Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
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Supporting Information

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SI1. NMR spectrums of target compounds (2 – 16)

SI2. NMR spectrums of intermediate compounds (17 – 41)

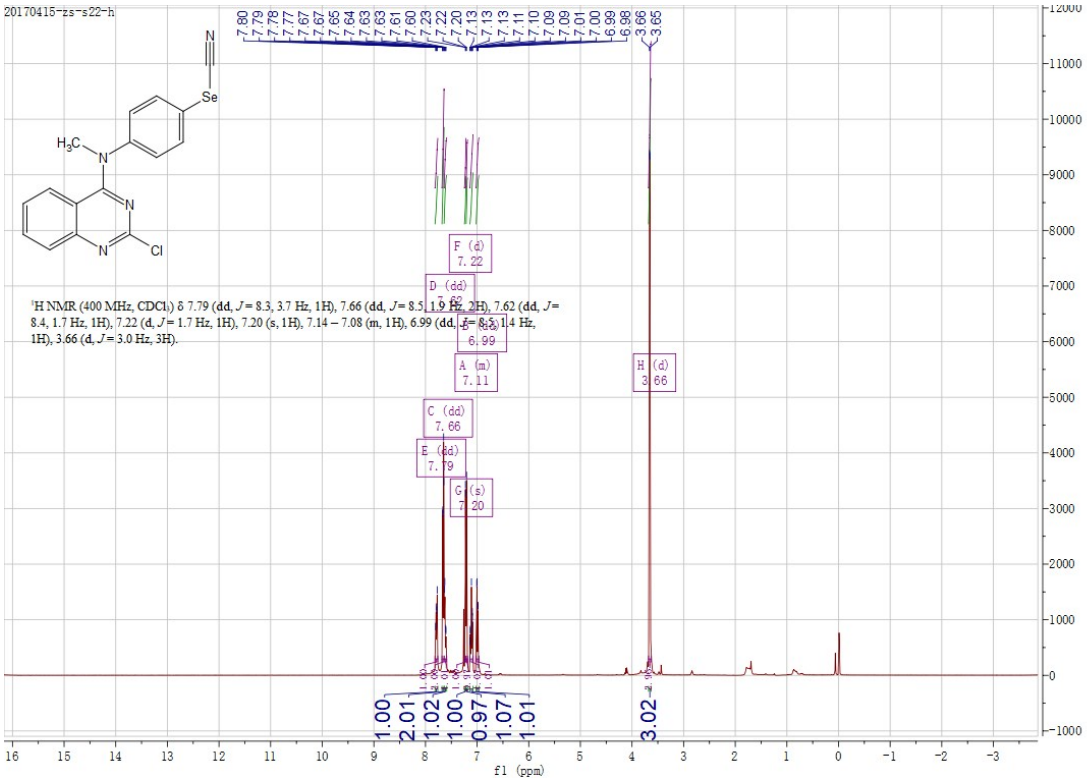
SI3. HPLC chromatograms of target compounds (42 – 49)

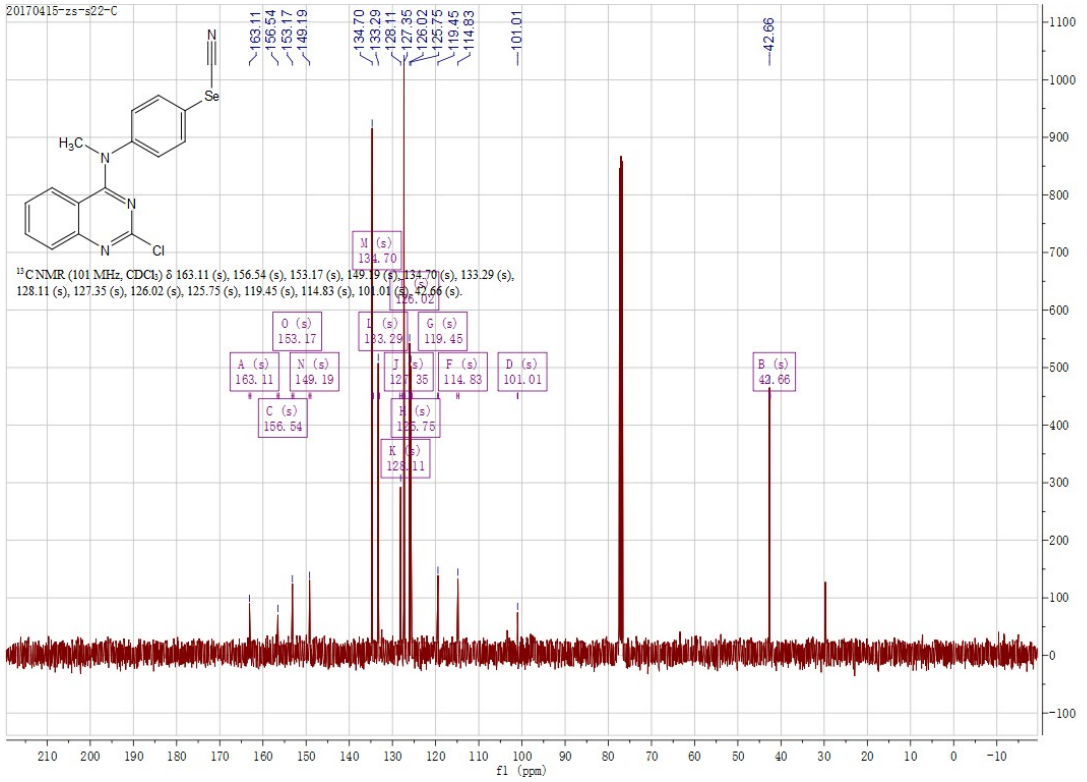
SI4. HR-MS of target compounds (50 – 59)

SI5. LR-MS of target compounds(60 – 74)

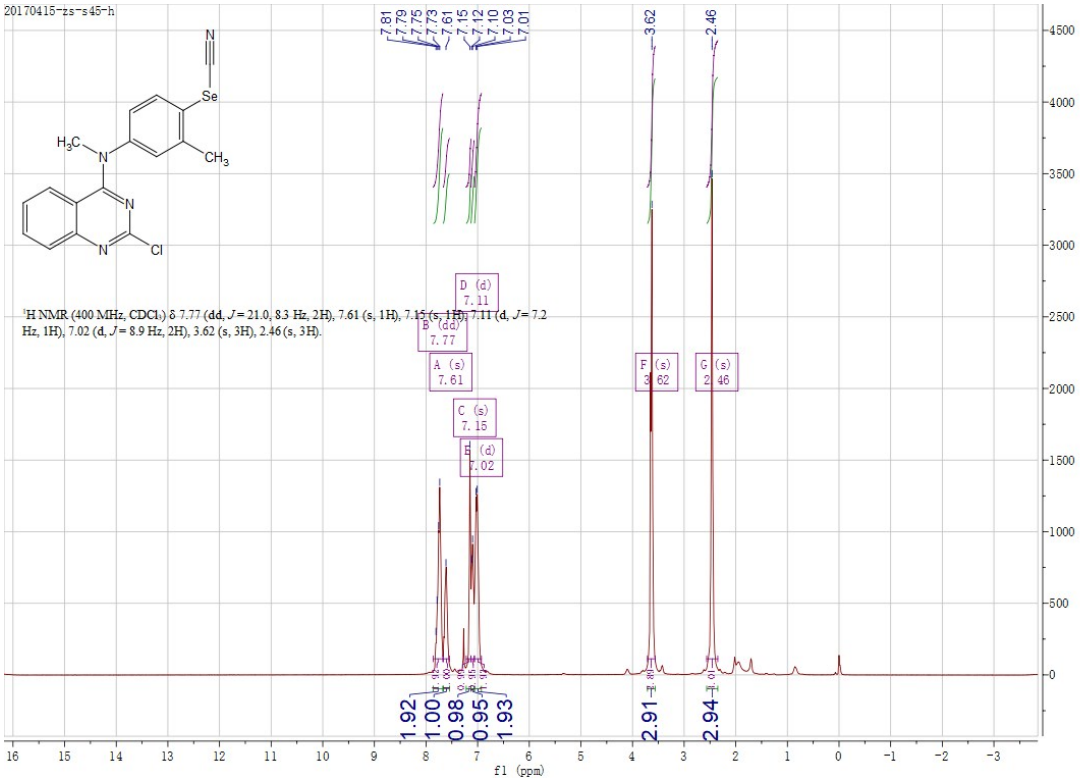
SI1. NMR spectrums of target compounds

5a

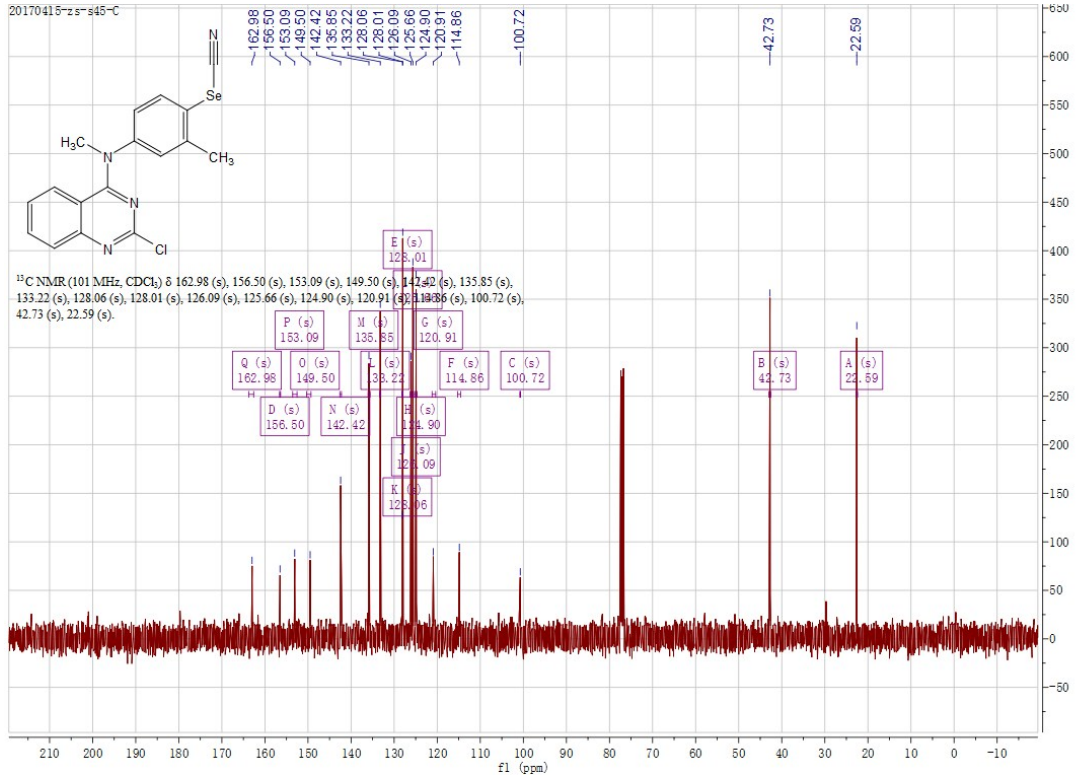




5b

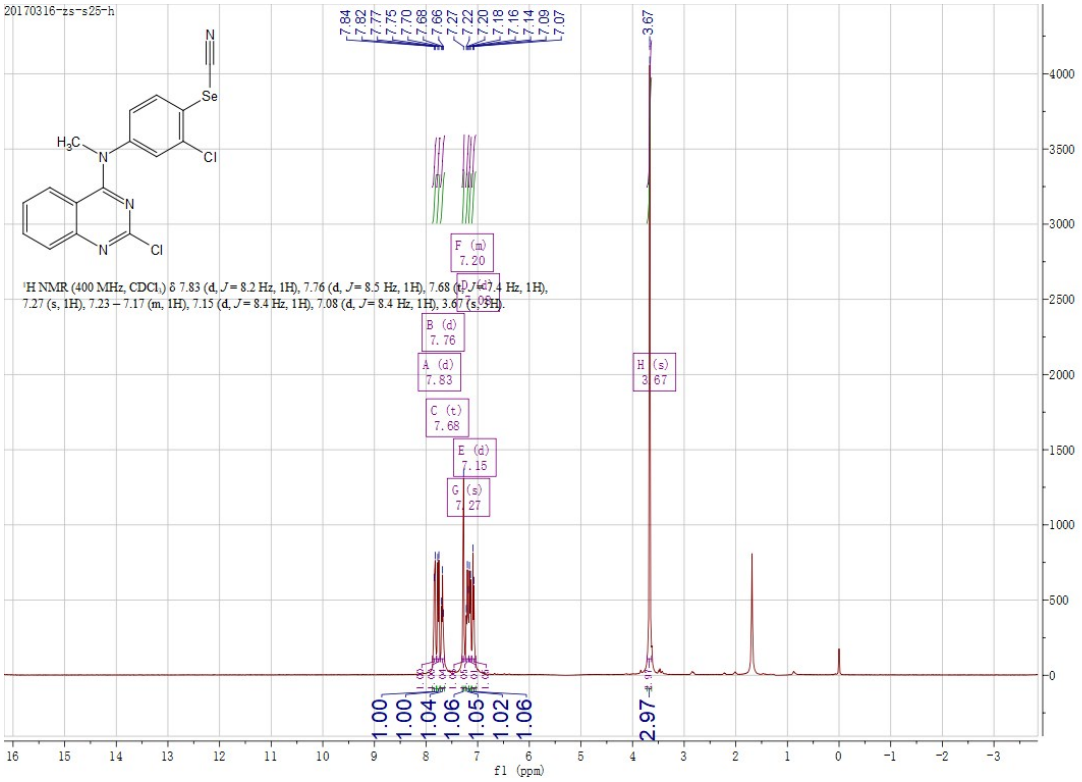


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, J = 21.0, 8.3 Hz, 2H), 7.61 (s, 1H), 7.15 (s, 1H), 7.11 (d, J = 7.2 Hz, 1H), 7.02 (d, J = 8.9 Hz, 2H), 3.62 (s, 3H), 2.46 (s, 3H).

