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Supporting Information

Dehydrogenation and Oxidative Coupling of Alcohol and Amines Catalyzed by Organosilicon-supported TiO_2@PMHSIPN

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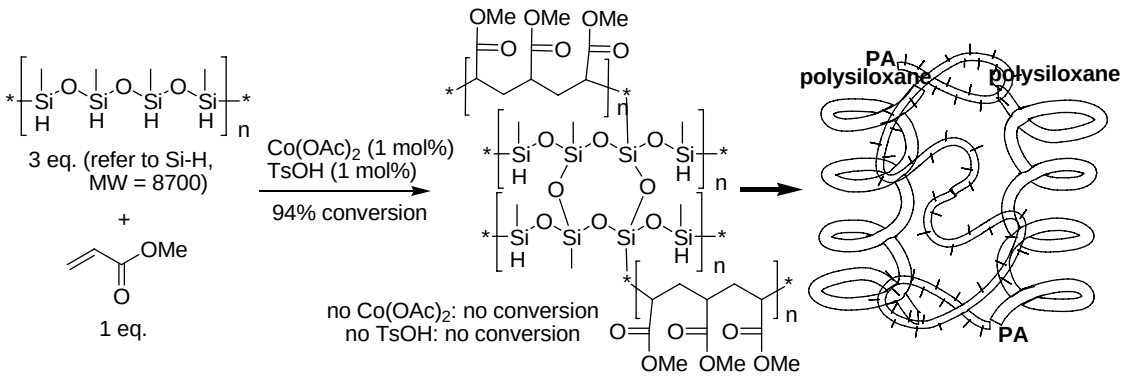
Experimental Section

1. General remarks

All the chemicals were of analytic reagent grade and were used as received without further purification. AP-grade methyl acrylate, $Co(OAc)_2$, TsOH, and chloroform were used as received. The molecular weight of PMHS was about 8684 g/mol. Attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy was performed on VERTEX70 IR (Bruker). The data were collected over 32 scans with a resolution of 4 cm^{-1} at room temperature. The morphology of the polymer fracture surface was characterized by scanning electron micrograph (SEM, Hitachi S3000N). Transmission electron microscopy (TEM) was carried out with the phosphotungstic acid staining method on a Hitachi H-7650 transmission electron microscope. Flash column chromatography was performed over silica (200-300 mesh). ^{1}H-NMR and ^{13}C-NMR spectra were recorded at 400, 500 and 100, 125 MHz, respectively on Advance (Brucker) 400 MHz Nuclear Magnetic Resonance Spectromer, and were referenced to the internal solvent signals. Thin layer chromatography was performed using silica gel; GF254 TLC plates and visualized with ultraviolet light. The product was confirmed by GC-MS, and usual spectroscopic methods (NMR).

2. Synthesis of PMHS/PA semi-IPN material (PMHS-based semi-interpenetrating networks, PMHSIPN)[1]

In a typical reaction, a PMHS/PEA semi-IPN was prepared as follows: ethyl acrylate (1.07 g), PMHS (2.01 g), TsOH (0.0184 g) and $Co(OAc)_2$ (0.026 g) were mixed in a reactor and stirred for 24 h at 70 °C. The resulting mixture was washed with the distilled water and dried for 24 h at 60 °C under vacuum.



Scheme S1.

3. Synthesis of TiO2@PMHSIPN Catalyst[2]

According to previous report[2], to a solution of PMHS/PEA semi-IPN (3 g, 25 mmol, calculated on the Si-H hydrogen content) dissolved in THF under nitrogen atmosphere, Ti(O*i*-Pr)$_4$ (25 mmol, 7.38 mL) was added dropwise, and stirred for 3 hours. Then the solvent was concentrated in vacuo, the residue was dried for 12 h at 60 ^{o}C under vacuum. After that, the HNO_3 aqueous solution (1 %, 25 mL) was added and stirred for a period of time, filtration, dried and then the faint yellow powder was obtained.

4. General Procedure for the Oxidation reaction/dehydrogenation of benzyl alcohol catalyzed by TiO_2@PMHSIPN

4-Methylbenzyl alcohol (**1g**, 1 mmol), TiO_2@PMHSIPN (2 mol% Ti), K_2CO_3 (20 mol%), 5-chloro-1-indanone (**3f,** 20 mol%), and 3 mL nitrobenzene were added into a 15 mL Schlenk tube under nitrogen, and stirred at 160 ^{o}C for 15 h. The mixture was extracted with 3×3 mL of ethyl acetate. The combined organic layer was dried with anhydrous sodium sulfate and concentrated by rotary evaporation. The residue was purified by flash column chromatography (10:1 hexanes and ethyl acetate) to give **2g** with 99% of yield. In this reaction, all the products were known[3] and have been confirmed by GC-MS, IR, and NMR.

5. General Procedure for the oxidative coupling of amines with alcohols catalyzed by TiO_2@PMHSIPN

o-Toluidine (**6a**, 1 mmol), benzyl alcohol (**1a**, 5 eq.), TiO_2@PMHSIPN (2 mol% Ti), and K_2CO_3 (20 mol%), were added into a 15 mL Schlenk tube under nitrogen, and then, were stirred at 160 ^oC for 12 h. The mixture was extracted by 3×3 mL of ethyl acetate. The extraction was dried with anhydrous sodium sulfate and concentrated by rotary evaporation. The residue was purified by recrystallization in ethanol to give **7a** with 99% of yield. In this TiO_2@PMHSIPN-catalyzed dehydrogenation-initiated of oxidative coupling of amines with benzyl alcohol, all the products were known[4] and have been confirmed by GC-MS, IR, and NMR.

6. General Procedure for the oxidative coupling of $TsNH_2$ with alcohols catalyzed by TiO_2@PMHSIPN

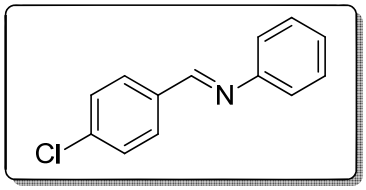
p-Toluenesulfonamide (**8a**, 1 mmol), benzyl alcohol (**1a**, 5 eq.), TiO_2@PMHSIPN (2 mol% Ti), and K_2CO_3 (20 mol%), were added into a 15 mL Schlenk tube under nitrogen. And then the reaction mixture were stirred at 160 ^oC for 12 h. The mixture was extracted by 3×3 mL of ethyl acetate. The extraction was dried with anhydrous sodium sulfate and concentrated by rotary evaporation. The residue was purified by recrystallization in ethanol to give **9a** with 99% of yield. In this TiO_2@PMHSIPN-catalyzed dehydrogenation-initiated of oxidative coupling of Ts-NH_2 with benzyl alcohol, all the products were known and have been confirmed by GC-MS, IR, and NMR.

7. General Procedure for the oxidative coupling of benzyl alcohol and benzene-1,2-diamine catalyzed by TiO_2@PMHSIPN

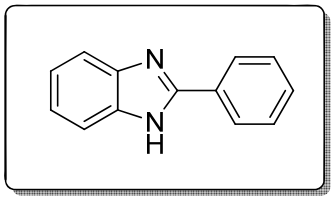
o-Phenylenediamine (**10a**, 1 mmol), benzyl alcohol (**1a**, 5 eq.), TiO_2@PMHSIPN (2 mol% Ti), and K_2CO_3 (20 mol%), were added into a 15 mL Schlenk tube under nitrogen. And then the reaction mixture were stirred at 160 ^oC for 12h. The mixture

was extracted by 3×3 mL of ethyl acetate. The extraction was dried with anhydrous sodium sulfate and concentrated by rotary evaporation. The residue was purified by flash column (5:1 hexanes and ethyl acetate) to give **11a** with 72% of yield. In this oxidative coupling of benzyl alcohol and benzene-1,2-diamine catalyzed by TiO2@PMHSIPN, all the products were known[5] and have been confirmed by GC-MS, IR, and NMR.

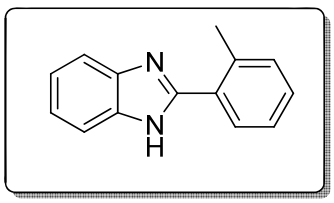
The characterization data of the representative compounds 7, 11, 13



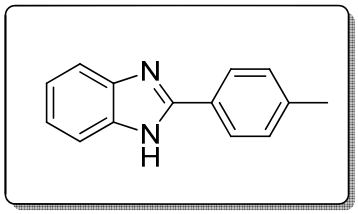
A white solid, 99% Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) : δ = 8.31 (s, 1H), 7.75 (m, 2H), 7.37 (d, J = 8.4 Hz, 2H), 7.33-7.37 (m, 4H), 7.15-7.21 (m, 3H); ^{13}C-NMR ($CDCl_3$, 125 MHz): 158.7, 151.8, 137.4, 134.9, 130.1, 129.3, 129.1, 126.3, 121.0 ; IR (v_{max}/cm^{-1}): 3081.1, 2875.9, 2570.7, 1944.3, 1908.3, 1880.6, 1703.0, 1490.5, 1189.4, 1168.5, 1012.8, 733.6, 710.2, 649.0.



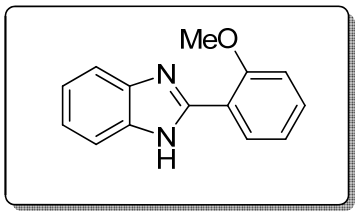
11a: A white solid, 72% Yield. ^{1}H-NMR (400 MHz, CD_3OD) : δ = 8.09 (d, J = 6.8 Hz, 2H), 7.60 (m, 2H), 7.51 (m, 3H), 7.25 (m, 2H), 4.90 (s, 1H) ; ^{13}C-NMR (CD_3OD, 100 MHz): 153.4, 131.4, 131.1, 130.1, 127.8, 123.9, 115.9 ; IR (v_{max}/cm^{-1}): 3105.9, 2180.6, 2097.2, 1523.7, 1462.9, 1412.8, 1310.8, 1276.1, 1224.2, 1112.7, 966.2, 745.3, 704.1.



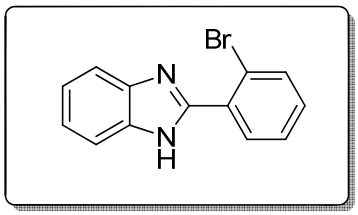
11b: A white solid, 93% Yield. ^{1}H-NMR (400 MHz, CD_3OD) : δ = 7.87 (t, J = 8.8 Hz, 2H), 7.58 (m, 2H), 7.36 (m, 1H), 7.23 (m, 3H), 5.08 (s, 1H), 2.38 (s, 3H); ^{13}C-NMR (CD_3OD, 125 MHz): 152.1, 138.6, 130.6, 129.5, 128.6, 127.0, 123.6, 122.4, 114.4, 20.1; IR (v_{max}/cm^{-1}): 3052.1, 2922.8, 2791.4, 2358.9, 1590.8, 1539.3, 1558.2, 1471.5, 1446.1, 1433.3, 1314.2, 1275.3, 974.8, 764.8, 742.6, 720.3.



11c: A white solid, 84% Yield. ^{1}H-NMR (400 MHz, CD_3OD) : δ = 7.97 (d, J = 8.0 Hz, 2H), 7.58 (m, 2H), 7.35 (d, J=8.4Hz, 2H), 7.24 (m, 2H), 4.85 (s, 1H), 2.41 (s, 3H); ^{13}C-NMR (CD_3OD, 125 MHz): 152.2, 140.5, 129.3, 126.8, 126.4, 122.4, 20.0; IR (v_{max}/cm^{-1}): 3647.7, 1716.5, 1683.4, 1652.5, 1635.4, 1456.5, 1418.5, 1270.1, 1119.7, 948.3, 818.7, 764.0, 740.7, 613.0, 529.9.

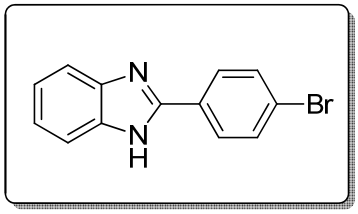


11d: A white solid, 78% Yield. ^{1}H-NMR (400 MHz, CD_3OD) : δ = 8.24 (m, 1H), 7.63 (m, 2H), 7.45 (m, 1H), 7.24 (m, 2H), 7.17 (d, J = 8.4 Hz, 1H), 7.10 (t, J = 7.6 HZ, 1H), 4.92 (s, 1H), 4.02 (s, 3H); ^{13}C-NMR (CD_3OD, 125 MHz): 157.3, 149.7, 138.0, 131.4, 129.6, 122.3, 120.8, 117.6, 114.5, 111.5, 54.9; IR (v_{max}/cm^{-1}): 3428.6, 3244.6, 3063.2, 2936.4, 1504.3, 1584.2, 1558.3, 1437.5, 1278.9, 1162.7, 1121.1, 1091.1, 1023.3, 747.8.

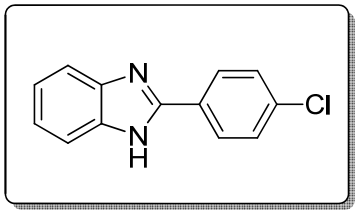


11f: A white solid, 69% Yield. ^{1}H-NMR (400 MHz, CD_3OD) : δ = 7.67 (d, J = 8.0 Hz, 1H), 7.60 (m, 1H), 7.52 (m, 2H), 7.40 (t, J = 7.6Hz, 1H), 7.32 (m, 1H), 7.19 (m, 2H),

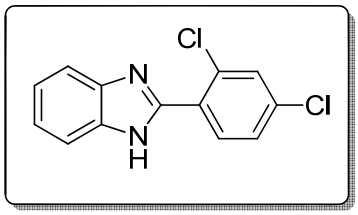
4.78 (s, 1H); ^{13}C-NMR (CD_3OD, 125 MHz): 151.0, 133.3, 132.1, 131.8, 131.2, 127.4, 122.6, 121.9, 114.7; IR (v_{max}/cm^{-1}): 3056.4, 1868.2, 1834.9, 1733.4, 1716.4, 1533.2, 1521.4, 1488.8, 1472.3, 1456.6, 1436.6, 1272.0, 1025.9, 742.5.



11g: A white solid, 68% Yield. ^{1}H-NMR (400 MHz, CD_3OD) : δ = 7.89 (m, 2H), 7.60 (m, 2H), 7.50 (m, 2H), 7.17 (m, 2H), 4.74 (s, 1H); ^{13}C-NMR (CD_3OD, 125 MHz): 150.9, 132.0, 128.8, 128.1, 124.1, 122.8; IR (v_{max}/cm^{-1}): 3468.9, 1558.6, 1540.8, 1553.0, 1521.7, 1489.1, 1473.0, 1457.3, 1416.7, 1261.8, 1069.5, 1009.9, 741.7.



11h: A white solid, 84% Yield. ^{1}H-NMR (400 MHz, CD_3OD) : δ = 8.06 (m, 2H), 7.61 (m, 2H), 7.56 (m, 2H), 7.27 (m, 2H), 4.84 (s, 1H); ^{13}C-NMR (CD_3OD, 125 MHz): 150.8, 135.9, 128.9, 128.4, 127.9, 122.7; IR (v_{max}/cm^{-1}): 3446.3, 3053.5, 2851.0, 2205.4, 2118.4, 1667.2, 1573.6, 1469.0, 1420.1, 1274.3, 1224.6, 1016.5, 832.3, 746.3.



11i: A white solid, 53% Yield. ^{1}H-NMR (400 MHz, CD_3OD) : δ = 7.82 (d, J = 8.4 Hz, 1H), 7.69 (d, J = 2.0 Hz, 1H), 7.65 (m, 2H), 7.50 - 7.53 (dd, J = 2.0 Hz, 1H), 7.31 (m, 2H), 4.76 (s, 1H); ^{13}C-NMR (CD_3OD, 125 MHz): 148.6, 136.4, 133.4, 132.7, 129.9, 128.3, 127.4, 122.9, 114.8; IR (v_{max}/cm^{-1}): 3058.5, 2128.8, 1684.1, 1506.0, 1487.3, 1359.1, 1187.6, 1104.2, 962.1, 924.4, 872.9, 860.1, 742.5.

References

[1] a) K. F. Yang, L. W. Xu, H. Wang, Faming Zhuanli Shenqing (Chinese Patent), CN 103289267, 2013. b) The polymethylhydrosiloxane (PMHS)-based semi-interpenetrating networks (PMHSIPN) was also a good supporter for palladium catalysis: H. Wang, L. Li, X. F. Bai, W. H. Deng, Z. J. Zheng, K. F. Yang, L. W. Xu, *Green Chem.* 2013, **15**, 2349-2355.

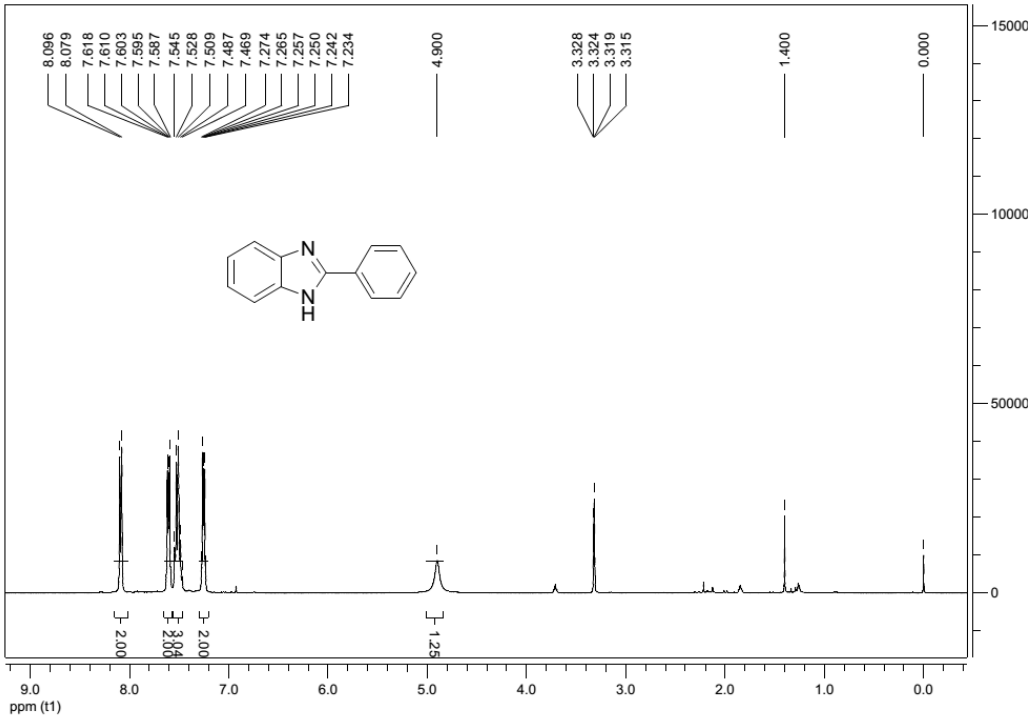
[2] H. Wang, K. F. Yang, L. Li, Y. Bai, Z. J. Zheng, W. Q. Zhang, L. W. Xu, *ChemCatChem* 2014, **6**, 580-591.

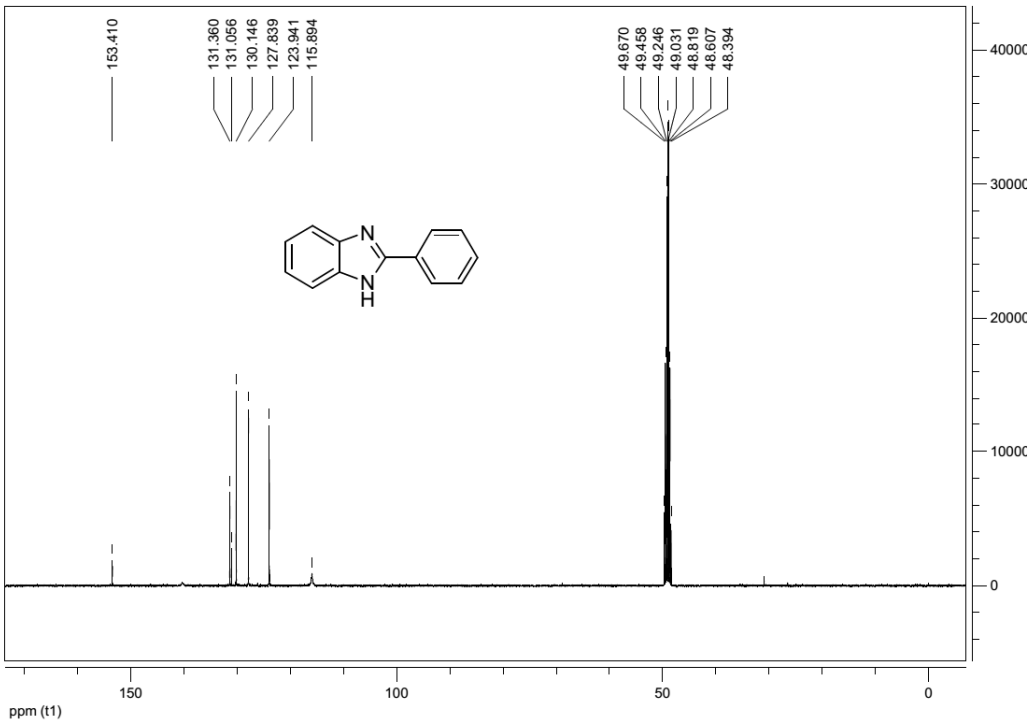
[3] R. K. Marella, C. K. P. Neeli, S. R. R. Kamaraju, D. R. Burri, *Catal. Sci. Tech.* 2012, **2**, 1833-1838.

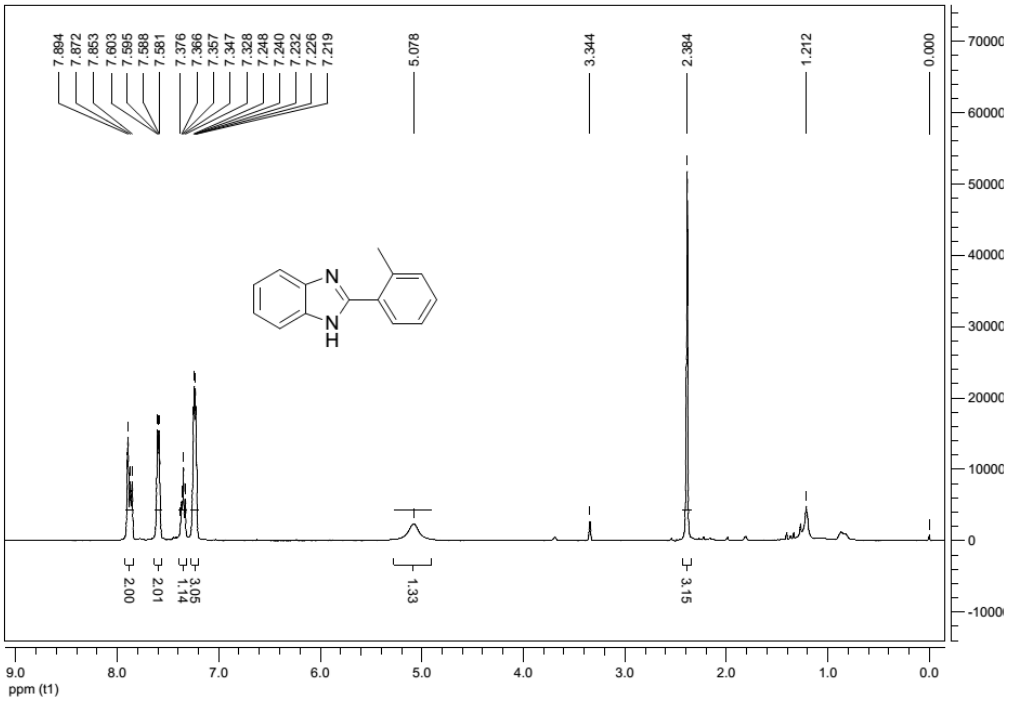
[4] a) Y. S. Lan, B. S. Liao, Y. H. Liu, S. M. Peng, S. T. Liu, *Eur. J. Org. Chem.* 2013, 5160-5164; b) L. Tang, H. Sun, Y. Li, Z. Zha, Z. Wang, *Green Chem.* 2012, **14**, 3423-3428.

[5] a) Y. Shiraishi, Y. Sugano, S. Tanaka, T. Hirrai, *Angew. Chem. Int. Ed.* 2010, **49**, 1656-1660; b) G. Li, J. Wang, B. Yuan, D. Zhang, Z. Lin, P. Li, H. Huang, *Tetrahedron Lett.* 2013, **54**, 6934-6936.

