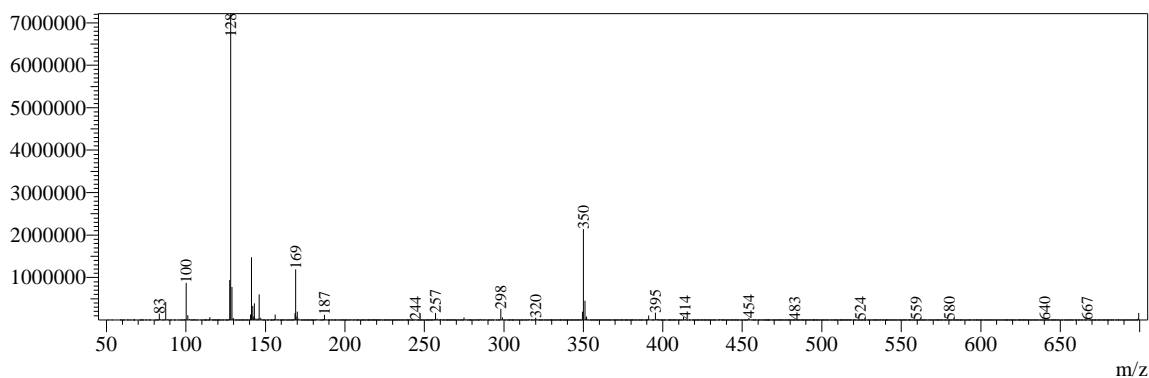


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	11.120	7568222	100.000
Total		7568222	100.000

MS Spectrum

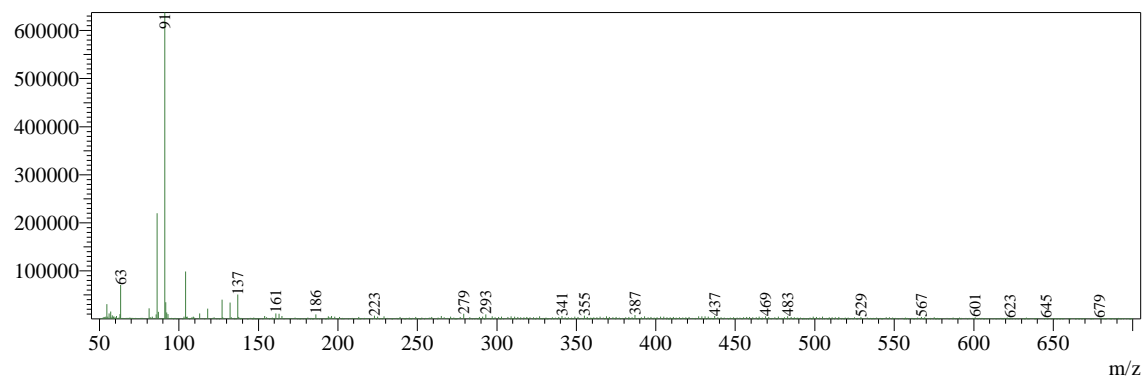
R.Time:11.120(Scan#:6673)
MassPeaks:128
Segment 1 - Event 1



R. Time: 11.121 (Scan#: 6674)

MassPeaks: 91

Segment 1 - Event 2





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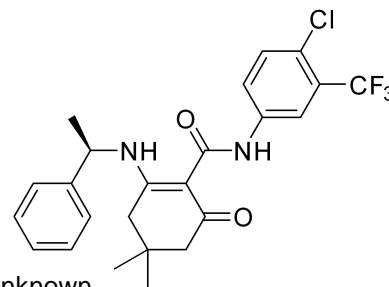
LabSolutions

Analysis Report

<Sample Information>

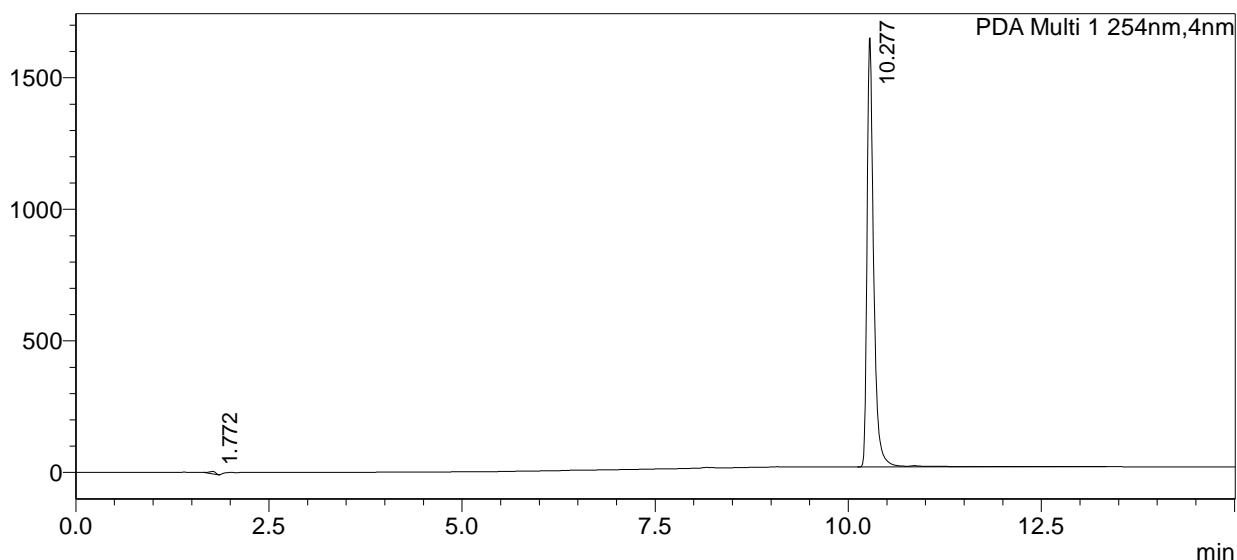
Sample Name : DWY-CXCR2-032R
 Sample ID : DWY-CXCR2-032R
 Data Filename : DWY-CXCR2-032R-Method2.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyangB.lcm
 Batch Filename :
 Vial # : 2-32
 Injection Volume : 10 uL
 Date Acquired : 2/3/2017 5:32:00 PM
 Date Processed : 2/3/2017 5:47:02 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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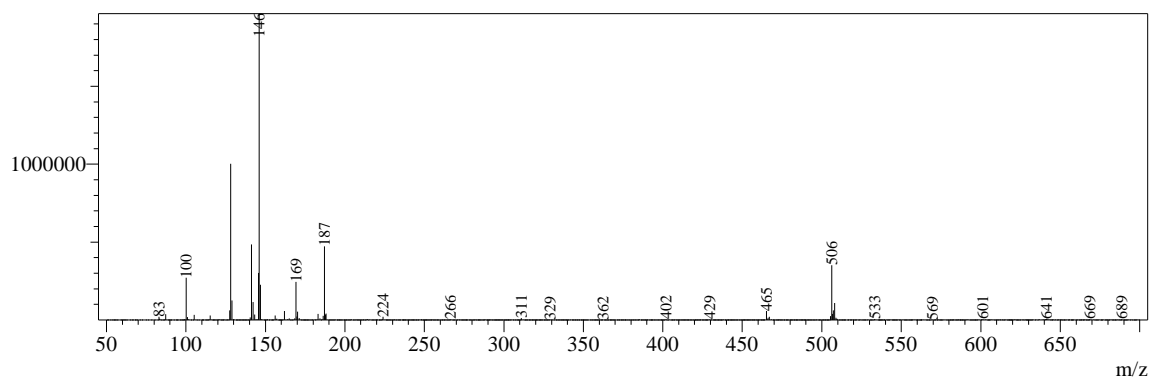
Peak Table

PDA Ch1 254nm

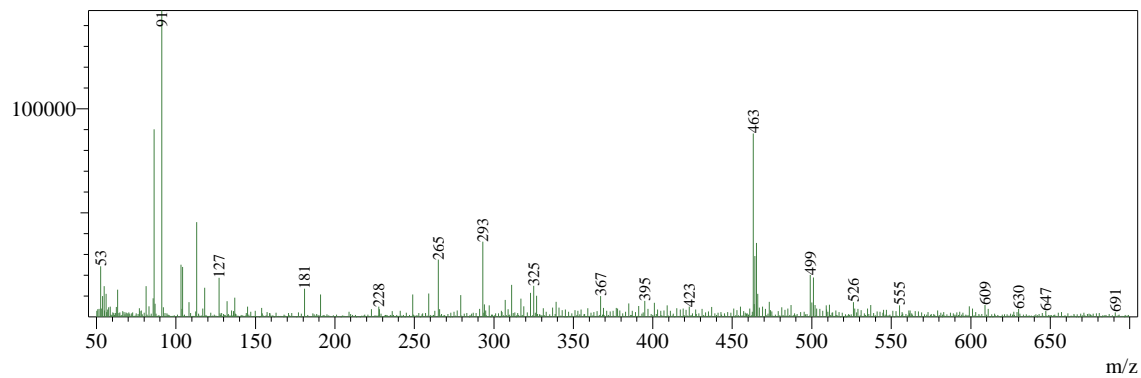
Peak#	Ret. Time	Area	Area%
1	1.772	49175	0.499
2	10.277	9797704	99.501
Total		9846879	100.000

MS Spectrum

R.Time:10.280(Scan#:6169)
 MassPeaks:146
 Segment 1 - Event 1



R.Time:10.281(Scan#:6170)
MassPeaks:91
Segment 1 - Event 2

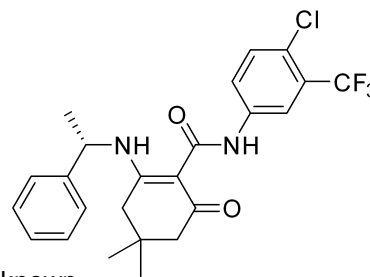


Analysis Report

<Sample Information>

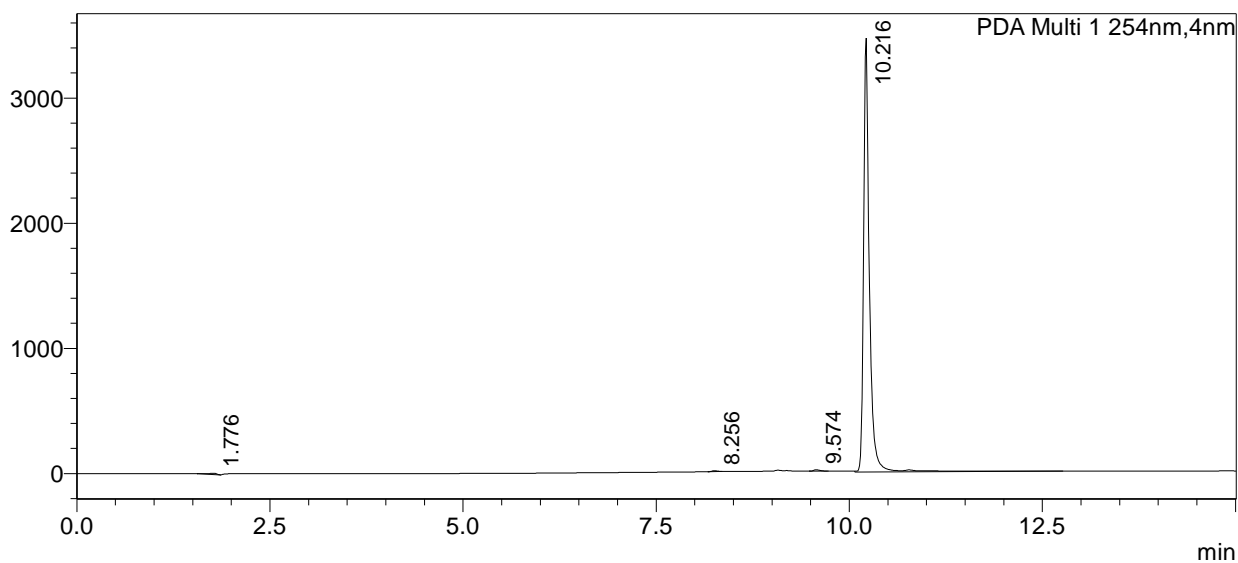
Sample Name : DWY-CXCR2-033S
 Sample ID : DWY-CXCR2-033S
 Data Filename : DWY-CXCR2-033S-Method2.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyangB.lcm
 Batch Filename :
 Vial # : 2-33
 Injection Volume : 10 uL
 Date Acquired : 2/3/2017 5:49:15 PM
 Date Processed : 2/3/2017 6:25:27 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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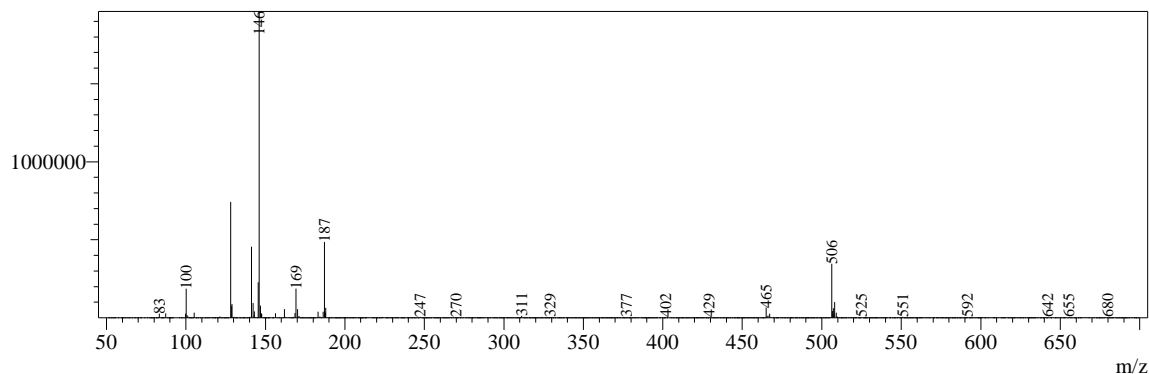
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	1.776	78416	0.427
2	8.256	31500	0.172
3	9.574	56462	0.308
4	10.216	18190230	99.094
Total		18356608	100.000