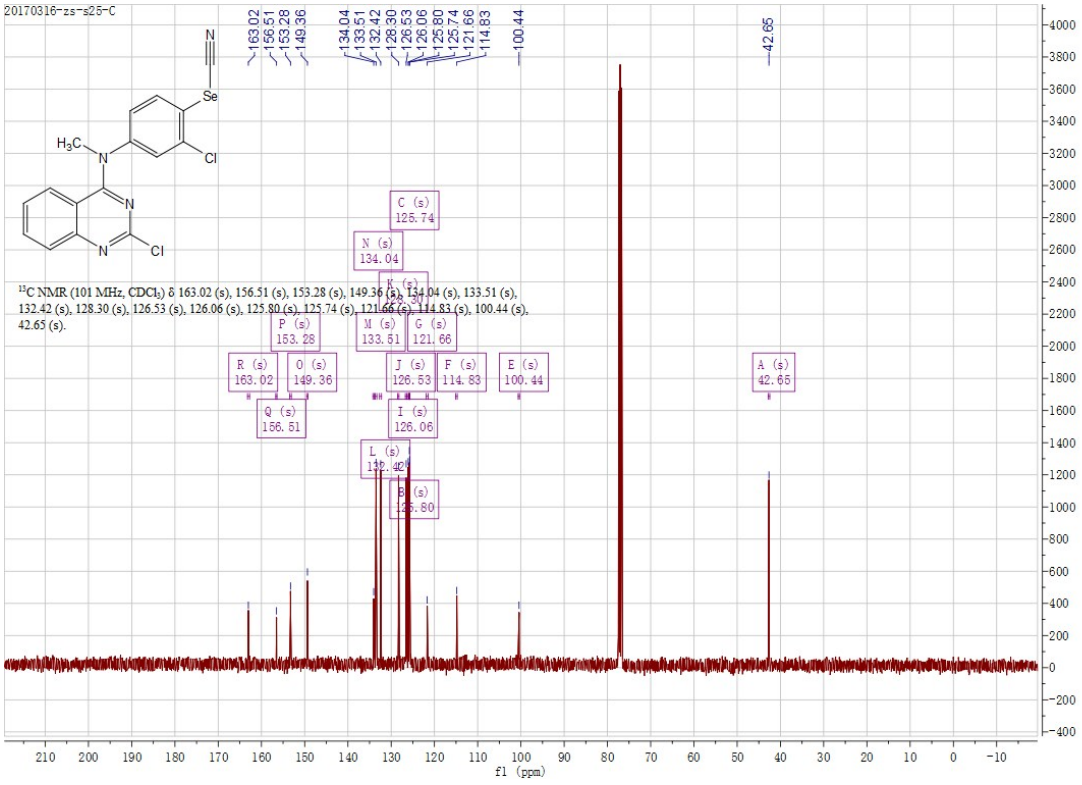


^{13}C NMR (101 MHz, $CDCl_3$) δ 162.98 (s), 156.50 (s), 153.09 (s), 149.50 (s), 142.42 (s), 135.85 (s), 133.22 (s), 128.06 (s), 128.01 (s), 126.09 (s), 125.66 (s), 124.90 (s), 120.91 (s), 114.86 (s), 100.72 (s), 42.73 (s), 22.59 (s).

5d

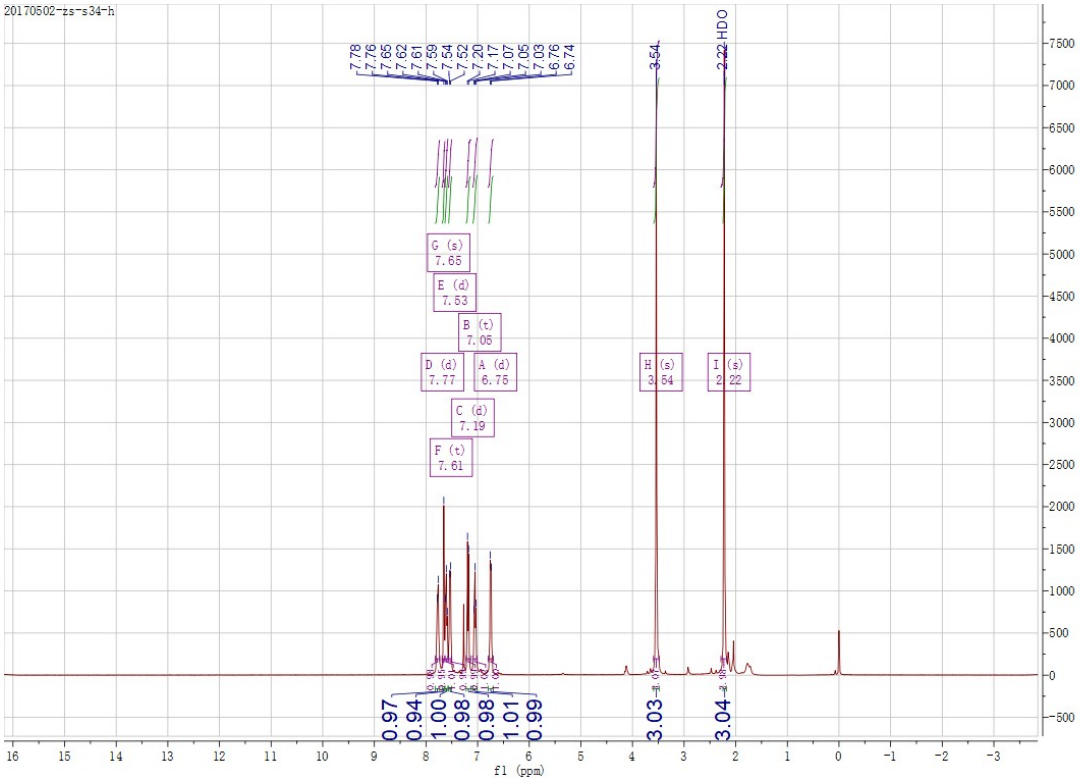


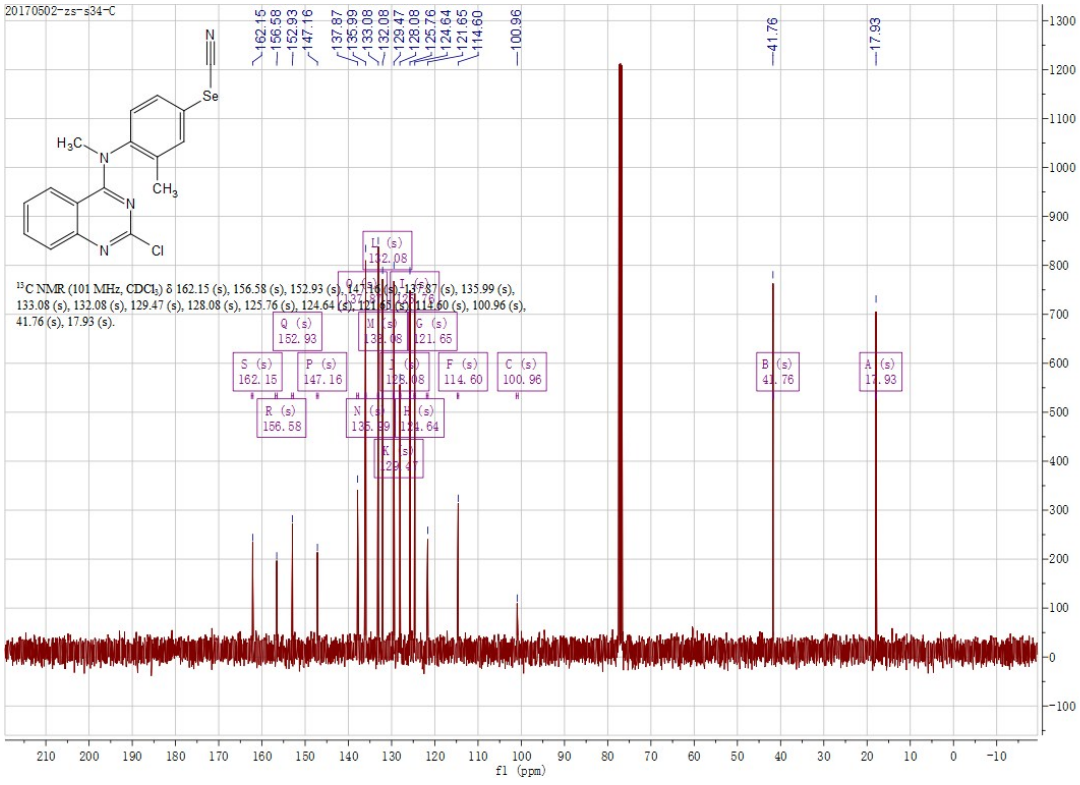
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.2 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 1H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.27 (s, 1H), 7.23 – 7.17 (m, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 3.67 (s, 3H).



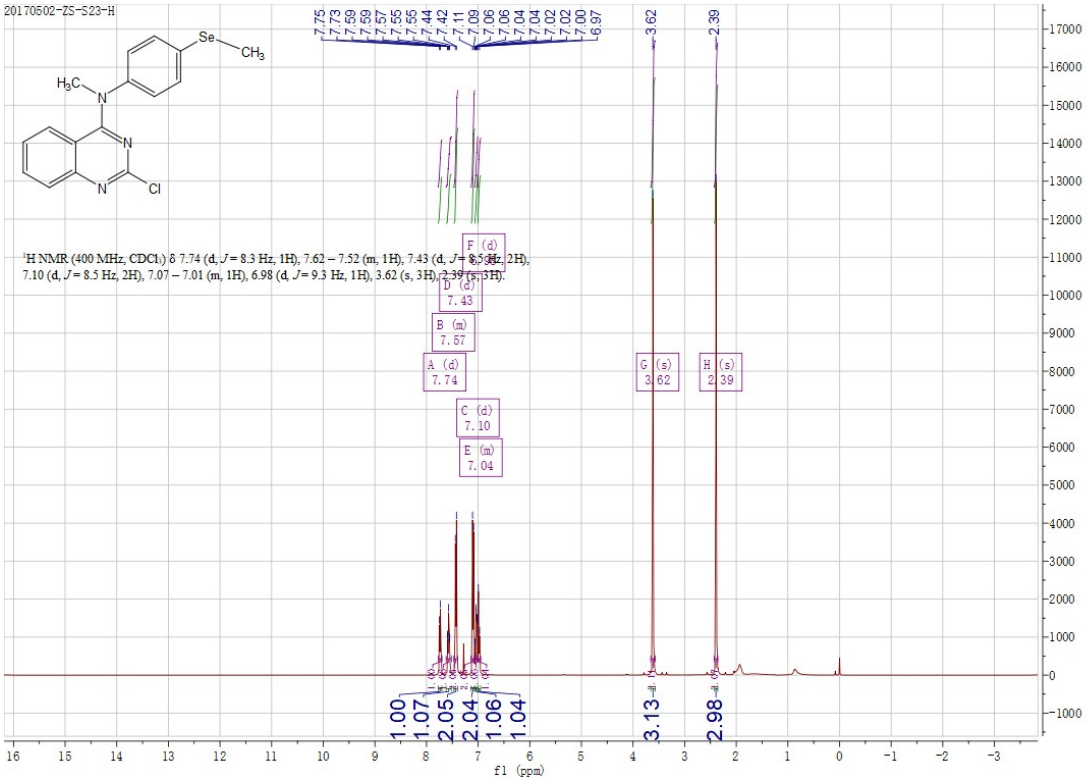
^{13}C NMR (101 MHz, $CDCl_3$) δ 163.02 (s), 156.51 (s), 153.28 (s), 149.36 (s), 134.04 (s), 133.51 (s), 132.42 (s), 128.30 (s), 126.53 (s), 126.06 (s), 125.80 (s), 125.74 (s), 121.66 (s), 114.83 (s), 100.44 (s), 42.65 (s).

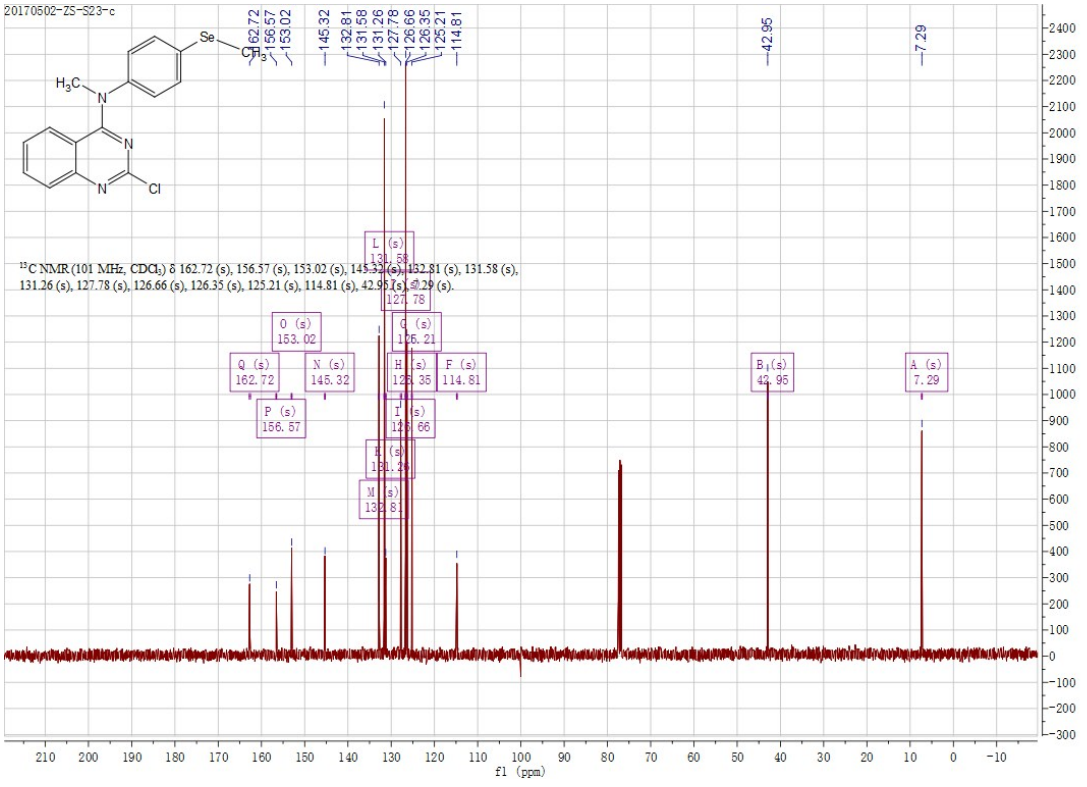
5f


20170502-zs-s34-h
7.78
7.76
7.65
7.62
7.61
7.59
7.54
7.52
7.20
7.17
7.07
7.05
7.03
6.76
6.74
3.54
2.22 HDO
G (s) 7.65
E (d) 7.53
B (t) 7.05
D (d) 7.77
A (d) 6.76
C (d) 7.19
F (t) 7.61
H (s) 3.54
I (s) 2.22
0.97
0.94
1.00
0.98
0.98
1.01
0.99
3.03
3.04
f1 (ppm)