8. NMR and GC-MS of representative products



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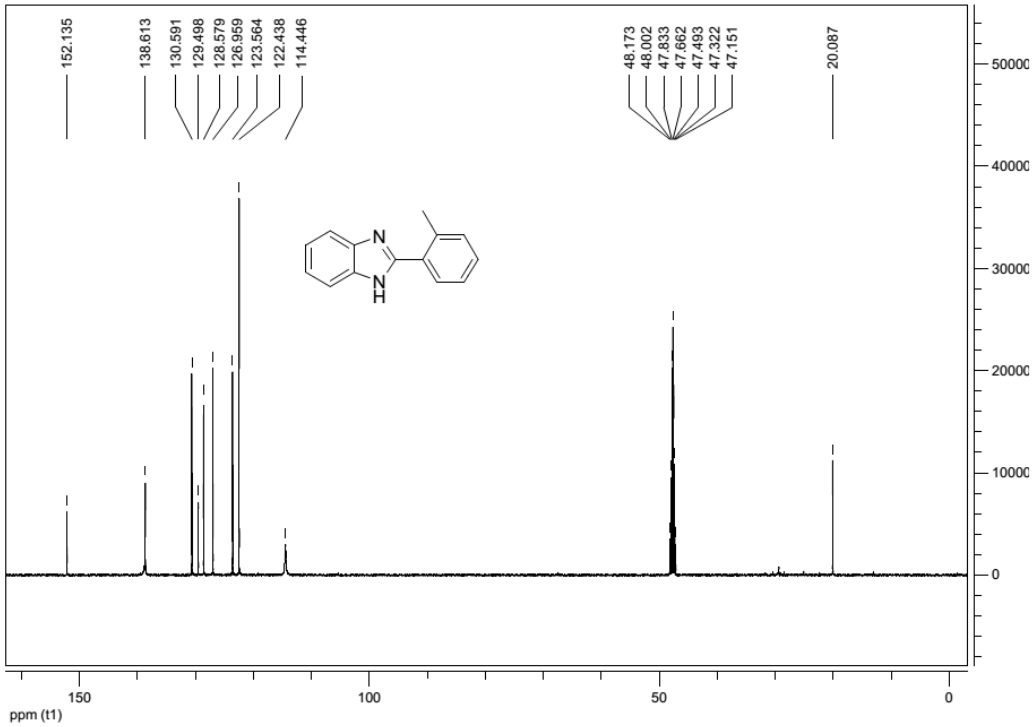
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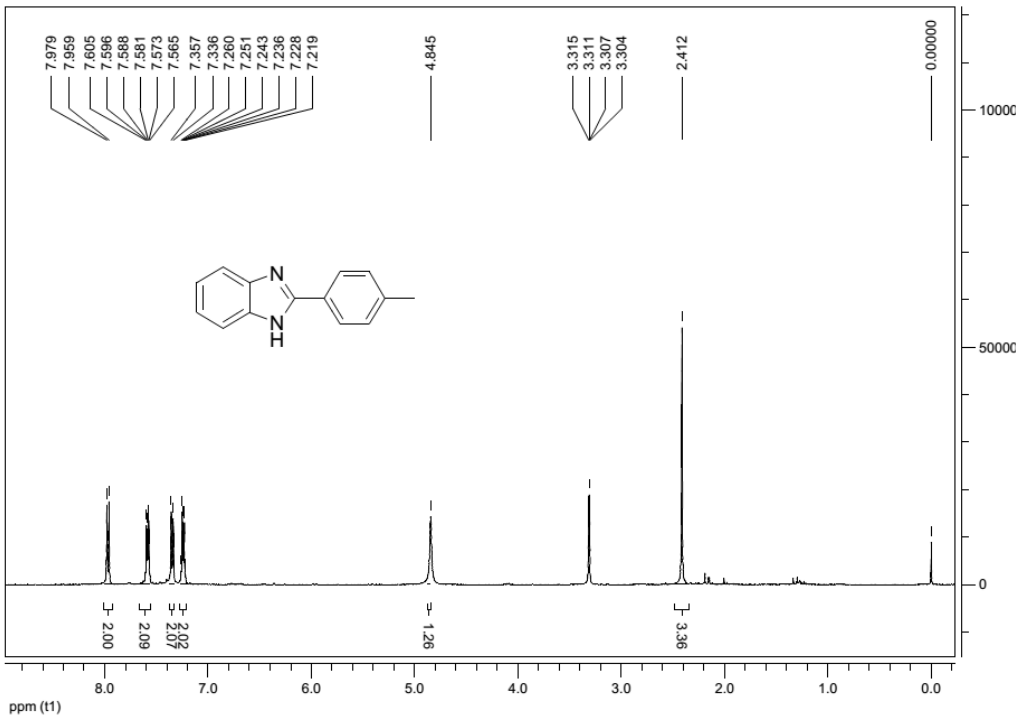
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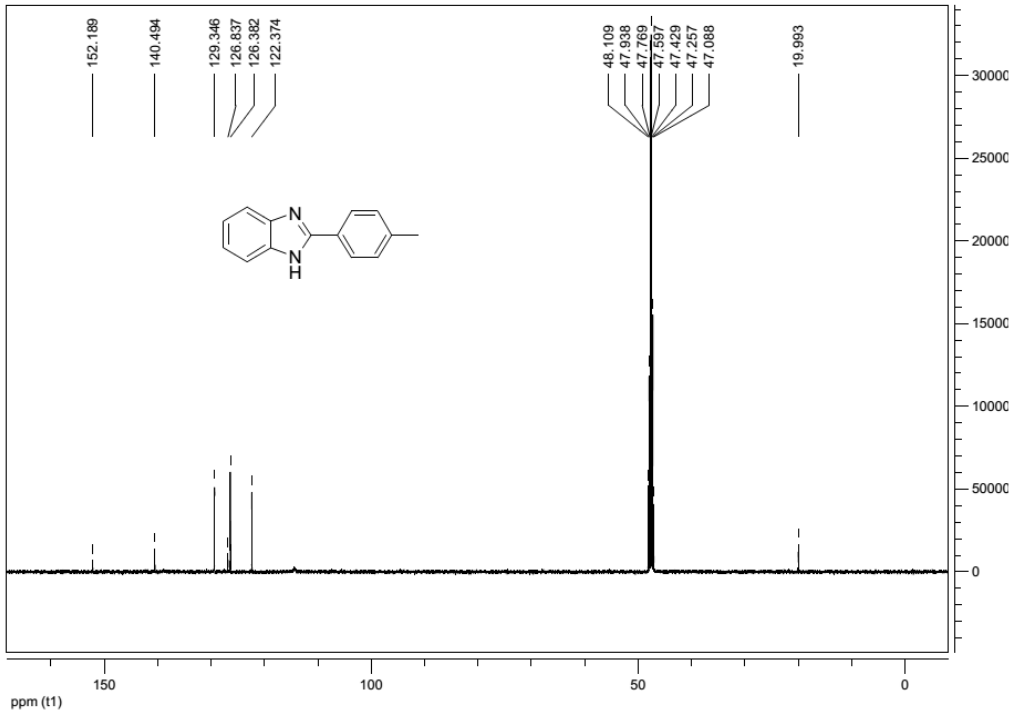
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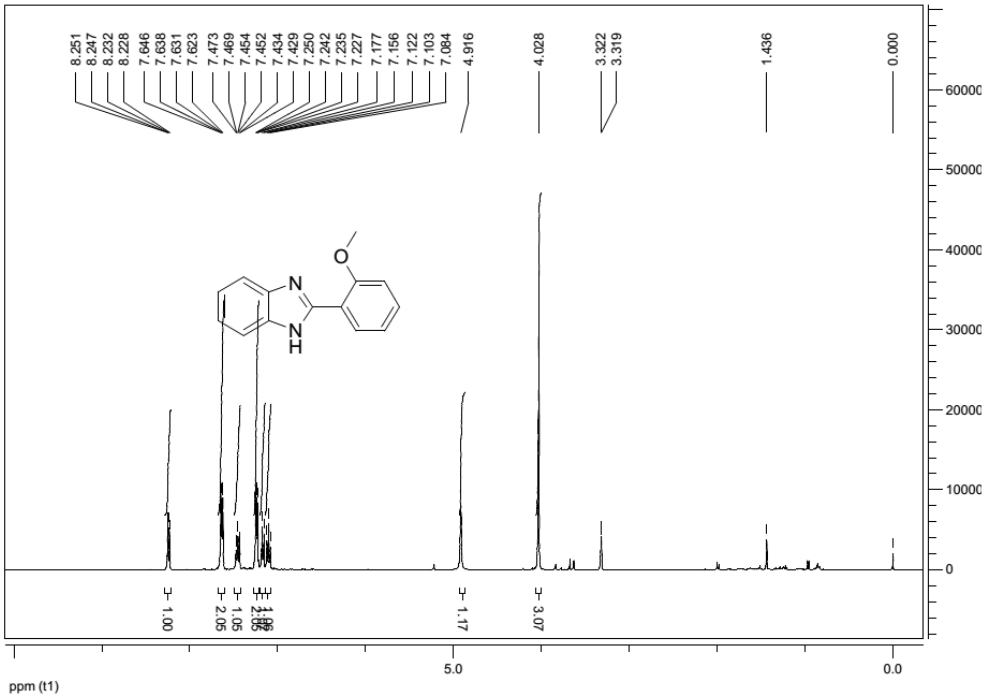
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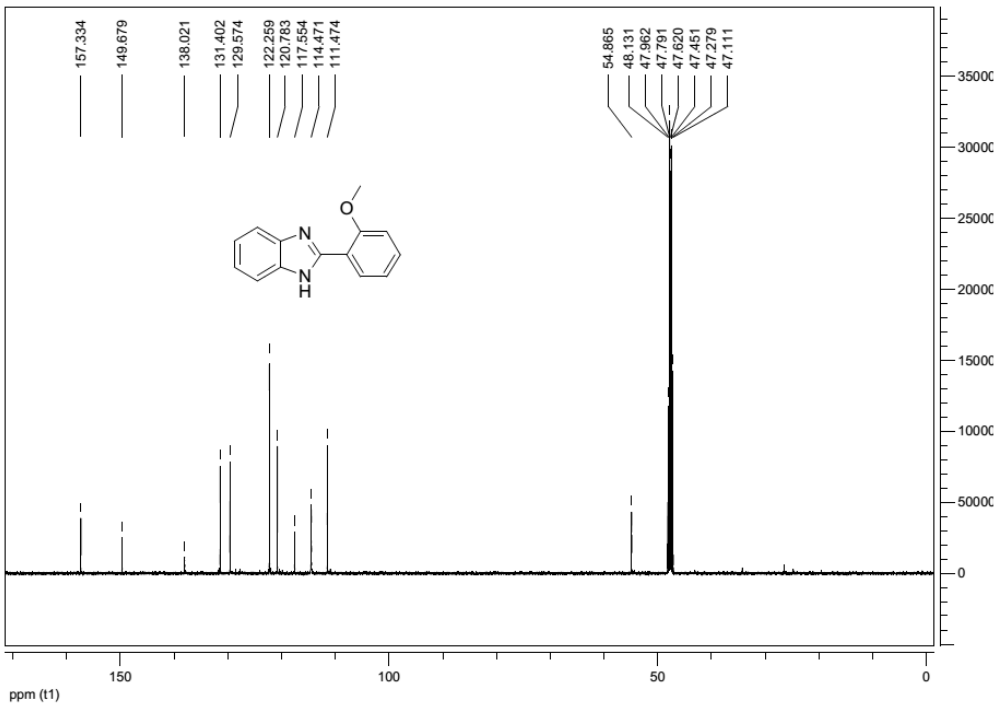
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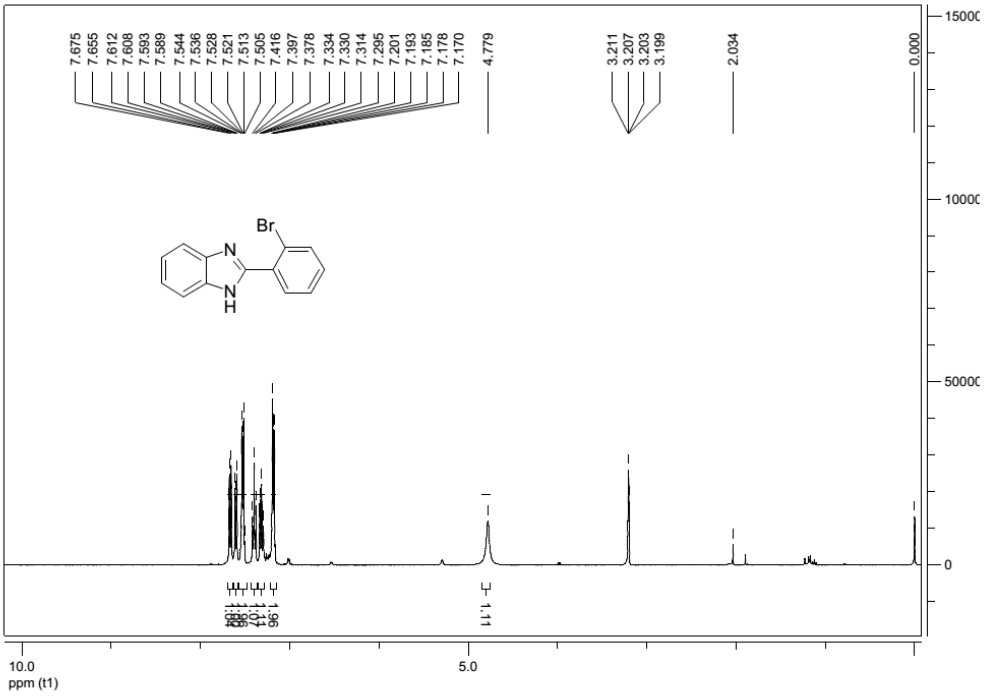
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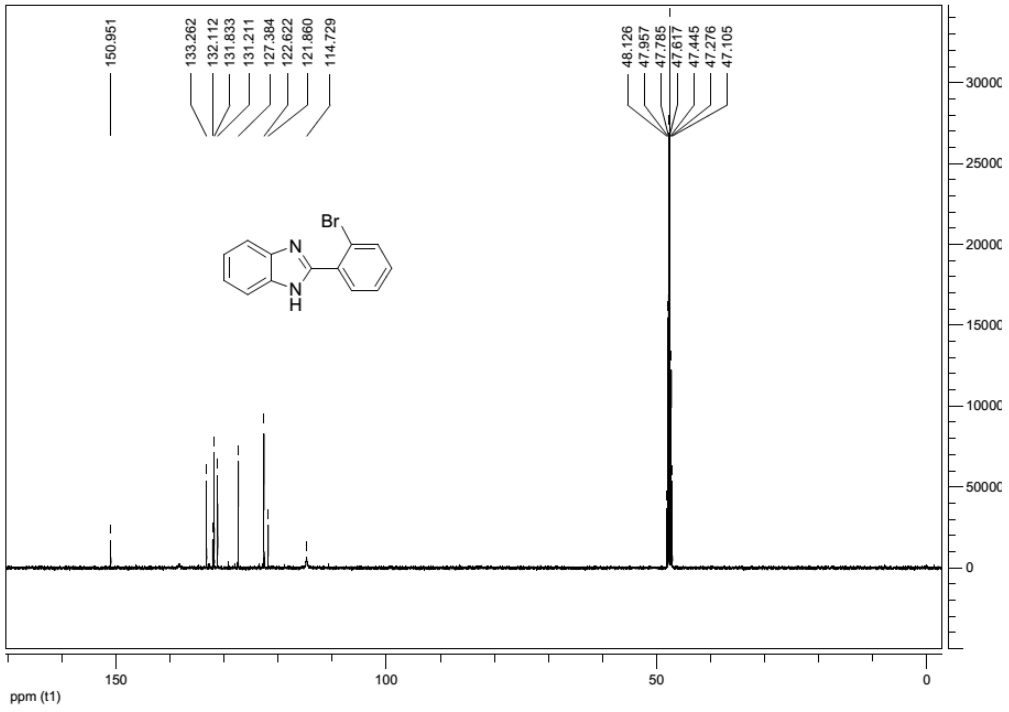
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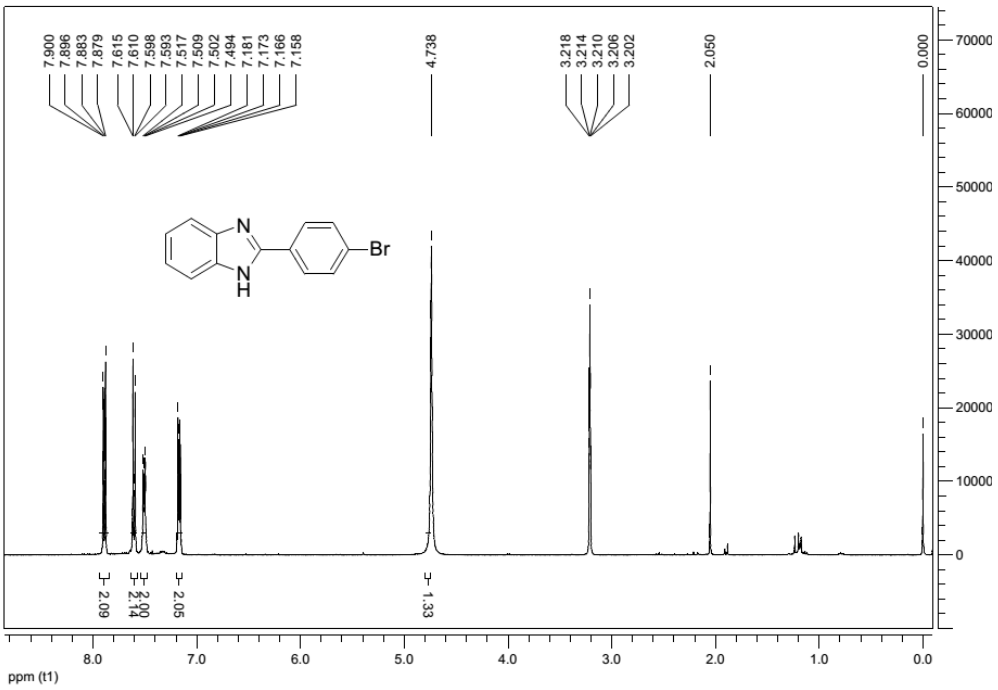
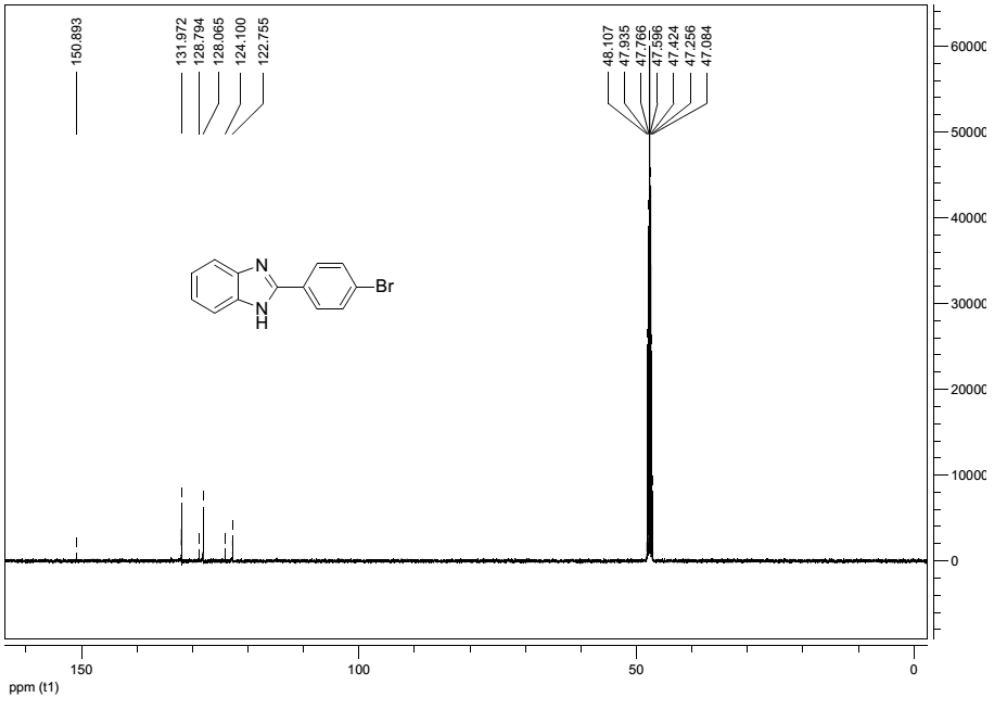
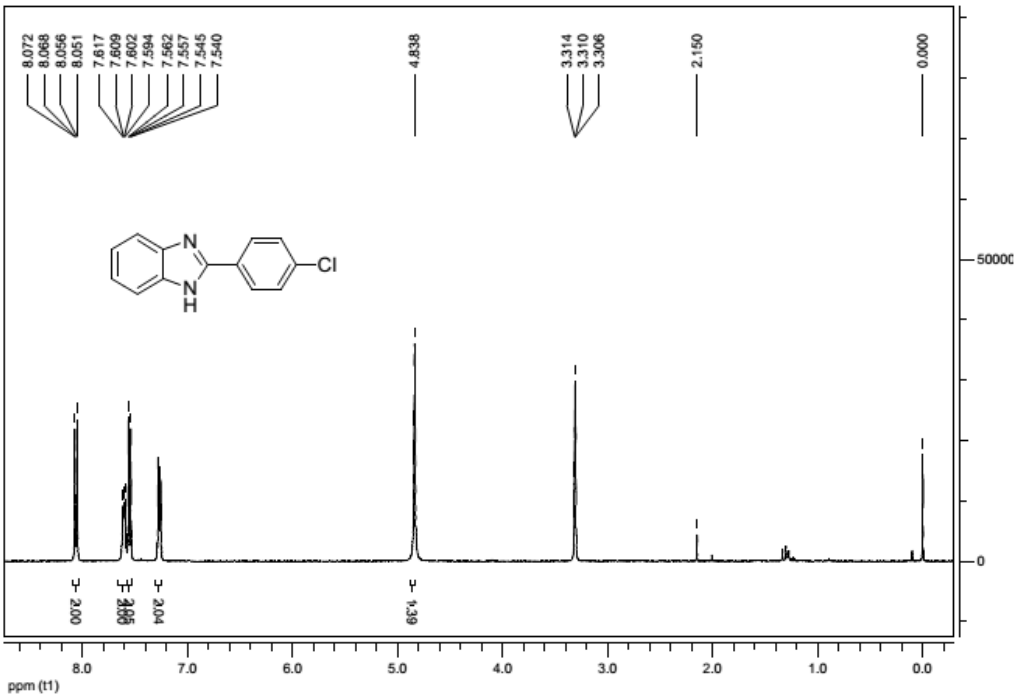
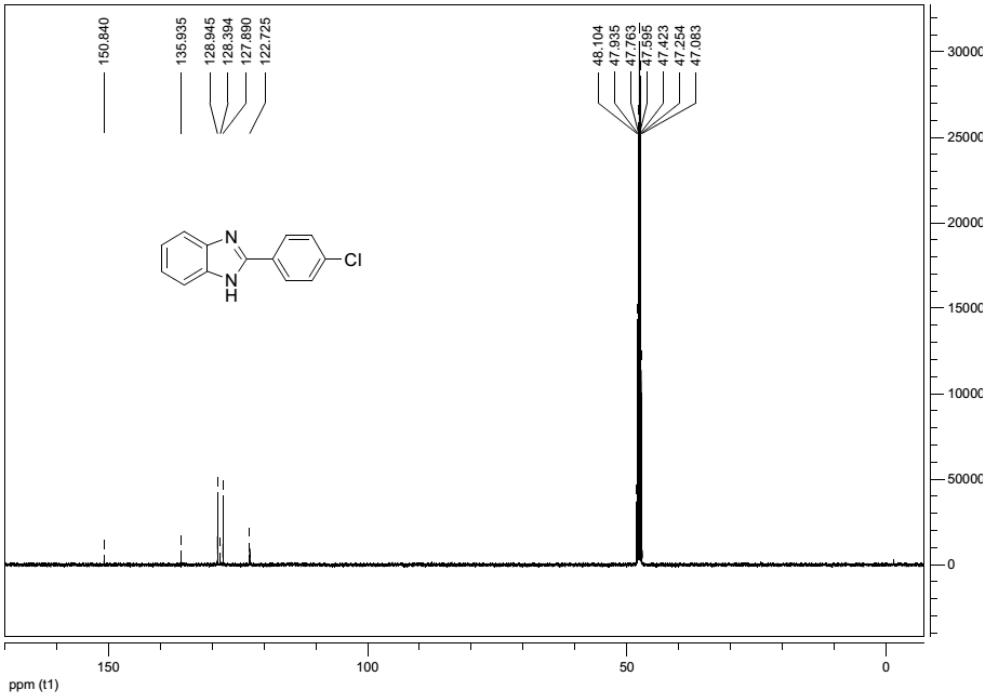
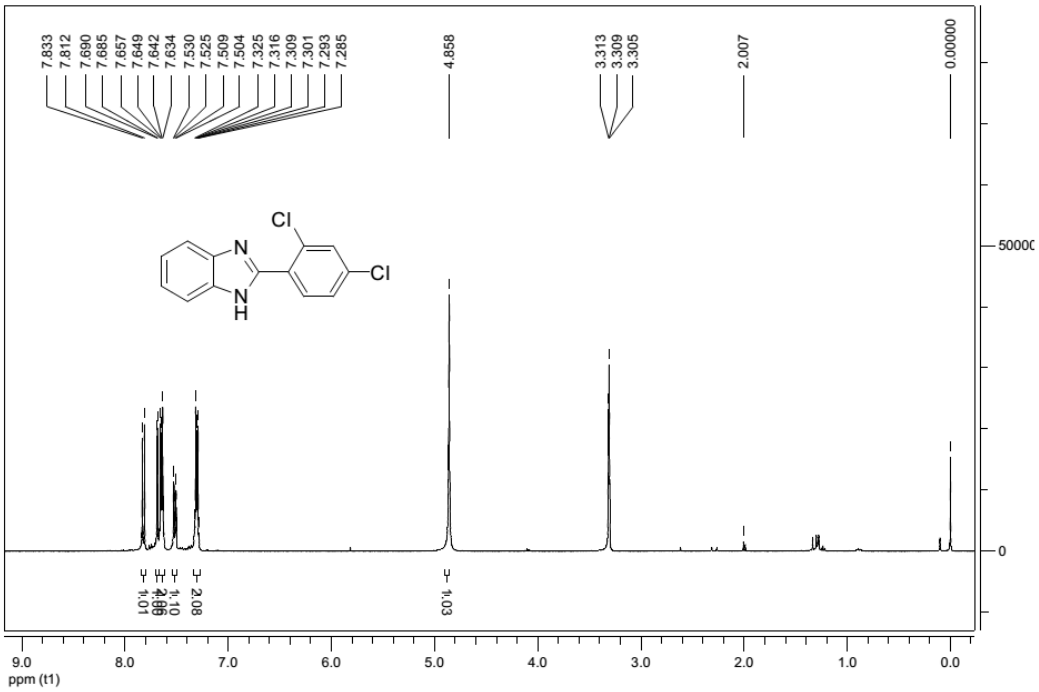
50
0
ppm (t1)

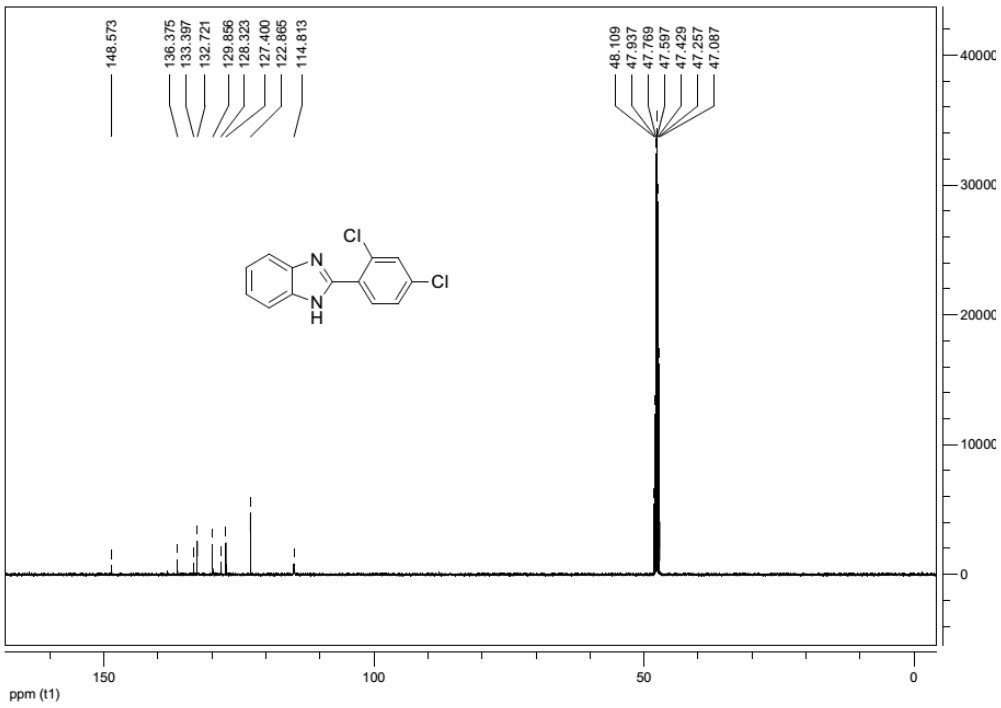

7.900
7.896
7.883
7.879
7.615
7.610
7.598
7.593
7.517
7.509
7.502
7.494
7.181
7.173
7.166
7.158
4.738
3.218
3.214
3.210
3.206
3.202
2.050
0.000
N
N
H
Br
2.09
2.14
2.00
2.05
1.33
ppm (t1)

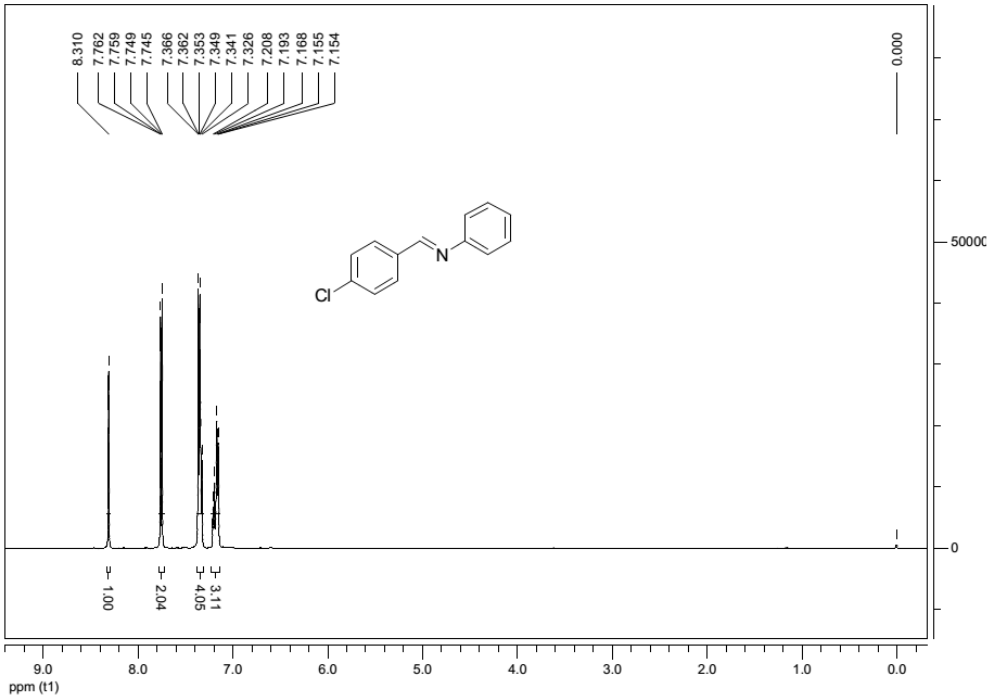

150.893
131.972
128.794
128.065
124.100
122.755
48.107
47.935
47.766
47.596
47.424
47.256
47.084
N
N
H
Br
ppm (t1)

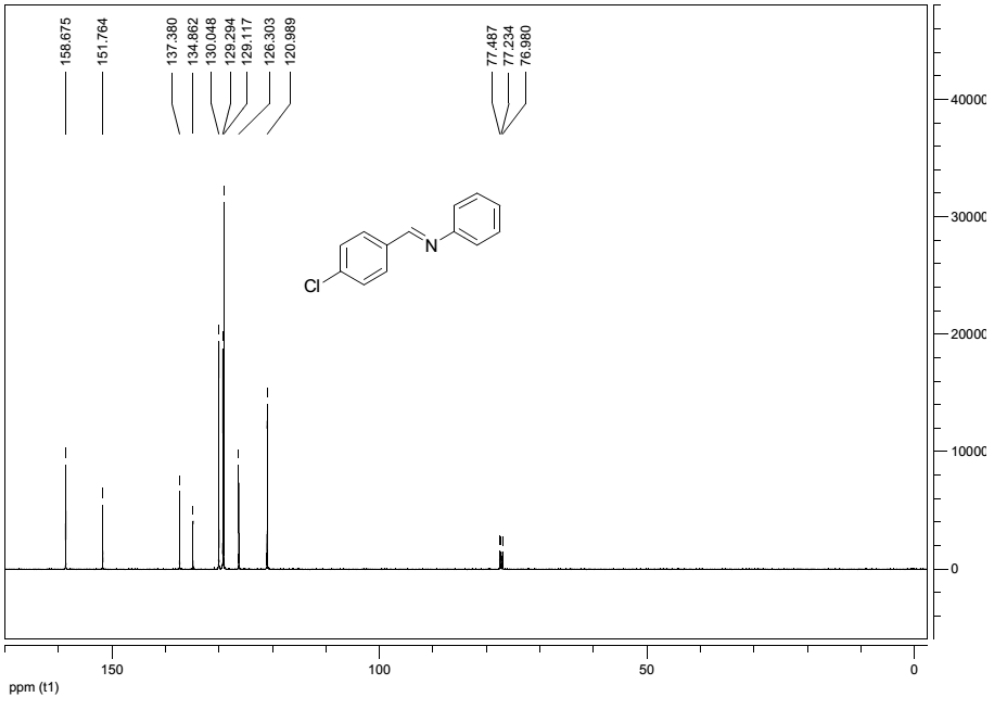

8.072
8.068
8.056
8.051
7.617
7.609
7.602
7.594
7.562
7.557
7.545
7.540
4.838
3.314
3.310
3.306
2.150
0.000
N
N
H
Cl
50000
0
2.00
4.04
1.39
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

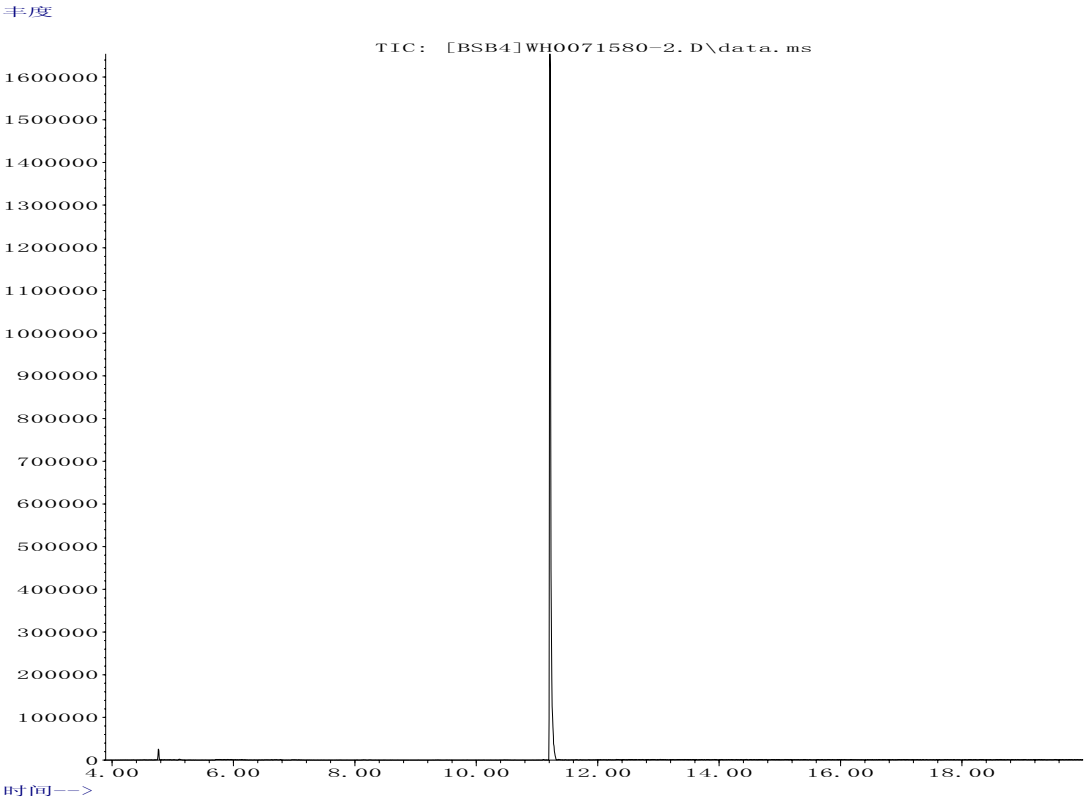

150.840
135.935
128.945
128.394
127.890
122.725
48.104
47.935
47.763
47.595
47.423
47.254
47.083
N
N
H
Cl
30000
25000
20000
15000
10000
5000
0
150
100
50
0
ppm (t1)


7.833
7.812
7.690
7.685
7.657
7.649
7.642
7.634
7.530
7.525
7.509
7.504
7.325
7.316
7.309
7.301
7.293
7.285
4.858
3.313
3.309
3.305
2.007
0.00000
Cl
N
N
H
Cl
50000
0
1.01
2.08
1.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

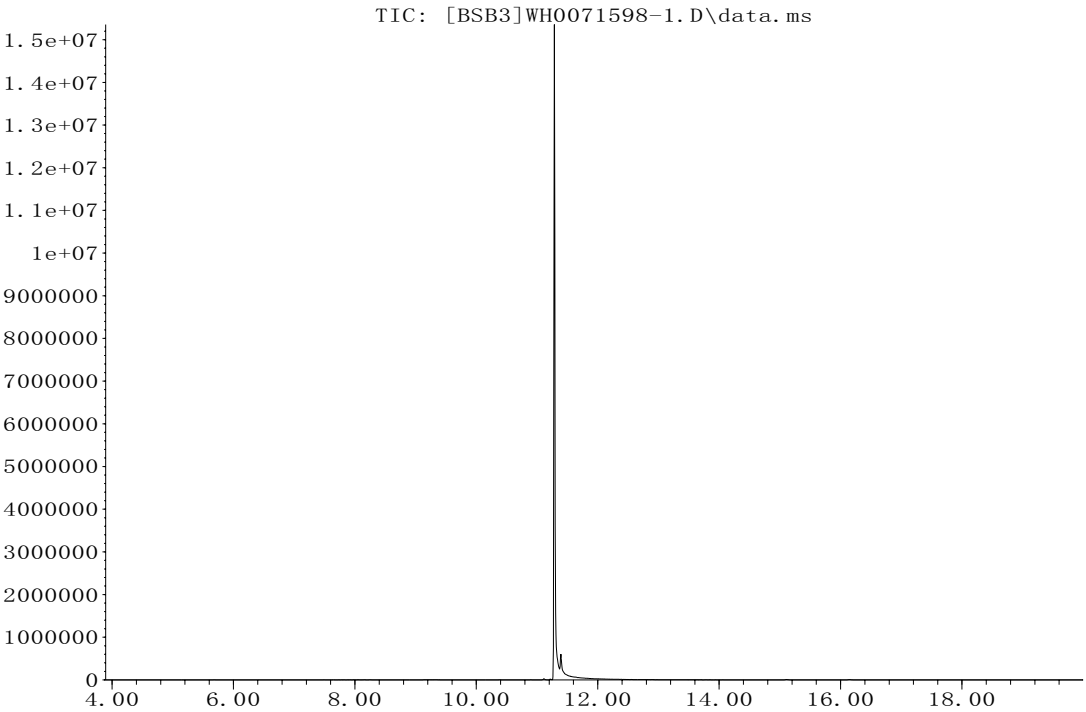

148.573
136.375
133.397
132.721
129.856
128.323
127.400
122.865
114.813
48.109
47.937
47.769
47.597
47.429
47.257
47.087
Cl
N
N
H
Cl
40000
30000
20000
10000
0
150
100
50
0
ppm (t1)


8.310
7.762
7.759
7.749
7.745
7.366
7.362
7.353
7.349
7.341
7.326
7.208
7.193
7.168
7.155
7.154
0.000
Cl
N
1.00
2.04
4.05
3.11
50000
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


158.675
151.764
137.380
134.862
130.048
129.294
129.117
126.303
120.989
77.487
77.234
76.980
Cl
N
40000
30000
20000
10000
0
150
100
50
0
ppm (t1)

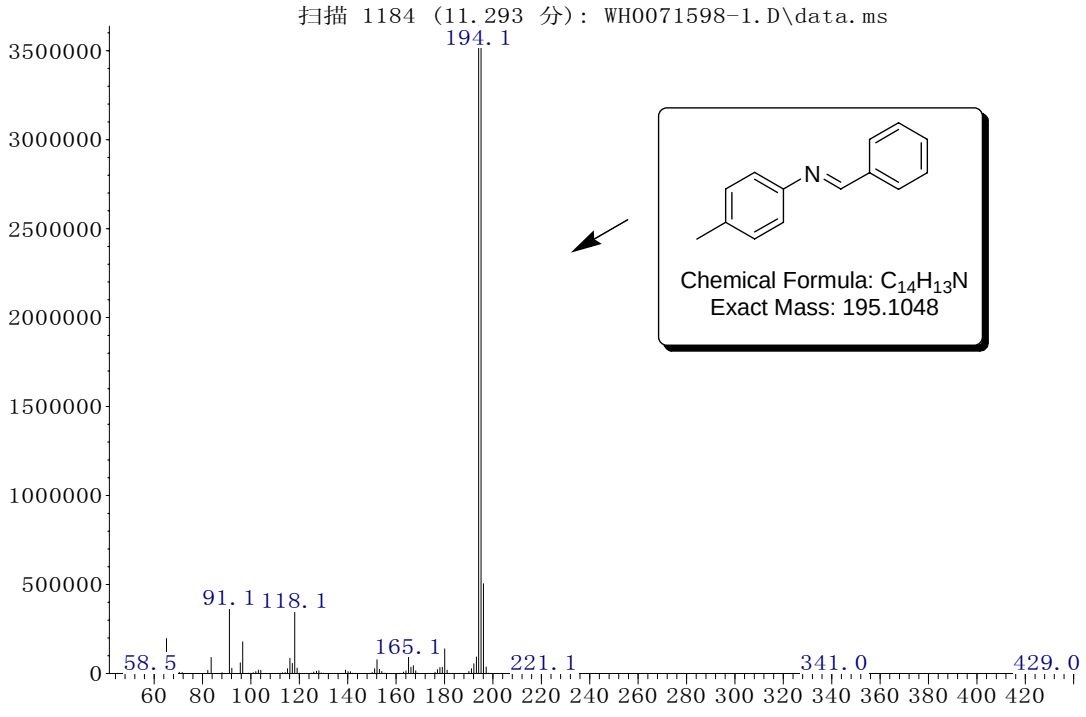

丰度
TIC: [BSB4]WH0071580-2.D\data.ms
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1173 (11.224 分): WH0071580-2.D\data.ms
194.1
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
N
Chemical Formula: C14H13N
Exact Mass: 195.1048
118.1
127.0
139.1
152.1
165.0
180.1
207.1
115 120 125 130 135 140 145 150 155 160 165 170 175 180 185 190 195 200 205 210
m/z-->