MS Spectrum

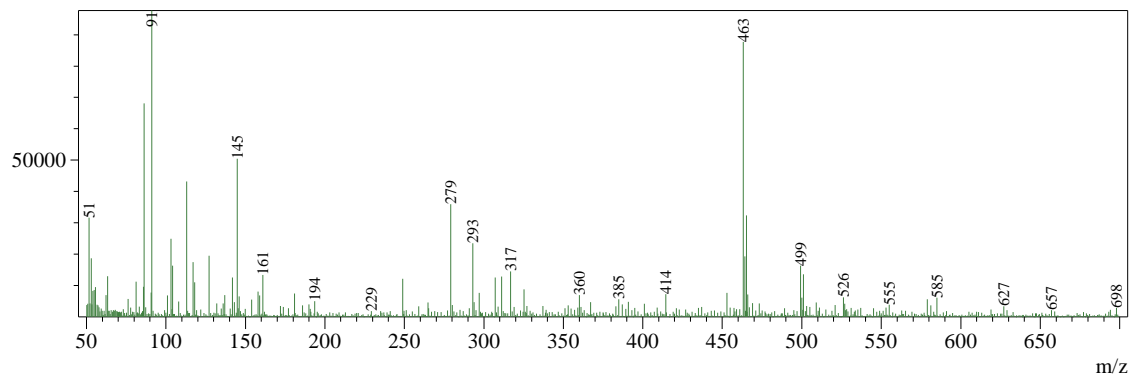
R.Time:10.213(Scan#:6129)
 MassPeaks:146
 Segment 1 - Event 1



R. Time:10.215(Scan#:6130)

MassPeaks:91

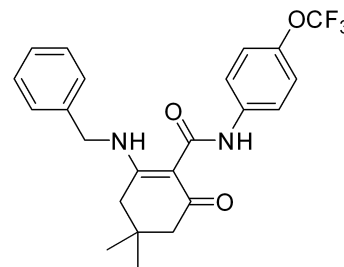
Segment 1 - Event 2



<Sample Information>

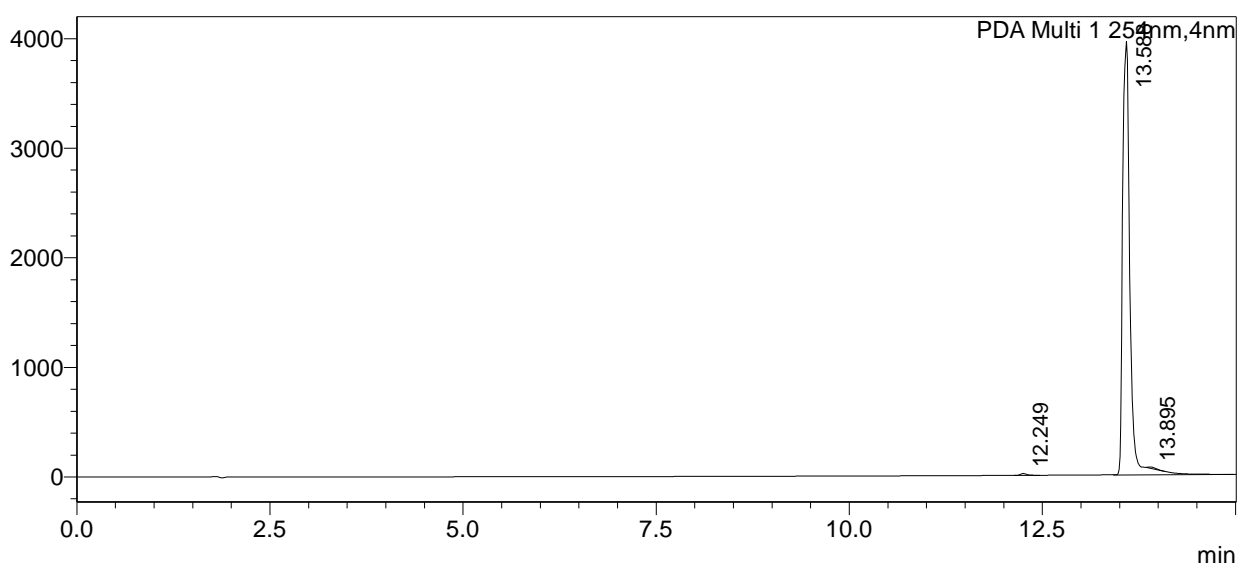
Sample Name : DWY-CXCR2-034
 Sample ID : DWY-CXCR2-034
 Data Filename : DWY-CXCR2-034(RE.lcd)
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 1-3
 Injection Volume : 10 uL
 Date Acquired : 2/17/2017 2:01:29 PM
 Date Processed : 2/17/2017 2:16:30 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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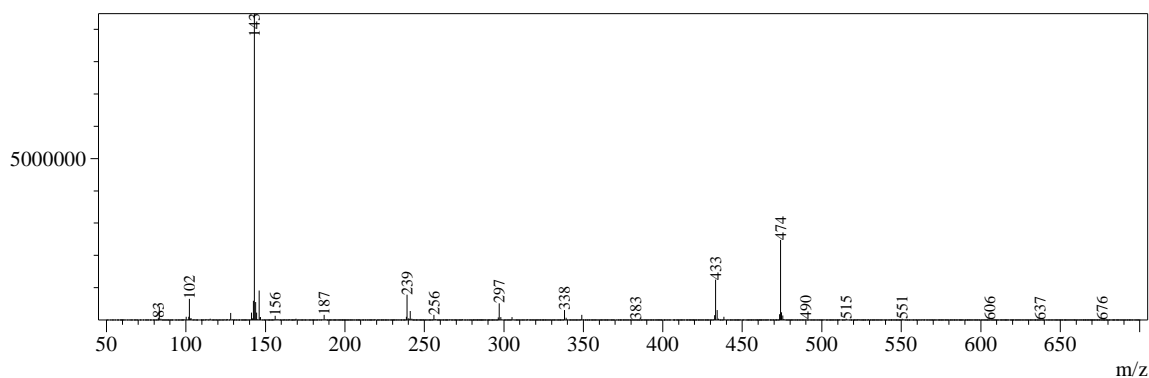
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	12.249	102111	0.388
2	13.588	26135589	99.358
3	13.895	66743	0.254
Total		26304443	100.000

MS Spectrum

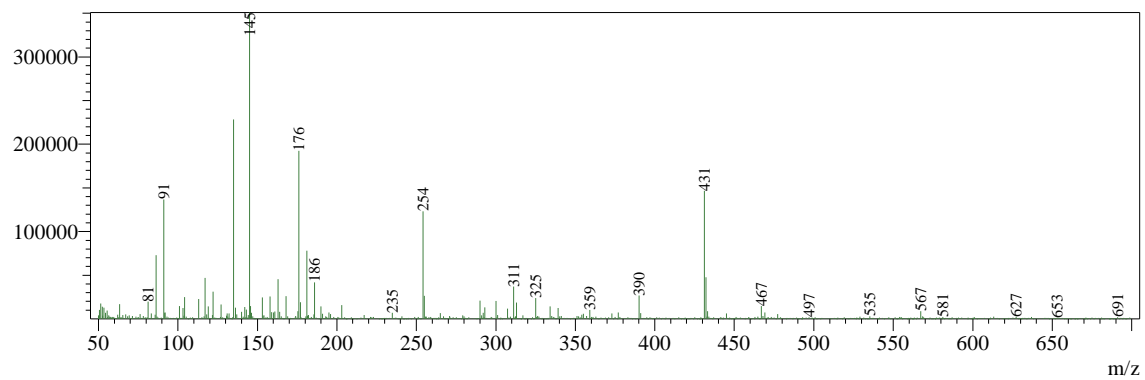
R.Time:13.587(Scan#:8153)
 MassPeaks:143
 Segment 1 - Event 1

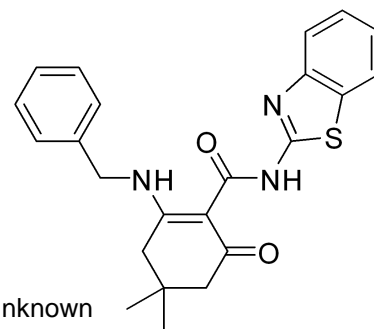


R. Time: 13.588(Scan#: 8154)

MassPeaks: 145

Segment 1 - Event 2





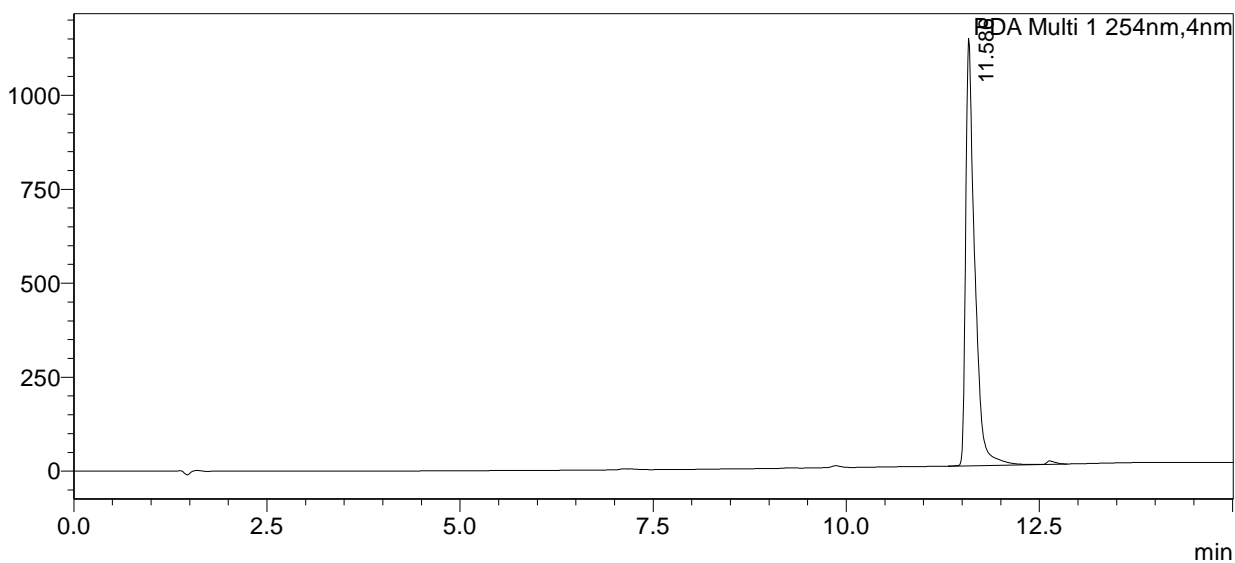
<Sample Information>

Sample Name : DWY-CXCR2-035
 Sample ID : DWY-CXCR2-035
 Data Filename : DWY-CXCR2-035.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 1-8
 Injection Volume : 10 uL
 Date Acquired : 2/20/2017 3:15:33 PM
 Date Processed : 2/20/2017 3:30:35 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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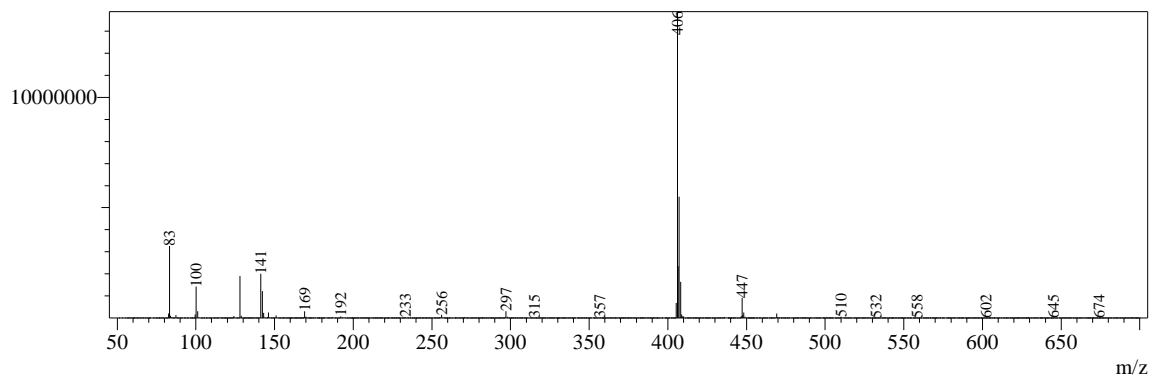
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	11.586	9280648	100.000
Total		9280648	100.000