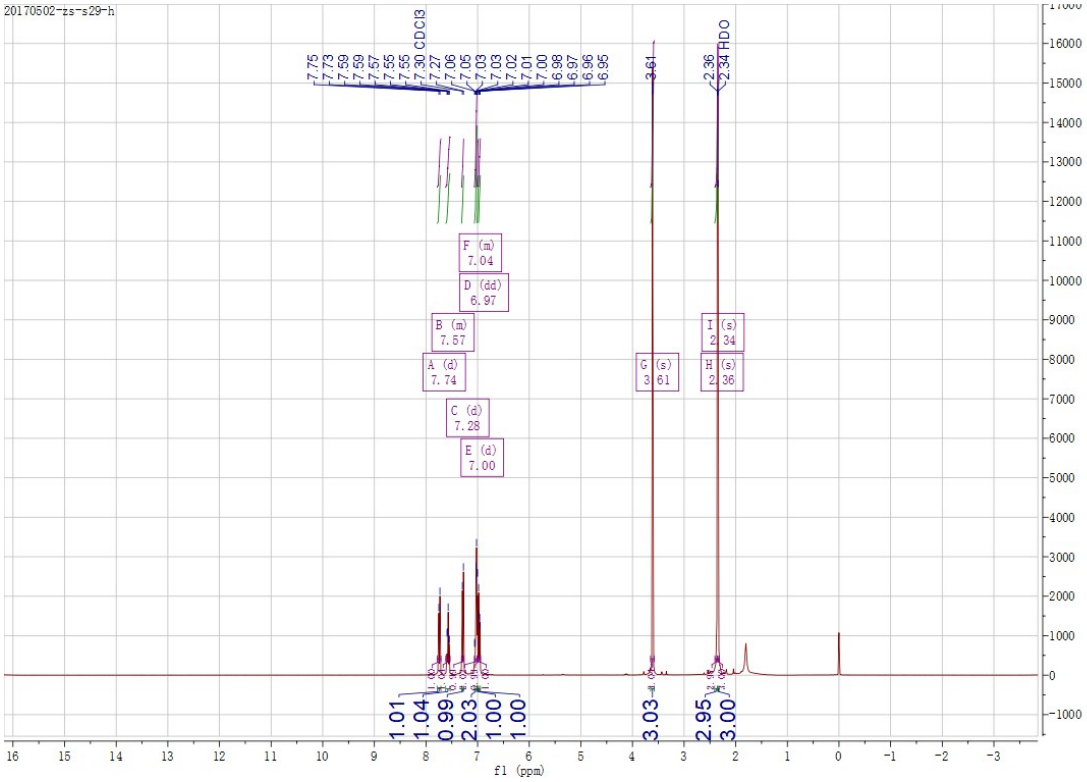

20170502-zs-s34-C
162.15
156.58
152.93
147.16
137.87
135.99
133.08
132.08
129.47
128.08
125.76
124.64
121.65
114.60
100.96
41.76
17.93
N
Se
H3C
N
CH3
N
N
Cl
13C NMR (101 MHz, CDCl3) δ 162.15 (s), 156.58 (s), 152.93 (s), 147.16 (s), 137.87 (s), 135.99 (s), 133.08 (s), 132.08 (s), 129.47 (s), 128.08 (s), 125.76 (s), 124.64 (s), 121.65 (s), 114.60 (s), 100.96 (s), 41.76 (s), 17.93 (s).
L (s) 132.08
Q (s) 152.93
M (s) 128.08
G (s) 121.65
S (s) 162.15
P (s) 147.16
J (s) 128.08
F (s) 114.60
C (s) 100.96
B (s) 41.76
A (s) 17.93
R (s) 156.58
H (s) 124.64
f1 (ppm)

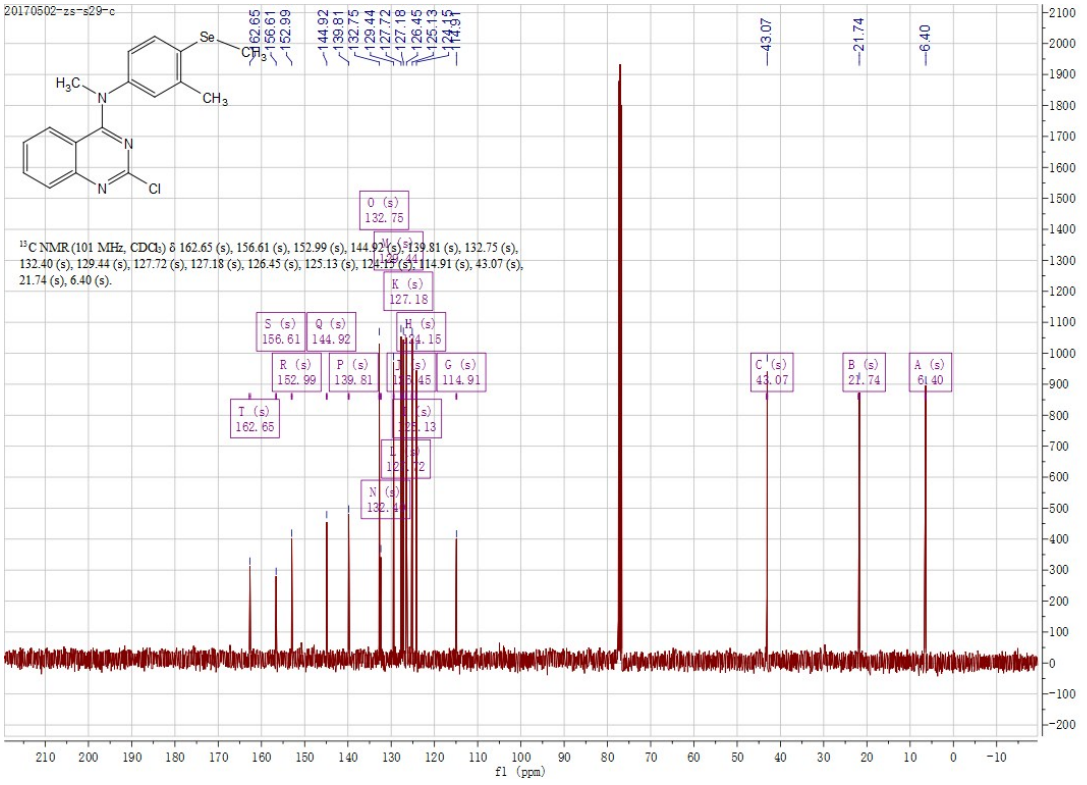
6a


20170502-ZS-S23-H
Se
CH3
H3C
N
N
N
Cl
7.75
7.73
7.59
7.57
7.55
7.44
7.42
7.11
7.09
7.06
7.04
7.02
6.97
3.62
2.39
F (d) 7.75
D (d) 7.43
B (m) 7.57
A (d) 7.74
C (d) 7.10
E (m) 7.04
G (s) 3.62
H (s) 2.39
1.00
1.07
2.05
2.04
1.06
1.04
3.13
2.98
f1 (ppm)

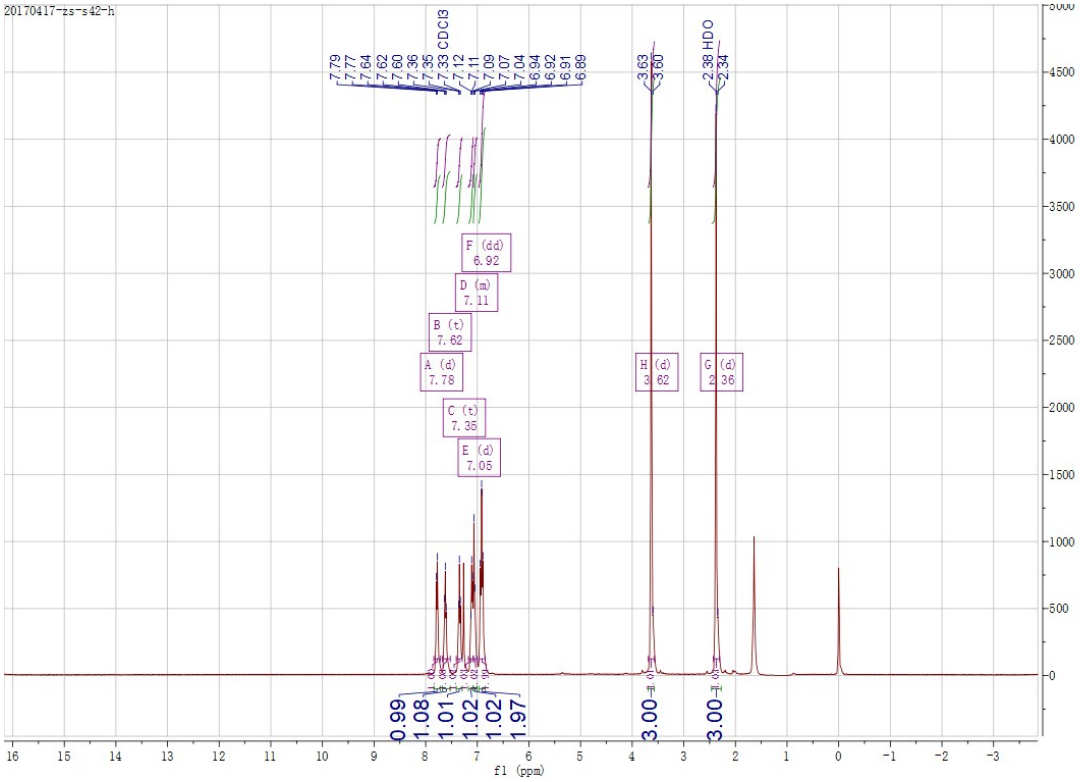

20170502-ZS-S23-c
Se
CH3
H3C
N
N
N
Cl
162.72
156.57
153.02
145.32
132.81
131.58
131.26
127.78
126.66
126.35
125.21
114.81
42.95
7.29
L (s) 132.81
O (s) 153.02
C (s) 126.21
Q (s) 162.72
N (s) 145.32
H (s) 126.35
F (s) 114.81
P (s) 156.57
I (s) 126.66
K (s) 131.26
M (s) 131.58
B1 (s) 42.95
A (s) 7.29
f1 (ppm)

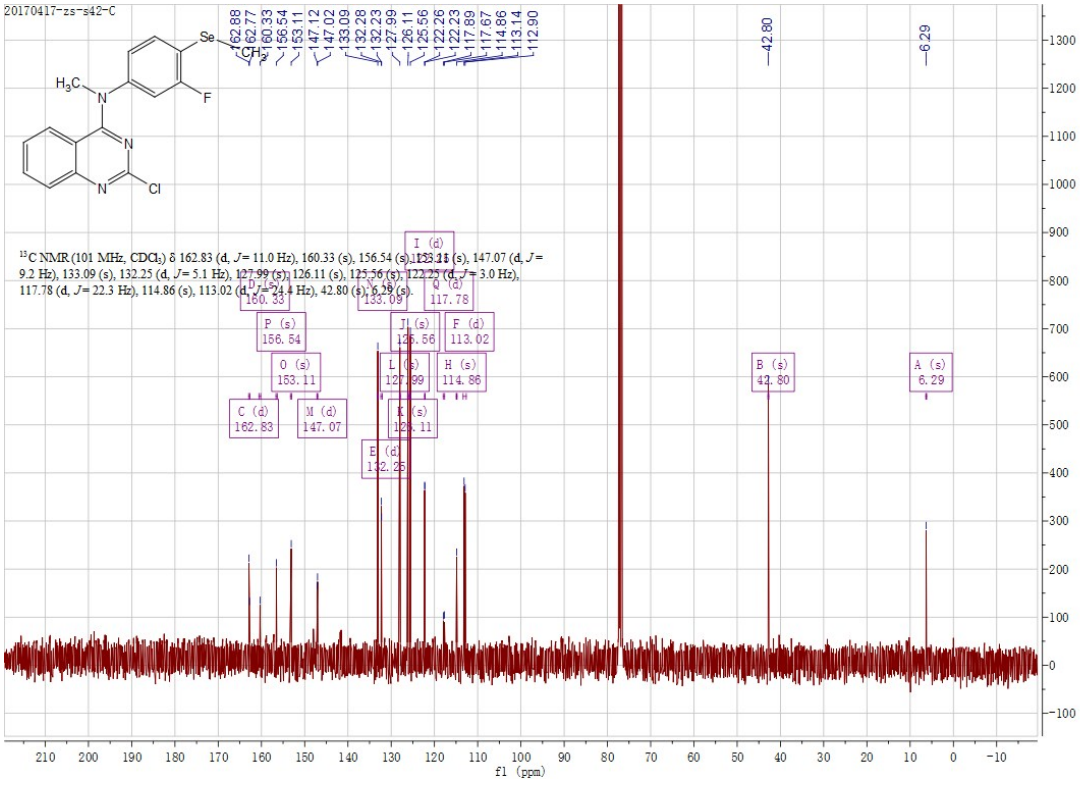
6b


20170502-zs-s29-h
CDCl3
HDO
F (m) 7.04
D (dd) 6.97
B (m) 7.57
A (d) 7.74
C (d) 7.28
E (d) 7.00
G (s) 3.61
I (s) 2.34
H (s) 2.36
1.01
1.04
0.99
2.03
1.00
1.00
3.03
2.95
3.00
f1 (ppm)