丰度


TIC: [BSB3]WH0071598-1.D\data.ms
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

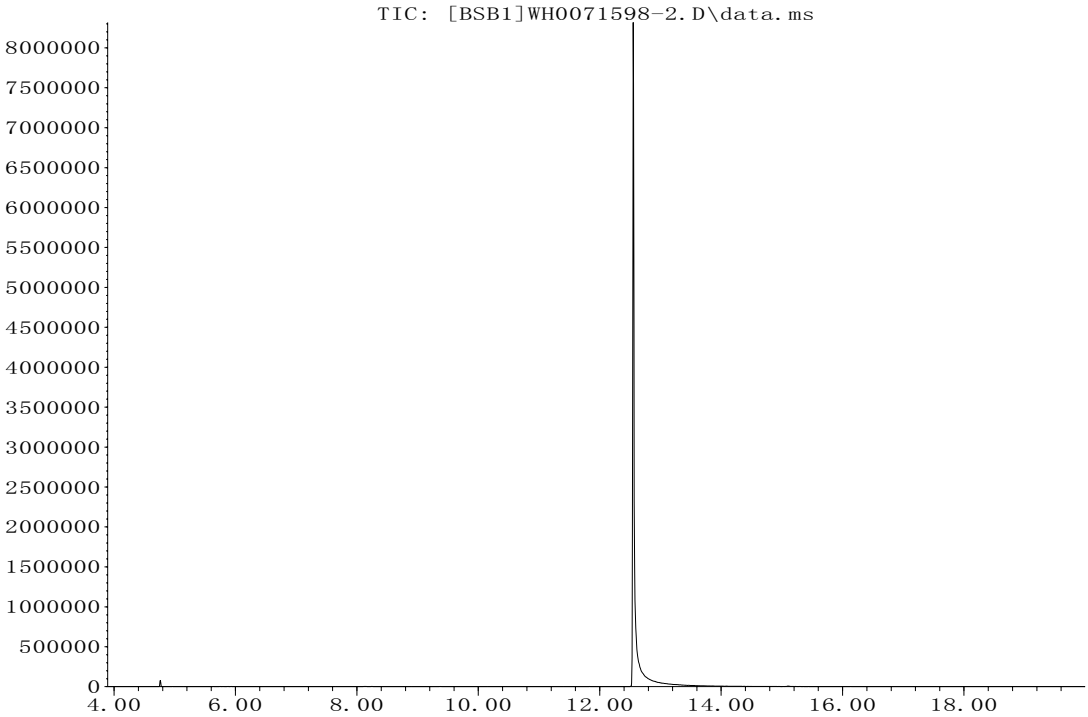
时间-->

丰度


扫描 1184 (11.293 分): WH0071598-1.D\data.ms
194.1
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
91.1
118.1
58.5
165.1
221.1
341.0
429.0
60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420
N
Chemical Formula: C14H13N
Exact Mass: 195.1048

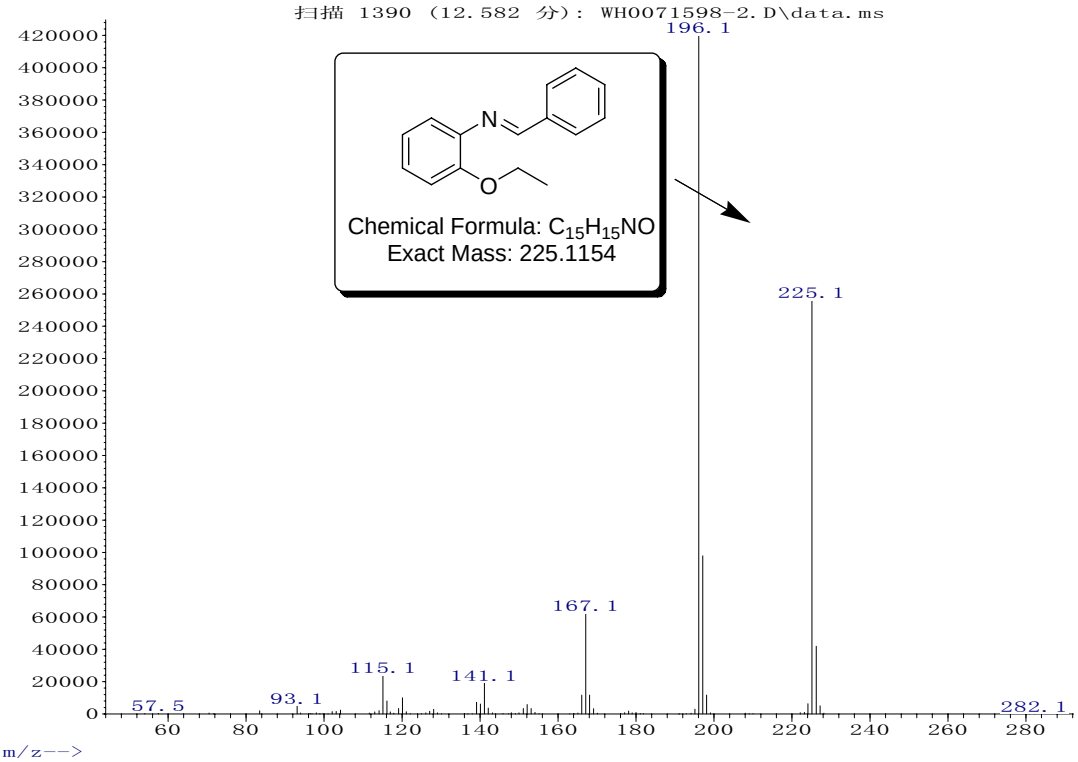
m/z-->

丰度


TIC: [BSB1]WH0071598-2.D\data.ms
8000000
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

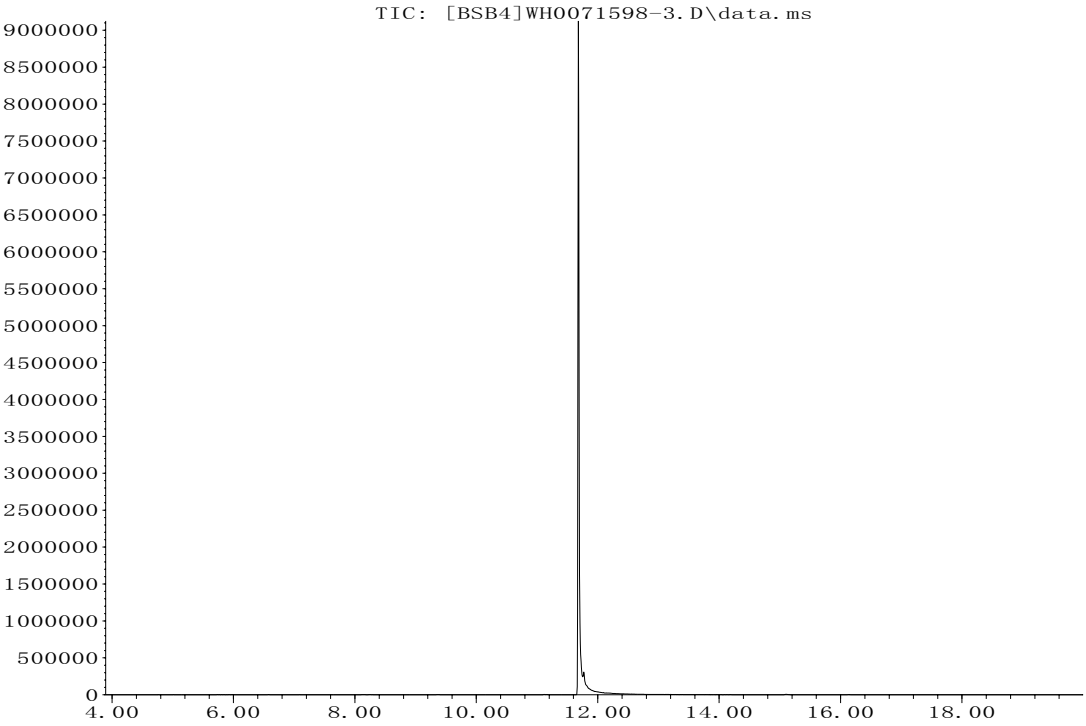
时间-->

丰度


扫描 1390 (12.582 分): WH0071598-2.D\data.ms
196.1
225.1
167.1
115.1
141.1
93.1
57.5
282.1
N
O
Chemical Formula: C15H15NO
Exact Mass: 225.1154
420000
400000
380000
360000
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
60
80
100
120
140
160
180
200
220
240
260
280

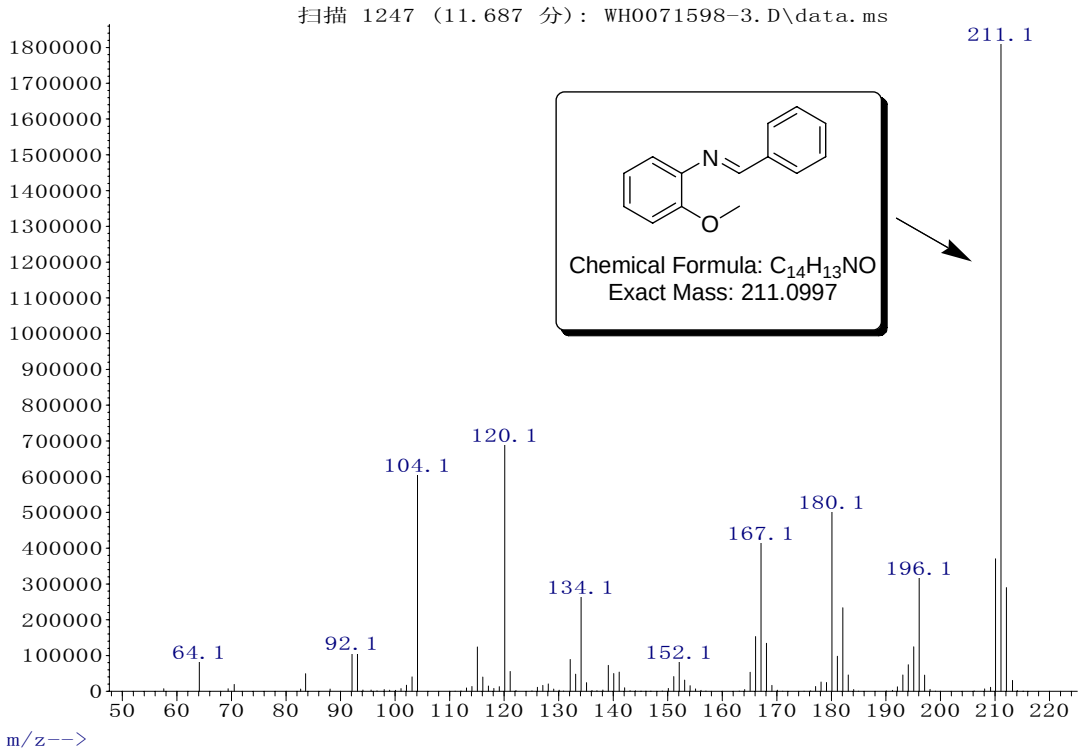
m/z-->

丰度


TIC: [BSB4]WH0071598-3.D\data.ms
9000000
8500000
8000000
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

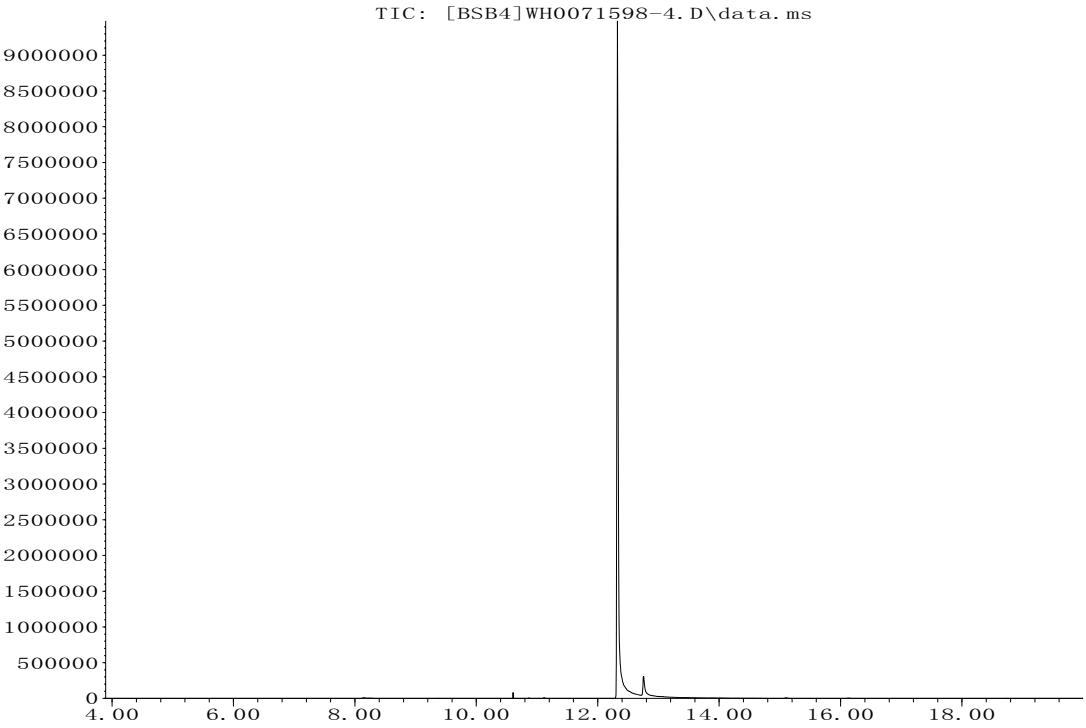
时间-->

丰度


扫描 1247 (11.687 分): WH0071598-3.D\data.ms
1800000
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
211.1
120.1
104.1
180.1
167.1
196.1
134.1
64.1
92.1
152.1
N
O
Chemical Formula: C14H13NO
Exact Mass: 211.0997

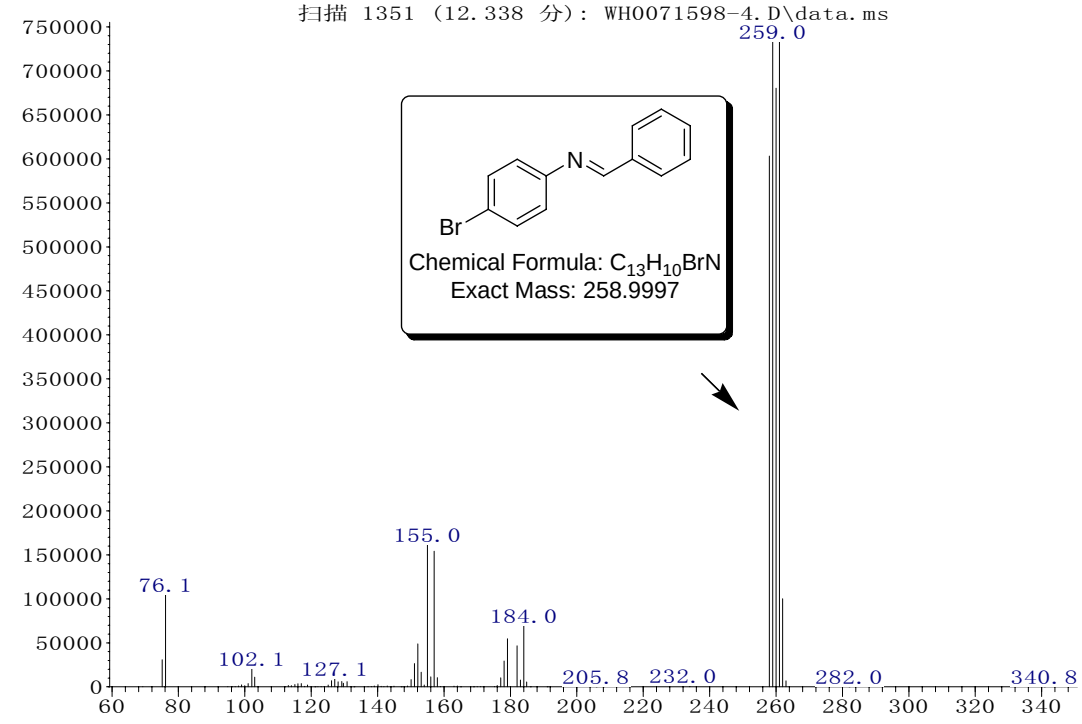
m/z-->

丰度


TIC: [BSB4]WH0071598-4.D\data.ms
9000000
8500000
8000000
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

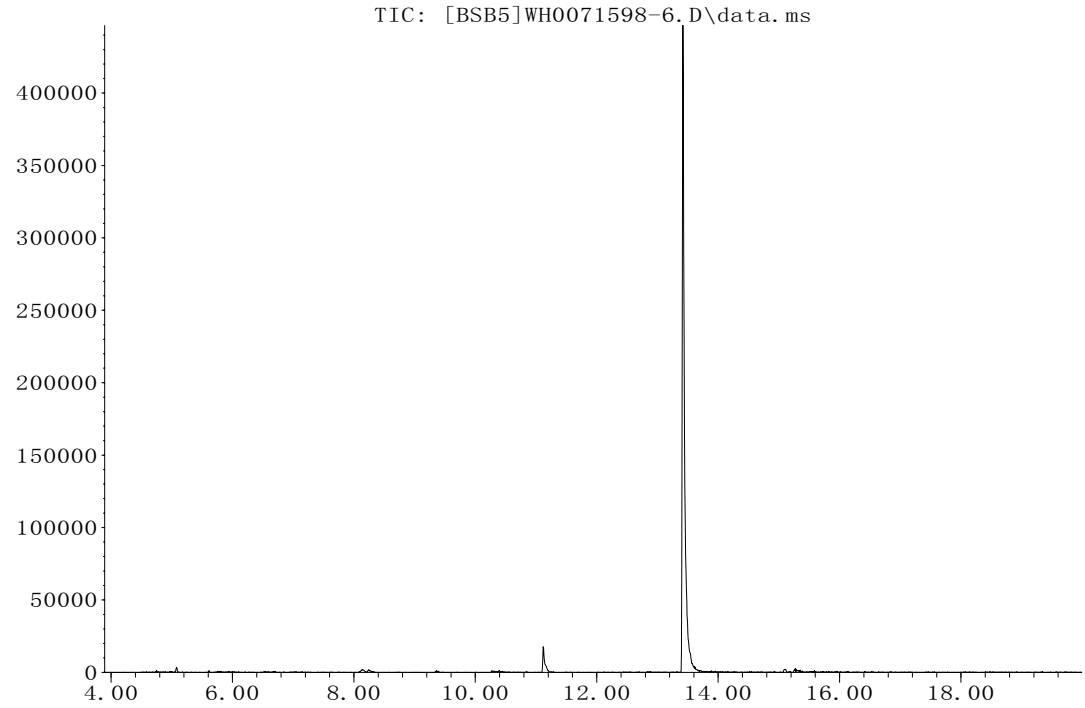
时间-->

丰度


扫描 1351 (12.338 分): WH0071598-4.D\data.ms
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
259.0
155.0
76.1
184.0
102.1
127.1
205.8
232.0
282.0
340.8
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
N
Br
Chemical Formula: C13H10BrN
Exact Mass: 258.9997

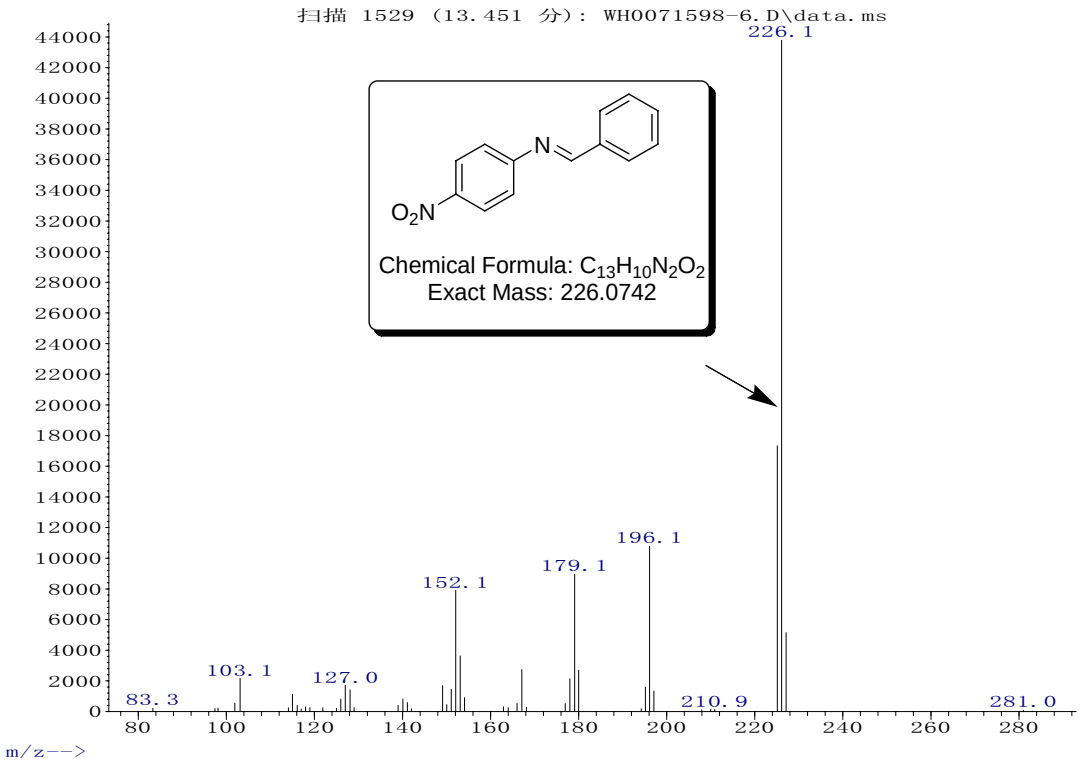
m/z-->

丰度

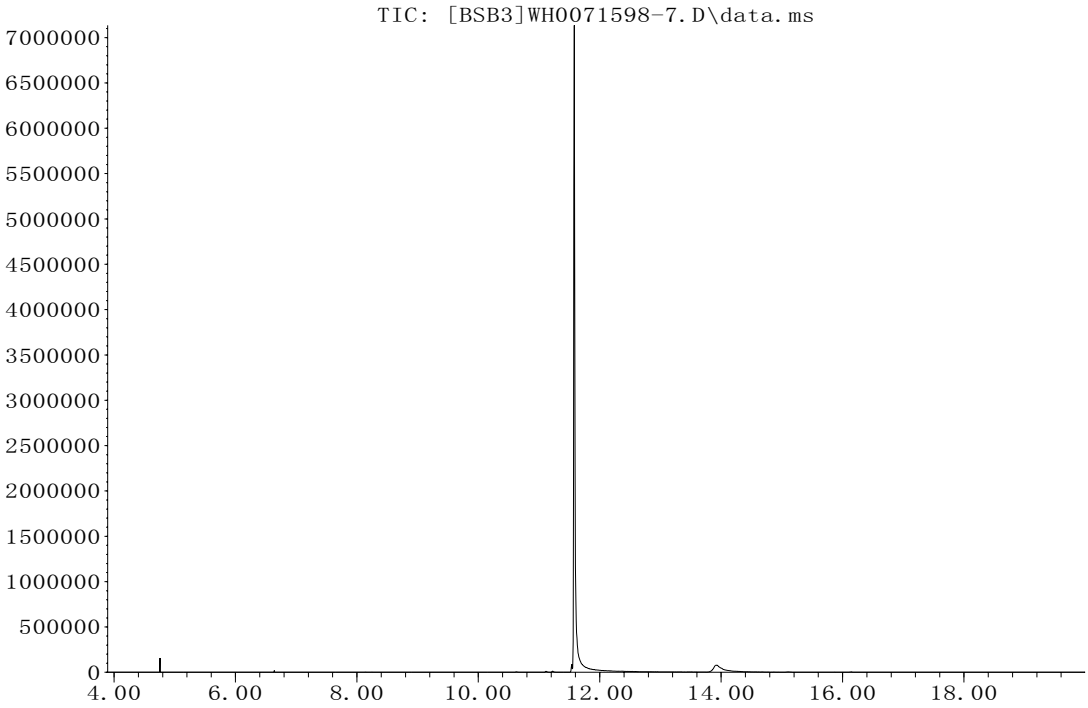

TIC: [BSB5]WH0071598-6.D\data.ms
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

时间-->

丰度

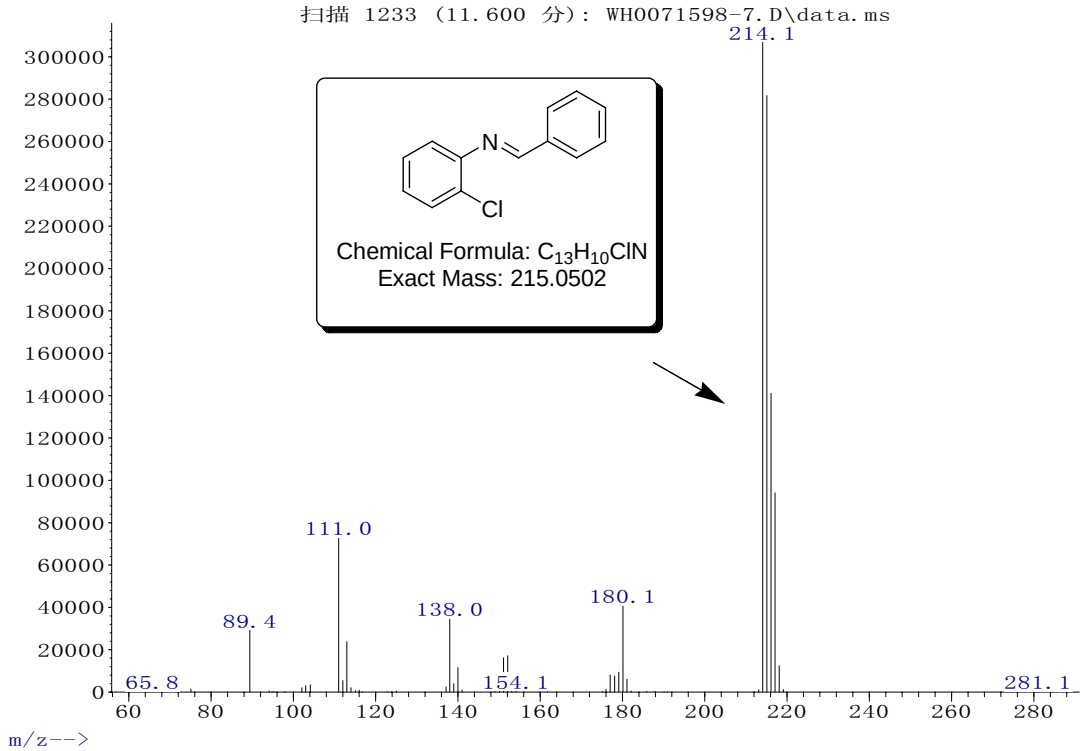

扫描 1529 (13.451 分): WH0071598-6.D\data.ms
226.1
196.1
179.1
152.1
103.1
127.0
83.3
210.9
281.0
N
O2N
Chemical Formula: C13H10N2O2
Exact Mass: 226.0742
m/z-->

丰度

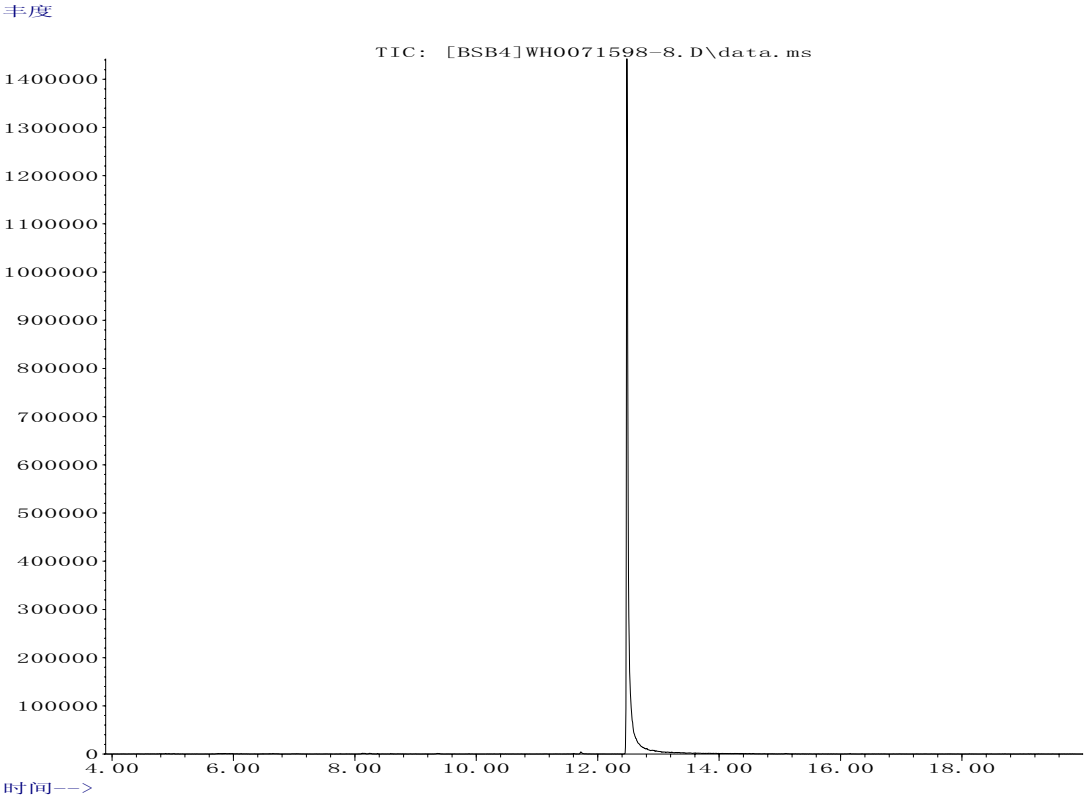

TIC: [BSB3]WH0071598-7.D\data.ms
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

时间-->

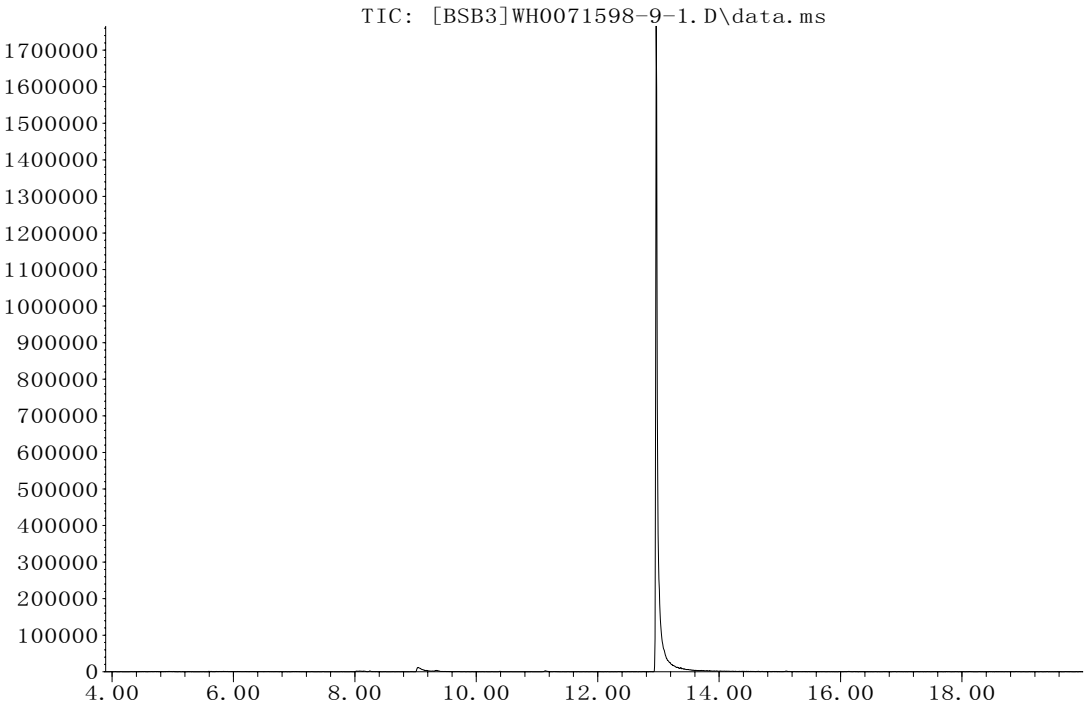
丰度


扫描 1233 (11.600 分): WH0071598-7.D\data.ms
214.1
N
Cl
Chemical Formula: C13H10ClN
Exact Mass: 215.0502
111.0
89.4
138.0
180.1
65.8
154.1
281.1
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
60
80
100
120
140
160
180
200
220
240
260
280

m/z-->

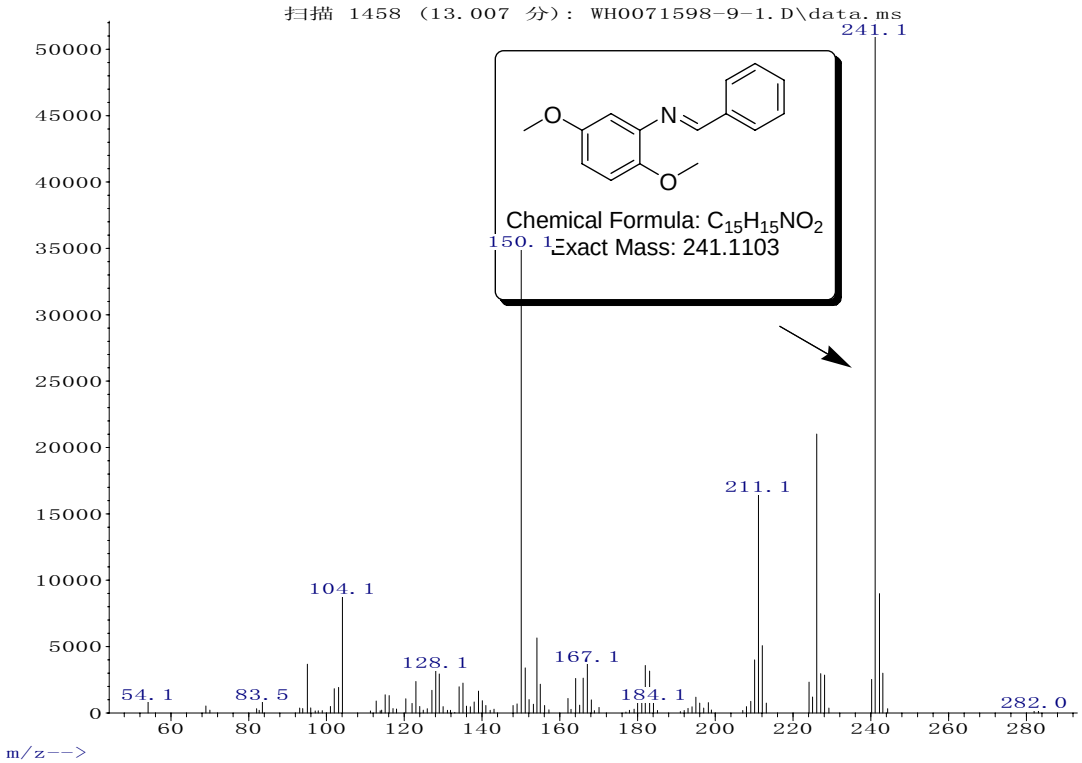

丰度
TIC: [BSB4]WH0071598-8.D\data.ms
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1378 (12.507 分): WH0071598-8.D\data.ms
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
249.0
214.1
145.0
172.0
111.0
94.2
185.9
Cl
N
Cl
Chemical Formula: C13H9Cl2N
Exact Mass: 249.0112
90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260
m/z-->
25 / 61