MS Spectrum

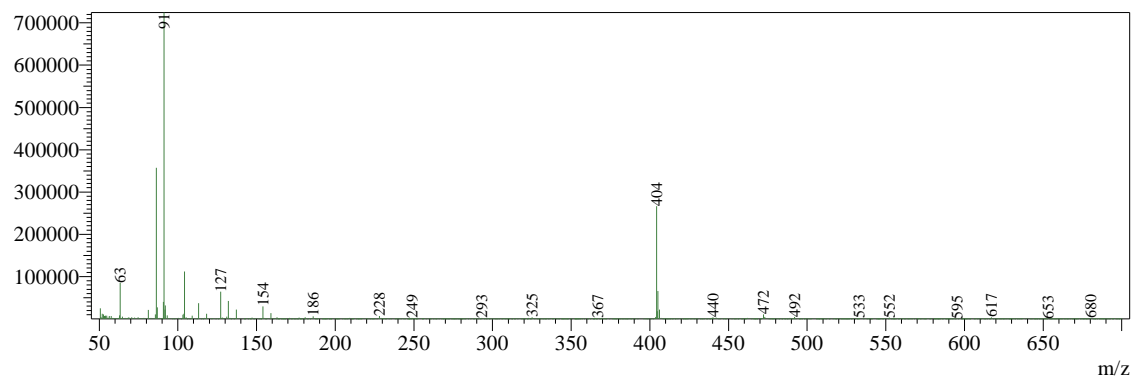
R.Time:11.583(Scan#:6951)
 MassPeaks:406
 Segment 1 - Event 1

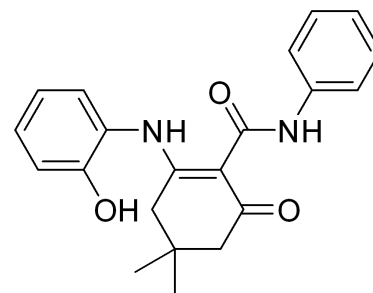


R.Time:11.585(Scan#:6952)

MassPeaks:91

Segment 1 - Event 2



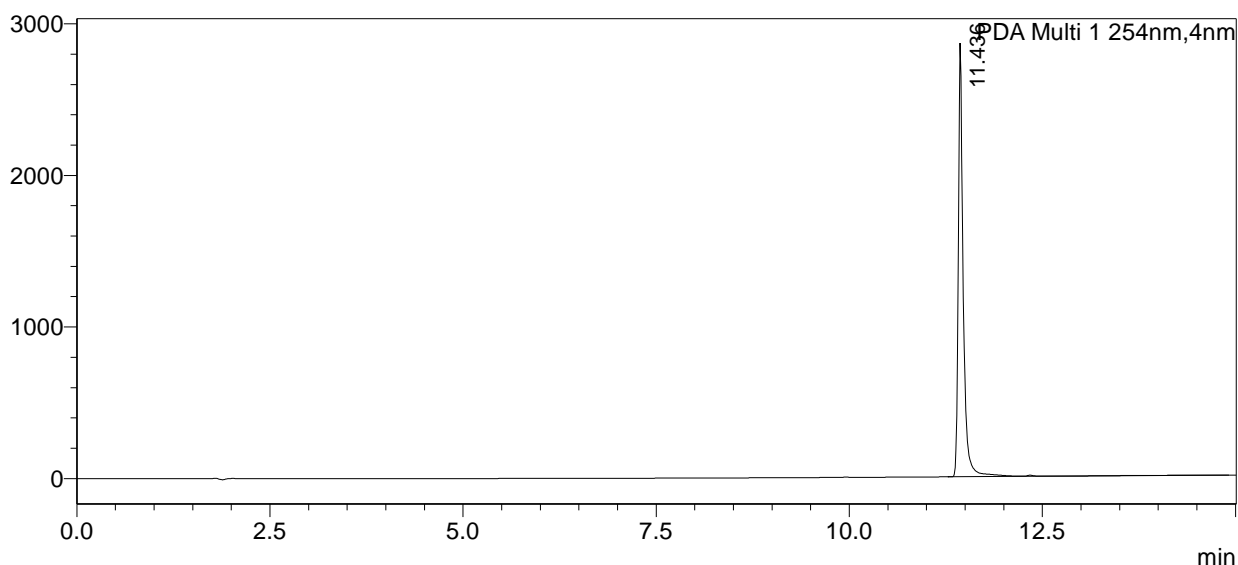


<Sample Information>

Sample Name	: DWY-CXCR2-036	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-036	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-036.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 1-30		
Injection Volume	: 10 uL		
Date Acquired	: 2/21/2017 3:00:53 PM		
Date Processed	: 2/21/2017 3:15:55 PM		

<Chromatogram>

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Peak Table

PDA Ch1 254nm

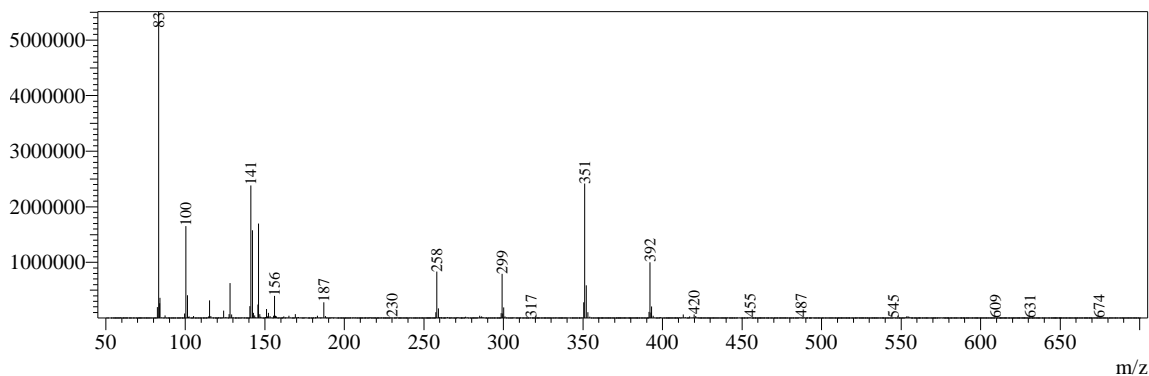
Peak#	Ret. Time	Area	Area%
1	11.436	12802908	100.000
Total		12802908	100.000

MS Spectrum

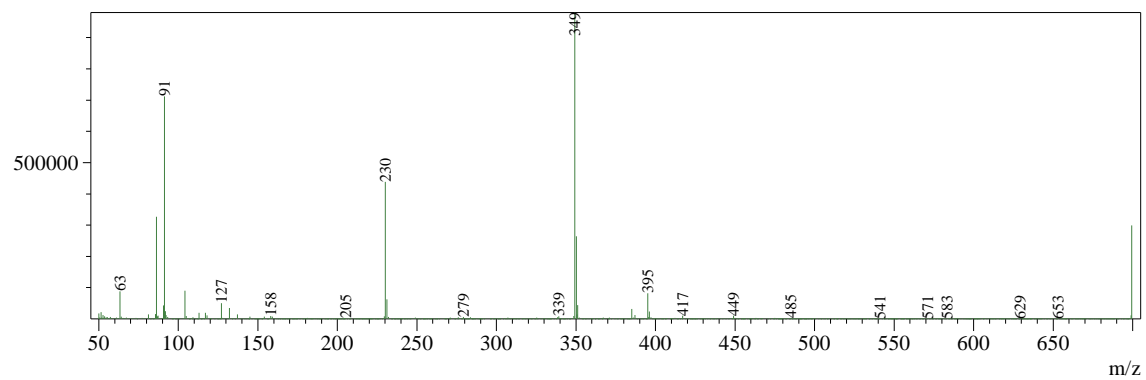
R.Time:11.433(Scan#:6861)

MassPeaks:83

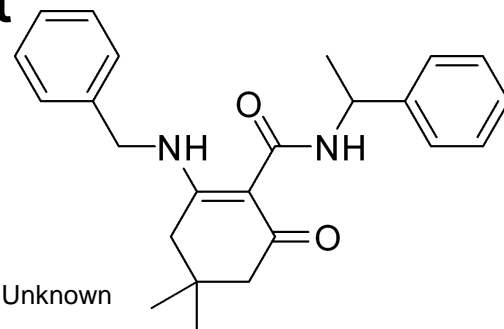
Segment 1 - Event 1



R.Time:11.435(Scan#:6862)
MassPeaks:349
Segment 1 - Event 2



Analysis Report



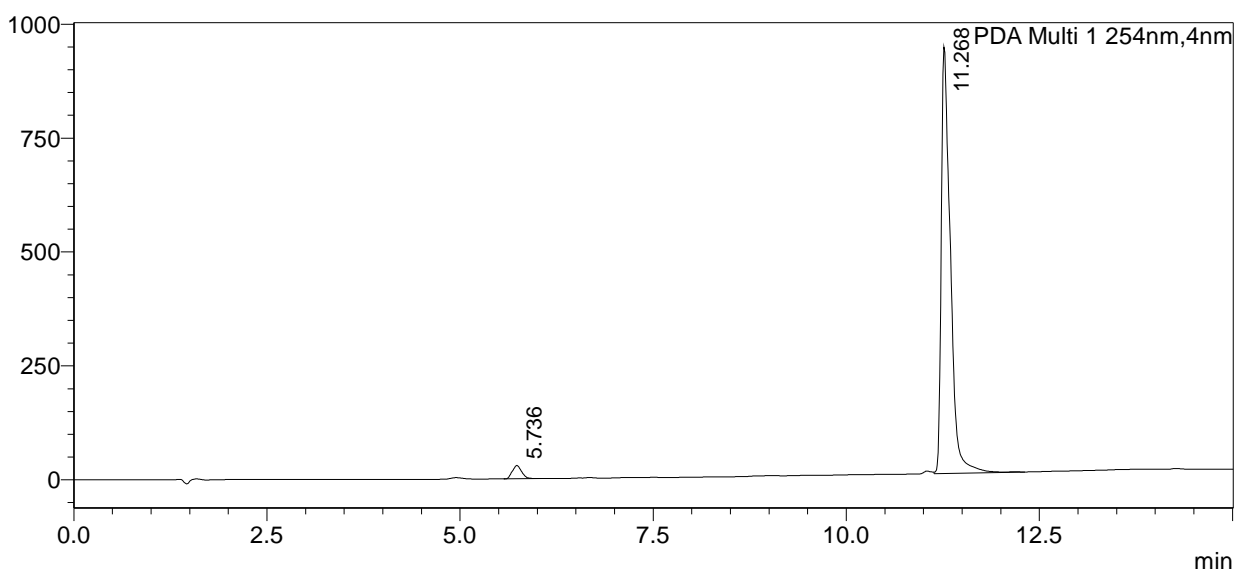
<Sample Information>

Sample Name : DWY-CXCR2-037
 Sample ID : DWY-CXCR2-037
 Data Filename : DWY-CXCR2-037(RE.lcd)
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 2-8
 Injection Volume : 10 uL
 Date Acquired : 2/24/2017 3:45:32 PM
 Date Processed : 2/24/2017 4:00:34 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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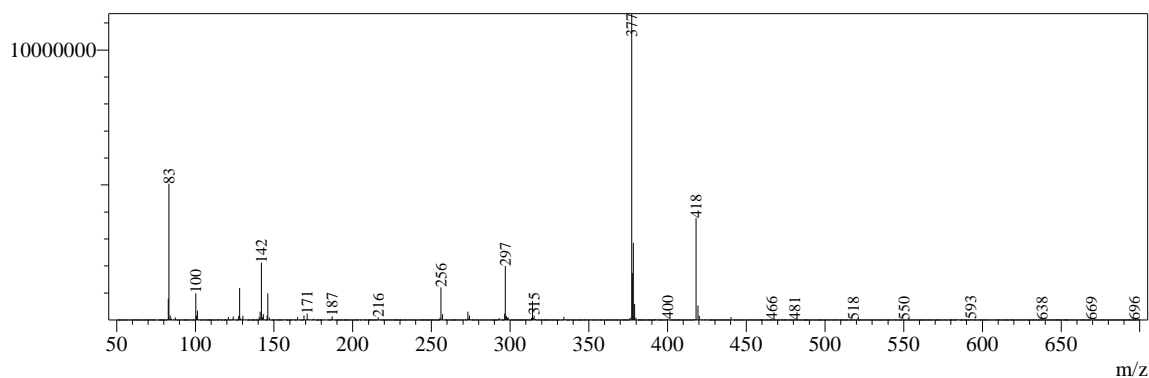