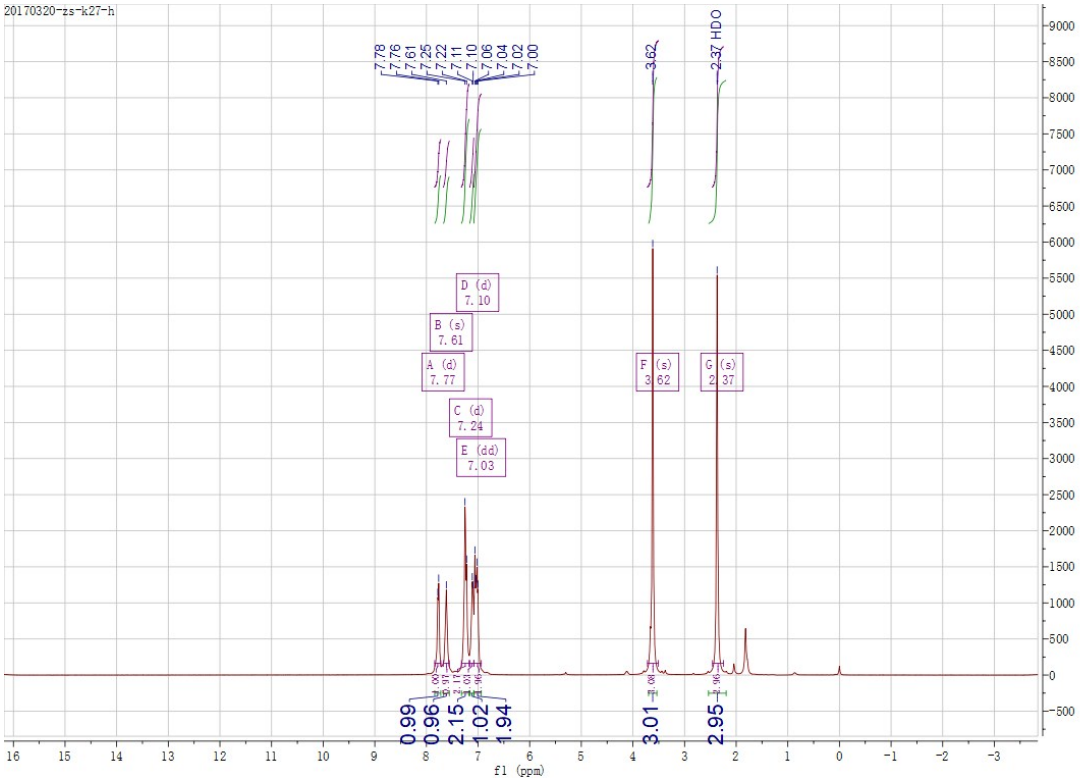

20170502-zs-s29-c
Se
CH3
H3C
N
CH3
N
N
Cl
13C NMR (101 MHz, CDCl3) δ 162.65 (s), 156.61 (s), 152.99 (s), 144.92 (s), 139.81 (s), 132.75 (s), 132.40 (s), 129.44 (s), 127.72 (s), 127.18 (s), 126.45 (s), 125.13 (s), 124.15 (s), 114.91 (s), 43.07 (s), 21.74 (s), 6.40 (s).
O (s) 132.75
K (s) 127.18
S (s) 156.61
Q (s) 144.92
H (s) 124.15
R (s) 152.99
P (s) 139.81
G (s) 114.91
T (s) 162.65
C (s) 43.07
B (s) 21.74
A (s) 6.40
f1 (ppm)

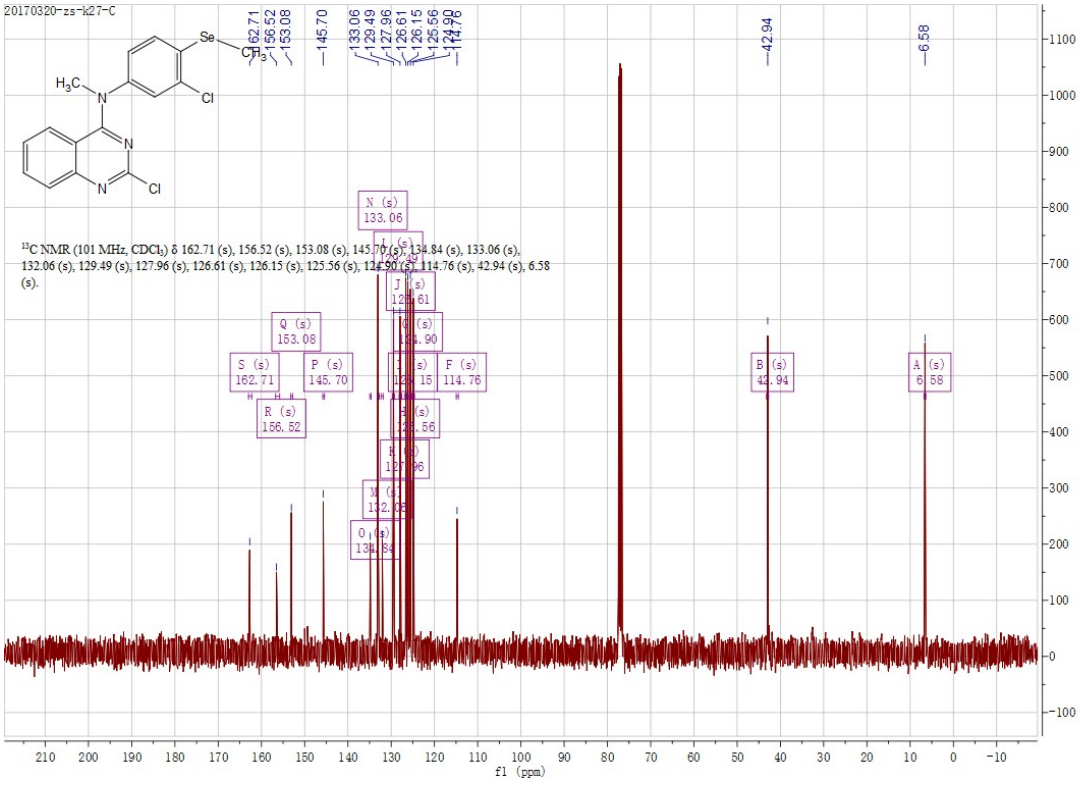
6c


20170417-zs-s42-h
7.79
7.77
7.64
7.62
7.60
7.36
7.35
7.33 CDCl3
7.12
7.11
7.09
7.07
7.04
6.94
6.92
6.91
6.89
3.63
3.60
2.38 HDO
2.34
F (dd) 6.92
D (m) 7.11
B (t) 7.62
A (d) 7.78
C (t) 7.35
E (d) 7.05
H (d) 3.62
G (d) 2.36
0.99
1.08
1.01
1.02
1.02
1.97
3.00
3.00
f1 (ppm)

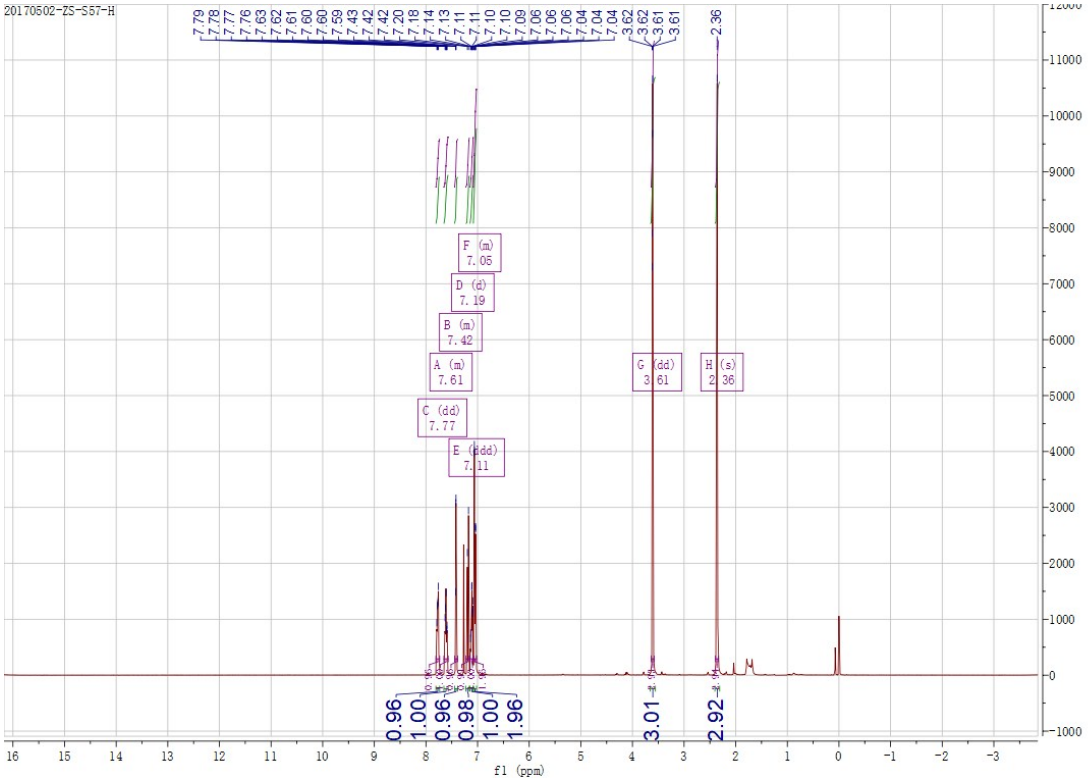

20170417-zs-s42-C
162.88
162.77
160.33
156.54
153.11
147.12
147.02
133.09
132.28
132.23
127.99
126.11
125.56
122.26
122.23
117.89
117.67
114.86
113.14
112.90
42.80
6.29
Se
CH2
H3C
N
F
N
N
Cl
13C NMR (101 MHz, CDCl3) δ 162.83 (d, J = 11.0 Hz), 160.33 (s), 156.54 (s), 153.11 (s), 147.07 (d, J = 9.2 Hz), 133.09 (s), 132.25 (d, J = 5.1 Hz), 127.99 (s), 126.11 (s), 125.56 (s), 122.25 (d, J = 3.0 Hz), 117.78 (d, J = 22.3 Hz), 114.86 (s), 113.02 (d, J = 24.4 Hz), 42.80 (s), 6.29 (s).
I (d) 153.11
Q (d) 117.78
P (s) 156.54
J (s) 125.56
F (d) 113.02
O (s) 153.11
L (s) 127.99
H (s) 114.86
C (d) 162.83
M (d) 147.07
K (s) 126.11
E (d) 132.25
B (s) 42.80
A (s) 6.29
f1 (ppm)

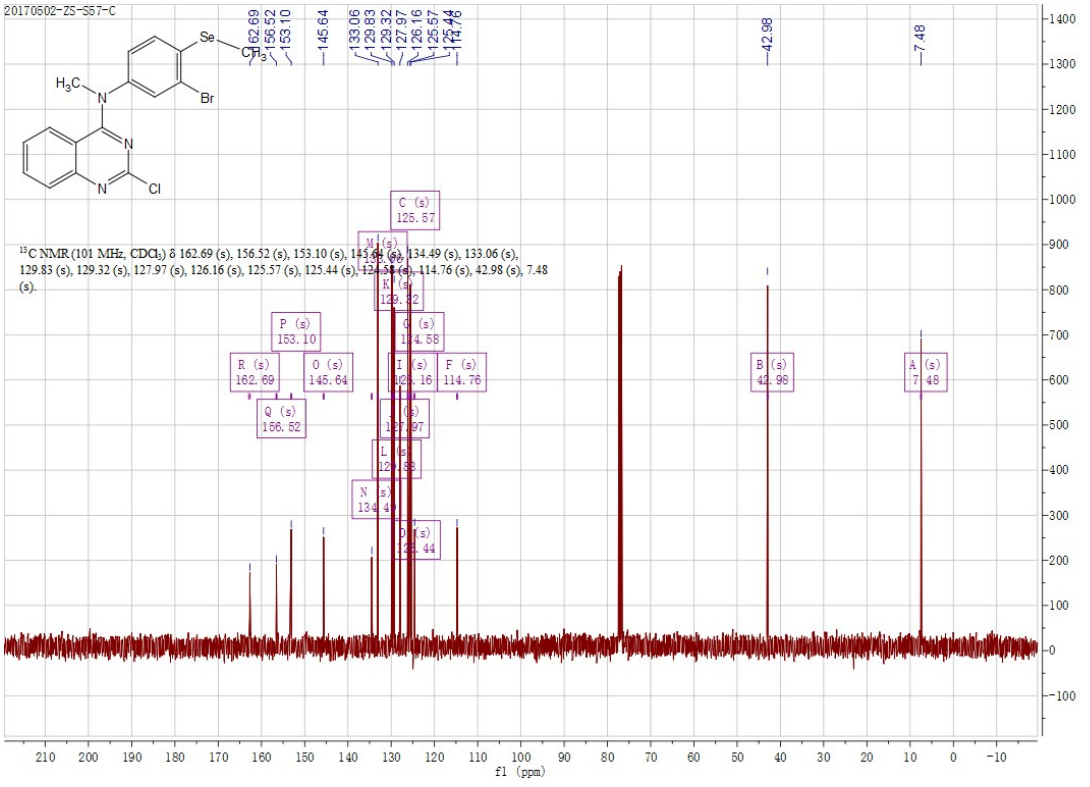
6d


20170320-zs-k27-h
7.78
7.76
7.61
7.25
7.22
7.11
7.10
7.06
7.04
7.02
7.00
3.62
2.37 HDO
D (d) 7.10
B (s) 7.61
A (d) 7.77
C (d) 7.24
E (dd) 7.03
F (s) 3.62
G (s) 2.37
0.99
0.96
2.15
1.02
1.94
3.01
2.95
f1 (ppm)