丰度

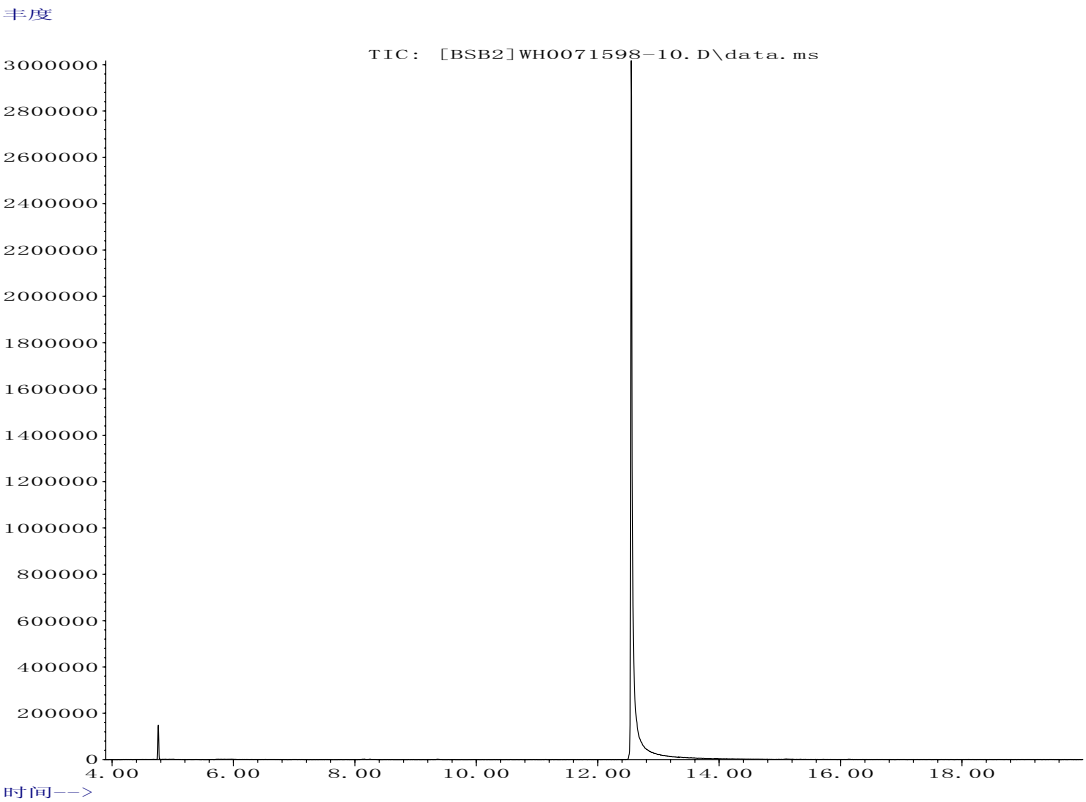

TIC: [BSB3]WH0071598-9-1.D\data.ms
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

时间-->

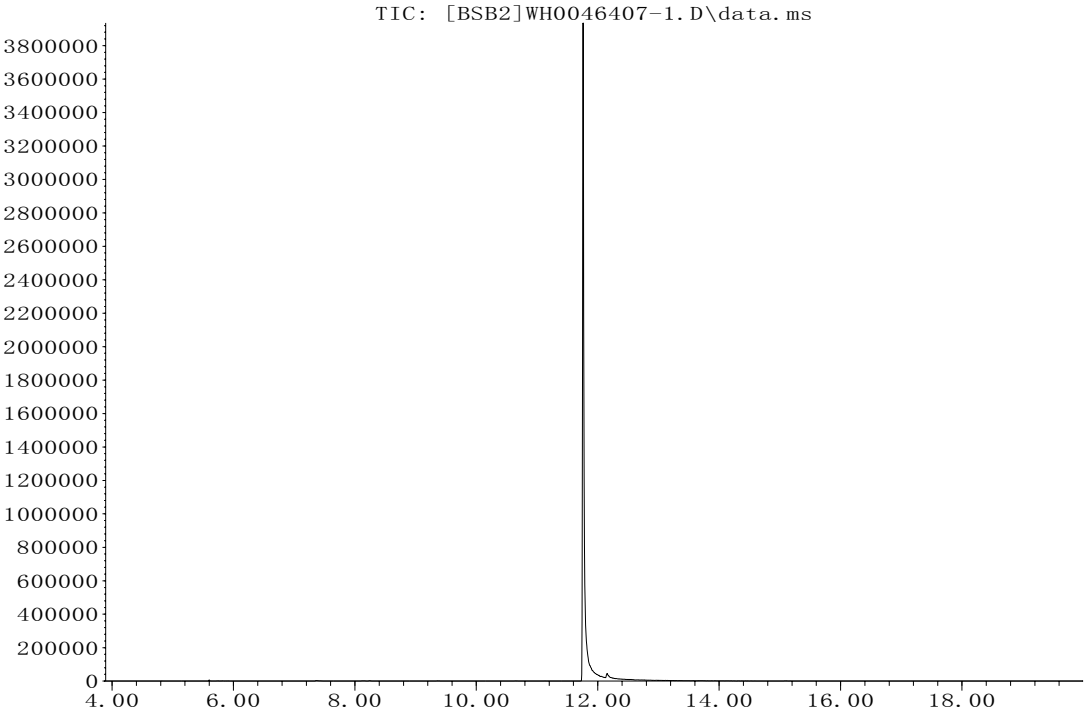
丰度


扫描 1458 (13.007 分): WH0071598-9-1.D\data.ms
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
241.1
150.1
211.1
104.1
128.1
167.1
184.1
54.1
83.5
282.0
60
80
100
120
140
160
180
200
220
240
260
280
O
N
O
Chemical Formula: C15H15NO2
Exact Mass: 241.1103

m/z-->

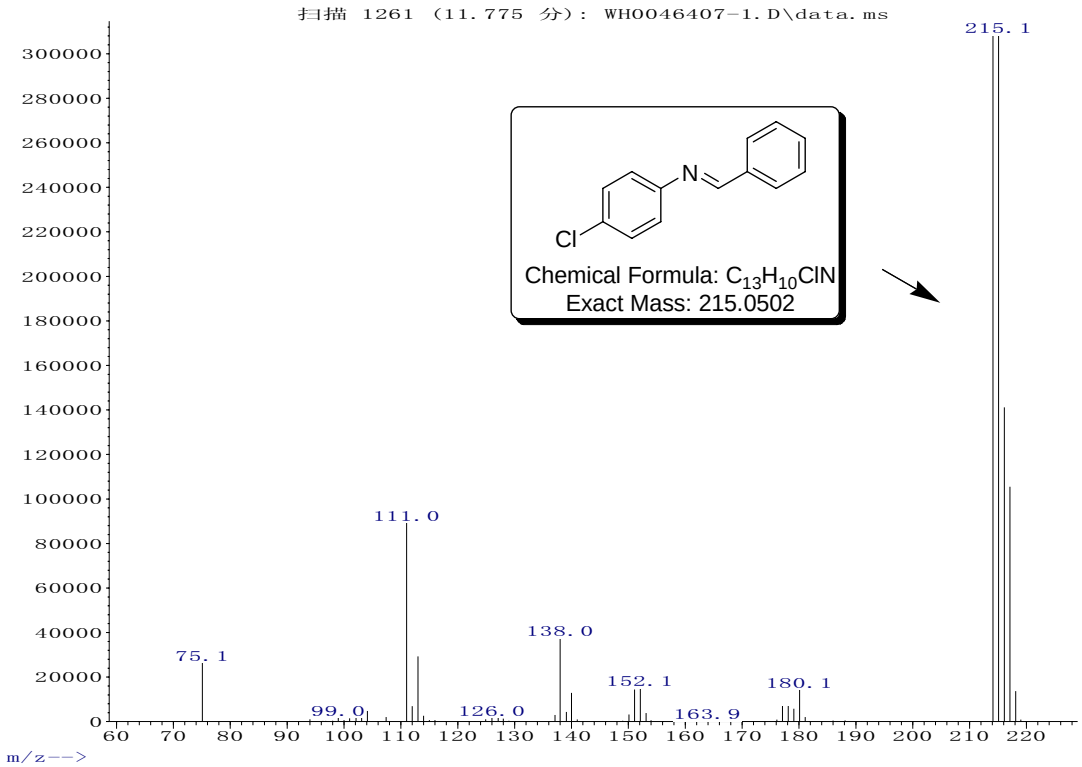

丰度
TIC: [BSB2]WH0071598-10.D\data.ms
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1390 (12.582 分): WH0071598-10.D\data.ms
196.1
225.1
167.1
115.1
141.1
54.0
70.6
93.0
282.0
Chemical Formula: C15H15NO
Exact Mass: 225.1154
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
60
80
100
120
140
160
180
200
220
240
260
280
m/z-->

丰度


TIC: [BSB2]WH0046407-1.D\data.ms
3800000
3600000
3400000
3200000
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

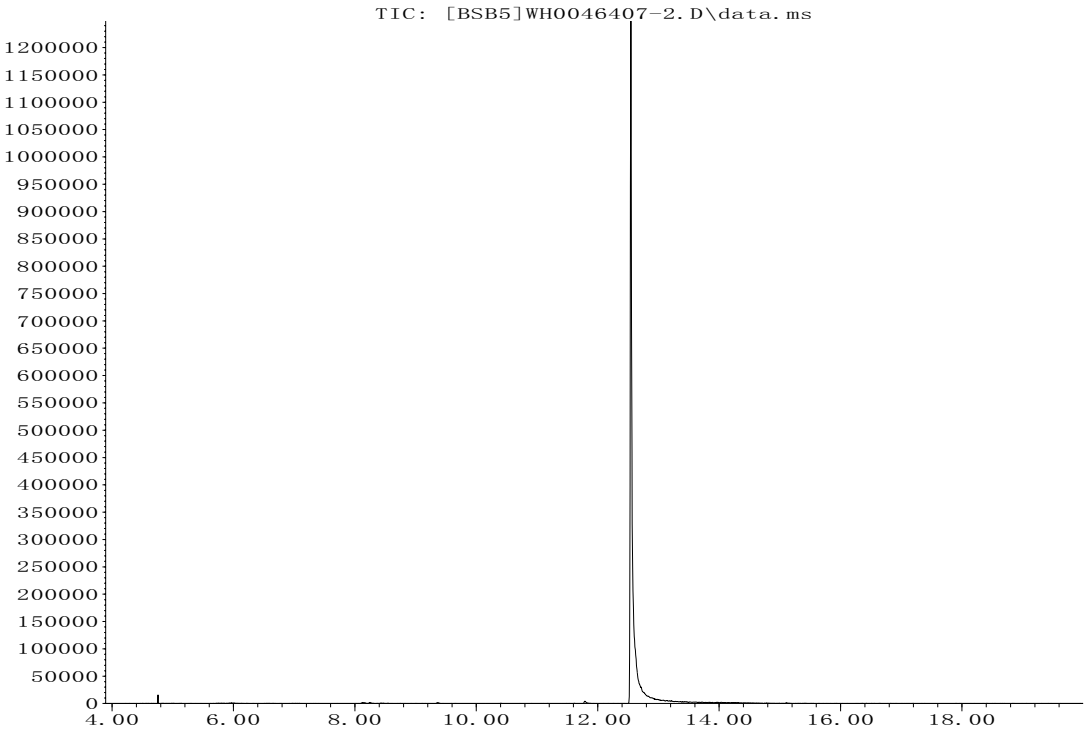
时间-->

丰度


扫描 1261 (11.775 分): WH0046407-1.D\data.ms
215.1
111.0
138.0
75.1
152.1
180.1
99.0
126.0
163.9
Cl
N
Chemical Formula: C13H10ClN
Exact Mass: 215.0502
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220

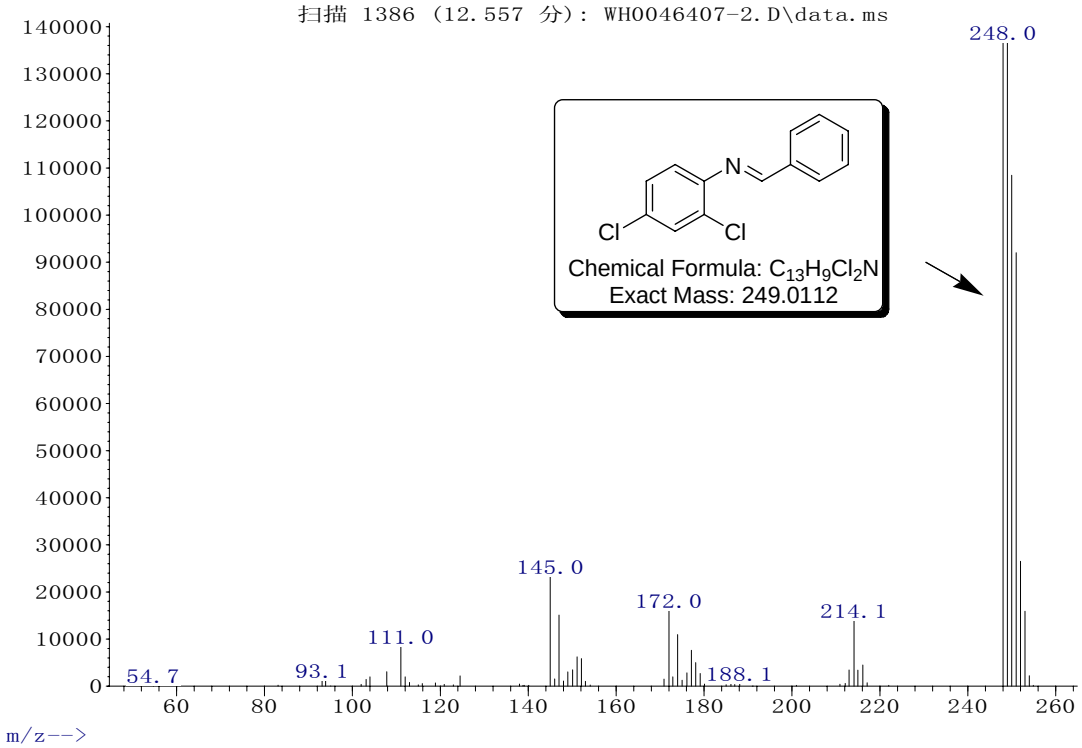
m/z-->

丰度

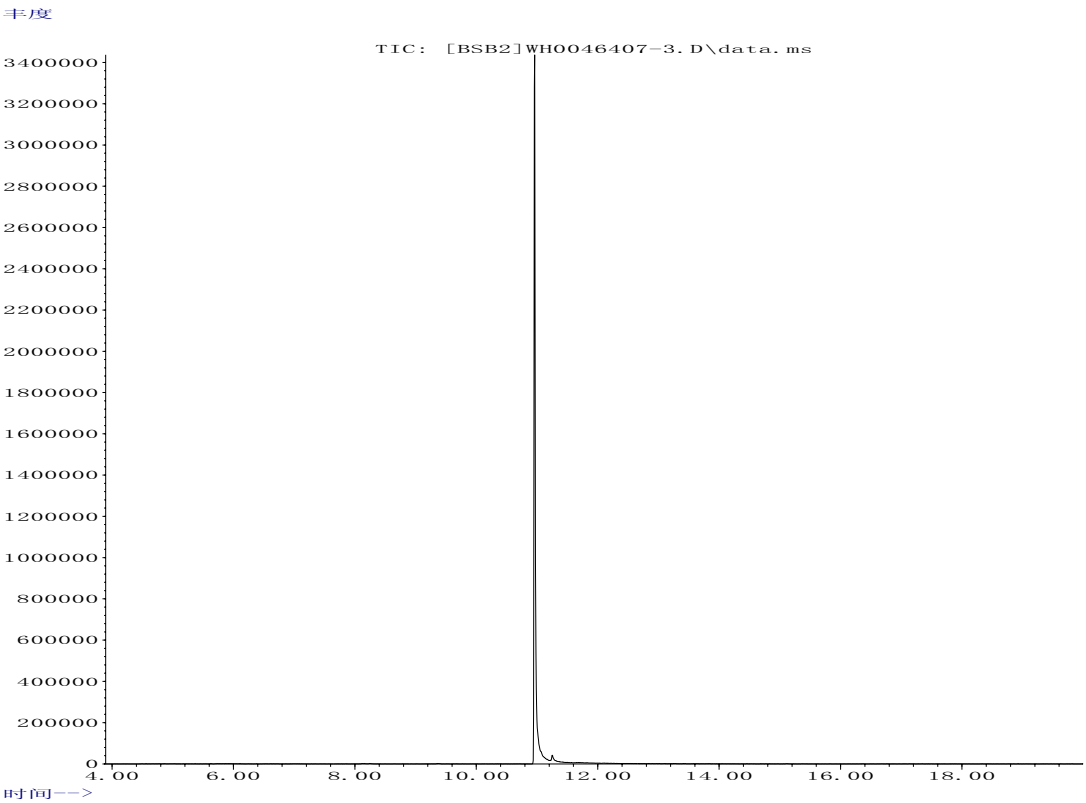

TIC: [BSB5]WH0046407-2.D\data.ms
1200000
1150000
1100000
1050000
1000000
950000
900000
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

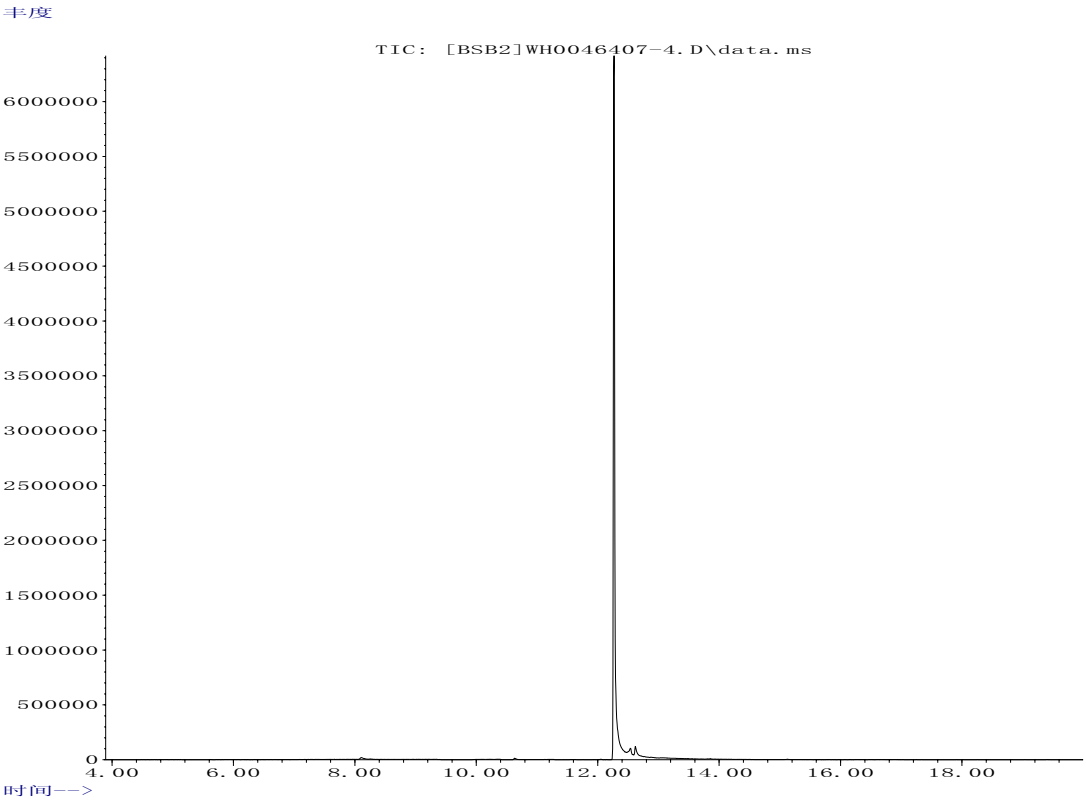
时间-->

丰度

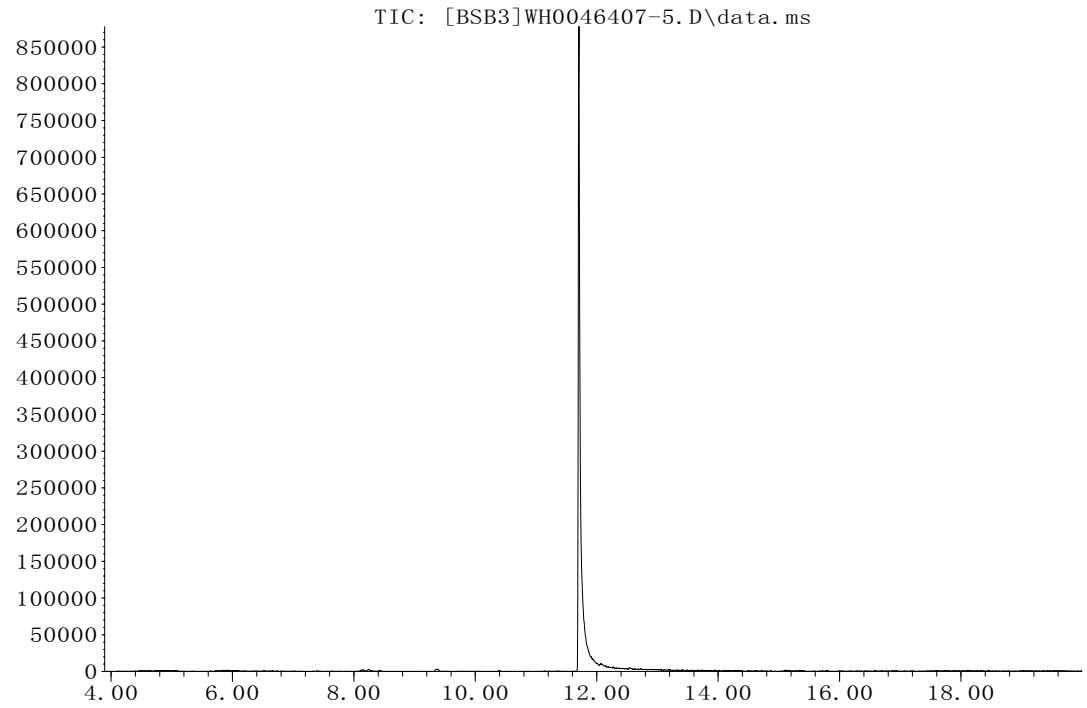

扫描 1386 (12.557 分): WH0046407-2.D\data.ms
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
248.0
145.0
172.0
214.1
111.0
54.7
93.1
188.1
60
80
100
120
140
160
180
200
220
240
260
N
Cl
Cl
Chemical Formula: C13H9Cl2N
Exact Mass: 249.0112

m/z-->


丰度
TIC: [BSB2]WH0046407-3.D\data.ms
3400000
3200000
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1134 (10.980 分): WH0046407-3.D\data.ms
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
195.1
118.1
96.6
83.6
71.4
128.1
139.1
152.1
167.1
178.1
N
Chemical Formula: C14H13N
Exact Mass: 195.1048
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
m/z-->

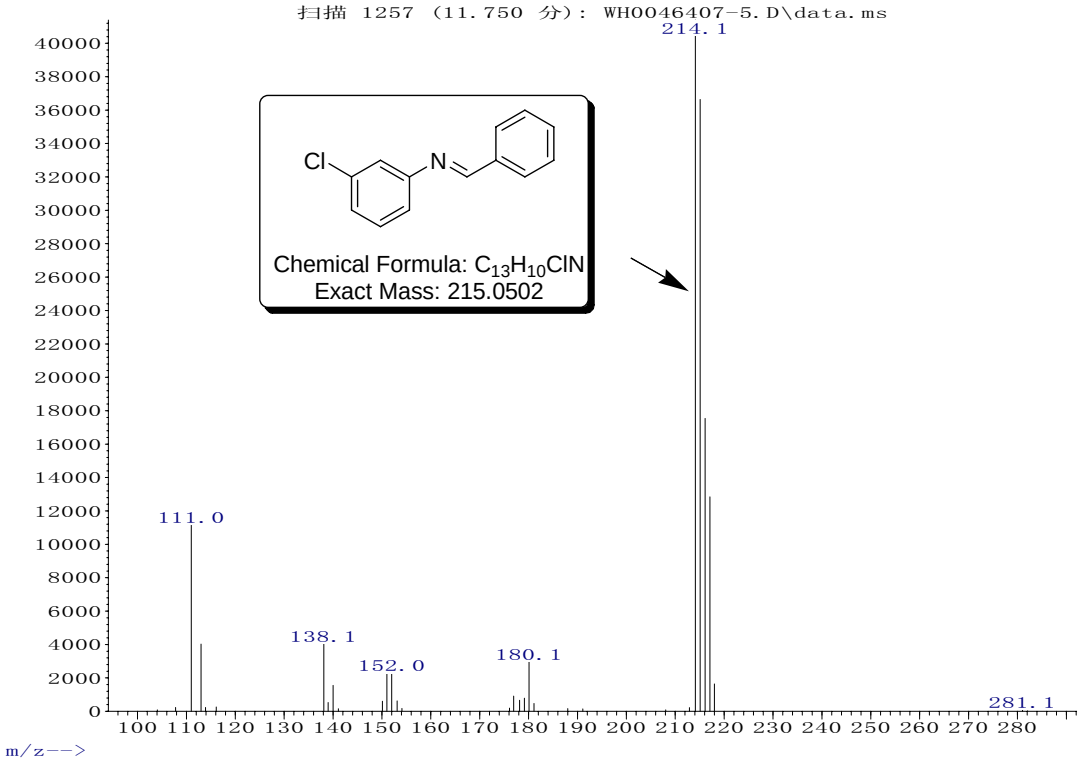

丰度
TIC: [BSB2]WH0046407-4.D\data.ms
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1341 (12.275 分): WH0046407-4.D\data.ms
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
259.0
155.0
76.1
180.1
104.1
127.1
207.1
232.0
80
100
120
140
160
180
200
220
240
260
m/z-->
Br
N
Chemical Formula: C13H10BrN
Exact Mass: 258.9997

丰度


TIC: [BSB3]WH0046407-5.D\data.ms
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

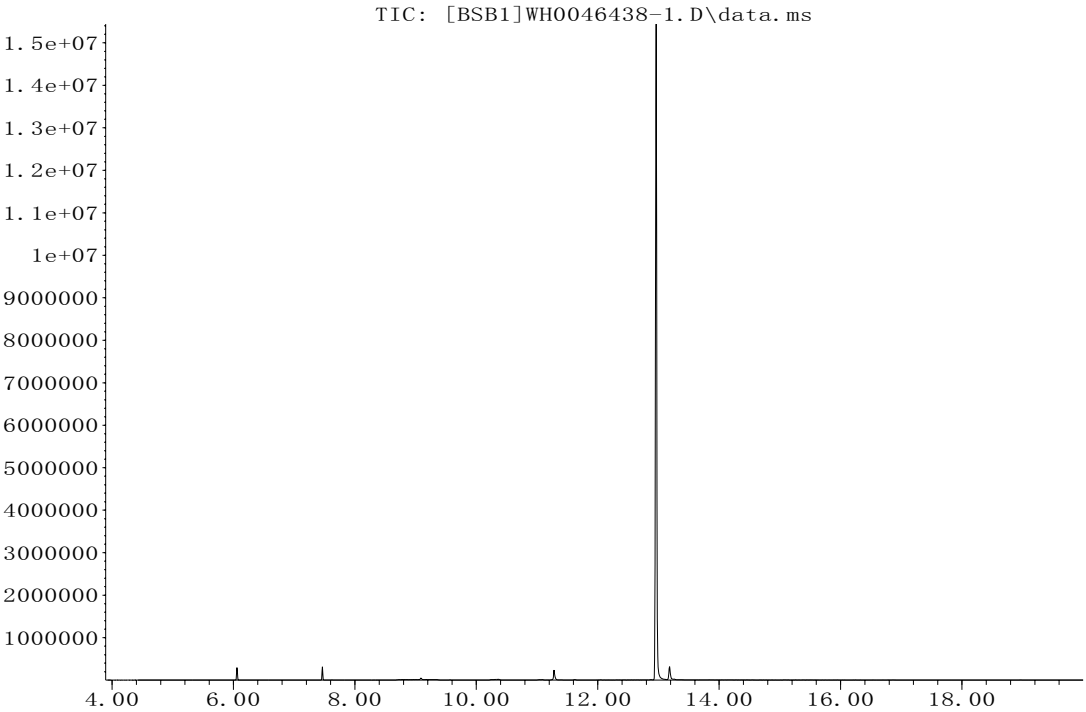
时间-->

丰度


扫描 1257 (11.750 分): WH0046407-5.D\data.ms
214.1
Cl
N
Chemical Formula: C13H10ClN
Exact Mass: 215.0502
111.0
138.1
152.0
180.1
281.1
40000
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280

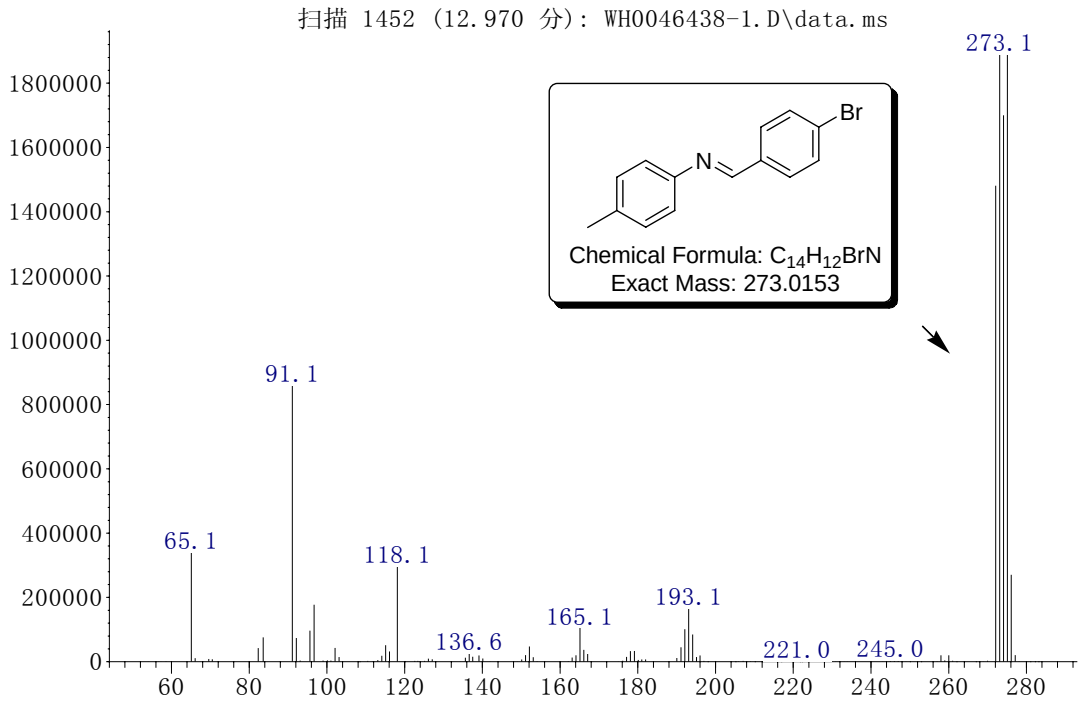
m/z-->

丰度


TIC: [BSB1]WH0046438-1.D\data.ms
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