Peak Table

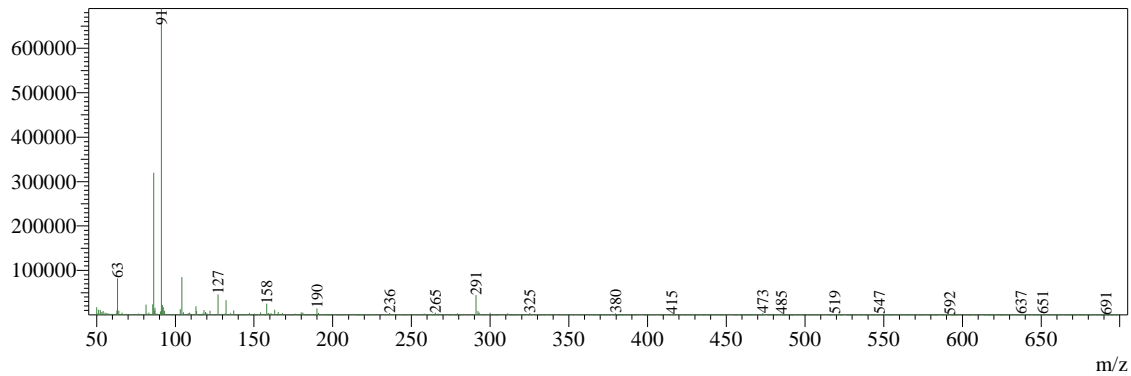
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	5.736	245946	3.106
2	11.268	7673015	96.894
Total		7918961	100.000

MS Spectrum

R.Time:11.267(Scan#:6761)
 MassPeaks:1044
 Segment 1 - Event 1



R.Time:11.268(Scan#:6762)
MassPeaks:1014
Segment 1 - Event 2





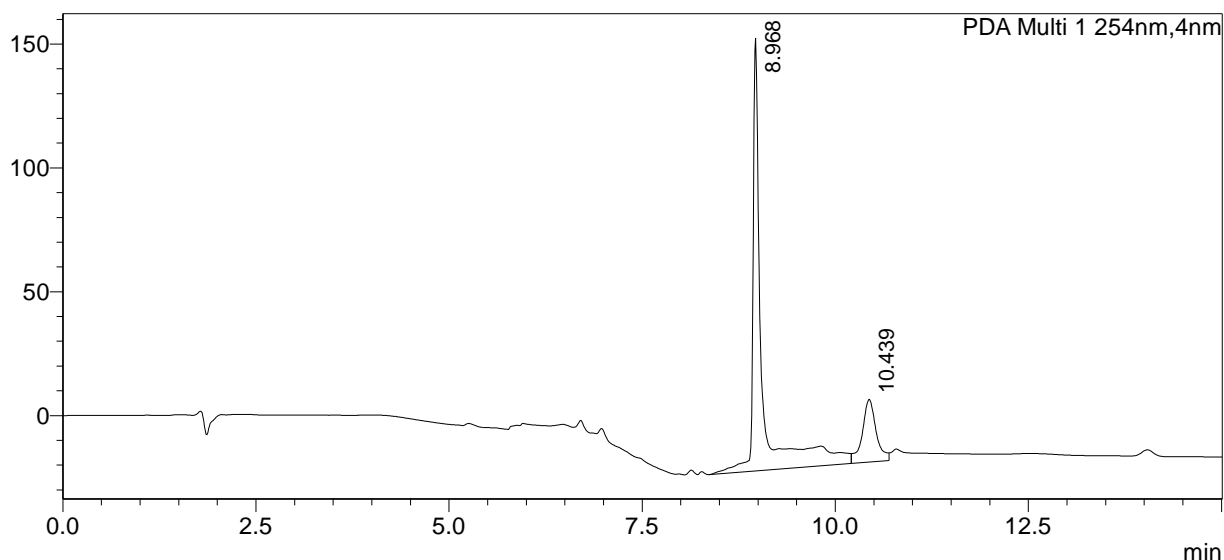
Analysis Report

<Sample Information>

Sample Name : DWY-CXCR2-039
Sample ID : DWY-CXCR2-039
Data Filename : DWY-CXCR2-039.lcd
Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyangB.lcm
Batch Filename :
Vial # : 3-22 Sample Type : Unknown
Injection Volume : 10 uL
Date Acquired : 2/28/2017 5:10:59 PM Acquired by : System Administrator
Date Processed : 2/28/2017 5:26:01 PM Processed by : System Administrator

<Chromatogram>

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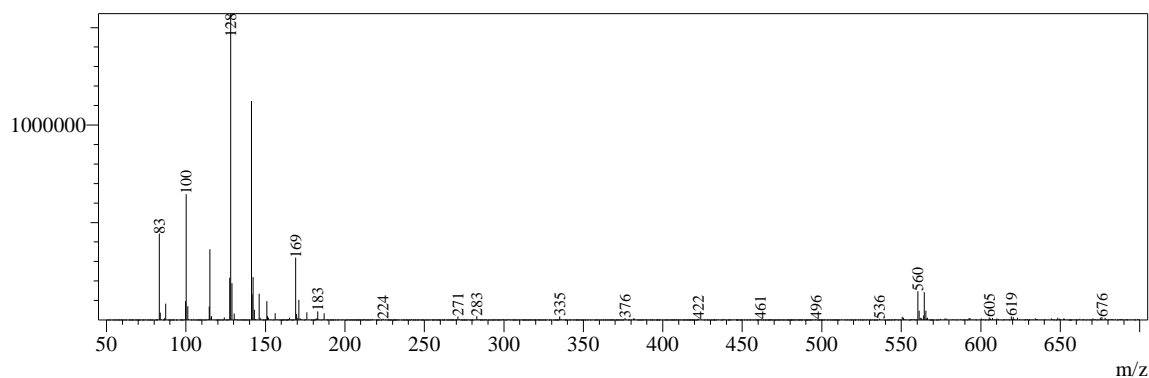


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	8.968	1387996	81.370
2	10.439	317780	18.630
Total		1705776	100.000

MS Spectrum

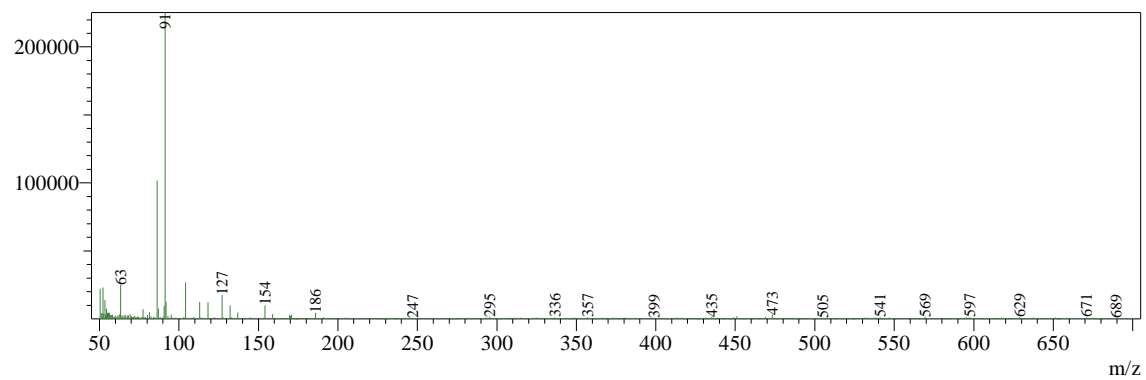
R.Time:8.967(Scan#:5381)
MassPeaks:128
Segment 1 - Event 1



R. Time:8.968(Scan#:5382)

MassPeaks:91

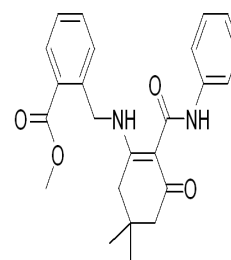
Segment 1 - Event 2



<Sample Information>

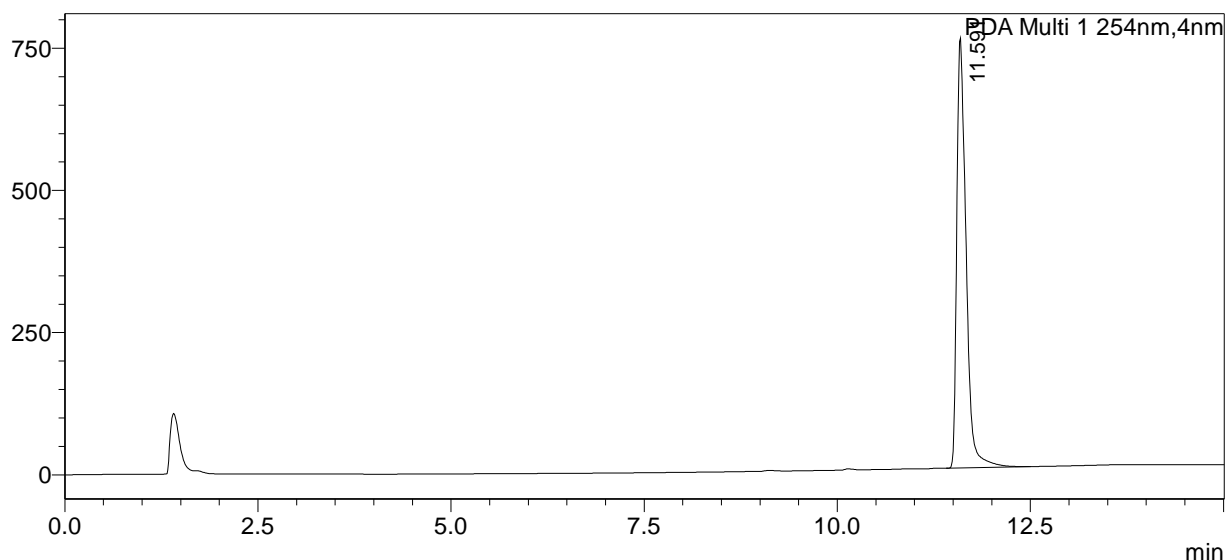
Sample Name : DWY-CXCR2-040
 Sample ID : DWY-CXCR2-040
 Data Filename : DWY-CXCR2-040.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 3-5
 Injection Volume : 10 uL
 Date Acquired : 4/10/2017 1:27:52 PM
 Date Processed : 4/10/2017 2:23:59 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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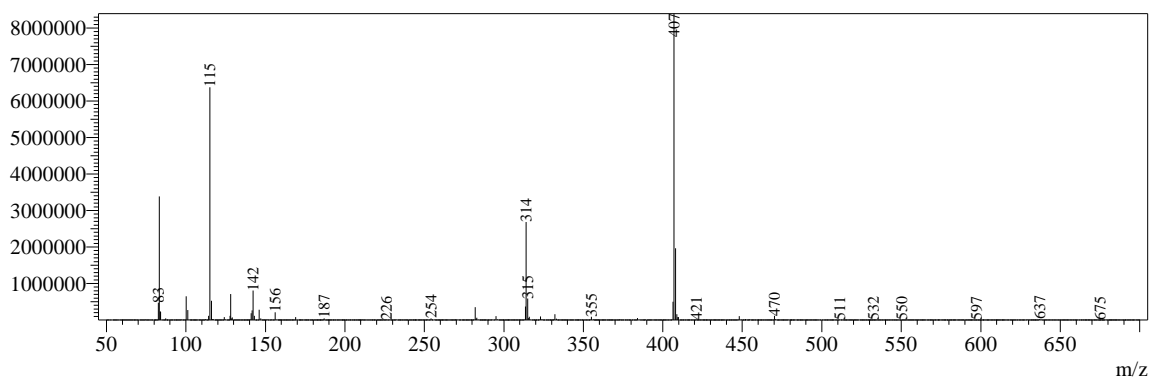
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	11.591	6336076	100.000
Total		6336076	100.000