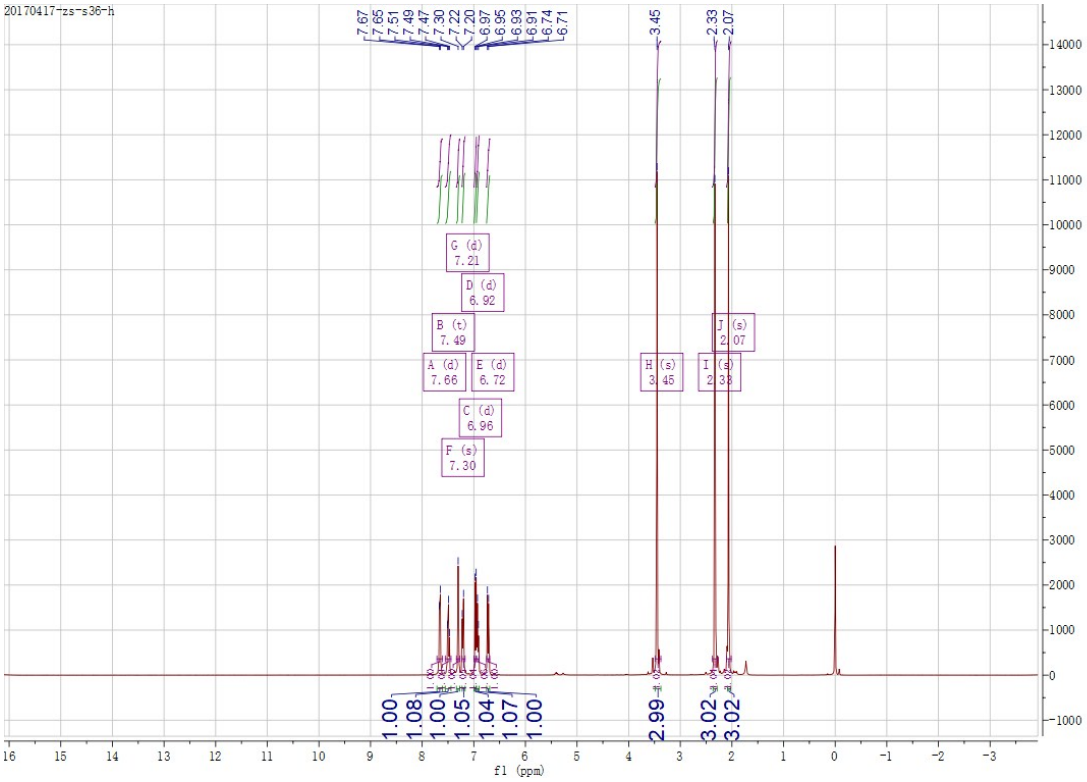

20170320-zs-k27-C
162.71
156.52
153.08
145.70
133.06
129.49
127.96
126.61
126.15
125.56
124.90
114.76
42.94
6.58
Se
CH3
H3C
N
Cl
N
N
Cl
13C NMR (101 MHz, CDCl3) δ 162.71 (s), 156.52 (s), 153.08 (s), 145.70 (s), 134.84 (s), 133.06 (s), 132.06 (s), 129.49 (s), 127.96 (s), 126.61 (s), 126.15 (s), 125.56 (s), 124.90 (s), 114.76 (s), 42.94 (s), 6.58 (s).
N (s) 133.06
Q (s) 153.08
S (s) 162.71
P (s) 145.70
F (s) 114.76
R (s) 156.52
B (s) 42.94
A (s) 6.58
f1 (ppm)

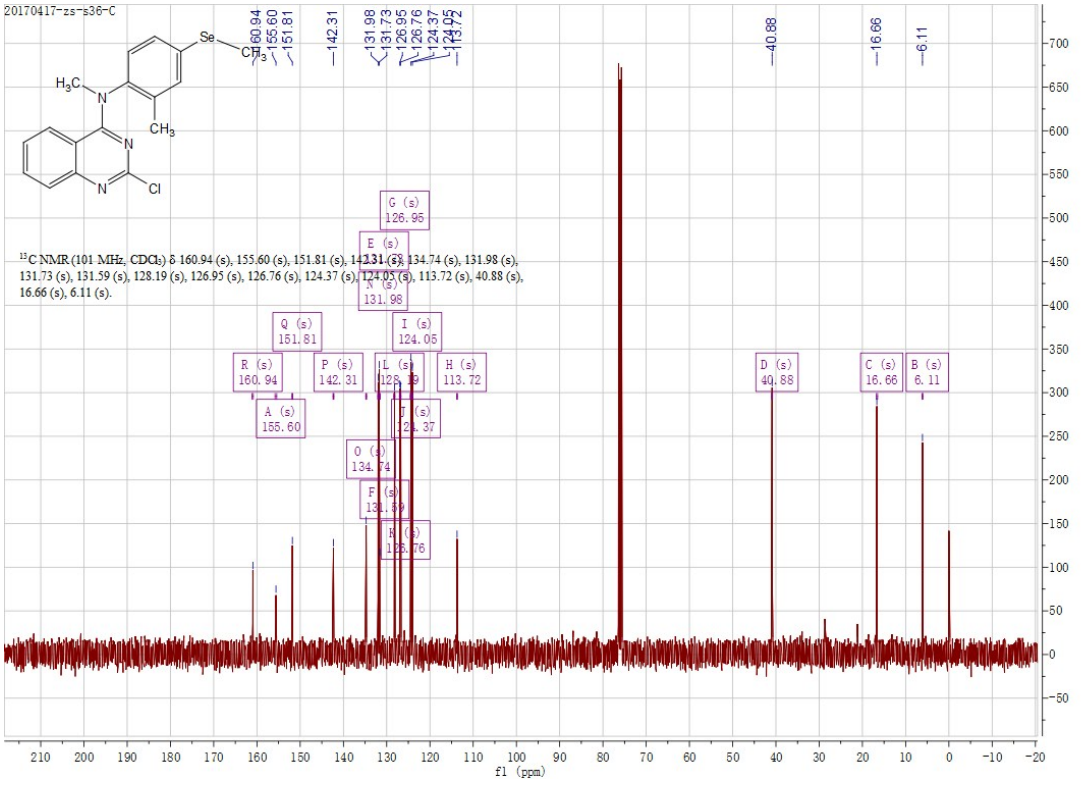
6e


20170502-ZS-S67-H
F (m) 7.05
D (d) 7.19
B (m) 7.42
A (m) 7.61
C (dd) 7.77
E (ddd) 7.11
G (dd) 3.61
H (s) 2.36
0.96
1.00
0.96
0.98
1.00
1.96
3.01
2.92
f1 (ppm)

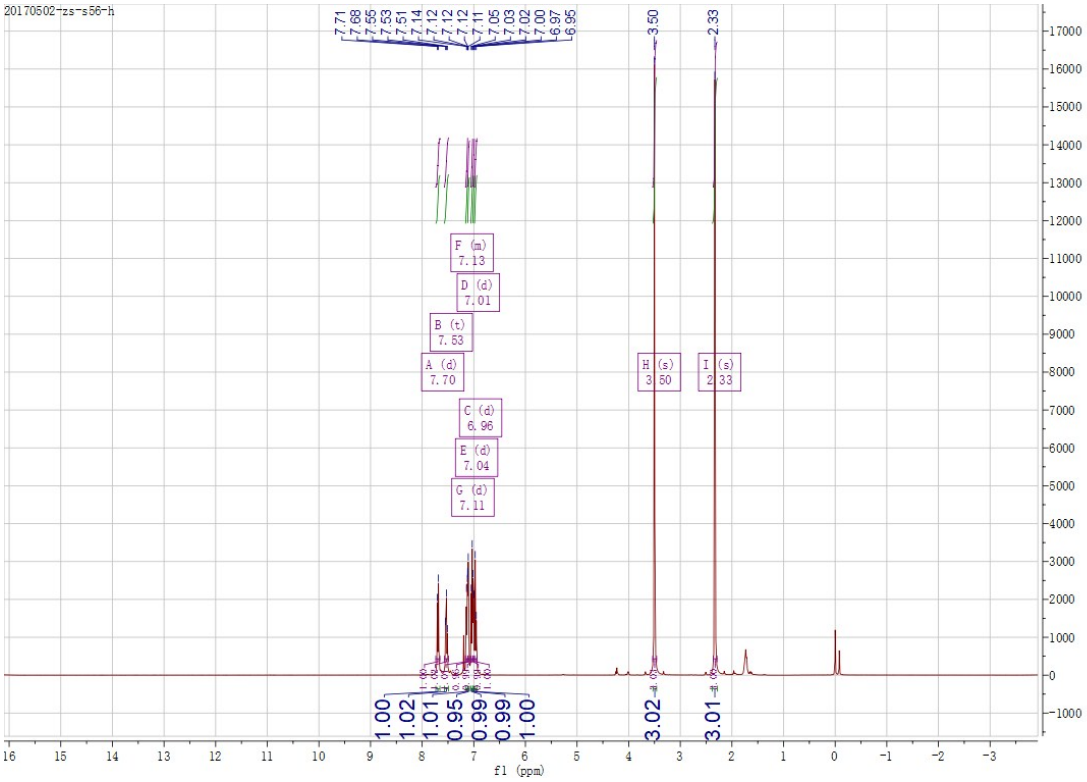

20170502-ZS-S67-C
Se
CH3
H3C
N
Br
N
N
Cl
C (s) 125.57
P (s) 153.10
R (s) 162.69
O (s) 145.64
Q (s) 156.52
I (s) 126.16
F (s) 114.76
B (s) 42.98
A (s) 7.48
f1 (ppm)

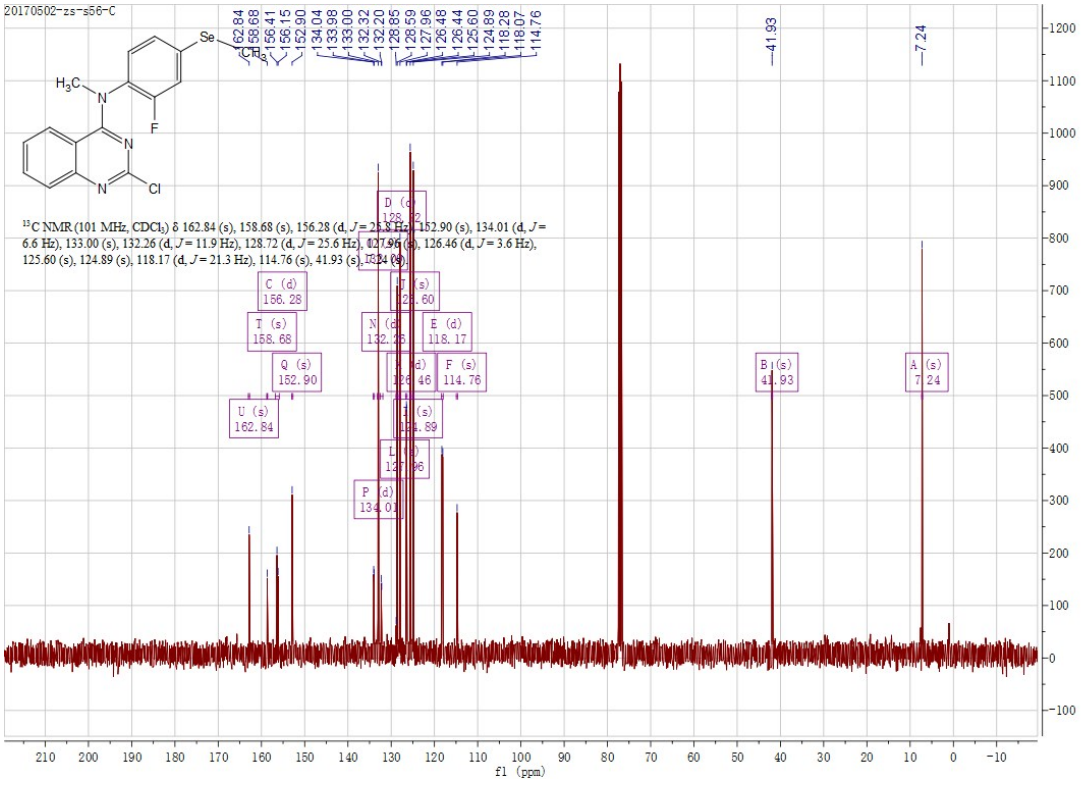
6f


20170417-zs-s36-h
7.67
7.66
7.51
7.49
7.47
7.30
7.22
7.20
6.97
6.95
6.93
6.91
6.74
6.71
3.45
2.33
2.07
G (d) 7.21
D (d) 6.92
B (t) 7.49
A (d) 7.66
E (d) 6.72
C (d) 6.96
F (s) 7.30
H (s) 3.45
I (s) 2.33
J (s) 2.07
1.00
1.08
1.00
1.05
1.04
1.07
1.00
2.99
3.02
3.02
f1 (ppm)

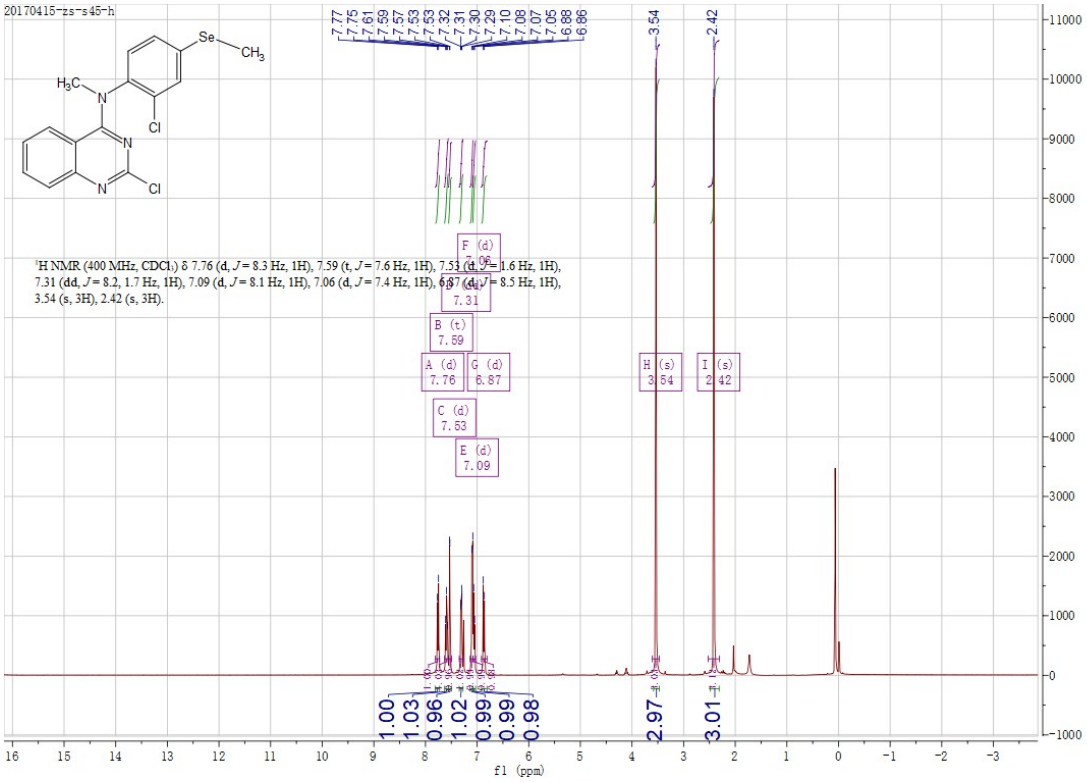

20170417-zs-s36-C
160.94
155.60
151.81
142.31
131.98
131.73
126.95
126.76
124.37
113.72
40.88
16.66
6.11
Se
CH3
H3C
N
CH3
N
N
Cl
13C NMR (101 MHz, CDCl3) δ 160.94 (s), 155.60 (s), 151.81 (s), 142.31 (s), 134.74 (s), 131.98 (s), 131.73 (s), 131.59 (s), 128.19 (s), 126.95 (s), 126.76 (s), 124.37 (s), 124.05 (s), 113.72 (s), 40.88 (s), 16.66 (s), 6.11 (s).
G (s) 126.96
E (s) 131.59
A (s) 131.98
Q (s) 151.81
I (s) 124.05
R (s) 160.94
P (s) 142.31
H (s) 113.72
A (s) 155.60
O (s) 134.74
D (s) 40.88
C (s) 16.66
B (s) 6.11
f1 (ppm)