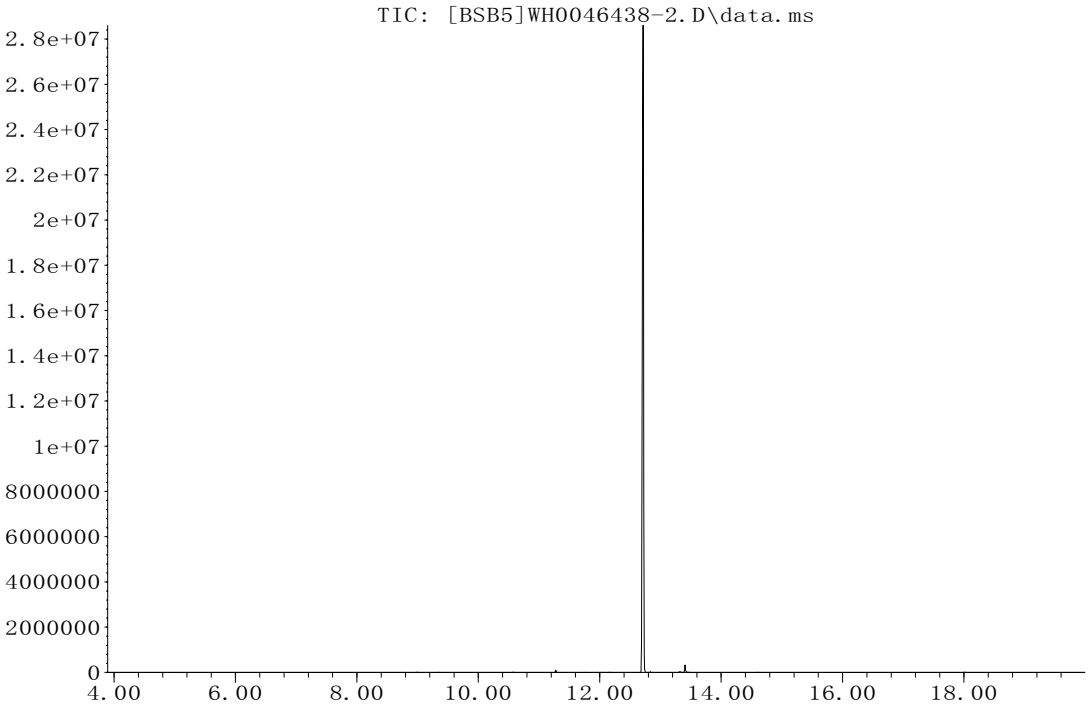
时间-->

丰度


扫描 1452 (12.970 分): WH0046438-1.D\data.ms
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
60
80
100
120
140
160
180
200
220
240
260
280
273.1
91.1
65.1
118.1
136.6
165.1
193.1
221.0
245.0
Br
N
Chemical Formula: C14H12BrN
Exact Mass: 273.0153

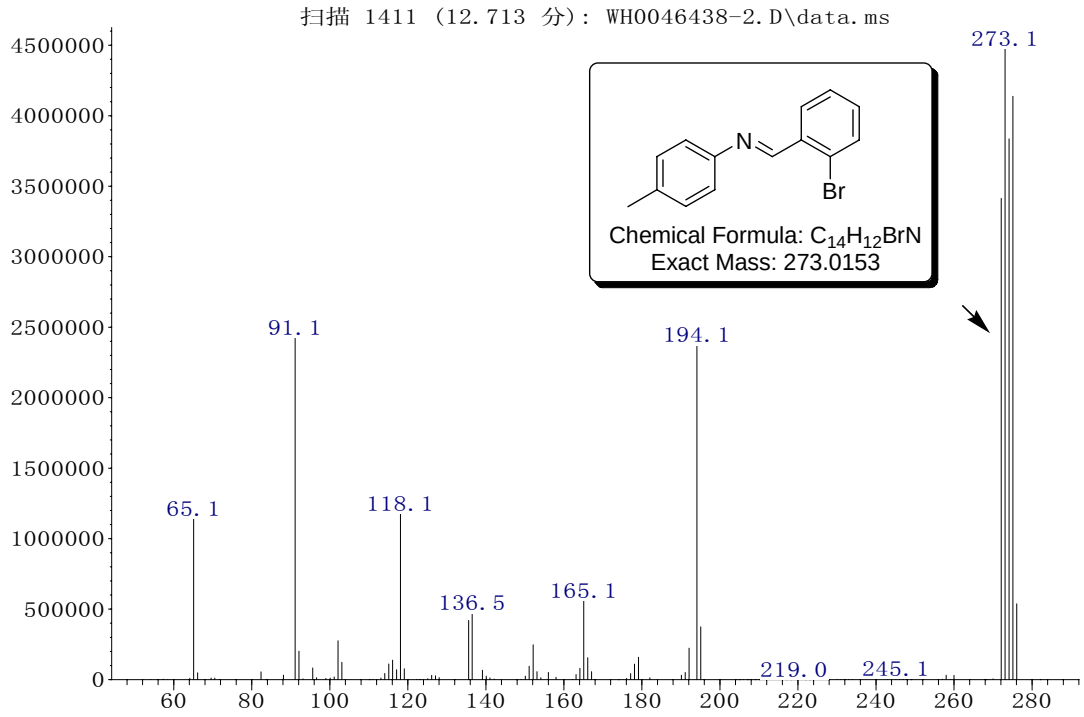
m/z-->

丰度


TIC: [BSB5]WH0046438-2.D\data.ms
2.8e+07
2.6e+07
2.4e+07
2.2e+07
2e+07
1.8e+07
1.6e+07
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

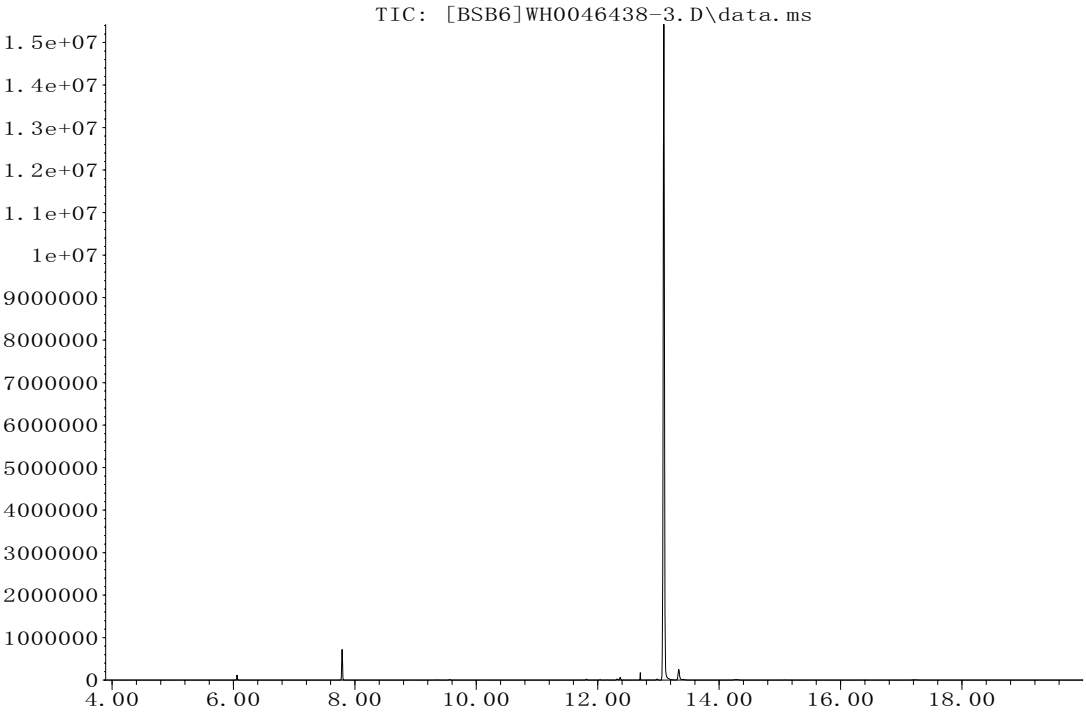
时间-->

丰度


扫描 1411 (12.713 分): WH0046438-2.D\data.ms
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
273.1
91.1
194.1
65.1
118.1
136.5
165.1
219.0
245.1
N
Br
Chemical Formula: C14H12BrN
Exact Mass: 273.0153
60
80
100
120
140
160
180
200
220
240
260
280

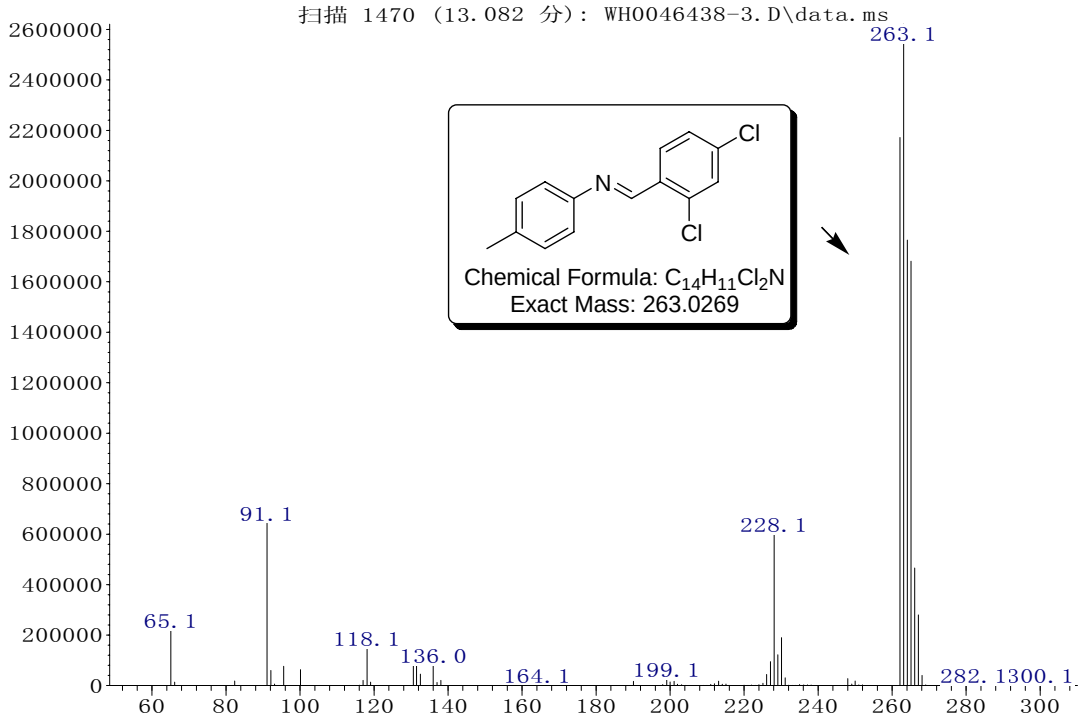
m/z-->

丰度

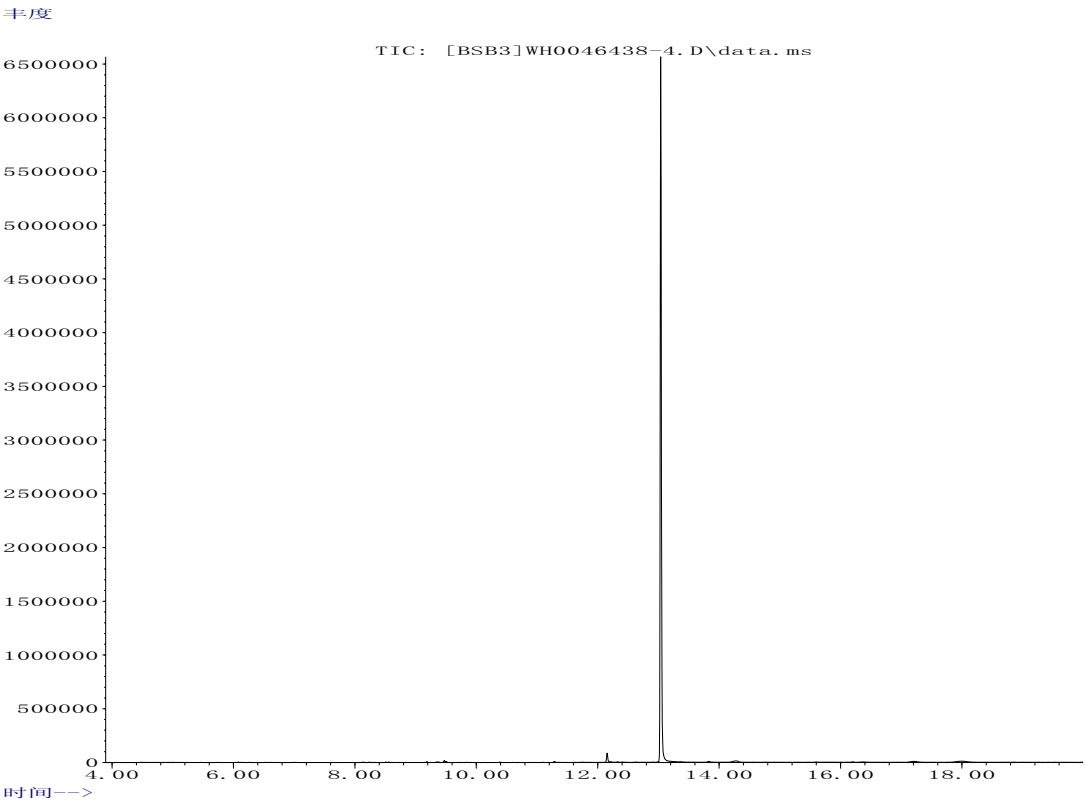

TIC: [BSB6]WH0046438-3.D\data.ms
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

时间-->

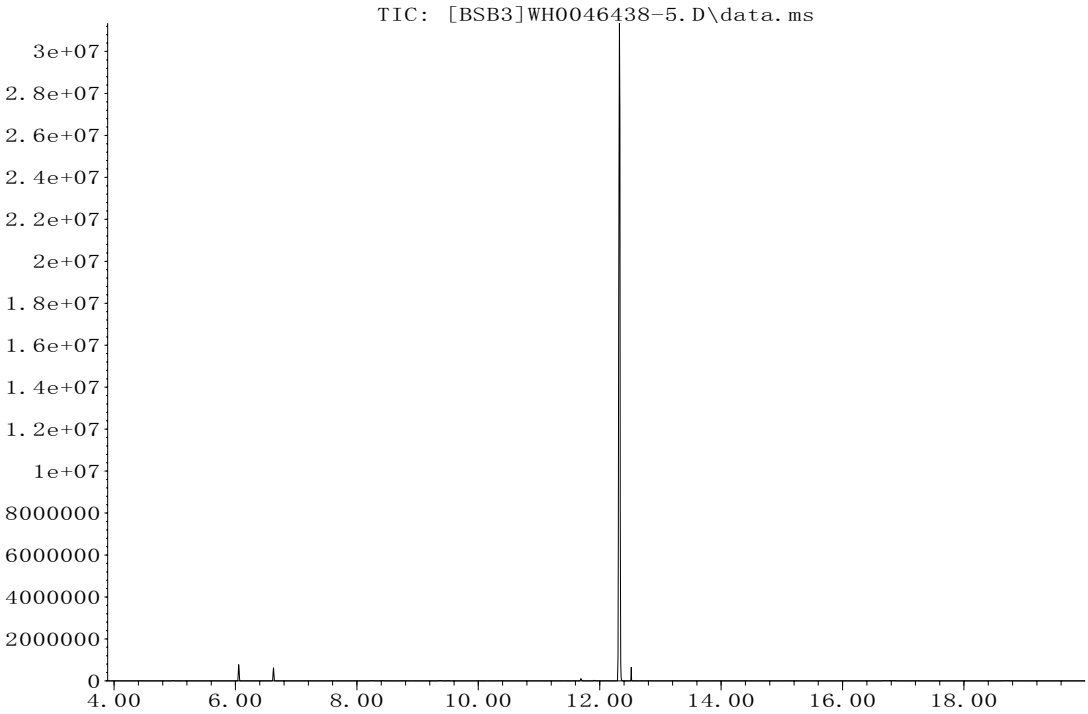
丰度


扫描 1470 (13.082 分): WH0046438-3.D\data.ms
263.1
228.1
91.1
65.1
118.1
136.0
164.1
199.1
282.1
300.1
Cl
N
Cl
Chemical Formula: C14H11Cl2N
Exact Mass: 263.0269
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
60
80
100
120
140
160
180
200
220
240
260
280
300

m/z-->

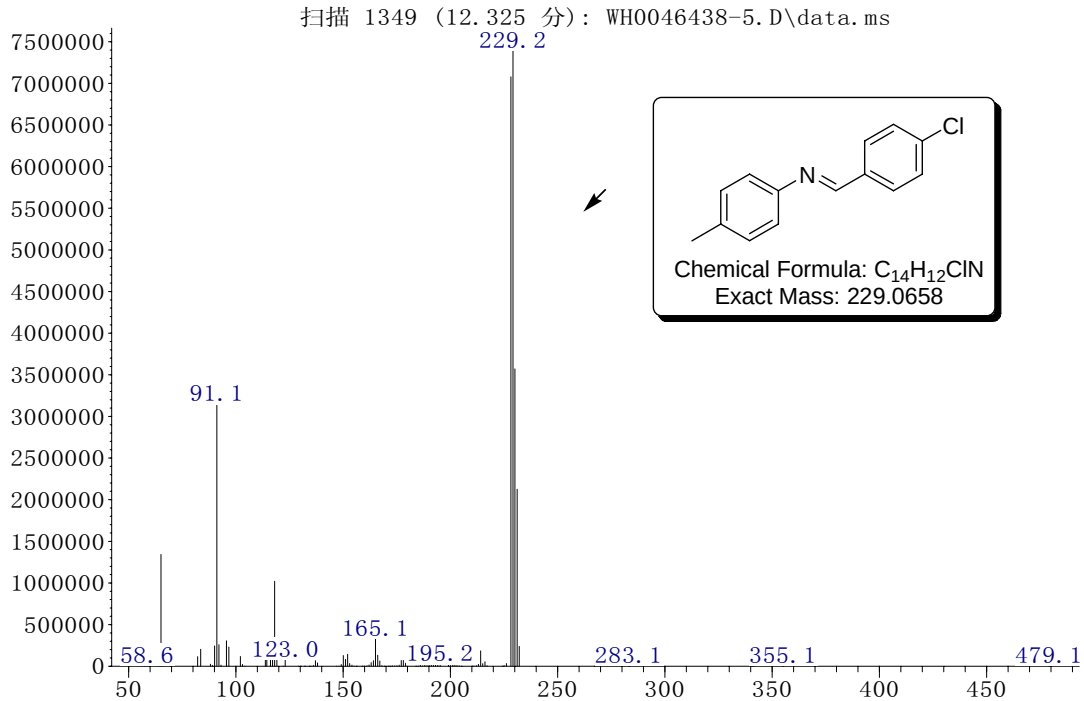

丰度
TIC: [BSB3]WH0046438-4.D\data.ms
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1464 (13.045 分): WH0046438-4.D\data.ms
263.1
800000
700000
600000
500000
400000
300000
200000
100000
0
91.1
118.1
228.1
65.1
138.0
165.1
191.1
283.1
309.0
Cl
N
Cl
Chemical Formula: C14H11Cl2N
Exact Mass: 263.0269
60
80
100
120
140
160
180
200
220
240
260
280
300
m/z-->

丰度

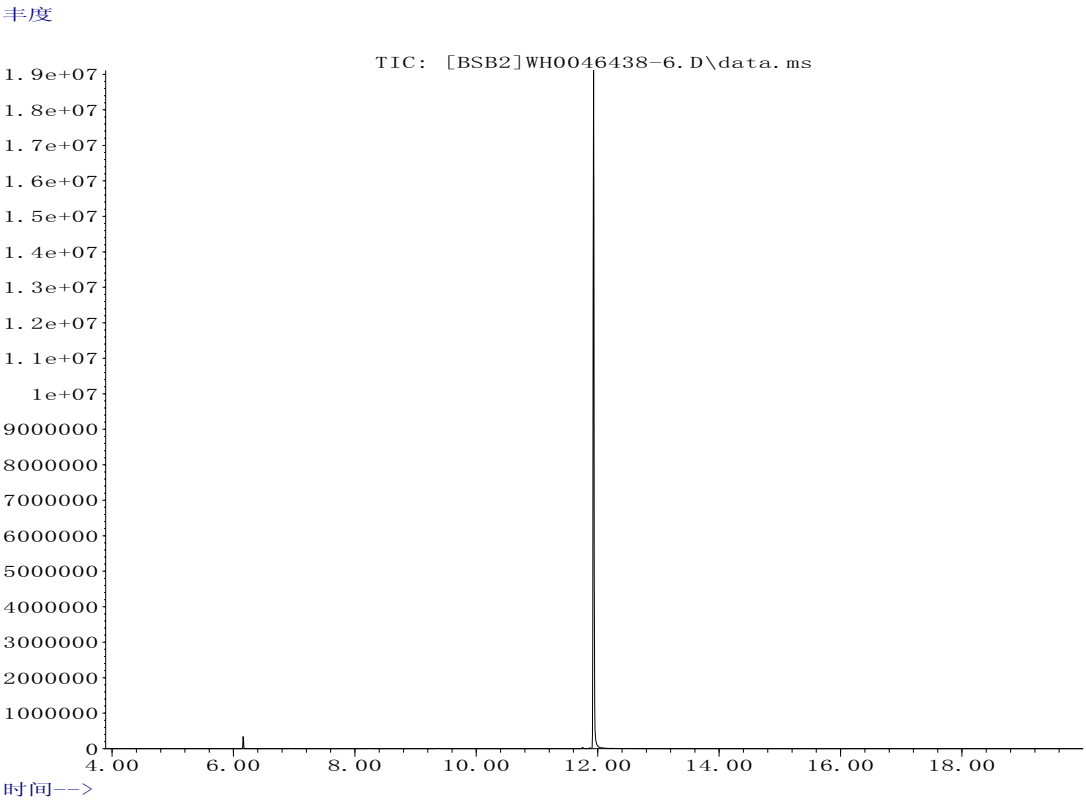

TIC: [BSB3]WH0046438-5.D\data.ms
3e+07
2.8e+07
2.6e+07
2.4e+07
2.2e+07
2e+07
1.8e+07
1.6e+07
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

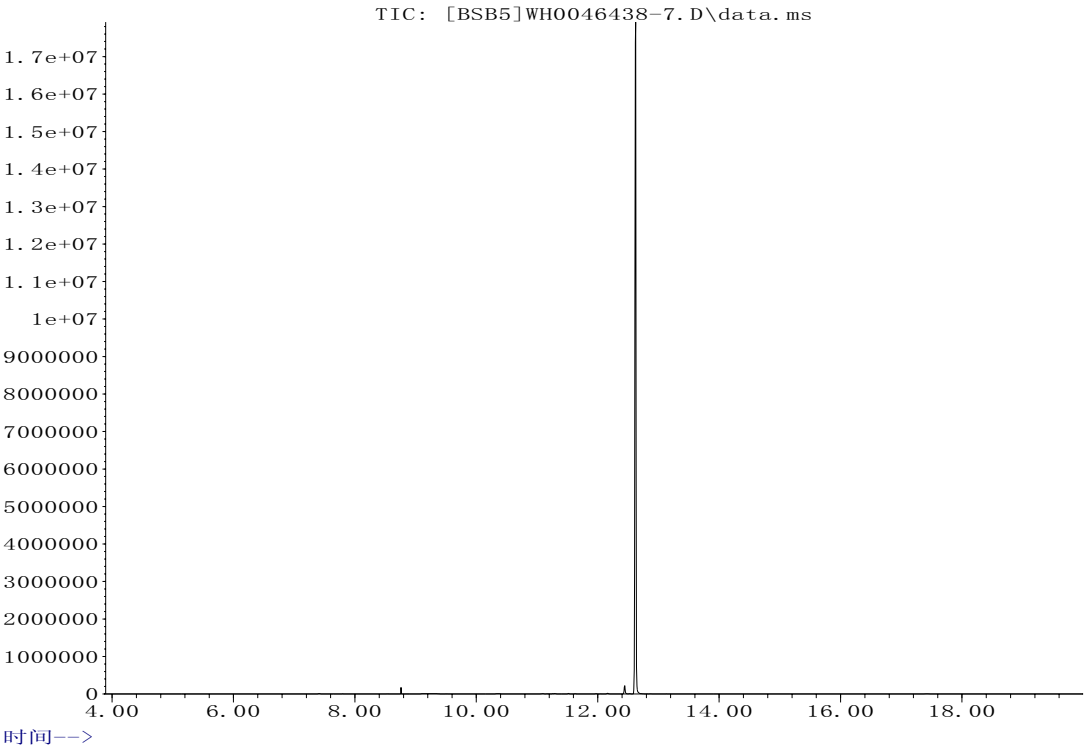
时间-->

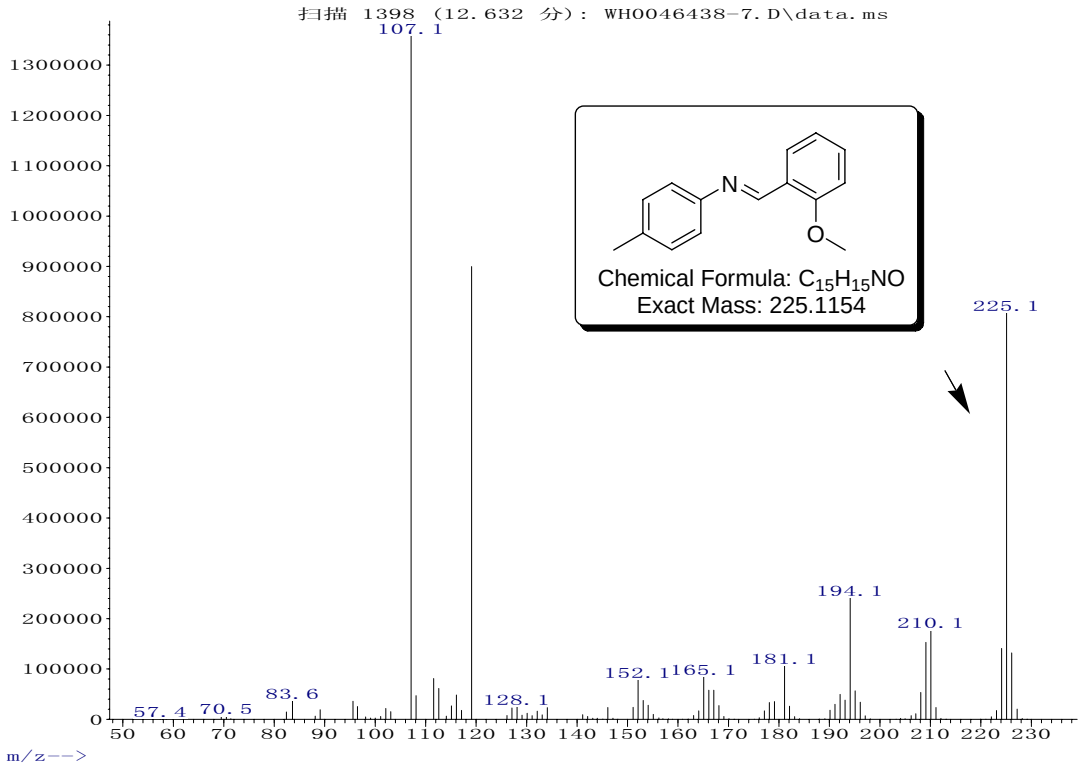
丰度


扫描 1349 (12.325 分): WH0046438-5.D\data.ms
229.2
91.1
58.6
123.0
165.1
195.2
283.1
355.1
479.1
Cl
N
Chemical Formula: C14H12ClN
Exact Mass: 229.0658
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
50
100
150
200
250
300
350
400
450

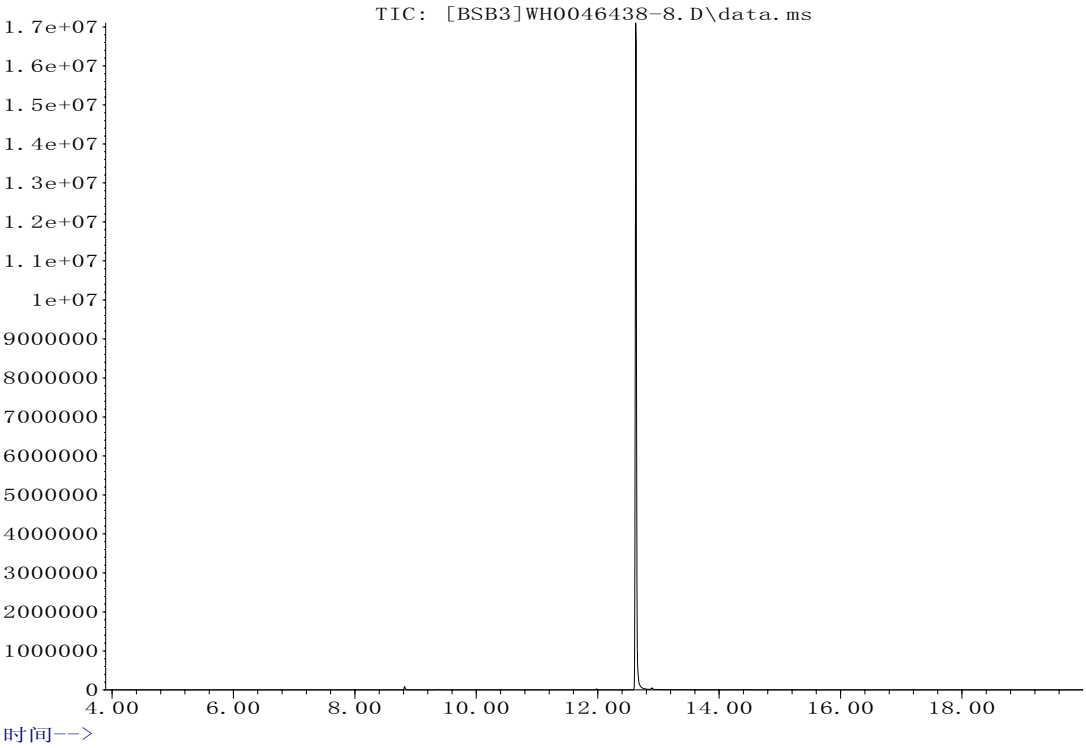
m/z-->

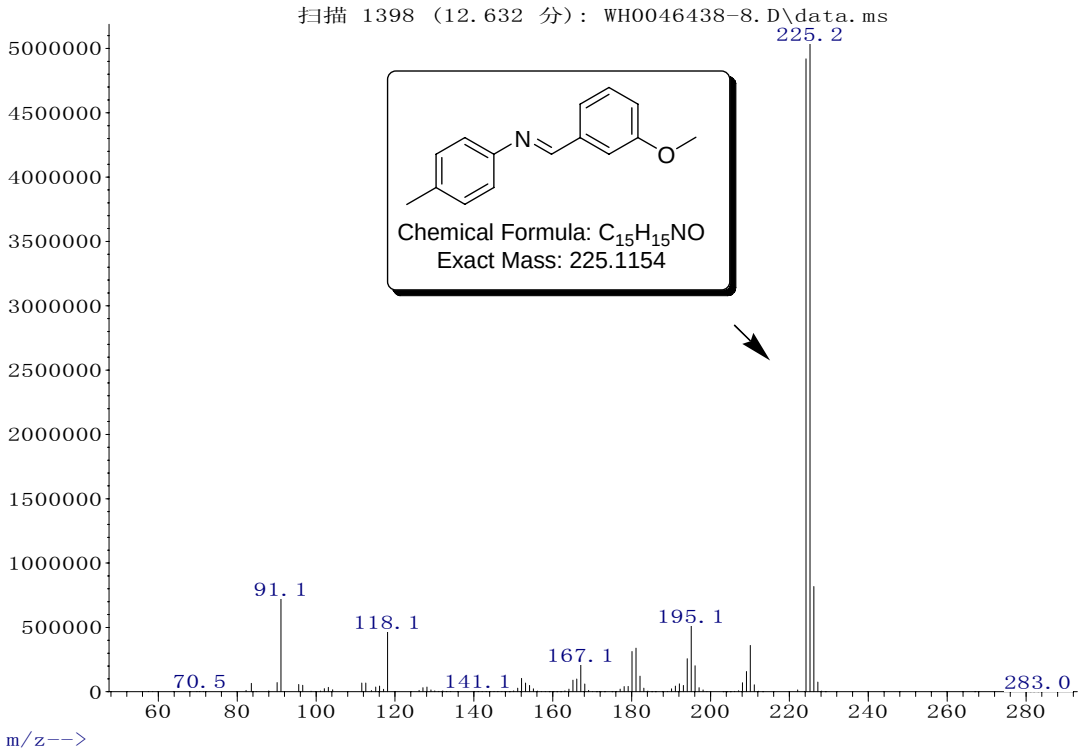

丰度
TIC: [BSB2]WH0046438-6.D\data.ms
1.9e+07
1.8e+07
1.7e+07
1.6e+07
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1286 (11.931 分): WH0046438-6.D\data.ms
208.2
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
65.1
90.1
118.1
139.1
165.1
191.1
239.3
283.1
60
80
100
120
140
160
180
200
220
240
260
280
m/z-->
Chemical Formula: C15H15N
Exact Mass: 209.1204


丰度
TIC: [BSB5]WH0046438-7.D\data.ms
1.7e+07
1.6e+07
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->