MS Spectrum

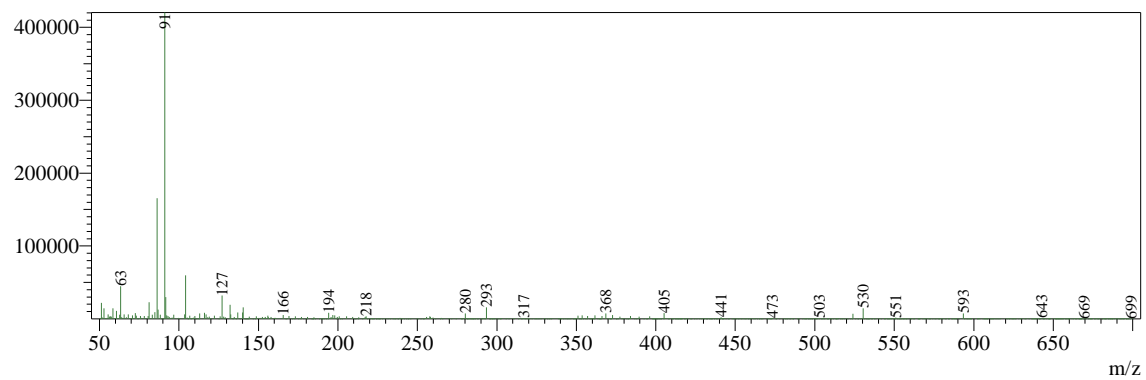
R.Time:11.590(Scan#:6955)
 MassPeaks:407
 Segment 1 - Event 1



R. Time: 11.591 (Scan#: 6956)

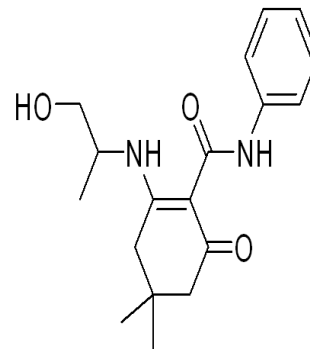
MassPeaks: 91

Segment 1 - Event 2



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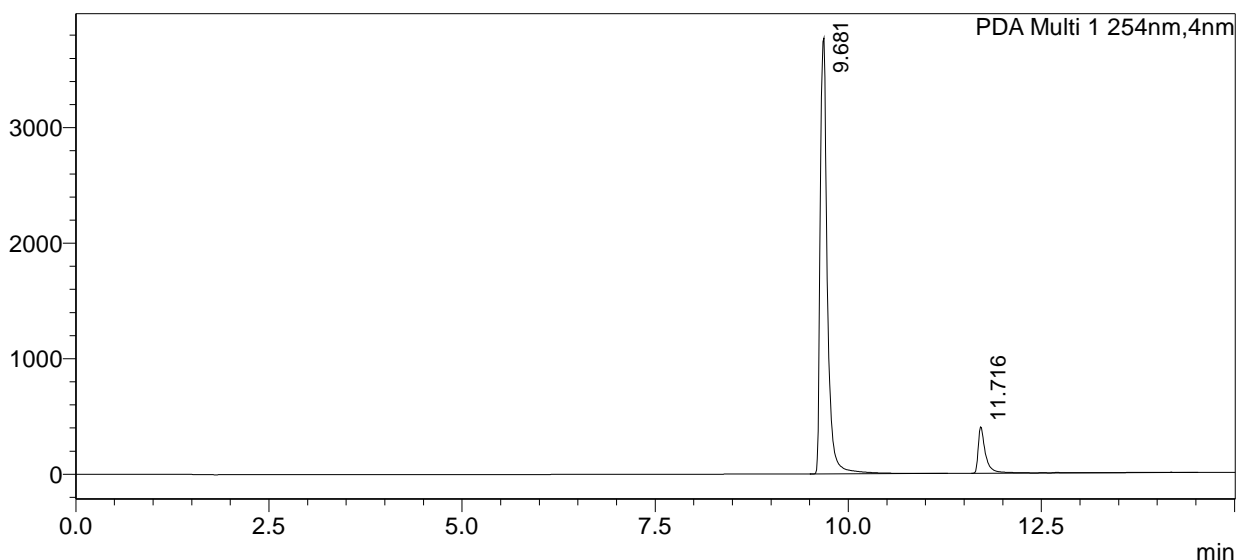
<Sample Information>

Sample Name : DWY-CXCR2-041
 Sample ID : DWY-CXCR2-041
 Data Filename : DWY-CXCR2-041.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 3-37
 Injection Volume : 20 uL
 Date Acquired : 7/10/2017 1:39:08 PM
 Date Processed : 7/10/2017 1:54:09 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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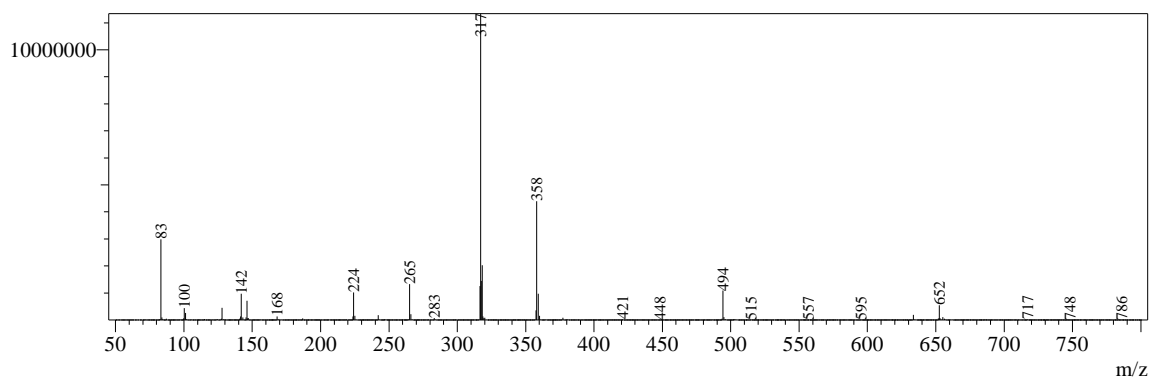


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	9.681	24115396	90.047
2	11.716	2665623	9.953
Total		26781018	100.000

MS Spectrum

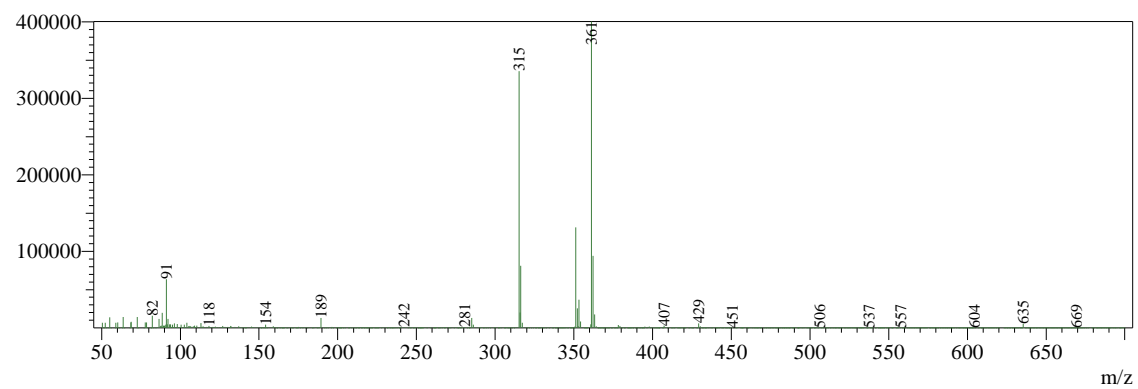
R.Time:9.680(Scan#:5809)
 MassPeaks:317
 Segment 1 - Event 1



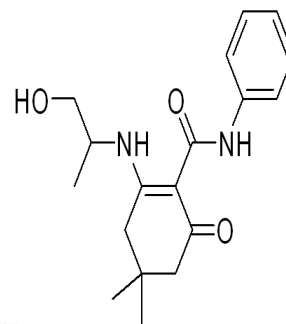
R. Time:9.682(Scan#:5810)

MassPeaks:361

Segment 1 - Event 2



Analysis Report

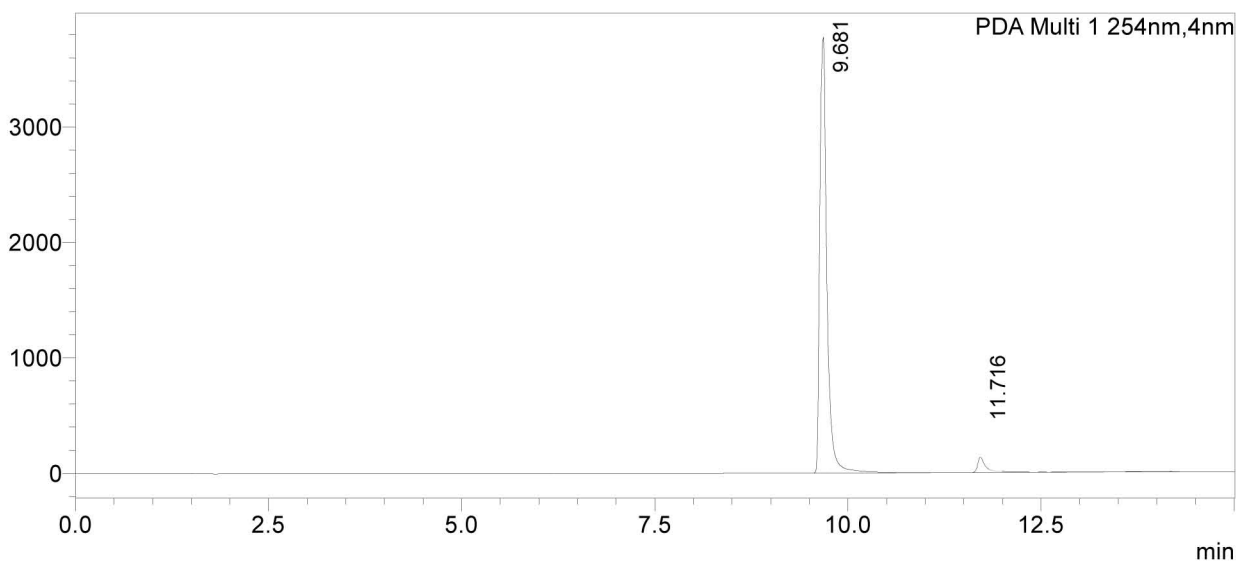


<Sample Information>

Sample Name	: DWY-CXCR2-041	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-041	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-041.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 3-37		
Injection Volume	: 20 uL		
Date Acquired	: 7/10/2017 1:39:08 PM		
Date Processed	: 7/10/2017 1:54:09 PM		