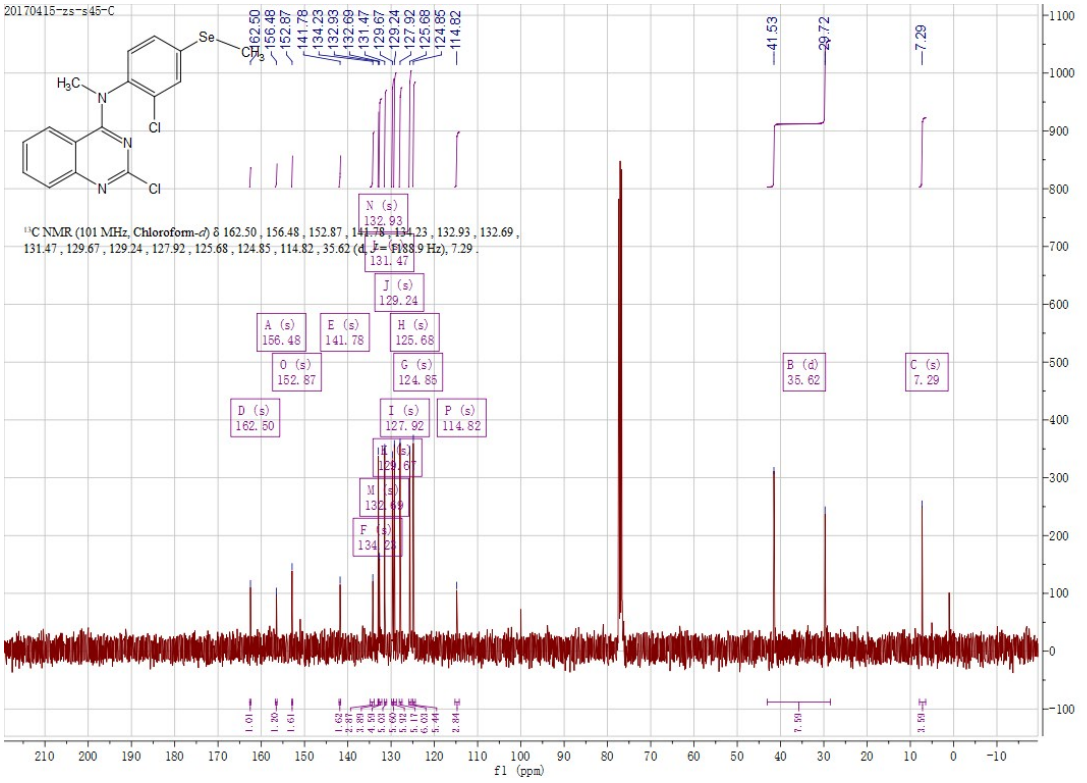
6g


20170502-zs-s66-h
7.71
7.68
7.55
7.53
7.51
7.14
7.12
7.12
7.12
7.11
7.05
7.03
7.02
7.00
6.97
6.95
3.50
2.33
F (m) 7.13
D (d) 7.01
B (t) 7.53
A (d) 7.70
C (d) 6.96
E (d) 7.04
G (d) 7.11
H (s) 3.50
I (s) 2.33
1.00
1.02
1.01
0.95
0.99
0.99
1.00
3.02
3.01
f1 (ppm)

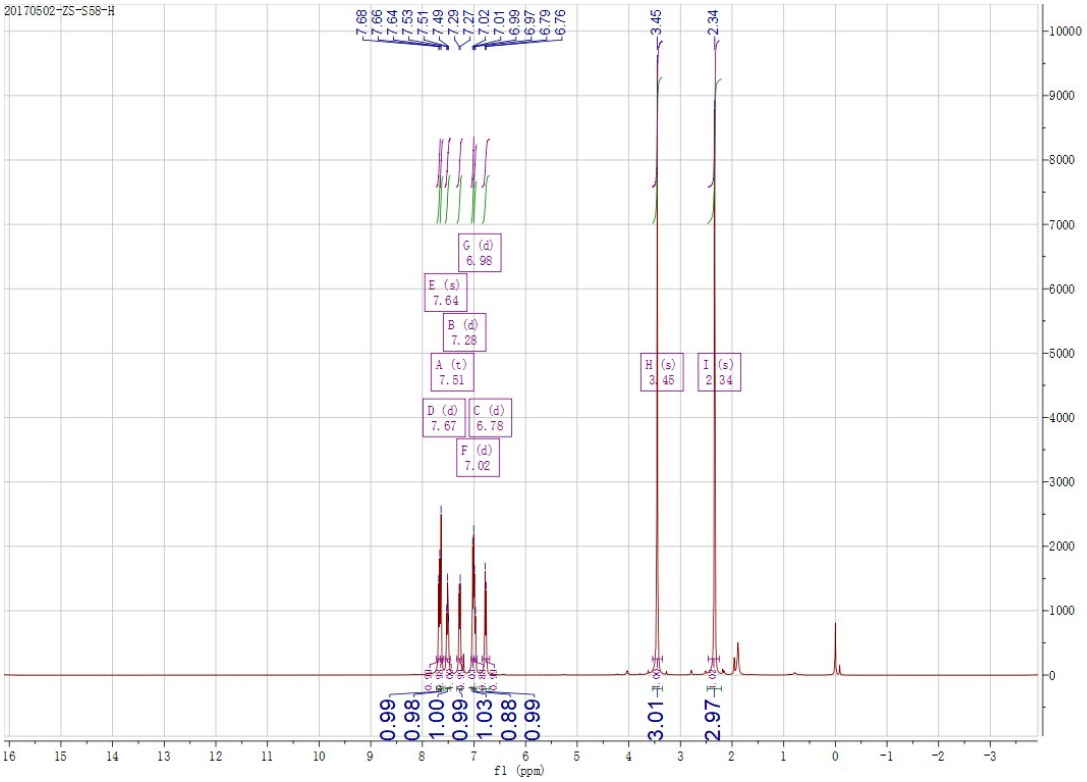

20170502-zs-s66-C
162.84
158.68
156.41
156.15
152.90
134.04
133.98
133.00
132.32
132.20
128.85
128.59
127.96
126.48
126.44
125.60
124.89
118.28
118.07
114.76
41.93
7.24
Se
(CH3)
H3C
N
F
N
N
Cl
13C NMR (101 MHz, CDCl3) δ 162.84 (s), 158.68 (s), 156.28 (d, J = 21.3 Hz), 152.90 (s), 134.01 (d, J = 6.6 Hz), 133.00 (s), 132.26 (d, J = 11.9 Hz), 128.72 (d, J = 25.6 Hz), 127.96 (s), 126.46 (d, J = 3.6 Hz), 125.60 (s), 124.89 (s), 118.17 (d, J = 21.3 Hz), 114.76 (s), 41.93 (s), 7.24 (s).
C (d) 156.28
T (s) 158.68
Q (s) 152.90
U (s) 162.84
B (s) 41.93
A (s) 7.24
f1 (ppm)

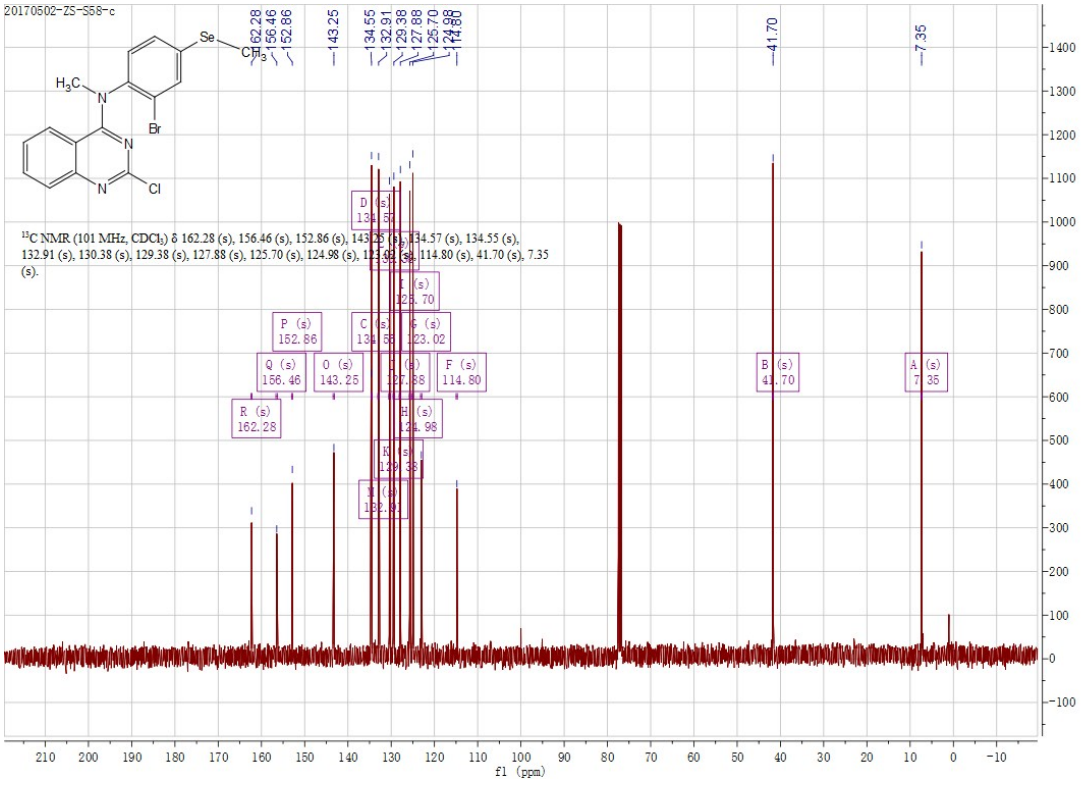
6h


20170415-zs-s45-h
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.76 (d, J = 8.3 Hz, 1H), 7.59 (t, J = 7.6 Hz, 1H), 7.53 (d, J = 1.6 Hz, 1H), 7.31 (dd, J = 8.2, 1.7 Hz, 1H), 7.09 (d, J = 8.1 Hz, 1H), 7.06 (d, J = 7.4 Hz, 1H), 6.87 (d, J = 8.5 Hz, 1H), 3.54 (s, 3H), 2.42 (s, 3H).
f1 (ppm)

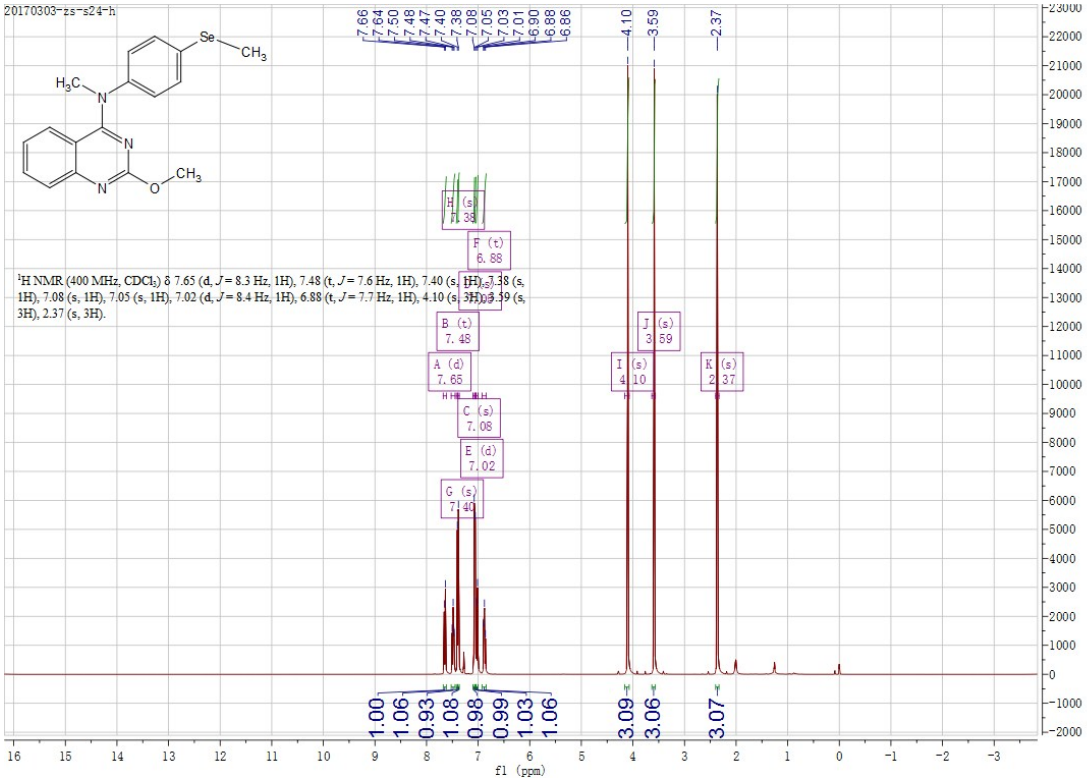

20170415-zs-s45-C
^{13}C NMR (101 MHz, Chloroform-d) δ 162.50 , 156.48 , 152.87 , 141.78 , 134.23 , 132.93 , 132.69 , 131.47 , 129.67 , 129.24 , 127.92 , 125.68 , 124.85 , 114.82 , 35.62 (d, J = 9188.9 Hz), 7.29 .
f1 (ppm)