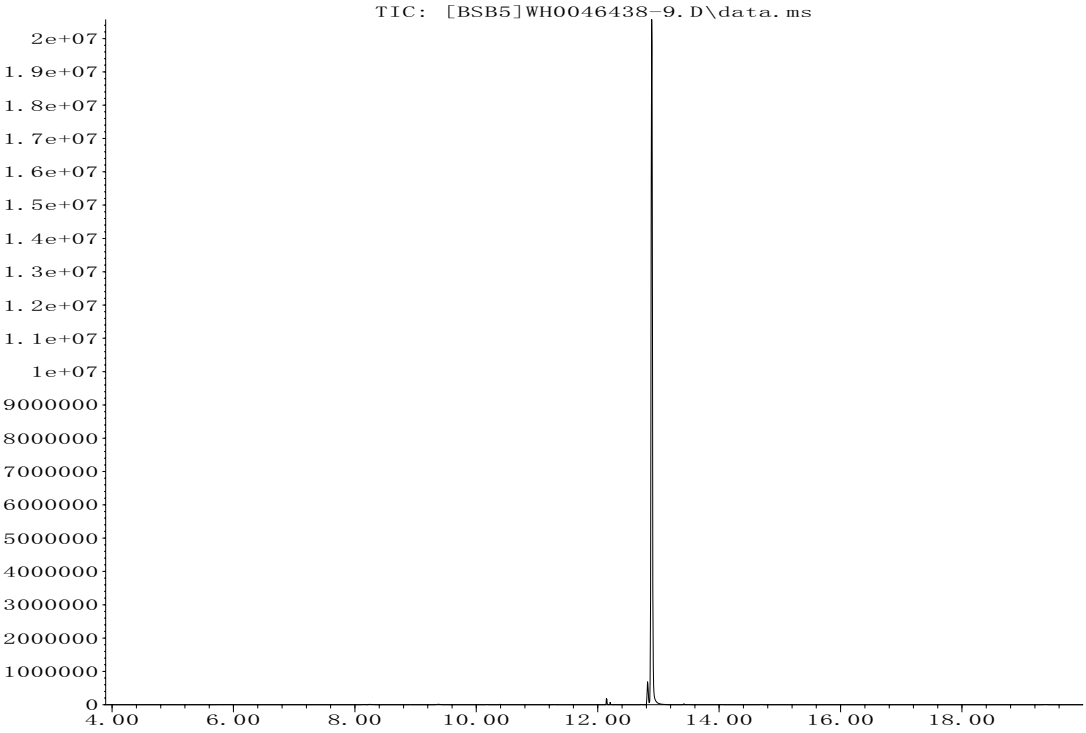

丰度
扫描 1398 (12.632 分): WH0046438-7.D\data.ms
107.1
225.1
194.1
210.1
181.1
152.1
165.1
128.1
83.6
57.4
70.5
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
m/z-->

N
O
Chemical Formula: C15H15NO
Exact Mass: 225.1154


丰度
TIC: [BSB3]WH0046438-8.D\data.ms
1.7e+07
1.6e+07
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->

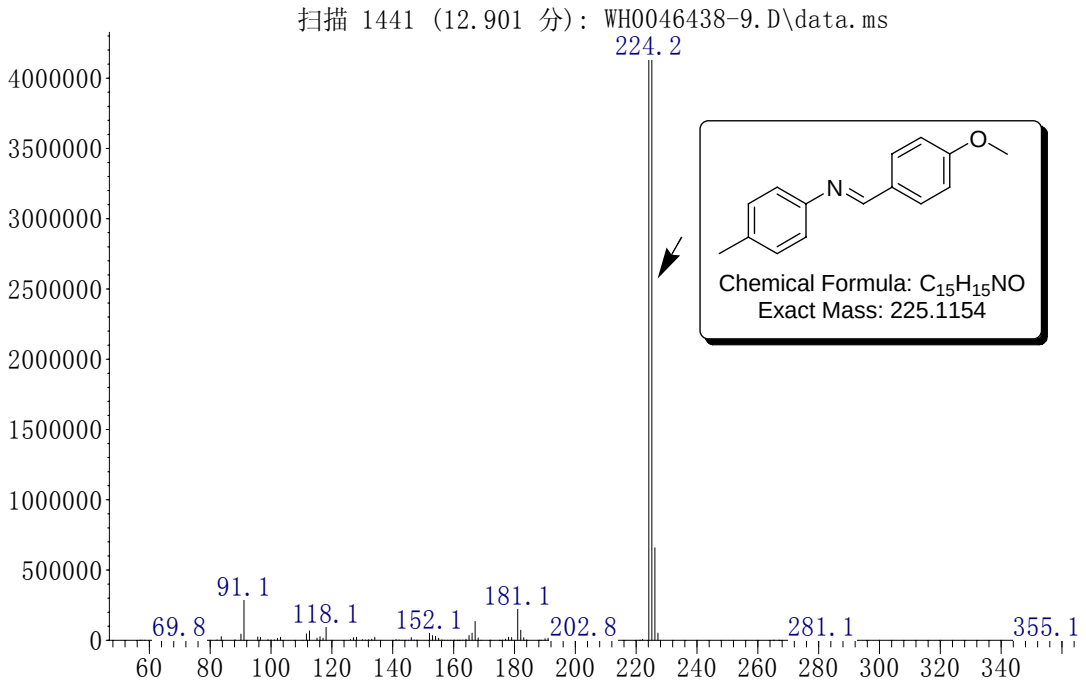

丰度
扫描 1398 (12.632 分): WH0046438-8.D\data.ms
225.2
N
O
Chemical Formula: C15H15NO
Exact Mass: 225.1154
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
91.1
118.1
195.1
167.1
70.5
141.1
283.0
60
80
100
120
140
160
180
200
220
240
260
280
m/z-->

丰度

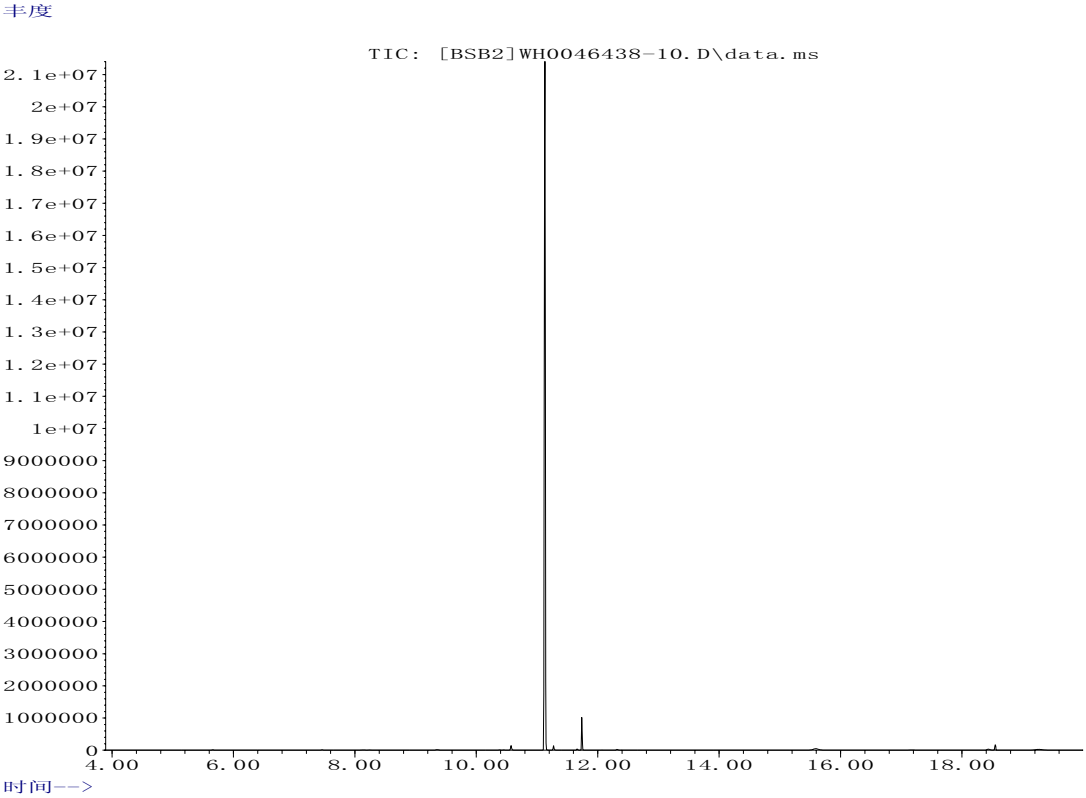

TIC: [BSB5]WH0046438-9.D\data.ms
2e+07
1.9e+07
1.8e+07
1.7e+07
1.6e+07
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

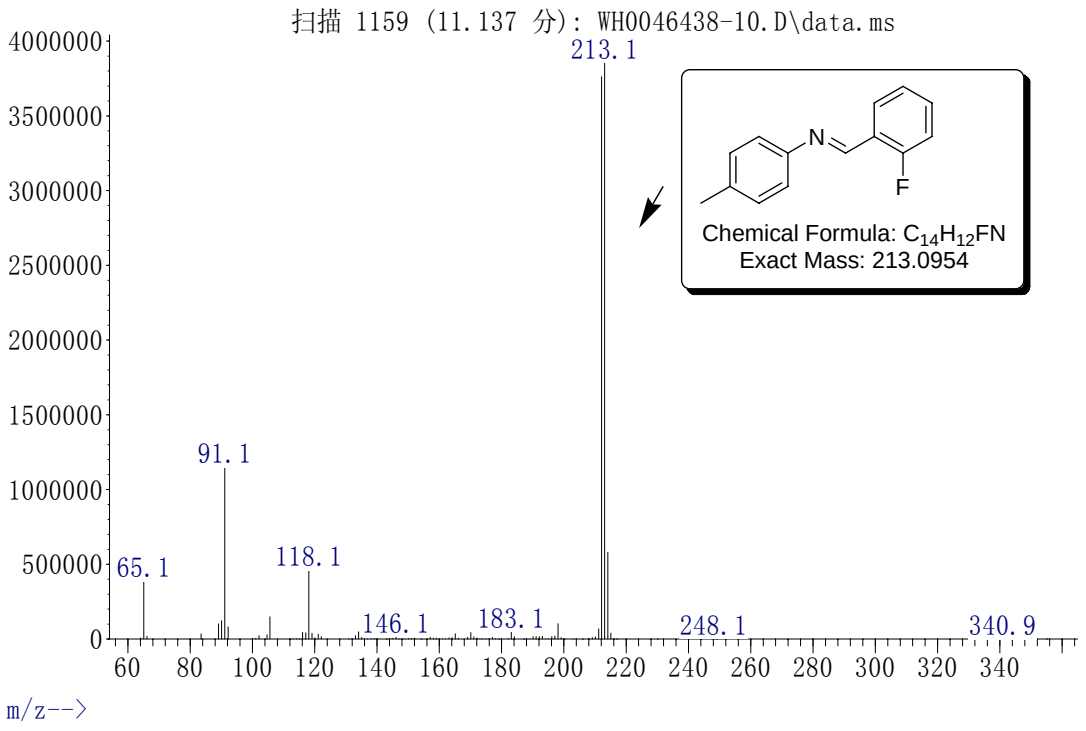
时间-->

丰度

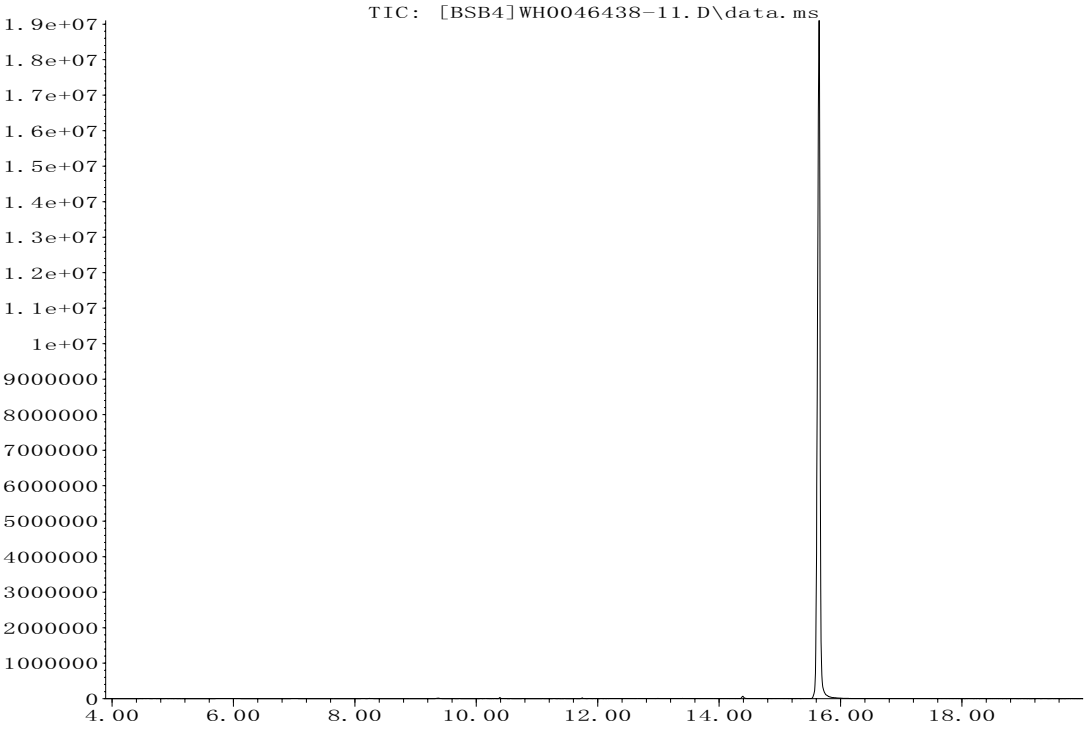

扫描 1441 (12.901 分): WH0046438-9.D\data.ms
224.2
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
91.1
69.8
118.1
152.1
181.1
202.8
281.1
355.1
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
O
N
Chemical Formula: C15H15NO
Exact Mass: 225.1154

m/z-->


丰度
TIC: [BSB2]WH0046438-10.D\data.ms
2.1e+07
2e+07
1.9e+07
1.8e+07
1.7e+07
1.6e+07
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->

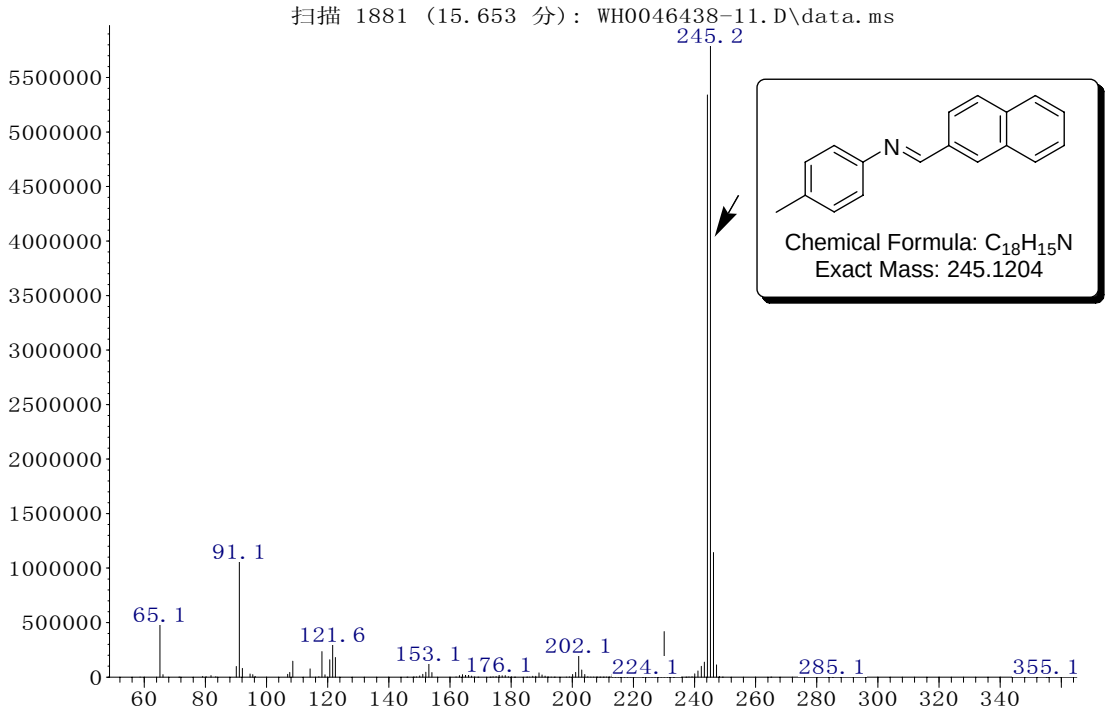

丰度
扫描 1159 (11.137 分): WH0046438-10.D\data.ms
213.1
91.1
65.1
118.1
146.1
183.1
248.1
340.9
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
m/z-->
N
F
Chemical Formula: C14H12FN
Exact Mass: 213.0954

丰度


TIC: [BSB4]WH0046438-11.D\data.ms
1.9e+07
1.8e+07
1.7e+07
1.6e+07
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

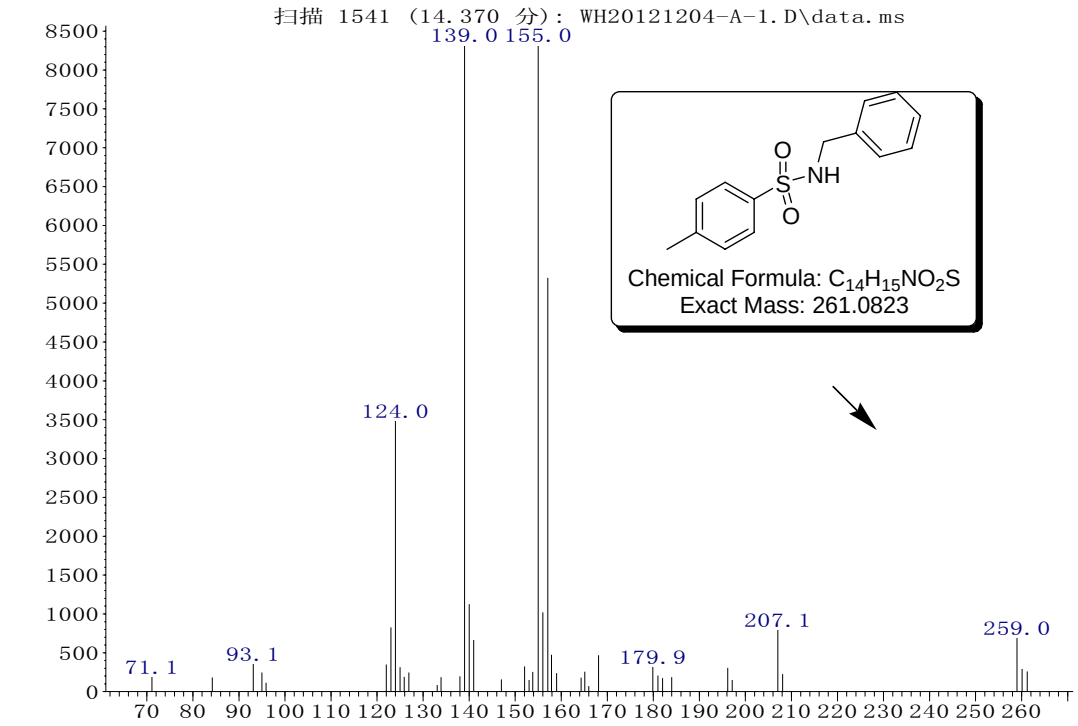
时间-->

丰度

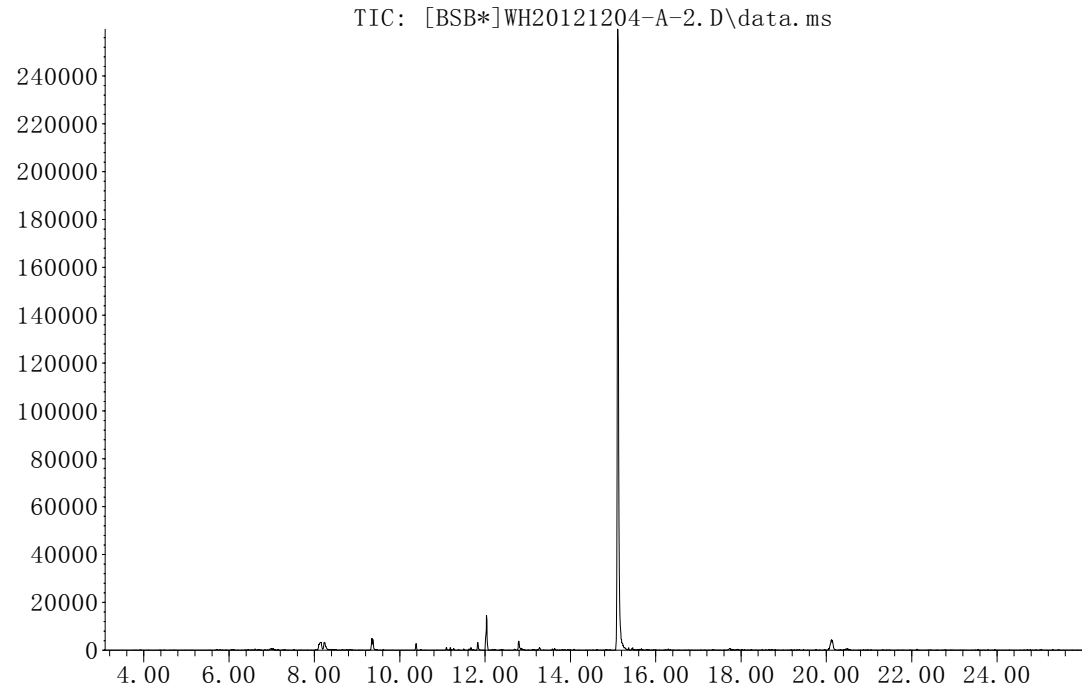

扫描 1881 (15.653 分): WH0046438-11.D\data.ms
245.2
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
91.1
65.1
121.6
153.1
176.1
202.1
224.1
285.1
355.1
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
N
Chemical Formula: C18H15N
Exact Mass: 245.1204

m/z-->

丰度

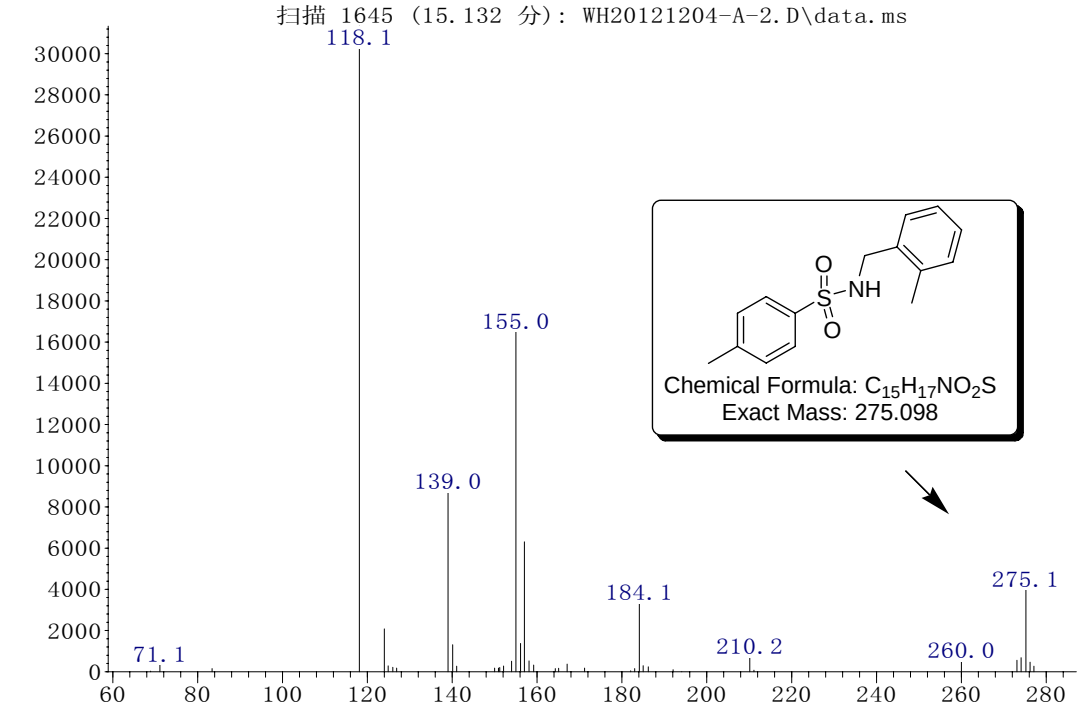

扫描 1541 (14.370 分): WH20121204-A-1.D\data.ms
139.0 155.0
124.0
207.1
259.0
71.1
93.1
179.9
Chemical Formula: C14H15NO2S
Exact Mass: 261.0823
m/z-->
丰度
扫描 1541 (14.370 分): WH20121204-A-1.D\data.ms
139.0 155.0
124.0
207.1
259.0
71.1
93.1
179.9
Chemical Formula: C14H15NO2S
Exact Mass: 261.0823
m/z-->

丰度


TIC: [BSB*]WH20121204-A-2.D\data.ms
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00

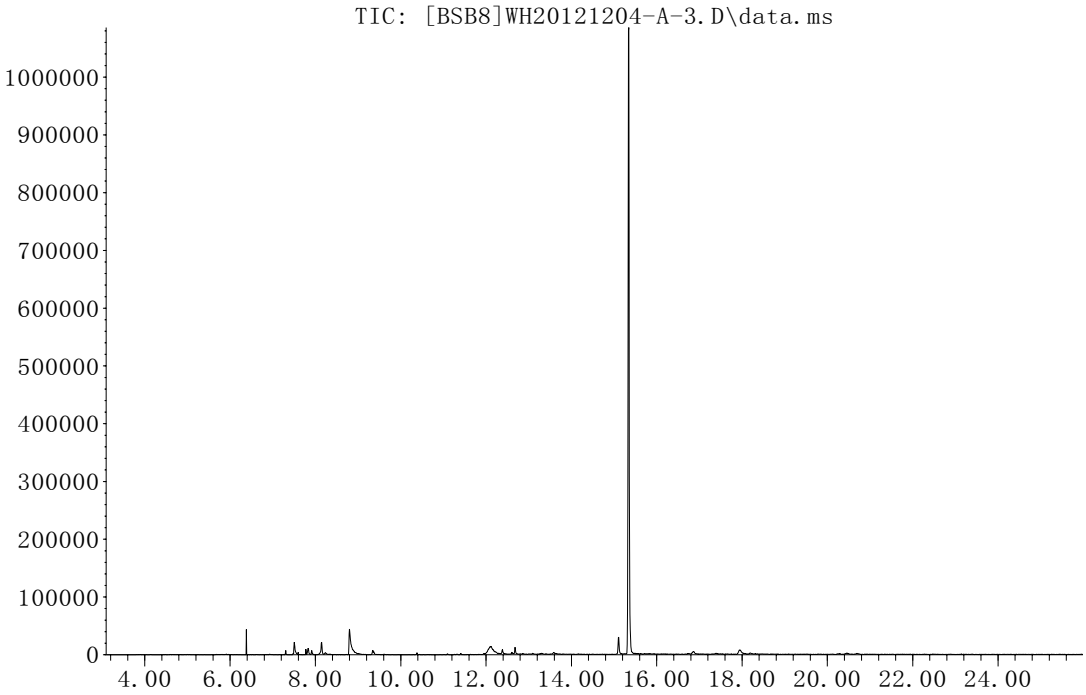
时间-->

丰度


扫描 1645 (15.132 分): WH20121204-A-2.D\data.ms
118.1
155.0
139.0
184.1
210.2
260.0
275.1
71.1
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
60
80
100
120
140
160
180
200
220
240
260
280
O
NH
S
O
Chemical Formula: C15H17NO2S
Exact Mass: 275.098

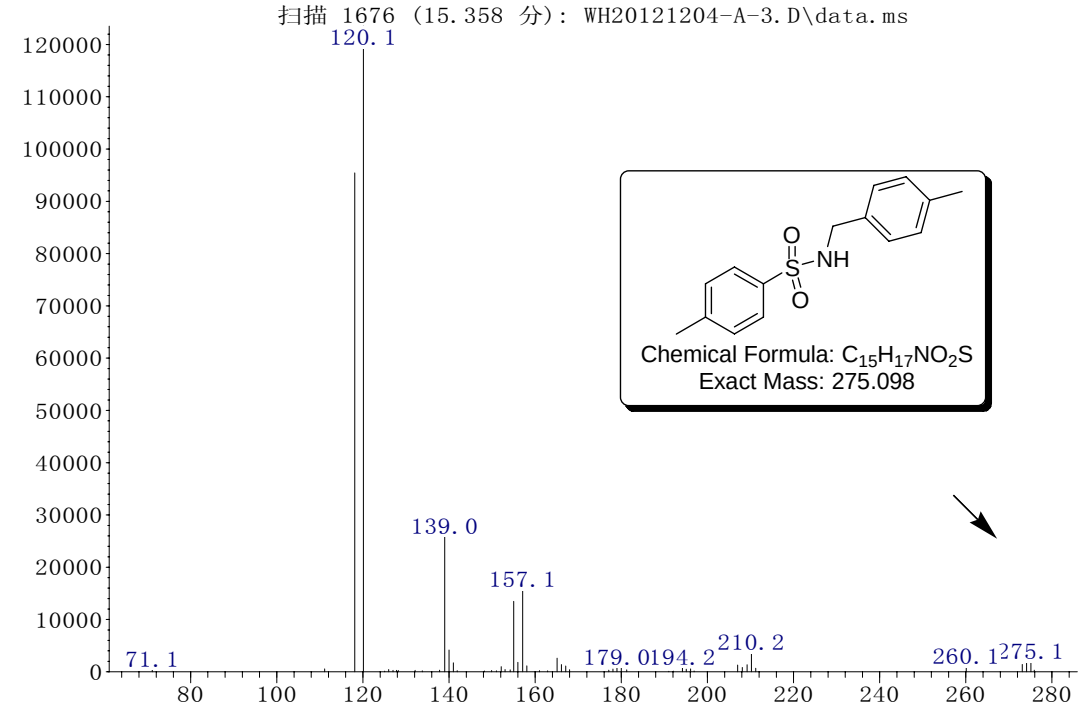
m/z-->

丰度


TIC: [BSB8]WH20121204-A-3.D\data.ms
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00

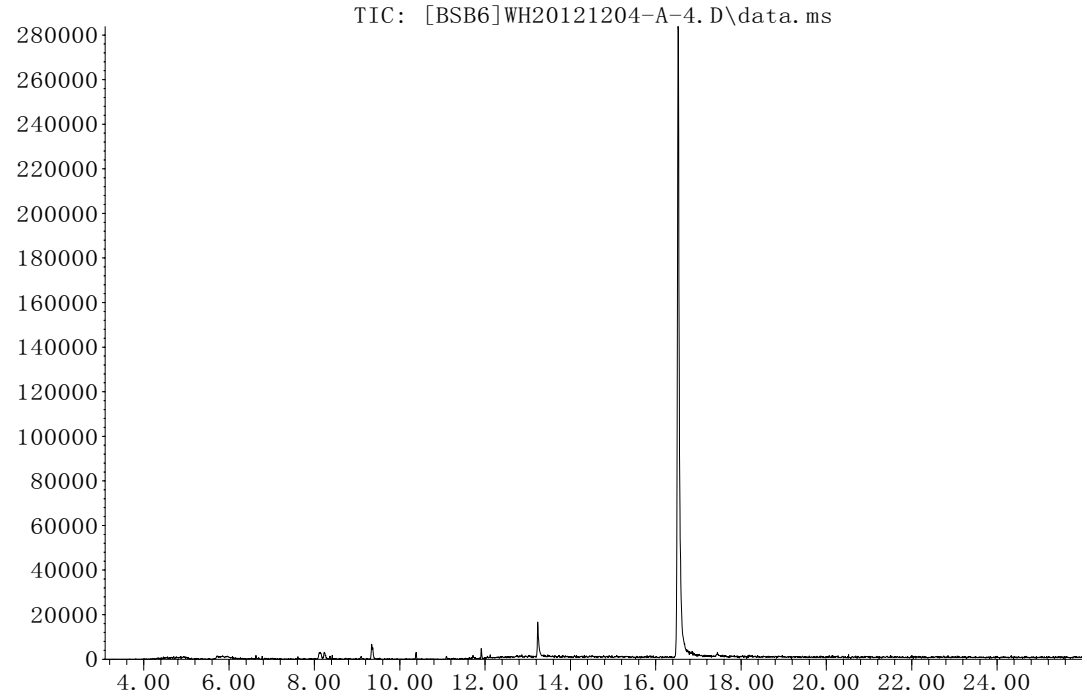
时间-->

丰度


扫描 1676 (15.358 分): WH20121204-A-3.D\data.ms
120.1
139.0
157.1
71.1
179.0
194.2
210.2
260.1
275.1
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
80
100
120
140
160
180
200
220
240
260
280
O
S
NH
O
Chemical Formula: C15H17NO2S
Exact Mass: 275.098

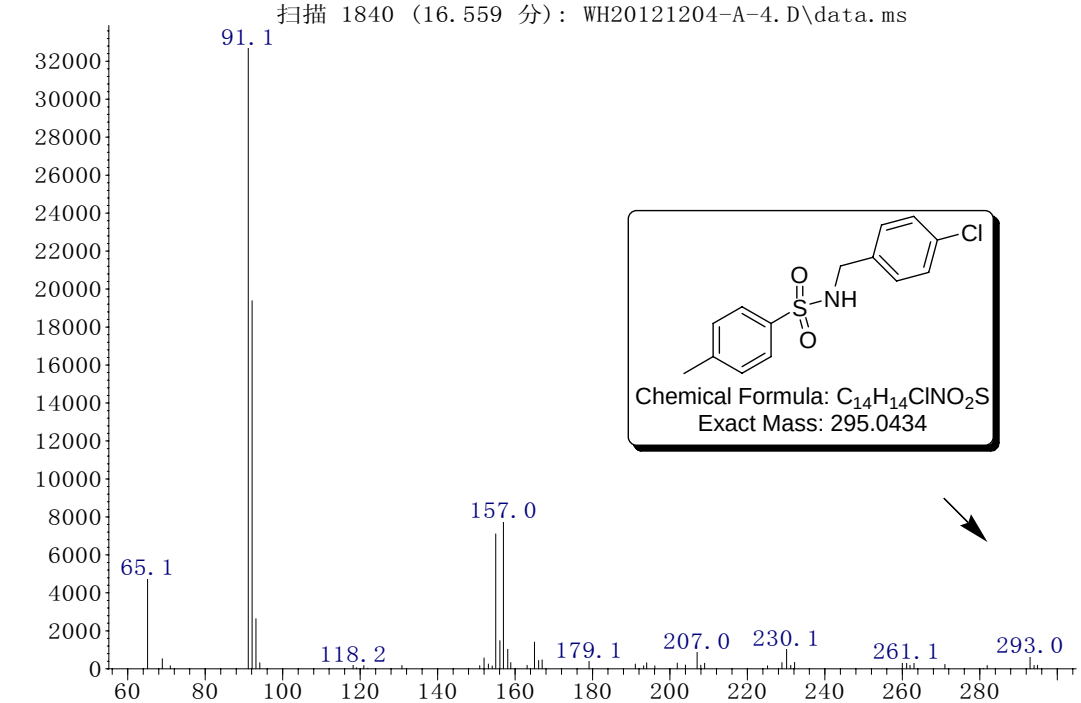
m/z-->

丰度


TIC: [BSB6]WH20121204-A-4.D\data.ms
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00