<Chromatogram>

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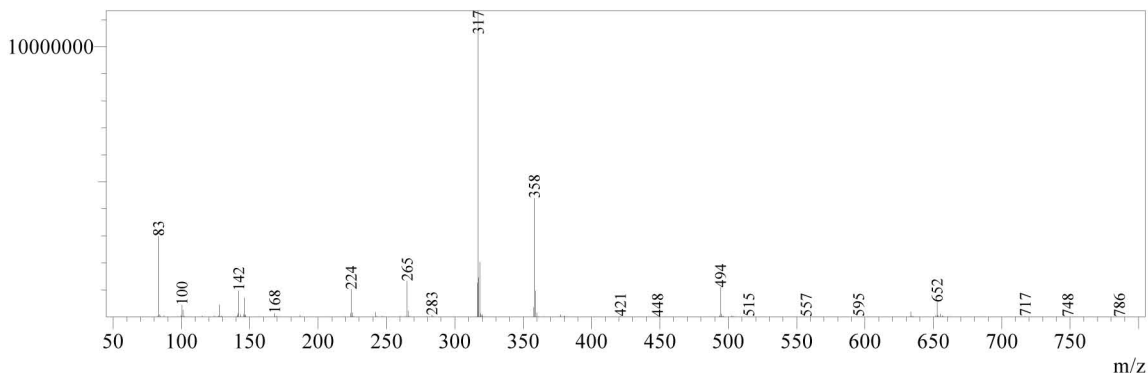


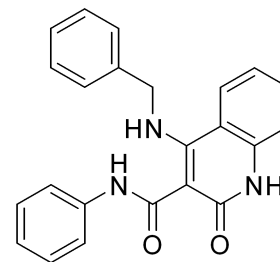
Peak Table

Peak#	Ret. Time	Area	Area%
1	9.681	24115396	97.047
2	11.716	2665623	2.953
Total		26781018	100.000

MS Spectrum

R.Time:9.680(Scan#:5809)
MassPeaks:317
Segment 1 - Event 1





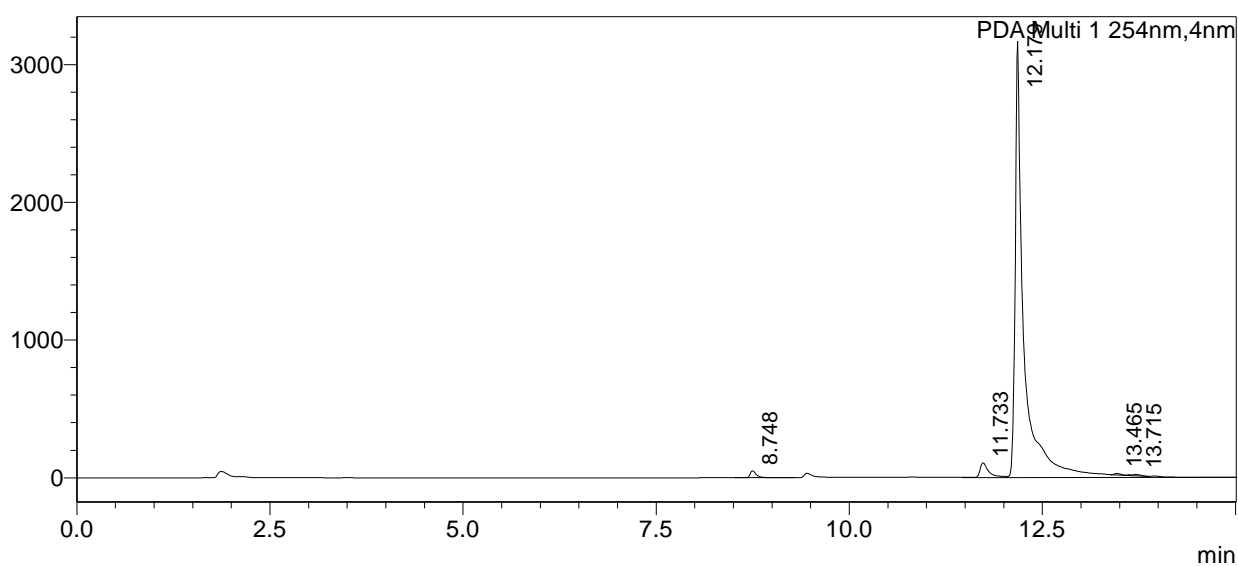
<Sample Information>

Sample Name : DWY-CXCR2-045
 Sample ID : DWY-CXCR2-045
 Data Filename : DWY-CXCR2-045(RE.lcd)
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 3-23
 Injection Volume : 10 uL
 Date Acquired : 4/20/2017 8:10:14 PM
 Date Processed : 4/20/2017 8:26:06 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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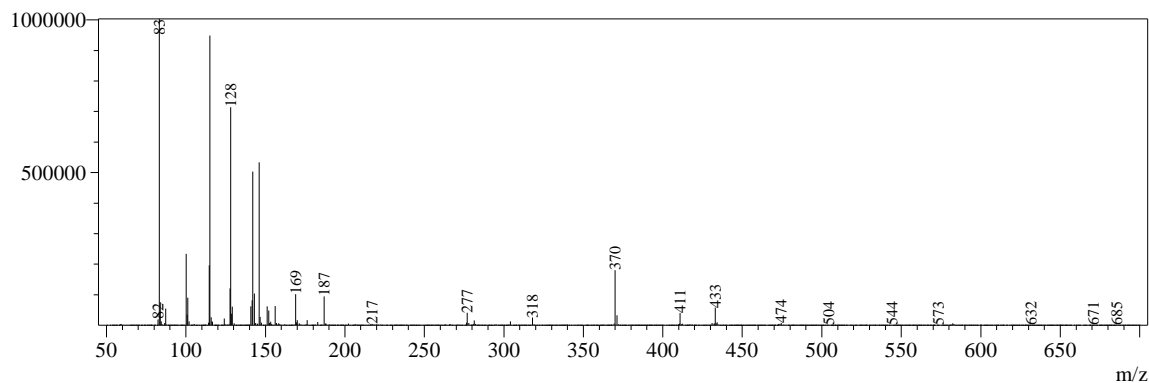
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	8.748	289366	1.086
2	11.733	857739	3.218
3	12.179	25362924	95.157
4	13.465	62042	0.233
5	13.715	81614	0.306
Total		26653686	100.000

MS Spectrum

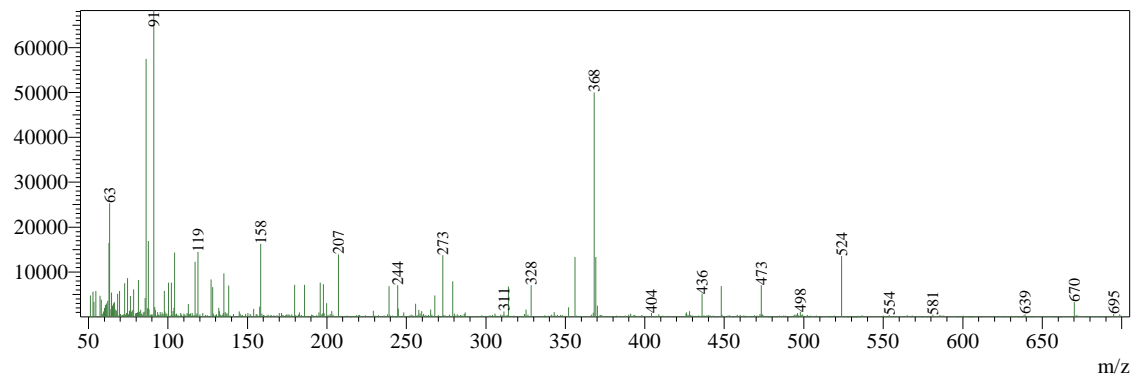
R.Time:12.177(Scan#:7307)
 MassPeaks:83
 Segment 1 - Event 1

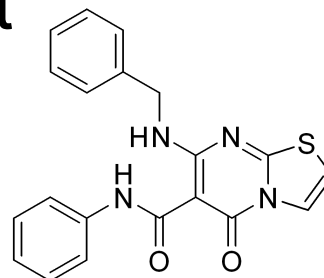


R.Time:12.178(Scan#:7308)

MassPeaks:91

Segment 1 - Event 2



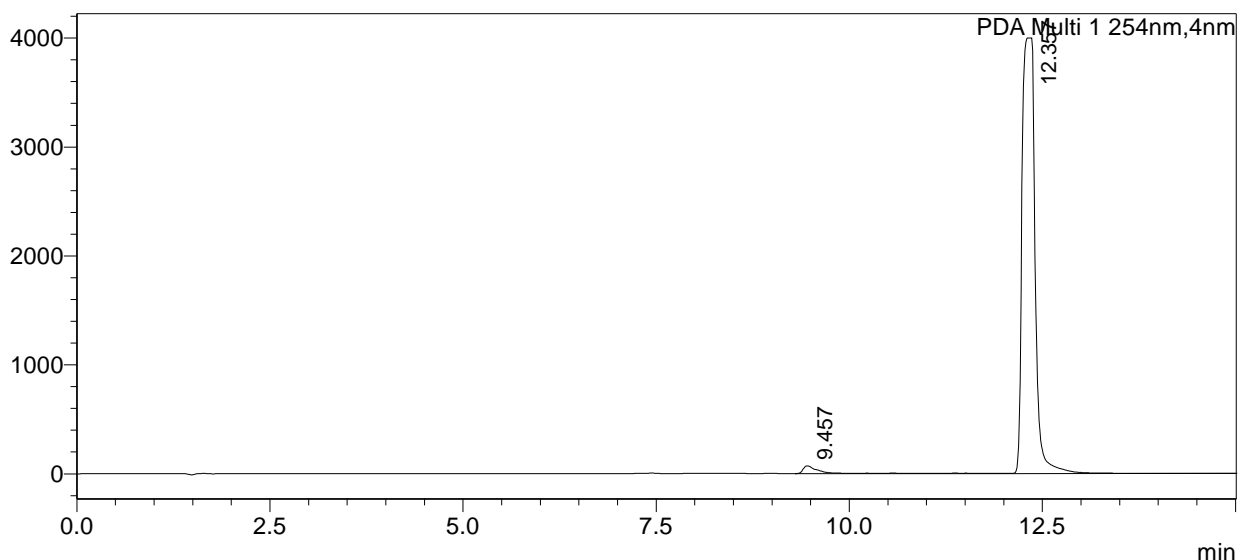


<Sample Information>

Sample Name	: DWY-CXCR2-049	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-049	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-049.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 3-1		
Injection Volume	: 25 uL		
Date Acquired	: 4/25/2017 2:52:47 PM		
Date Processed	: 4/25/2017 3:07:49 PM		

<Chromatogram>

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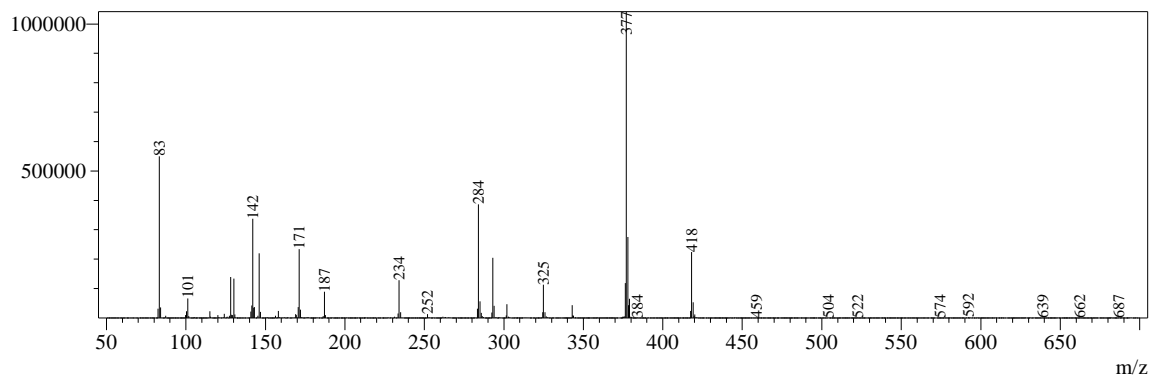


Peak Table

Peak#	Ret. Time	Area	Area%
1	9.457	1039874	2.184
2	12.357	46564630	97.816
Total		47604504	100.000