6i

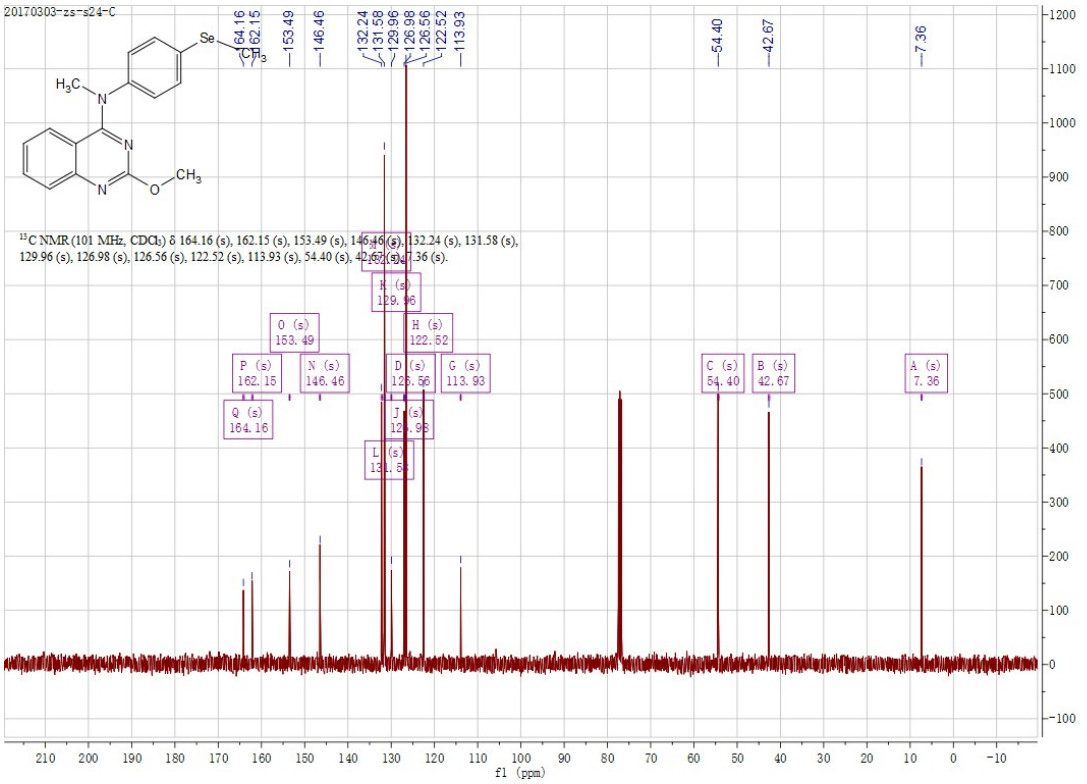

20170502-ZS-S58-H
7.68
7.66
7.64
7.53
7.51
7.49
7.29
7.27
7.02
7.01
6.99
6.97
6.79
6.76
3.45
2.34
G (d) 6.98
E (s) 7.64
B (d) 7.28
A (t) 7.51
D (d) 7.67
C (d) 6.78
F (d) 7.02
H (s) 3.45
I (s) 2.34
0.99
0.98
1.00
0.99
1.03
0.88
0.99
3.01
2.97
f1 (ppm)


20170502-ZS-S58-c
62.28
156.46
152.86
143.25
134.55
132.91
129.38
127.88
125.70
124.98
114.80
41.70
7.35
Se
CH3
H3C
N
Br
N
N
Cl
13C NMR (101 MHz, CDCl3) δ 162.28 (s), 156.46 (s), 152.86 (s), 143.25 (s), 134.57 (s), 134.55 (s), 132.91 (s), 130.38 (s), 129.38 (s), 127.88 (s), 125.70 (s), 124.98 (s), 123.02 (s), 114.80 (s), 41.70 (s), 7.35 (s).
D (s) 134.55
P (s) 152.86
Q (s) 156.46
O (s) 143.25
F (s) 114.80
R (s) 162.28
B (s) 41.70
A (s) 7.35
f1 (ppm)

7a

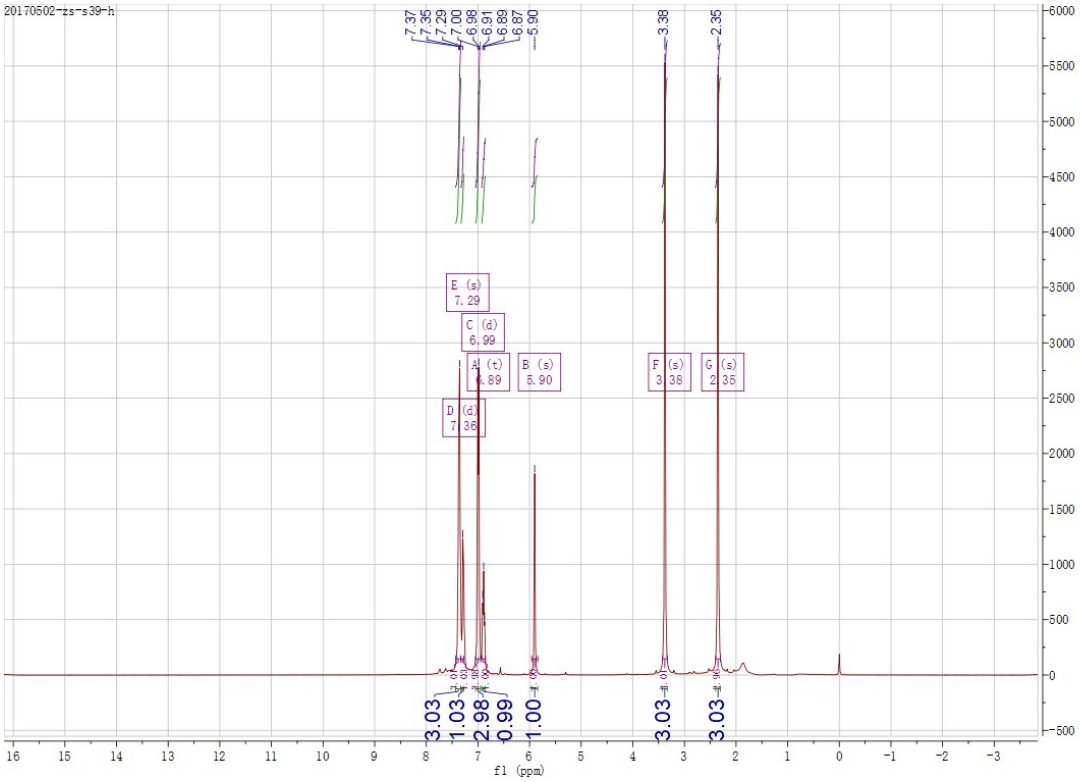


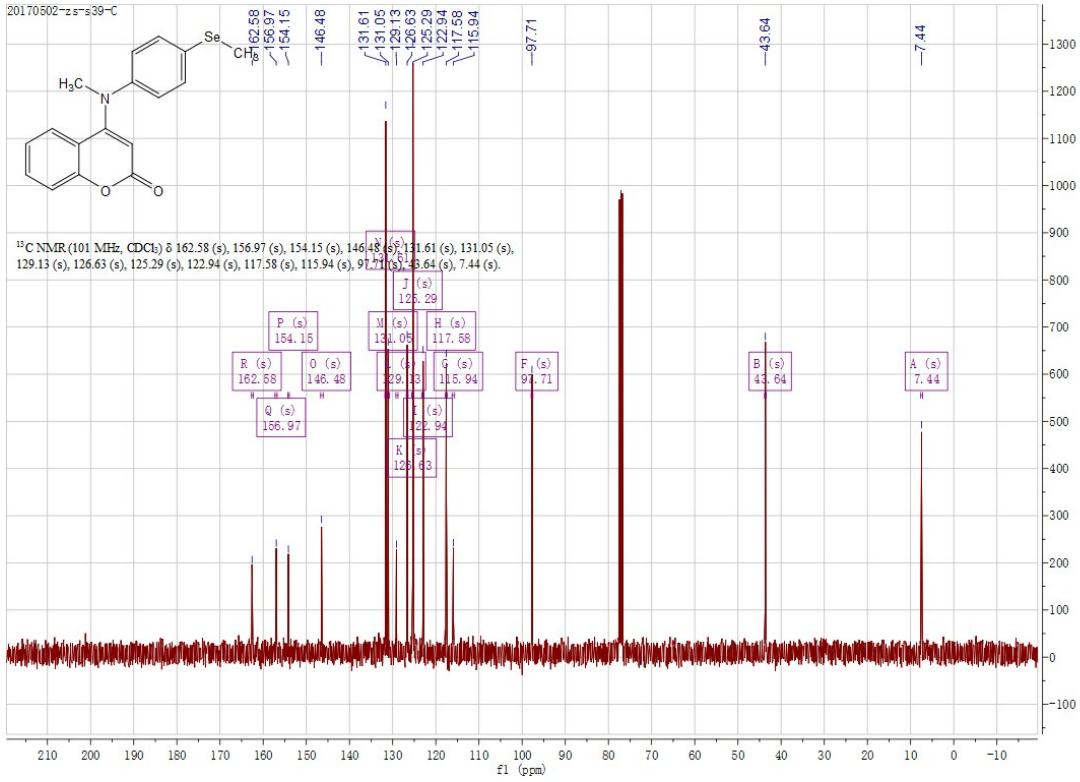
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 8.3 Hz, 1H), 7.48 (t, J = 7.6 Hz, 1H), 7.40 (s, 1H), 7.38 (s, 1H), 7.08 (s, 1H), 7.05 (s, 1H), 7.02 (d, J = 8.4 Hz, 1H), 6.88 (t, J = 7.7 Hz, 1H), 4.10 (s, 3H), 3.59 (s, 3H), 2.37 (s, 3H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 164.16 (s), 162.15 (s), 153.49 (s), 146.46 (s), 132.24 (s), 131.58 (s), 129.96 (s), 126.98 (s), 126.56 (s), 122.52 (s), 113.93 (s), 54.40 (s), 42.67 (s), 7.36 (s).

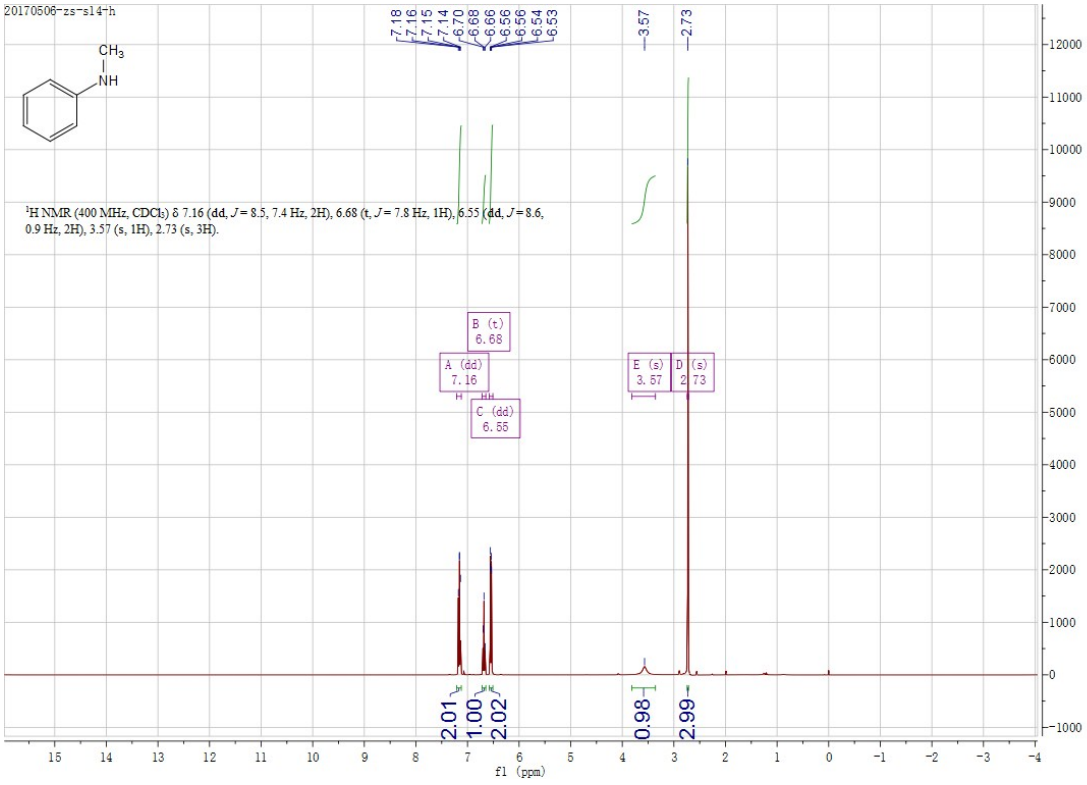
10

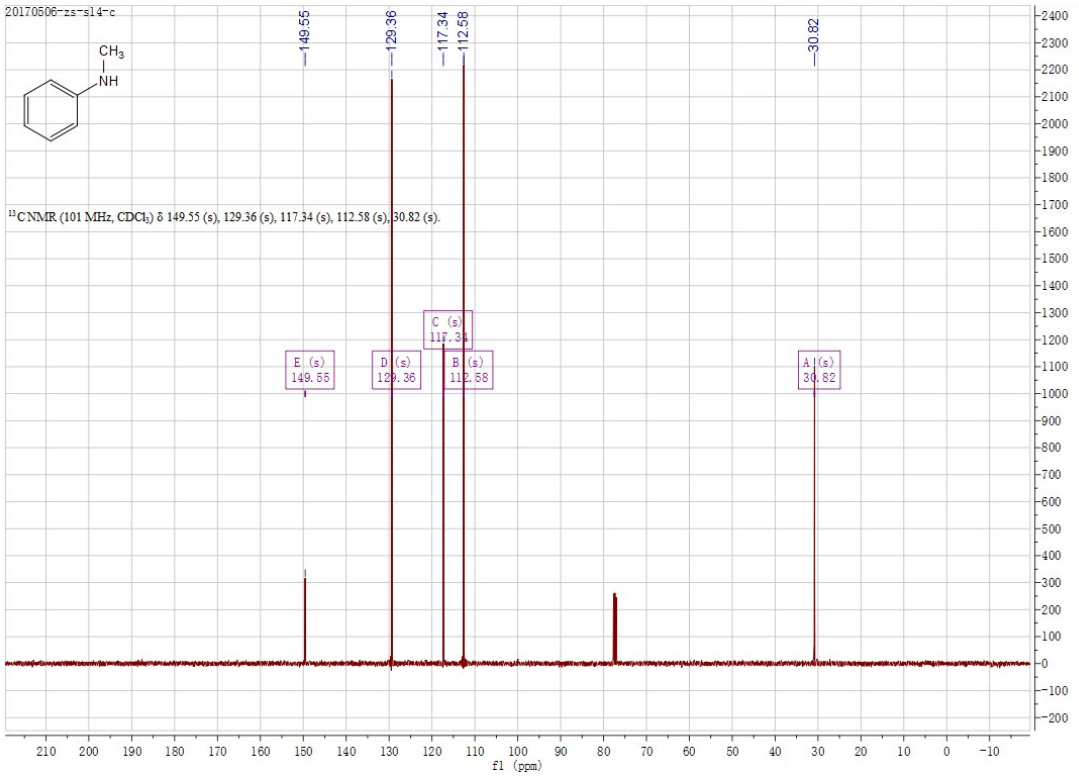

20170502-zs-s39-h
7.37
7.35
7.29
7.00
6.98
6.91
6.89
6.87
5.90
3.38
2.35
E (s) 7.29
C (d) 6.99
A (t) 6.89
B (s) 5.90
F (s) 3.38
G (s) 2.35
D (d) 7.36
3.03
1.03
2.98
0.99
1.00
3.03
3.03
f1 (ppm)