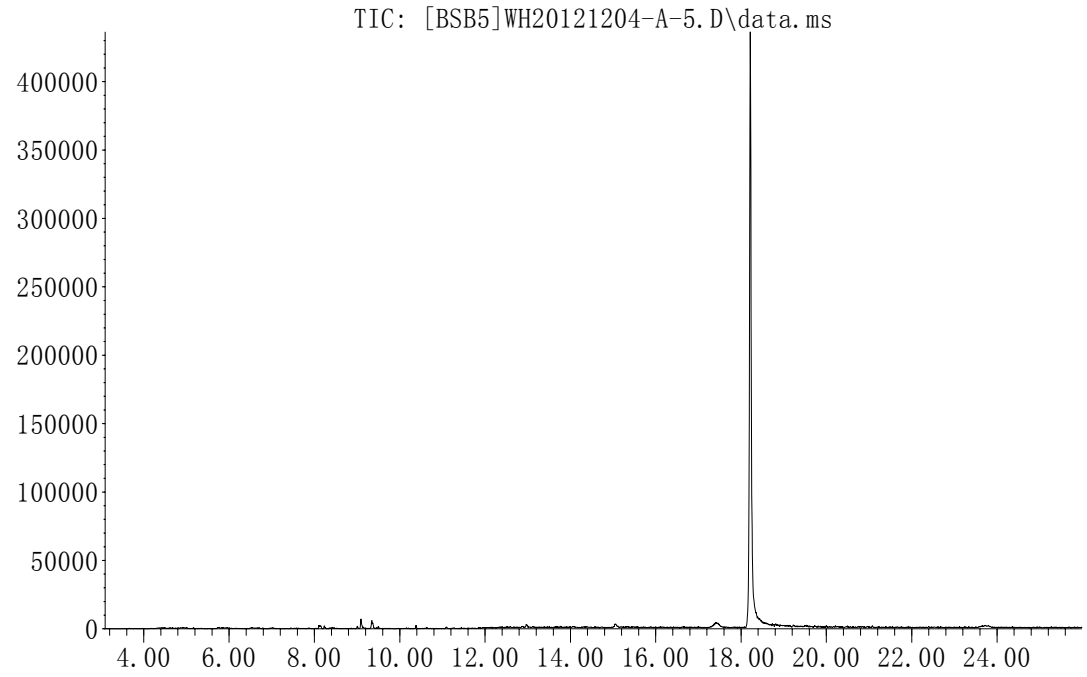
时间-->

丰度


扫描 1840 (16.559 分): WH20121204-A-4.D\data.ms
91.1
157.0
65.1
118.2
179.1
207.0
230.1
261.1
293.0
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
60
80
100
120
140
160
180
200
220
240
260
280
Cl
O
NH
S
O
Chemical Formula: C14H14ClNO2S
Exact Mass: 295.0434

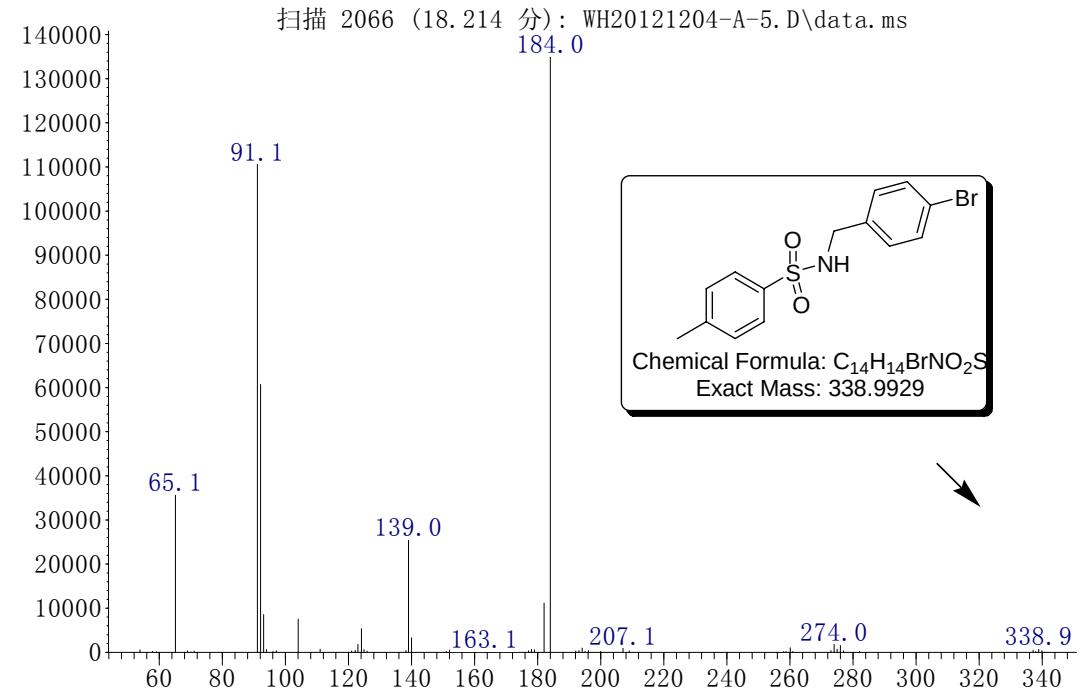
m/z-->

丰度


TIC: [BSB5]WH20121204-A-5.D\data.ms
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00

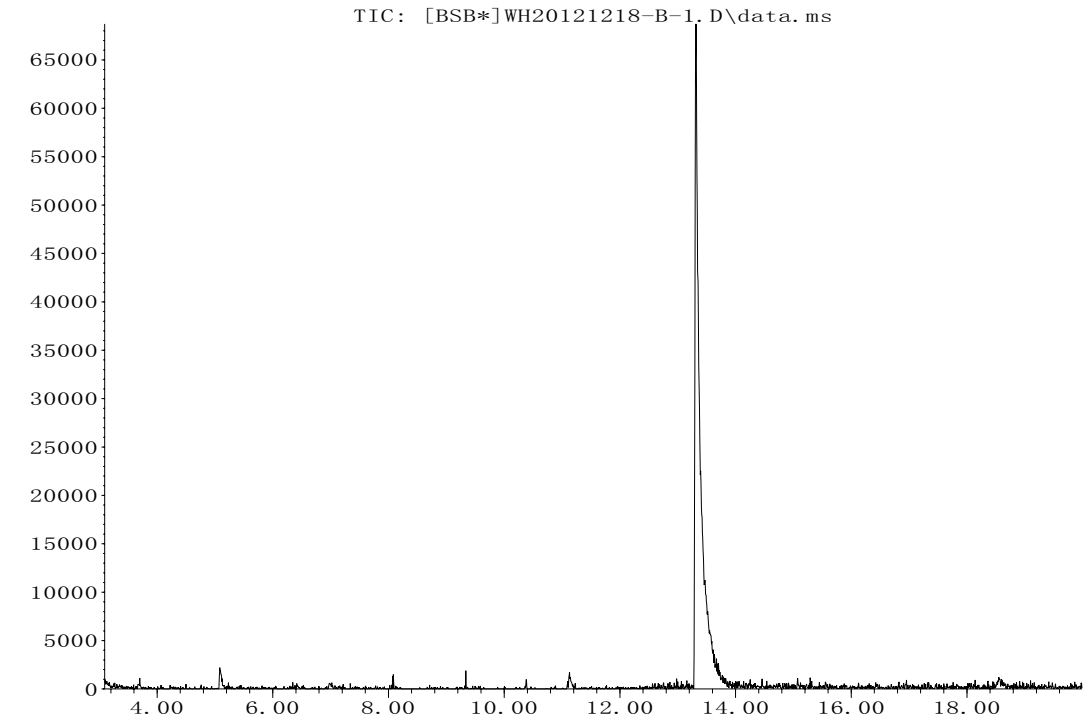
时间-->

丰度


扫描 2066 (18.214 分): WH20121204-A-5.D\data.ms
184.0
91.1
65.1
139.0
163.1
207.1
274.0
338.9
Br
O
NH
S
O
Chemical Formula: C14H14BrNO2S
Exact Mass: 338.9929
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340

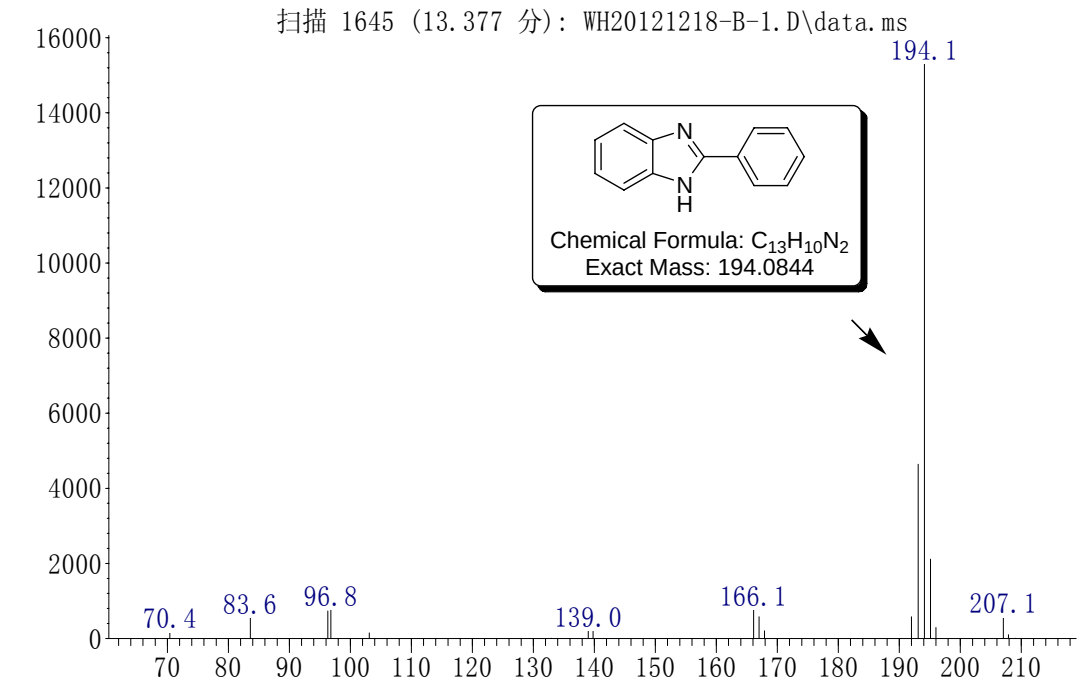
m/z-->

丰度


TIC: [BSB*]WH20121218-B-1.D\data.ms
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

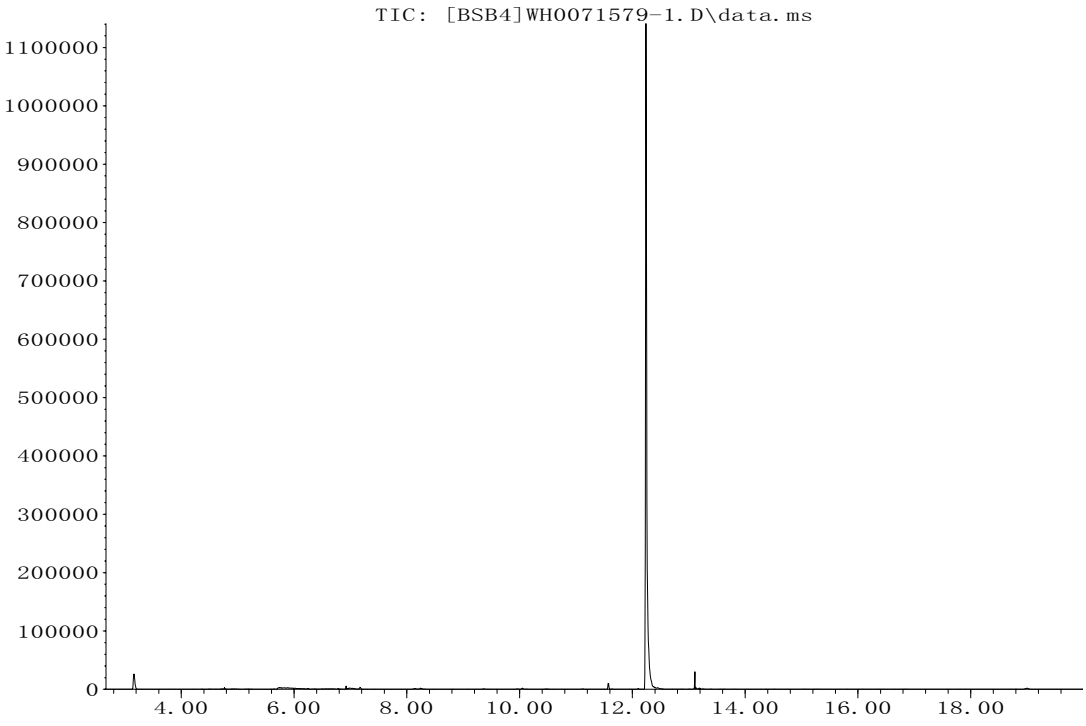
时间-->

丰度


扫描 1645 (13.377 分): WH20121218-B-1.D\data.ms
194.1
N
N
H
Chemical Formula: C13H10N2
Exact Mass: 194.0844
16000
14000
12000
10000
8000
6000
4000
2000
0
70.4
83.6
96.8
139.0
166.1
207.1
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

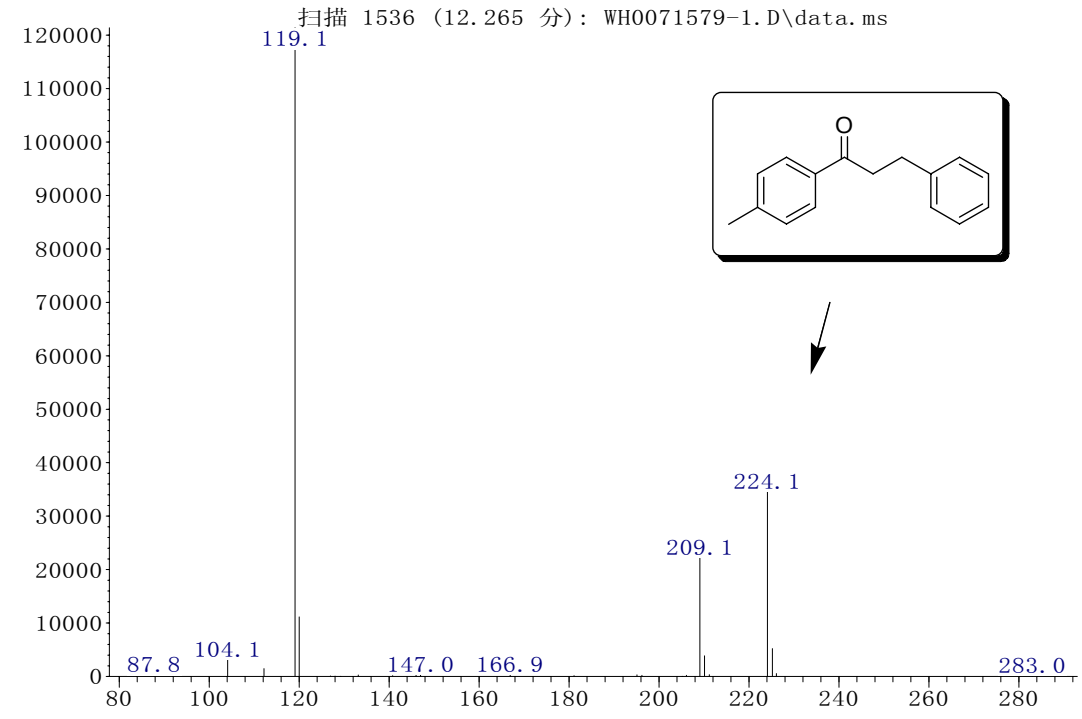
m/z-->

丰度


TIC: [BSB4]WH0071579-1.D\data.ms
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

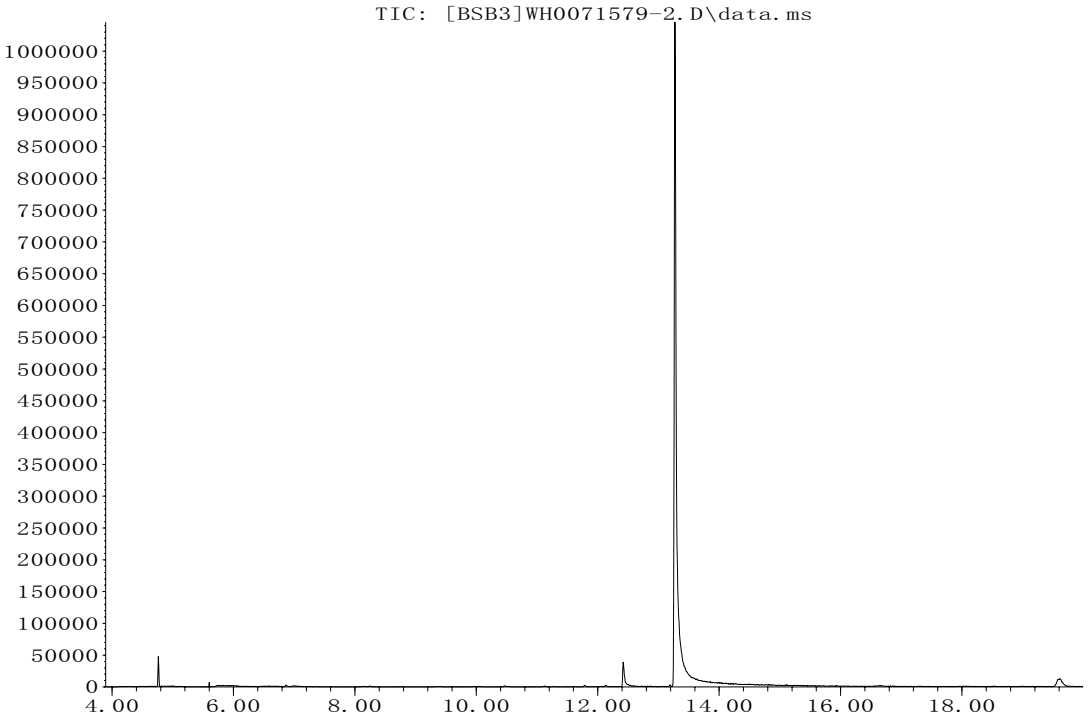
时间-->

丰度


扫描 1536 (12.265 分): WH0071579-1.D\data.ms
119.1
224.1
209.1
87.8
104.1
147.0
166.9
283.0
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
80
100
120
140
160
180
200
220
240
260
280
O

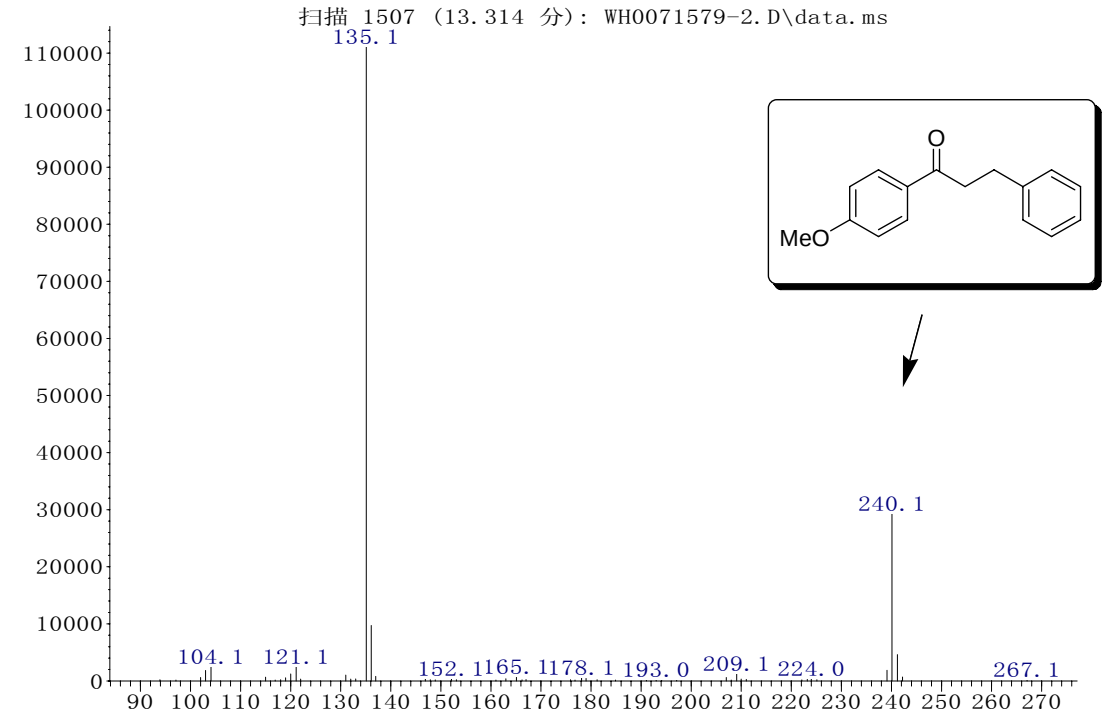
m/z-->

丰度


TIC: [BSB3]WH0071579-2.D\data.ms
1000000
950000
900000
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

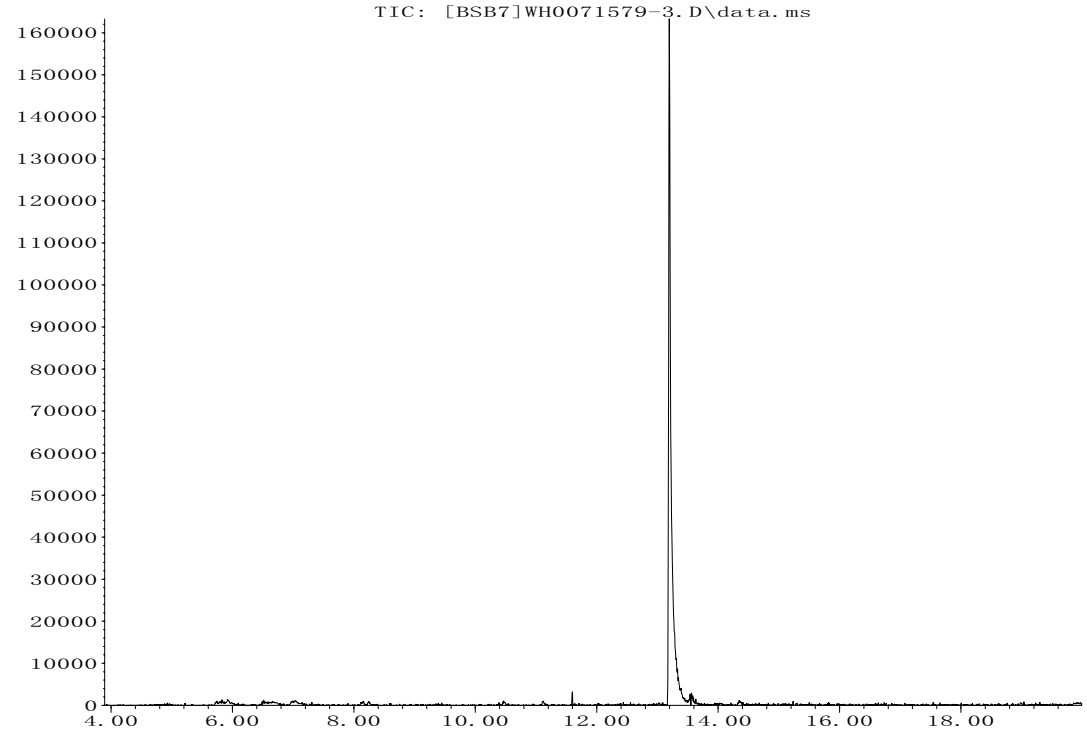
时间-->

丰度


扫描 1507 (13.314 分): WH0071579-2.D\data.ms
135.1
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
O
MeO
240.1
104.1
121.1
152.1
165.1
178.1
193.0
209.1
224.0
267.1
90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270

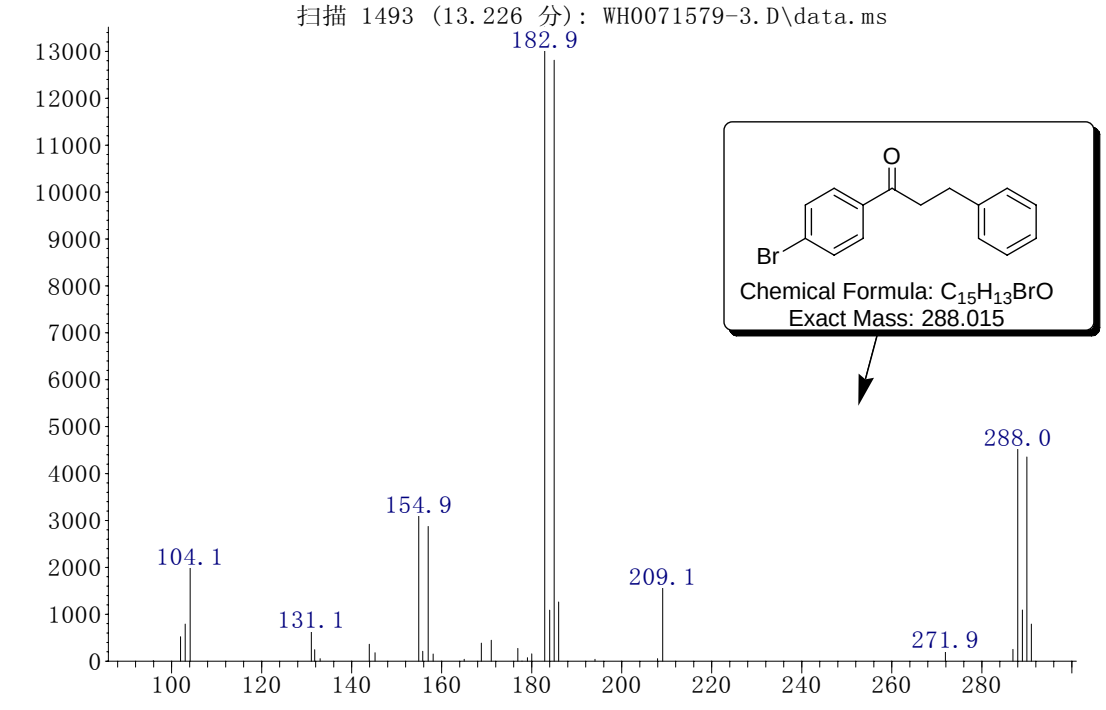
m/z-->

丰度


TIC: [BSB7]WH0071579-3.D\data.ms
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

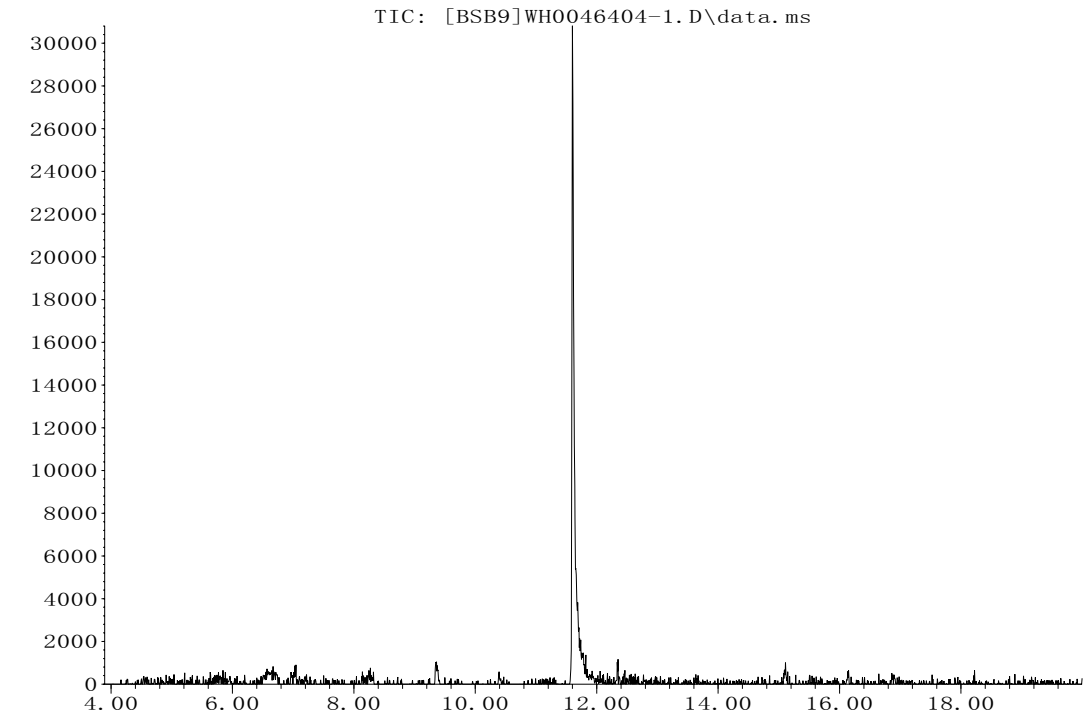
时间-->

丰度


扫描 1493 (13.226 分): WH0071579-3.D\data.ms
182.9
288.0
154.9
104.1
209.1
131.1
271.9
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
100
120
140
160
180
200
220
240
260
280
O
Br
Chemical Formula: C15H13BrO
Exact Mass: 288.015

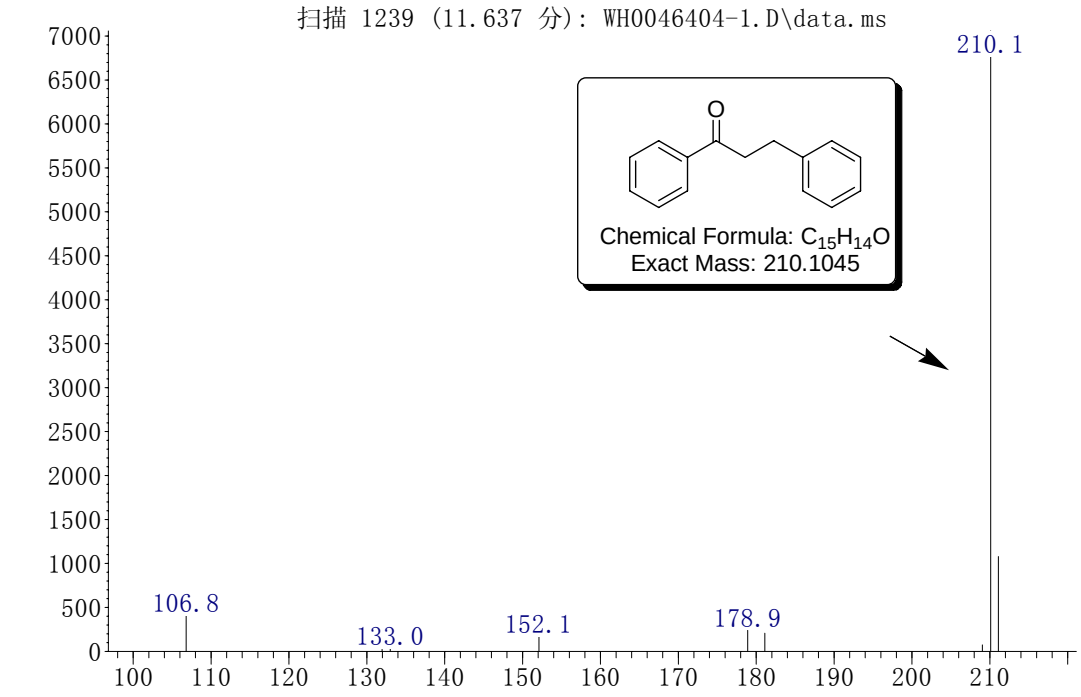
m/z-->

丰度

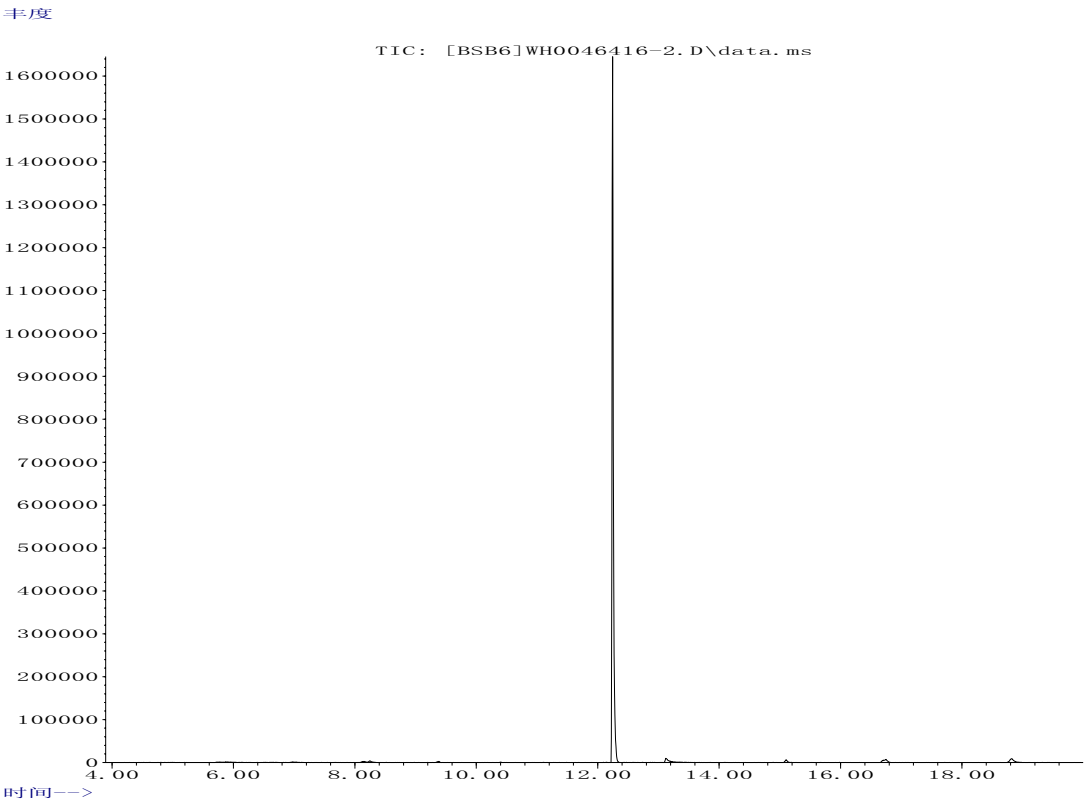

TIC: [BSB9]WH0046404-1.D\data.ms
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