MS Spectrum

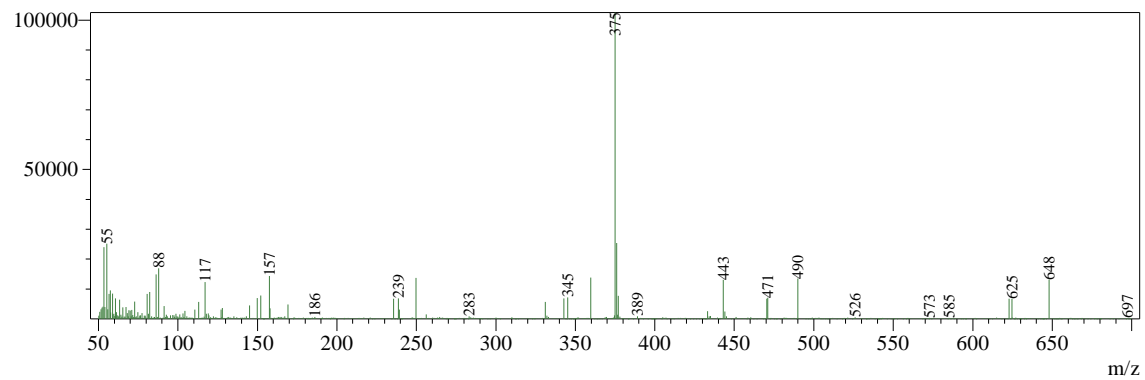
R.Time:12.357(Scan#:7415)
MassPeaks:377
Segment 1 - Event 1

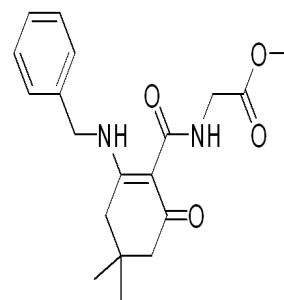


R. Time:12.358(Scan#:7416)

MassPeaks:375

Segment 1 - Event 2





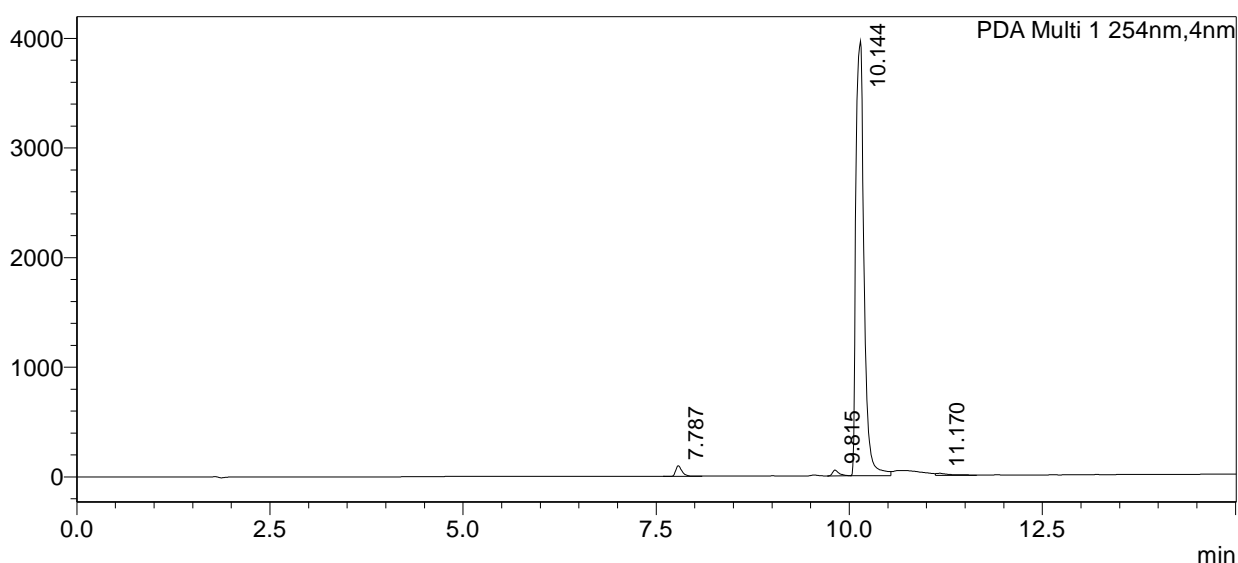
<Sample Information>

Sample Name : DWY-CXCR2-050
 Sample ID : DWY-CXCR2-050
 Data Filename : DWY-CXCR2-050(1.lcd)
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 1-28
 Injection Volume : 10 uL
 Date Acquired : 5/21/2017 5:05:01 PM
 Date Processed : 5/21/2017 5:20:47 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

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Peak Table

PDA Ch1 254nm

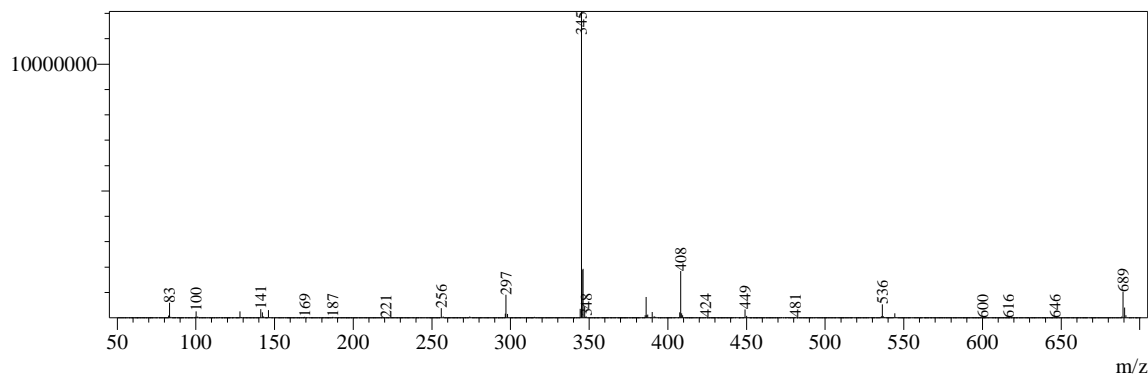
Peak#	Ret. Time	Area	Area%
1	7.787	554162	1.836
2	9.815	313049	1.037
3	10.144	29060905	96.271
4	11.170	258471	0.856
Total		30186586	100.000

MS Spectrum

R. Time: 10.143 (Scan#: 6087)

MassPeaks: 345

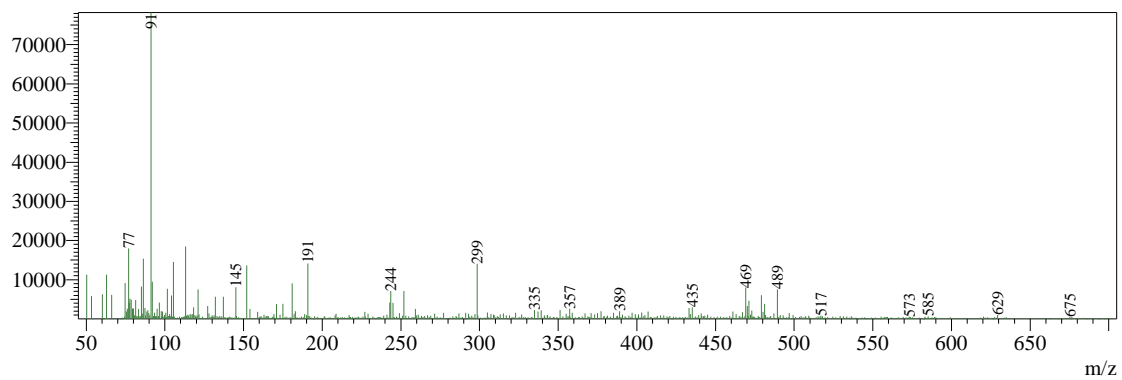
Segment 1 - Event 1



R. Time: 10.145 (Scan#: 6088)

Mass Peaks: 91

Segment 1 - Event 2



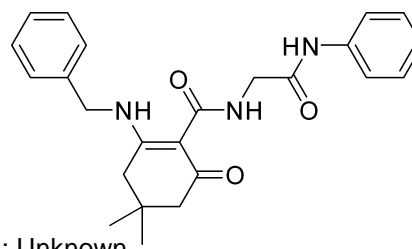
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<Sample Information>

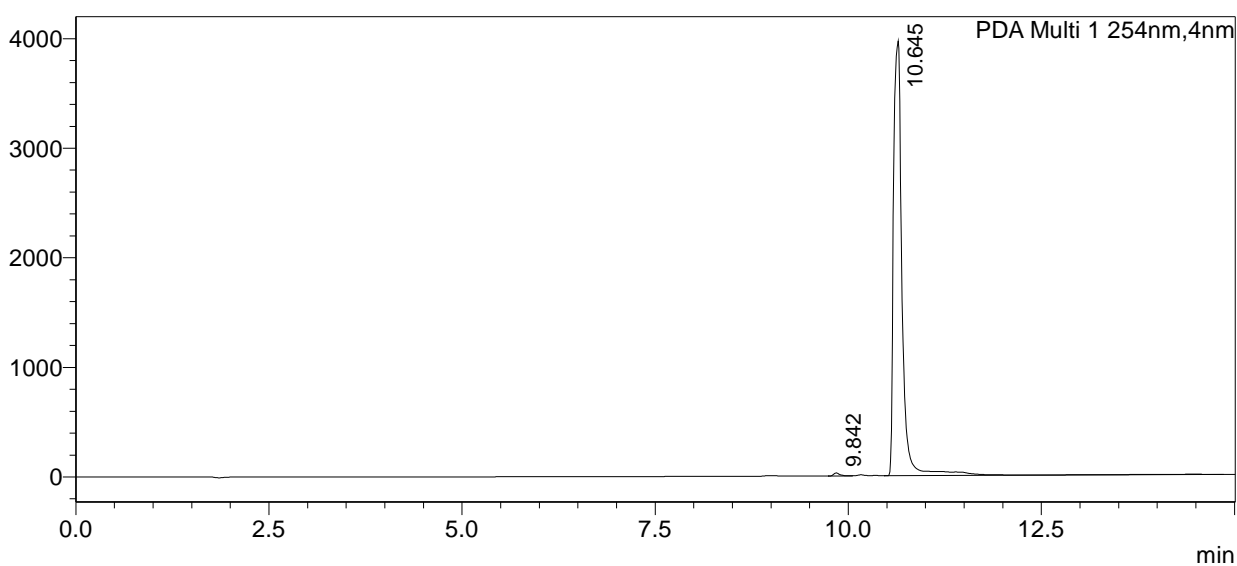
Sample Name : DWY-CXCR2-051
 Sample ID : DWY-CXCR2-051
 Data Filename : DWY-CXCR2-051(2.lcd)
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 3-54
 Injection Volume : 20 uL
 Date Acquired : 5/25/2017 6:26:24 PM
 Date Processed : 5/25/2017 6:41:26 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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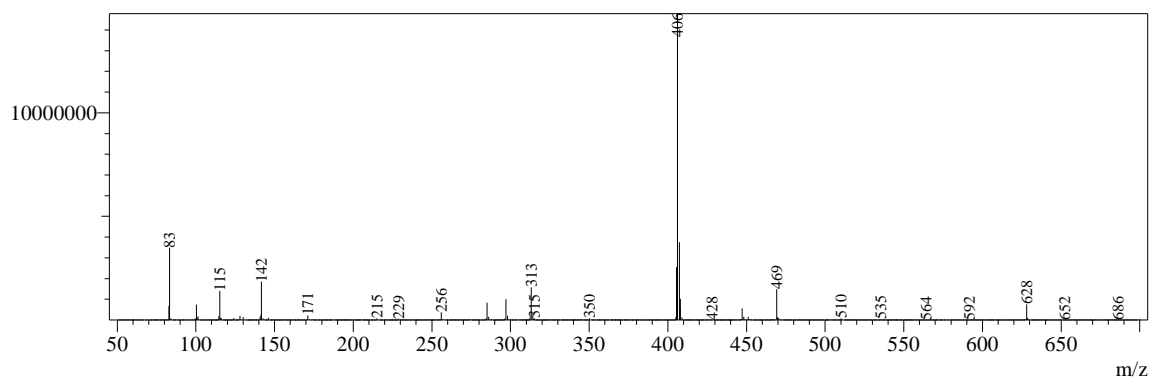
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	9.842	160078	0.512
2	10.645	31127141	99.488
Total		31287219	100.000

MS Spectrum

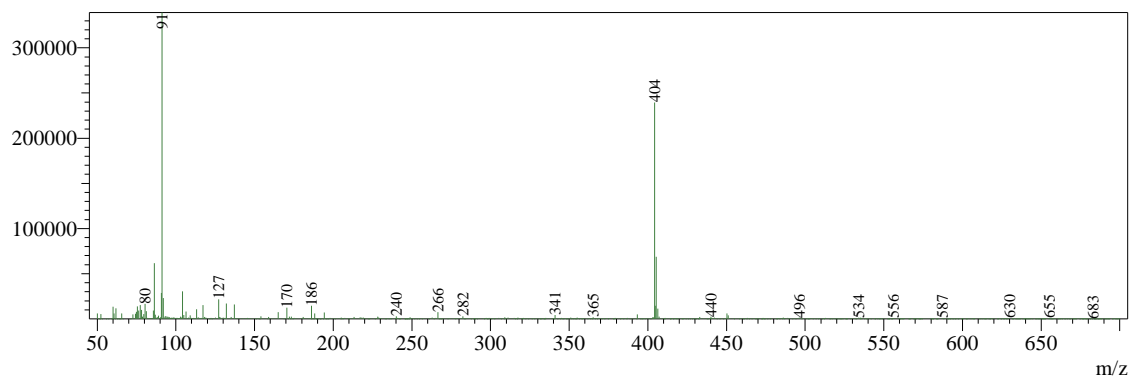
R.Time:10.643(Scan#:6387)
 MassPeaks:406
 Segment 1 - Event 1



R. Time:10.645(Scan#:6388)

MassPeaks:91

Segment 1 - Event 2



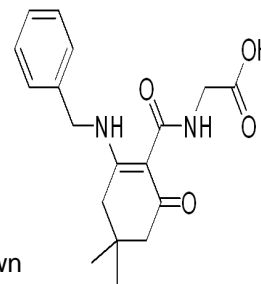
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<Sample Information>

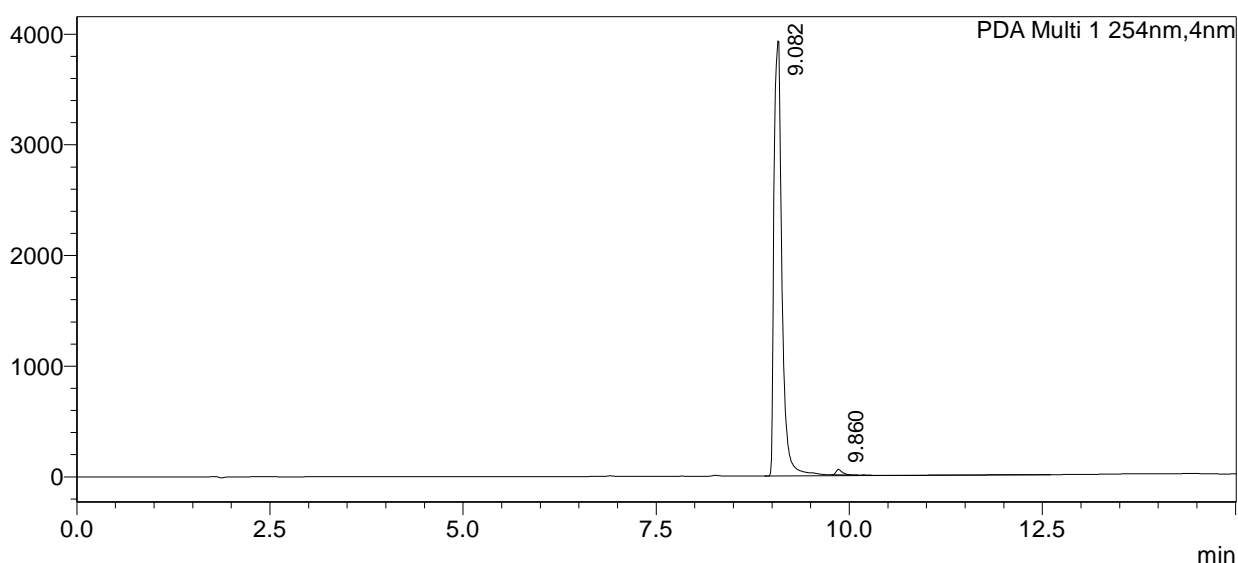
Sample Name : DWY-CXCR2-052
 Sample ID : DWY-CXCR2-052
 Data Filename : DWY-CXCR2-052.lcd
 Method Filename : LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm
 Batch Filename :
 Vial # : 1-36
 Injection Volume : 10 uL
 Date Acquired : 5/24/2017 11:11:42 AM
 Date Processed : 5/24/2017 11:26:44 AM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

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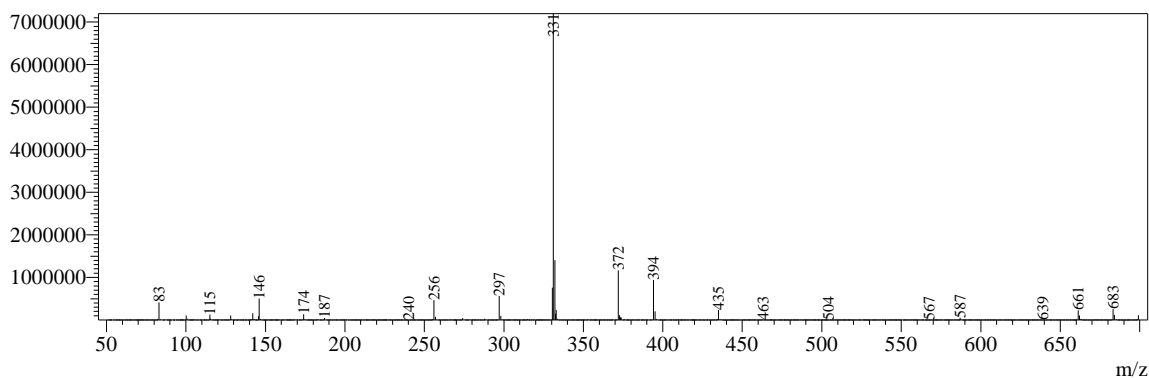
Peak Table

PDA Ch1 254nm

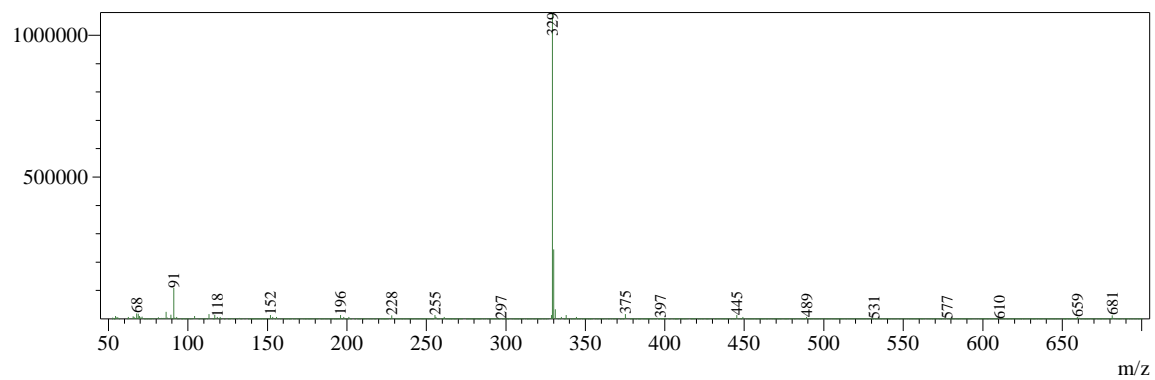
Peak#	Ret. Time	Area	Area%
1	9.082	28283724	98.993
2	9.860	287800	1.007
Total		28571524	100.000

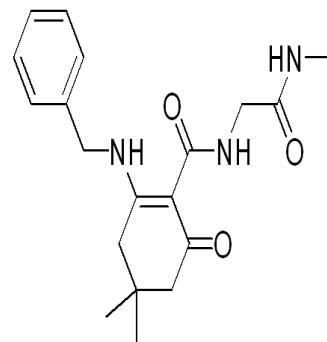
MS Spectrum

R.Time:9.080(Scan#:5449)
 MassPeaks:331
 Segment 1 - Event 1



R. Time:9.081(Scan#:5450)
MassPeaks:329
Segment 1 - Event 2



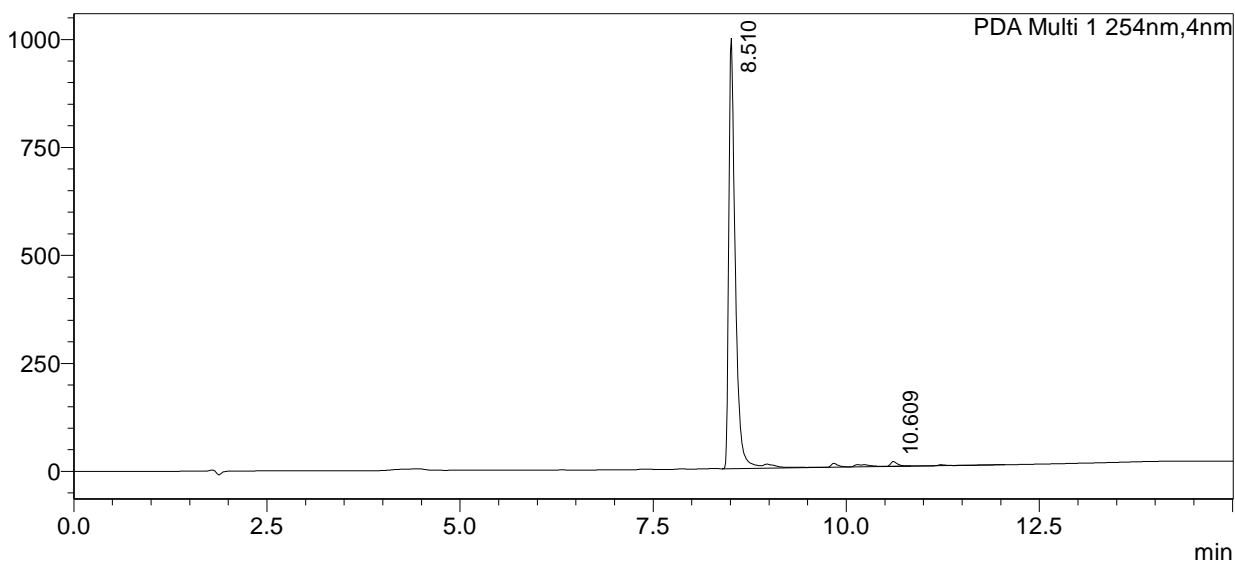


<Sample Information>

Sample Name	: DWY-CXCR2-053	Sample Type	: Unknown
Sample ID	: DWY-CXCR2-053	Acquired by	: System Administrator
Data Filename	: DWY-CXCR2-053.lcd	Processed by	: System Administrator
Method Filename	: LCMS_10_95_15min-CH3CN_pos_neg_weiyang.lcm		
Batch Filename	:		
Vial #	: 3-17		
Injection Volume	: 10 uL		
Date Acquired	: 5/26/2017 9:53:13 AM		
Date Processed	: 5/26/2017 10:43:26 AM		

<Chromatogram>

mAU

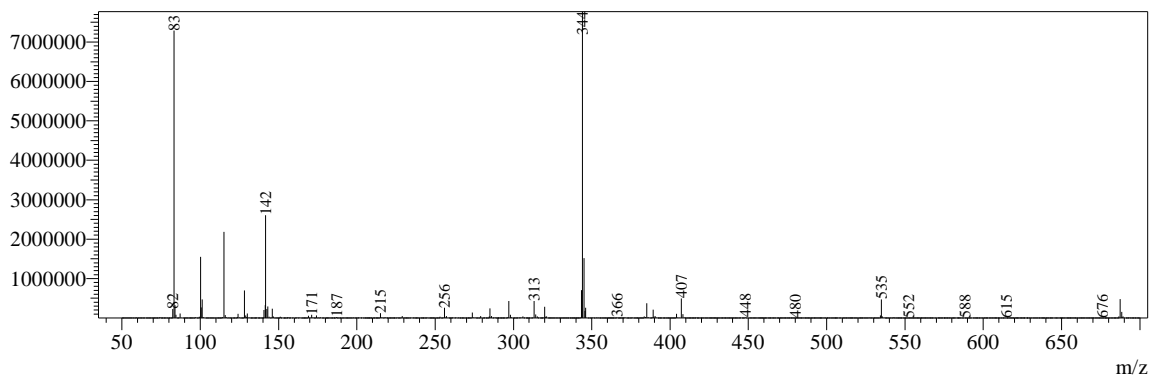


Peak Table

PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	8.510	5861667	98.815
2	10.609	70292	1.185
Total		5931959	100.000

MS Spectrum

R.Time:8.510(Scan#:5107)
MassPeaks:344
Segment 1 - Event 1



R.Time:8.511(Scan#:5108)
MassPeaks:91
Segment 1 - Event 2