时间-->

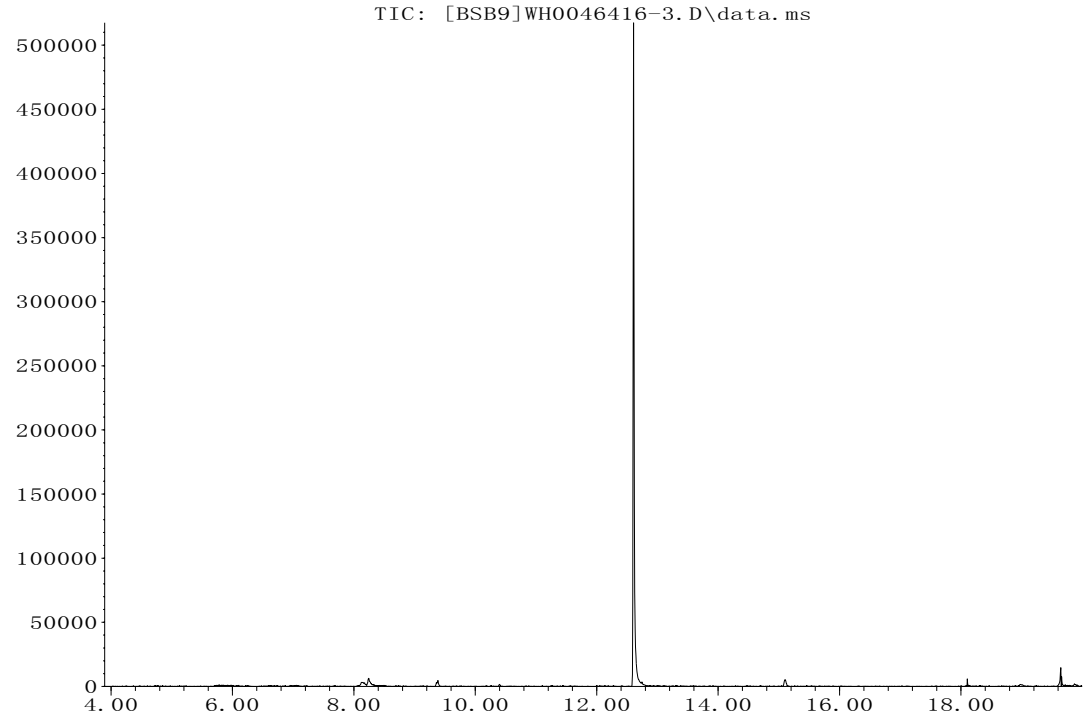
丰度


扫描 1239 (11.637 分): WH0046404-1.D\data.ms
210.1
O
Chemical Formula: C15H14O
Exact Mass: 210.1045
106.8
133.0
152.1
178.9
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
100
110
120
130
140
150
160
170
180
190
200
210

m/z-->

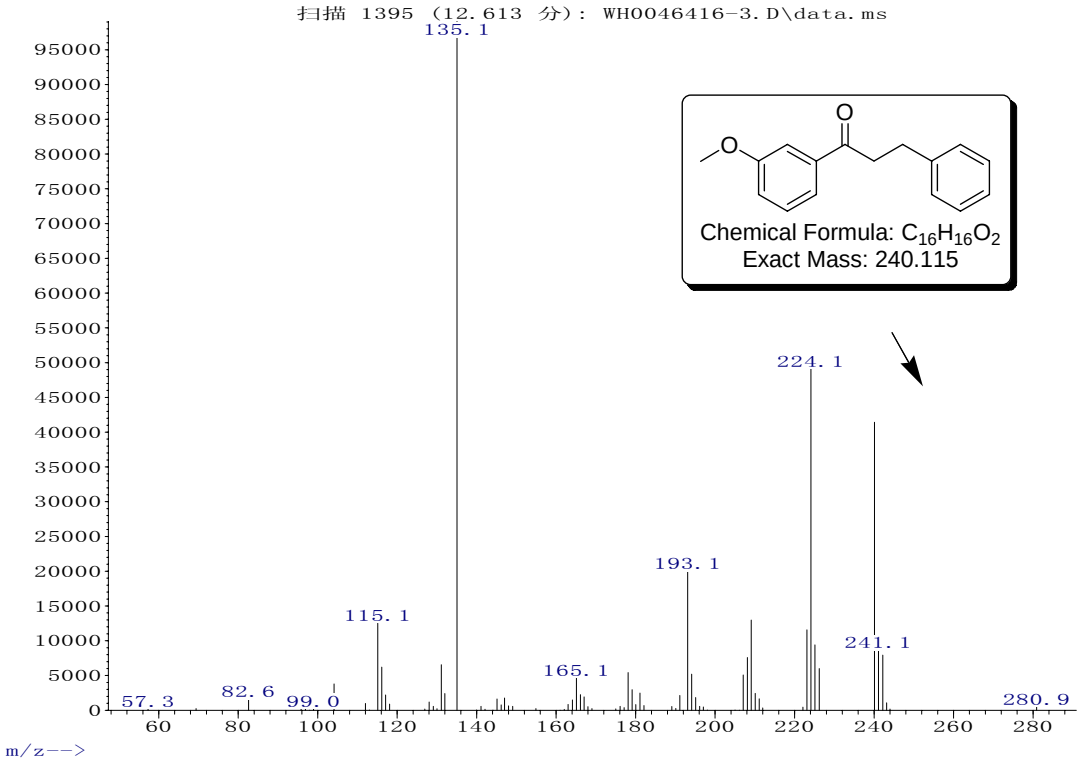

丰度
TIC: [BSB6]WH0046416-2.D\data.ms
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1339 (12.263 分): WH0046416-2.D\data.ms
119.1
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
O
Chemical Formula: C16H16O
Exact Mass: 224.1201
224.1
209.1
81.8
145.0
282.0
80
100
120
140
160
180
200
220
240
260
280
m/z-->

丰度

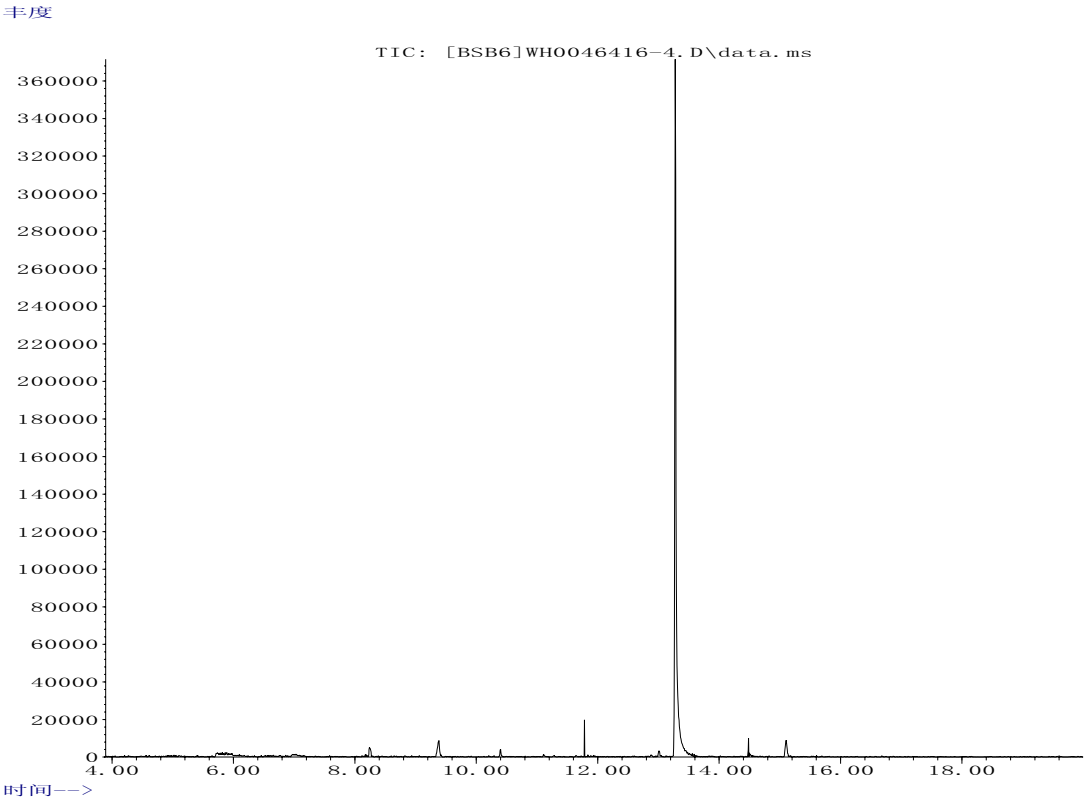

TIC: [BSB9]WH0046416-3.D\data.ms
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

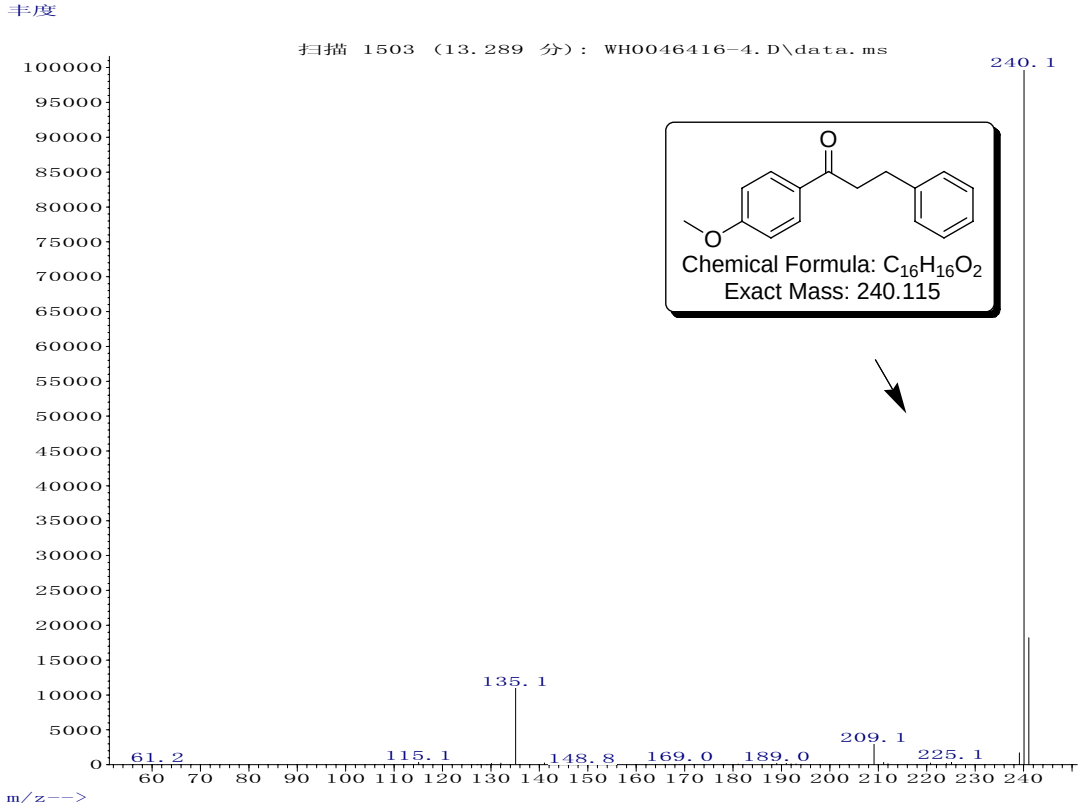
时间-->

丰度

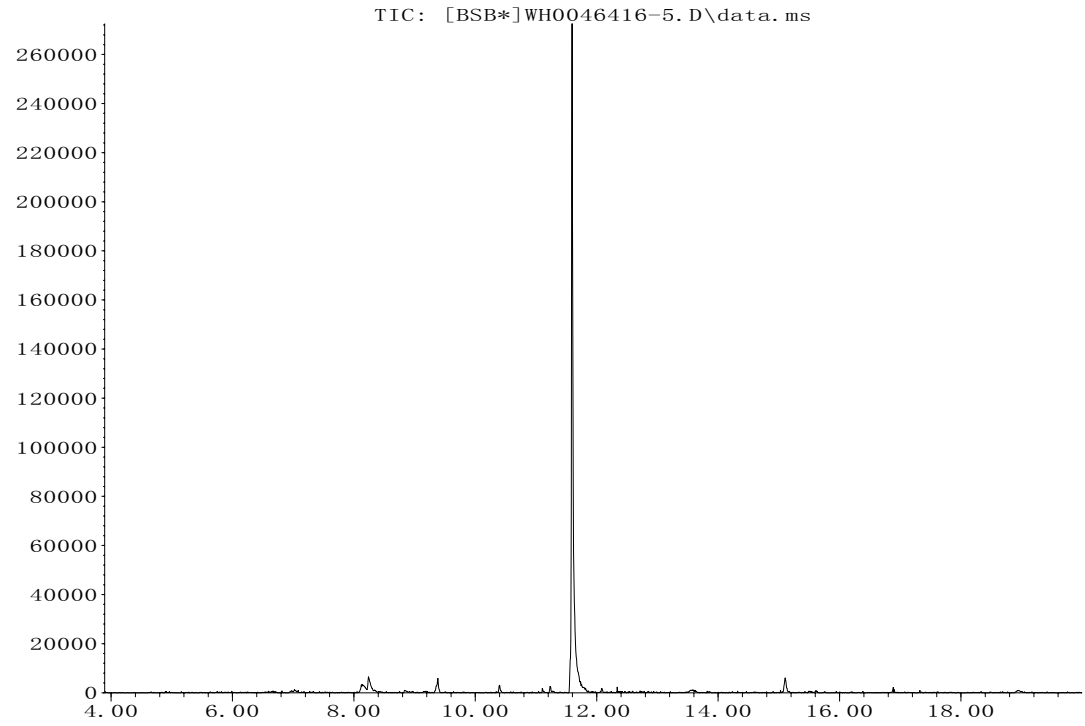

扫描 1395 (12.613 分): WH0046416-3.D\data.ms
135.1
224.1
193.1
115.1
241.1
165.1
82.6
99.0
57.3
280.9
95000
90000
85000
80000
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
60
80
100
120
140
160
180
200
220
240
260
280
O
O
Chemical Formula: C16H16O2
Exact Mass: 240.115

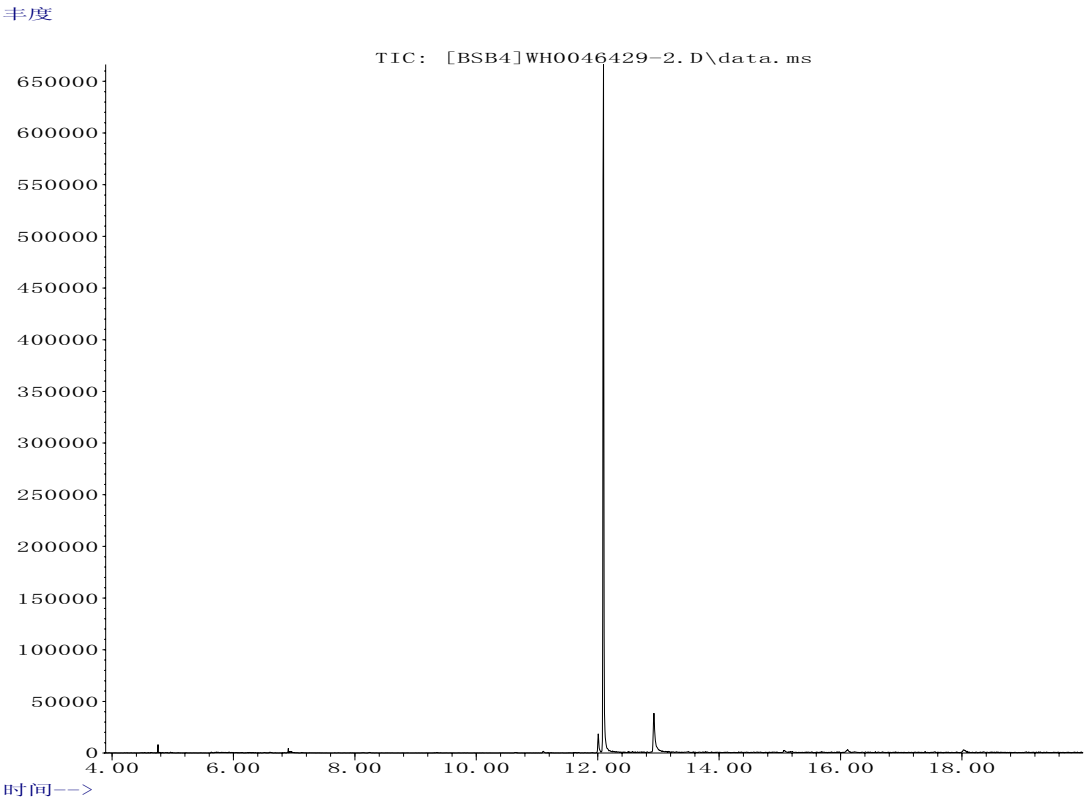
m/z-->


丰度
TIC: [BSB6]WH0046416-4.D\data.ms
360000
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->

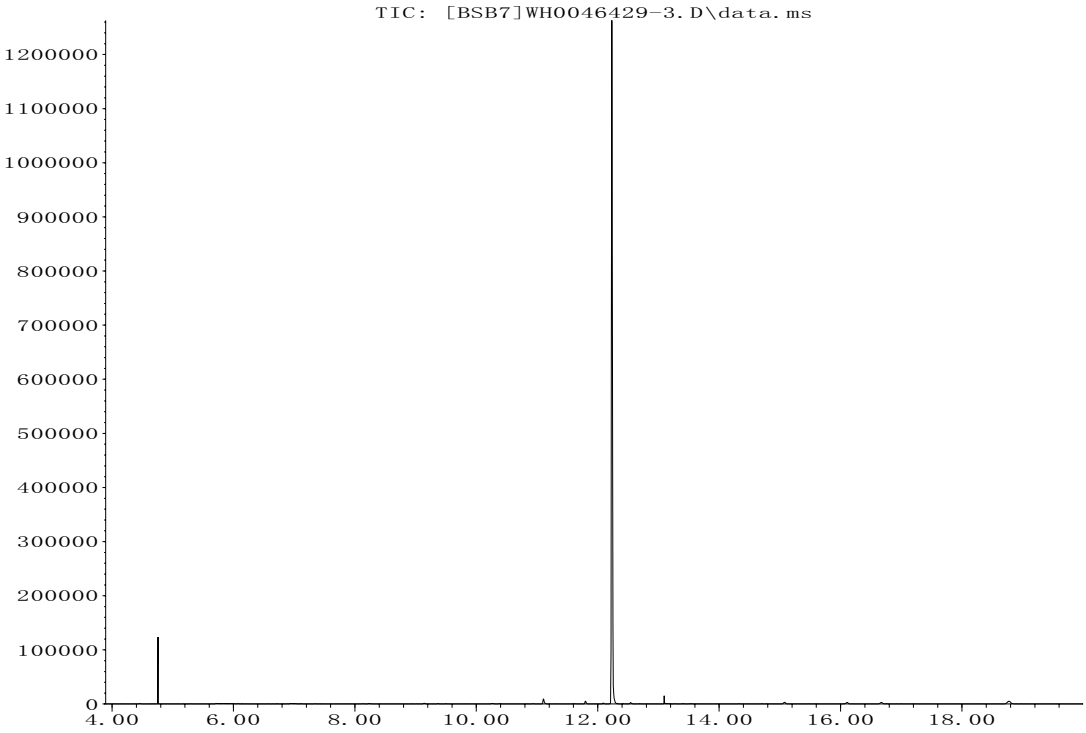

丰度
扫描 1503 (13.289 分): WH0046416-4.D\data.ms
100000
95000
90000
85000
80000
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
240.1
135.1
209.1
61.2
115.1
148.8
169.0
189.0
225.1
60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240
m/z-->
O
O
Chemical Formula: C16H16O2
Exact Mass: 240.115

丰度


TIC: [BSB*]WH0046416-5.D\data.ms
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1235 (11.612 分): WH0046416-5.D\data.ms
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
210.1
95.0
118.0
133.0
152.9
167.1
181.1
194.1
O
Chemical Formula: C15H14O
Exact Mass: 210.1045
90
100
110
120
130
140
150
160
170
180
190
200
210
m/z-->

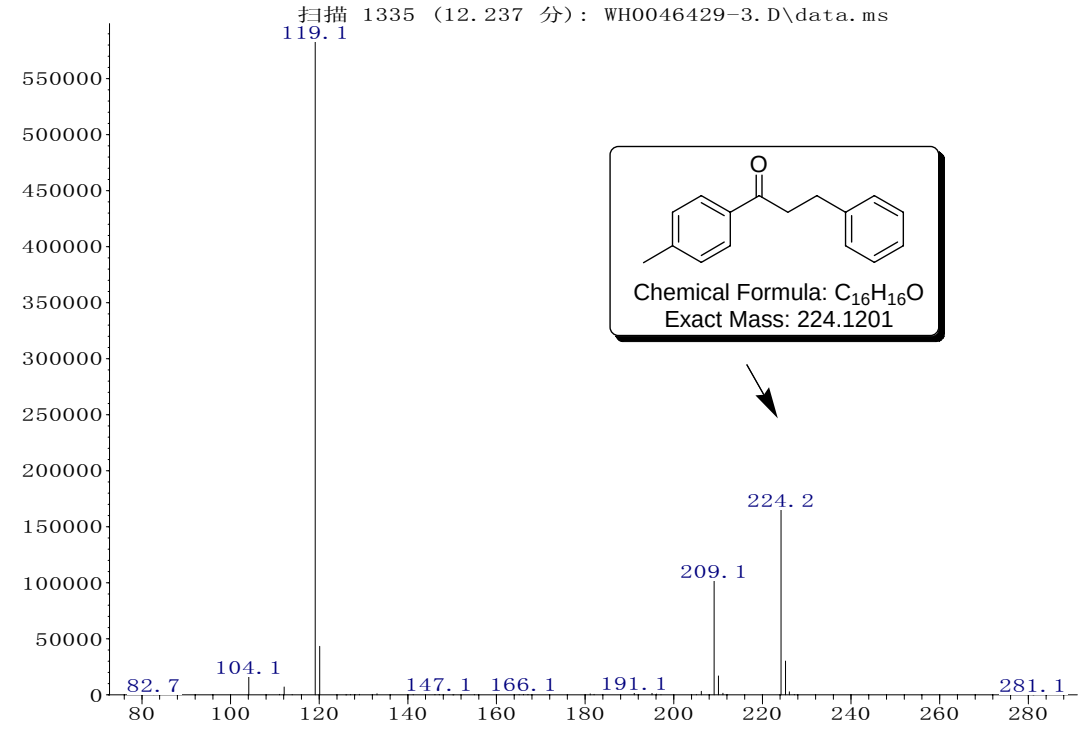

丰度
TIC: [BSB4]WH0046429-2.D\data.ms
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1314 (12.106 分): WH0046429-2.D\data.ms
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
224.2
119.1
131.1
145.2
165.1
178.1
191.0
209.2
O
Chemical Formula: C16H16O
Exact Mass: 224.1201
110
120
130
140
150
160
170
180
190
200
210
220
230
m/z-->

丰度


TIC: [BSB7]WH0046429-3.D\data.ms
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

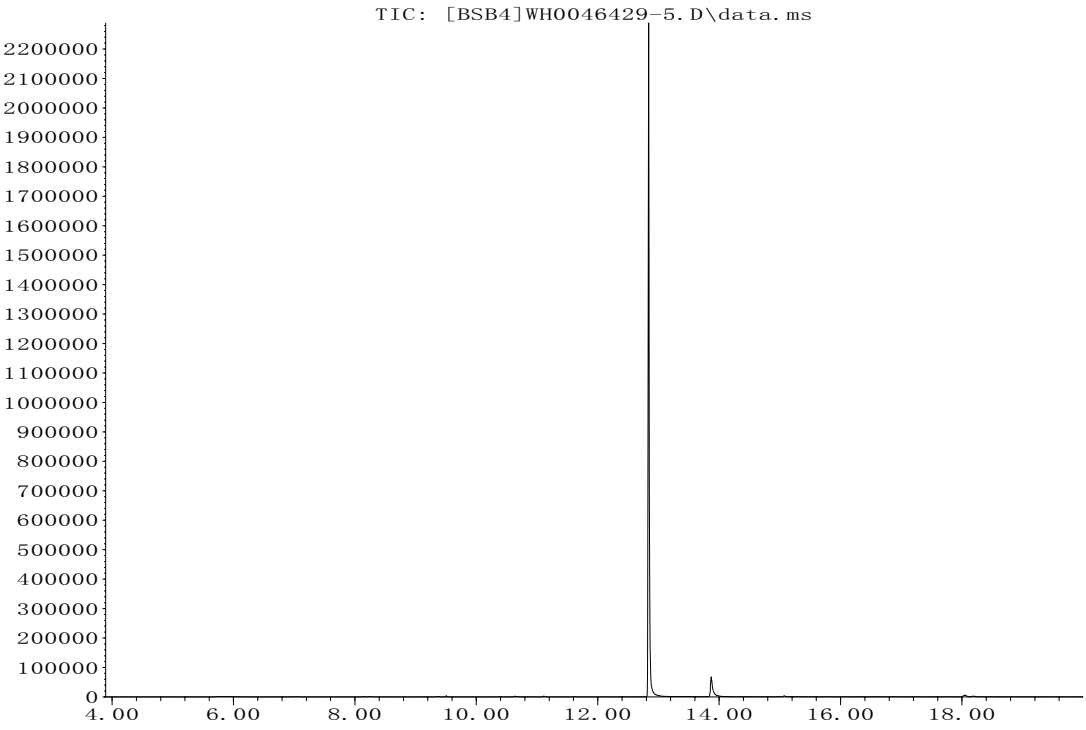
时间-->

丰度


扫描 1335 (12.237 分): WH0046429-3.D\data.ms
119.1
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
82.7
104.1
147.1
166.1
191.1
209.1
224.2
281.1
80
100
120
140
160
180
200
220
240
260
280
O
Chemical Formula: C16H16O
Exact Mass: 224.1201

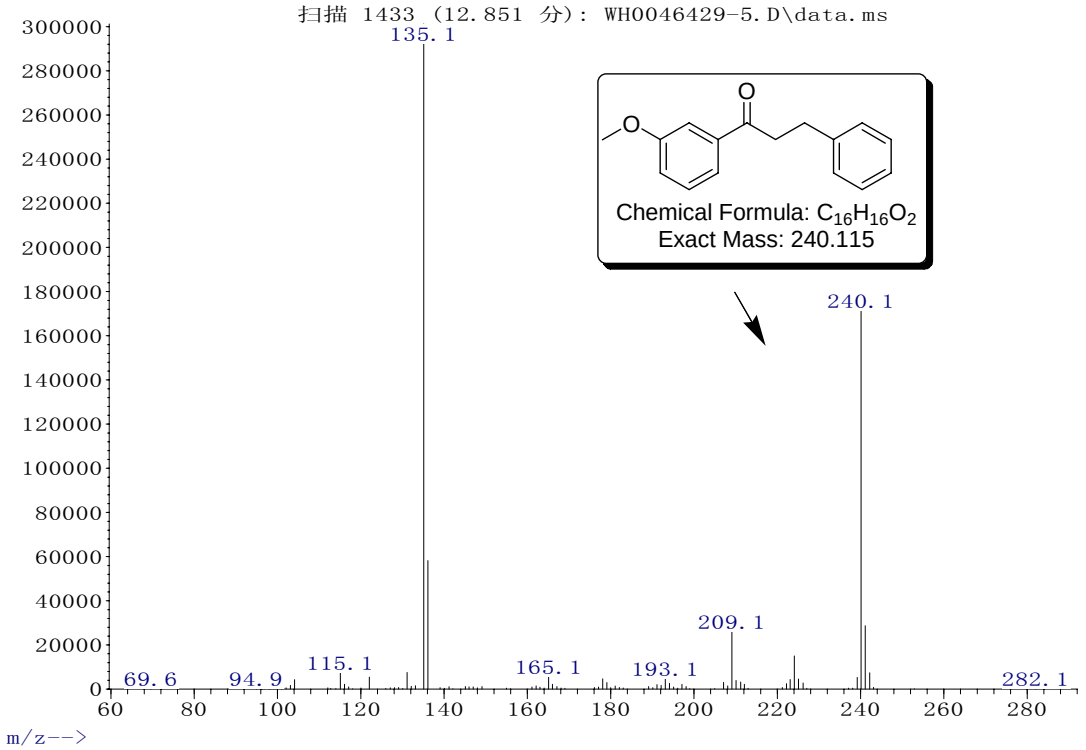
m/z-->

丰度

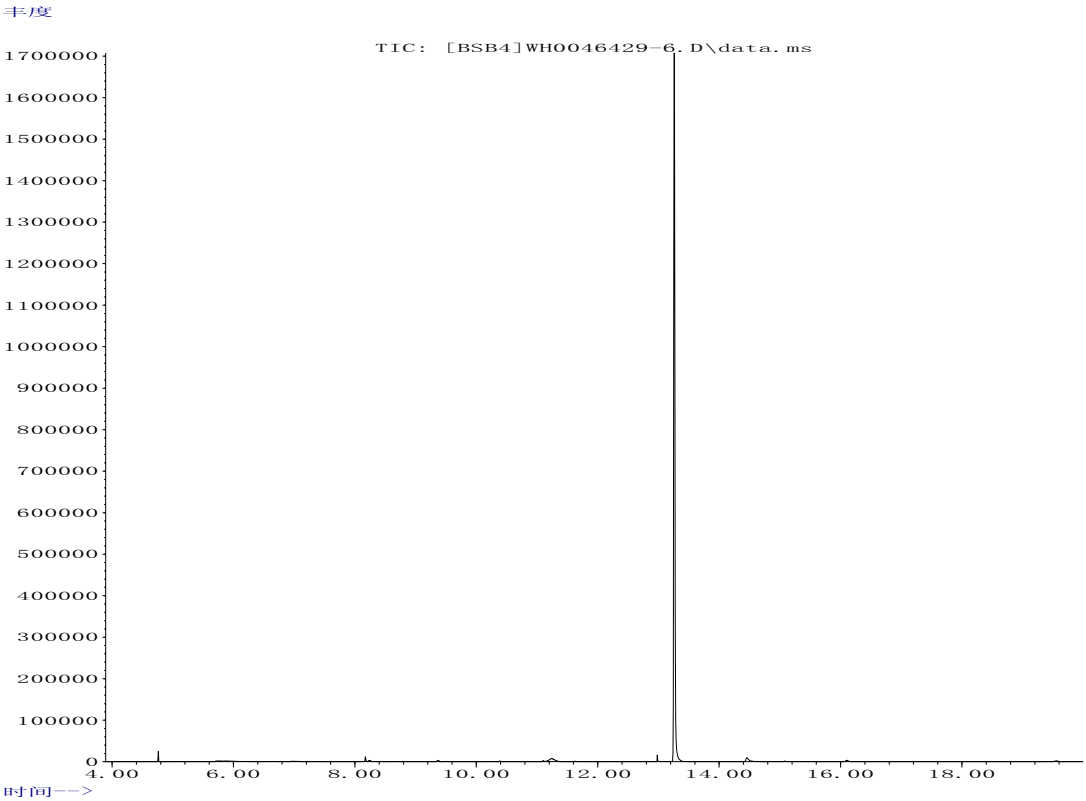

TIC: [BSB4]WH0046429-5.D\data.ms
2200000
2100000
2000000
1900000
1800000
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

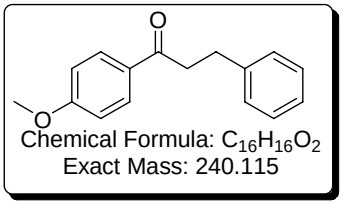
时间-->

丰度


扫描 1433 (12.851 分): WH0046429-5.D\data.ms
135.1
O
O
Chemical Formula: C16H16O2
Exact Mass: 240.115
240.1
209.1
69.6
94.9
115.1
165.1
193.1
282.1
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
60
80
100
120
140
160
180
200
220
240
260
280

m/z-->


丰度
TIC: [BSB4]WH0046429-6.D\data.ms
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时间-->
丰度
扫描 1499 (13.263 分): WH0046429-6.D\data.ms
135.1
240.1
82.9
104.1
161.1
182.1
209.1
282.9
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
60
80
100
120
140
160
180
200
220
240
260
280
m/z-->


O
O
Chemical Formula: C16H16O2
Exact Mass: 240.115