20170502-zs-s39-C
162.58
156.97
154.15
146.48
131.61
131.05
129.13
126.63
125.29
122.94
117.58
115.94
97.71
43.64
7.44
Se
CH2
H3C
N
O
O
13C NMR (101 MHz, CDCl3) δ 162.58 (s), 156.97 (s), 154.15 (s), 146.48 (s), 131.61 (s), 131.05 (s), 129.13 (s), 126.63 (s), 125.29 (s), 122.94 (s), 117.58 (s), 115.94 (s), 97.71 (s), 43.64 (s), 7.44 (s).
P (s) 154.15
R (s) 162.58
O (s) 146.48
Q (s) 156.97
M (s) 131.05
H (s) 117.58
G (s) 115.94
F (s) 97.71
B (s) 43.64
A (s) 7.44
f1 (ppm)

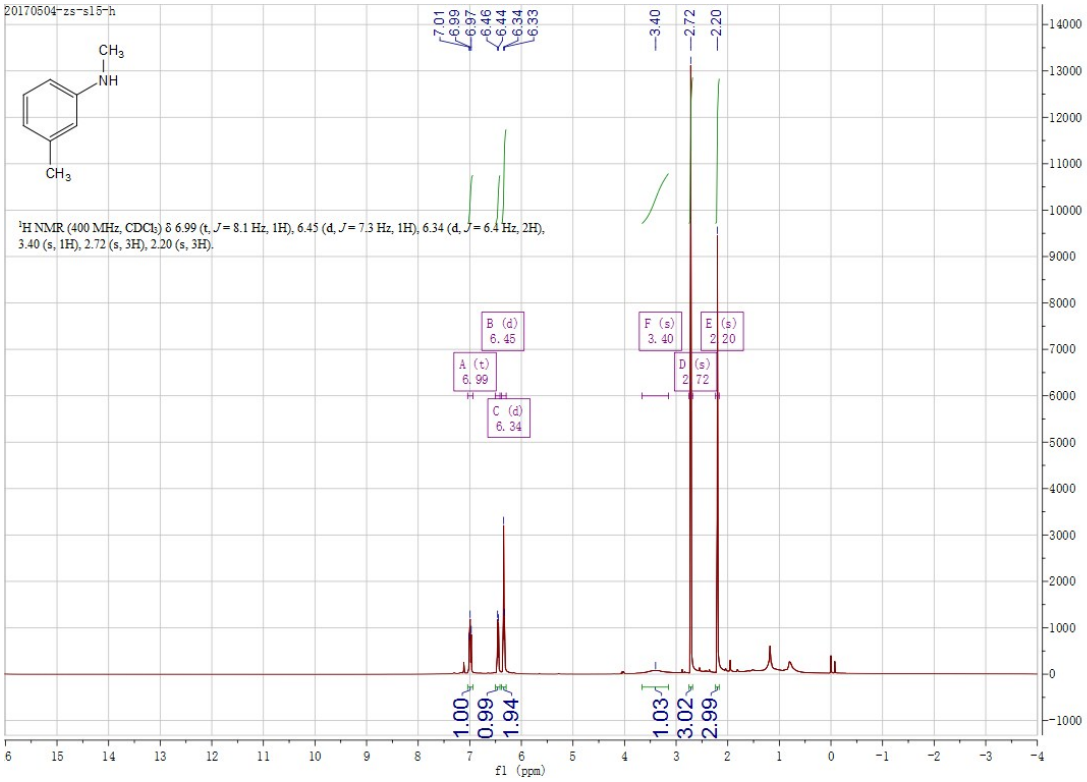
SI2. NMR spectrums of intermediate compounds

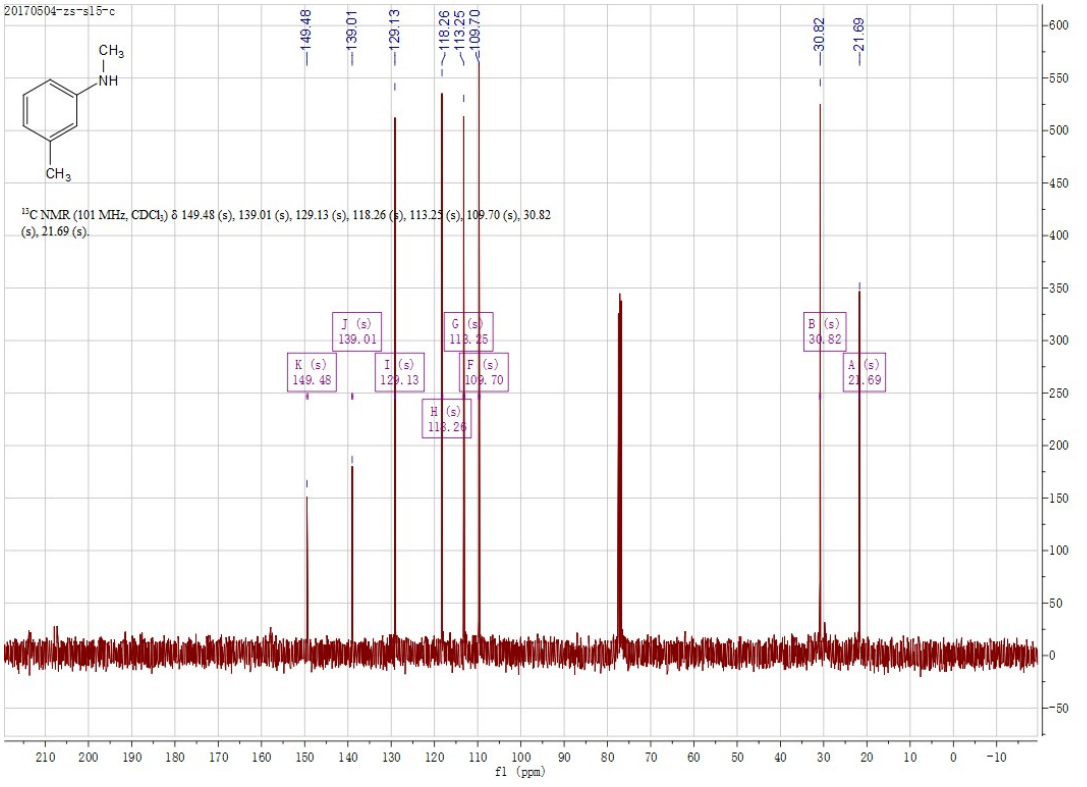
2a



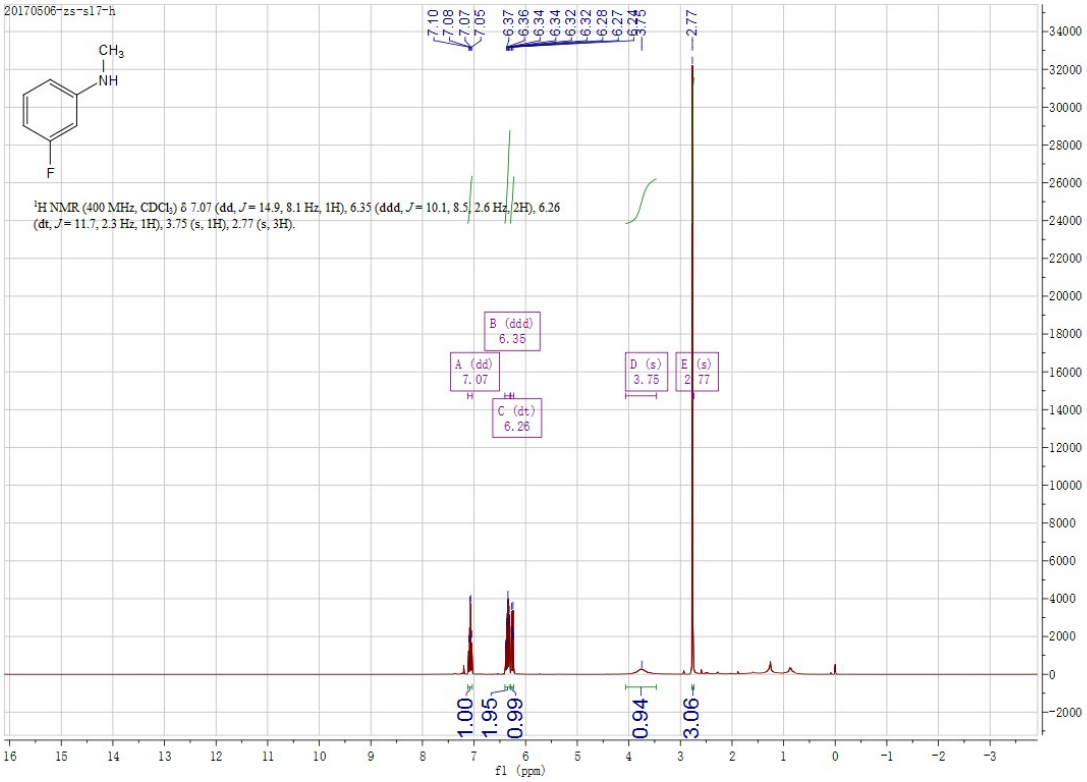


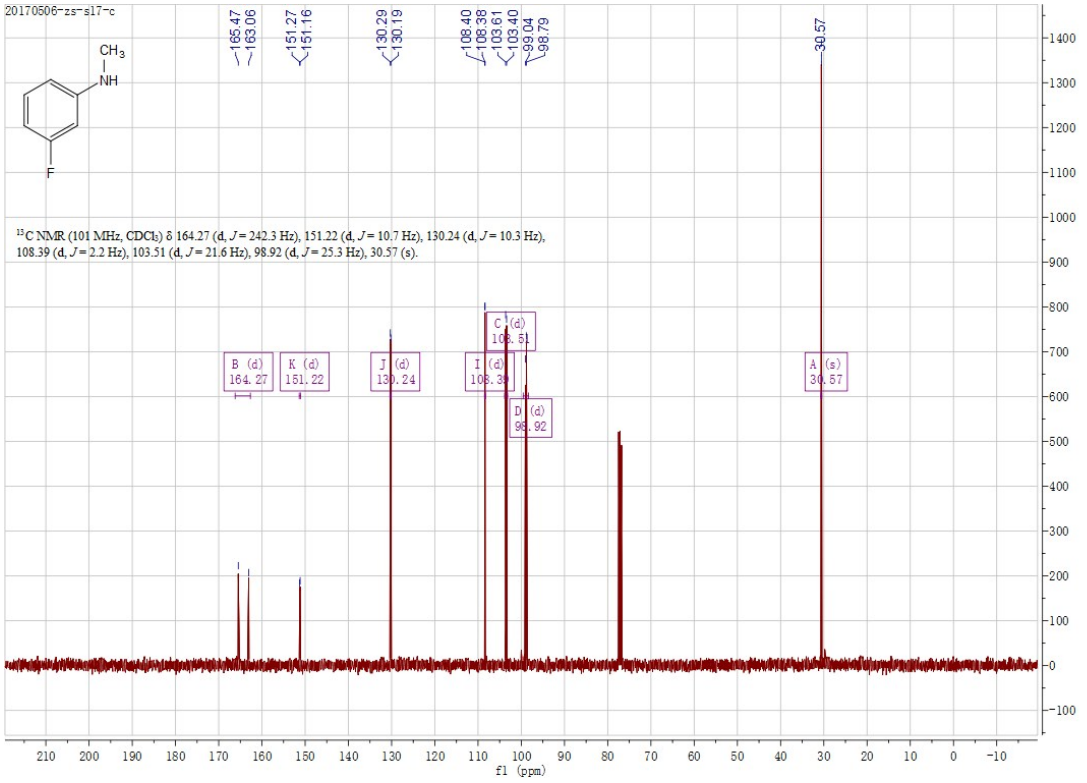
2b


20170504-zs-s15-h
CH3
NH
CH3
7.01
6.99
6.97
6.46
6.44
6.34
6.33
3.40
2.72
2.20
1H NMR (400 MHz, CDCl3) δ 6.99 (t, J = 8.1 Hz, 1H), 6.45 (d, J = 7.3 Hz, 1H), 6.34 (d, J = 6.4 Hz, 2H), 3.40 (s, 1H), 2.72 (s, 3H), 2.20 (s, 3H).
B (d) 6.45
A (t) 6.99
C (d) 6.34
F (s) 3.40
D (s) 2.72
E (s) 2.20
1.00
0.99
1.94
1.03
3.02
2.99
f1 (ppm)

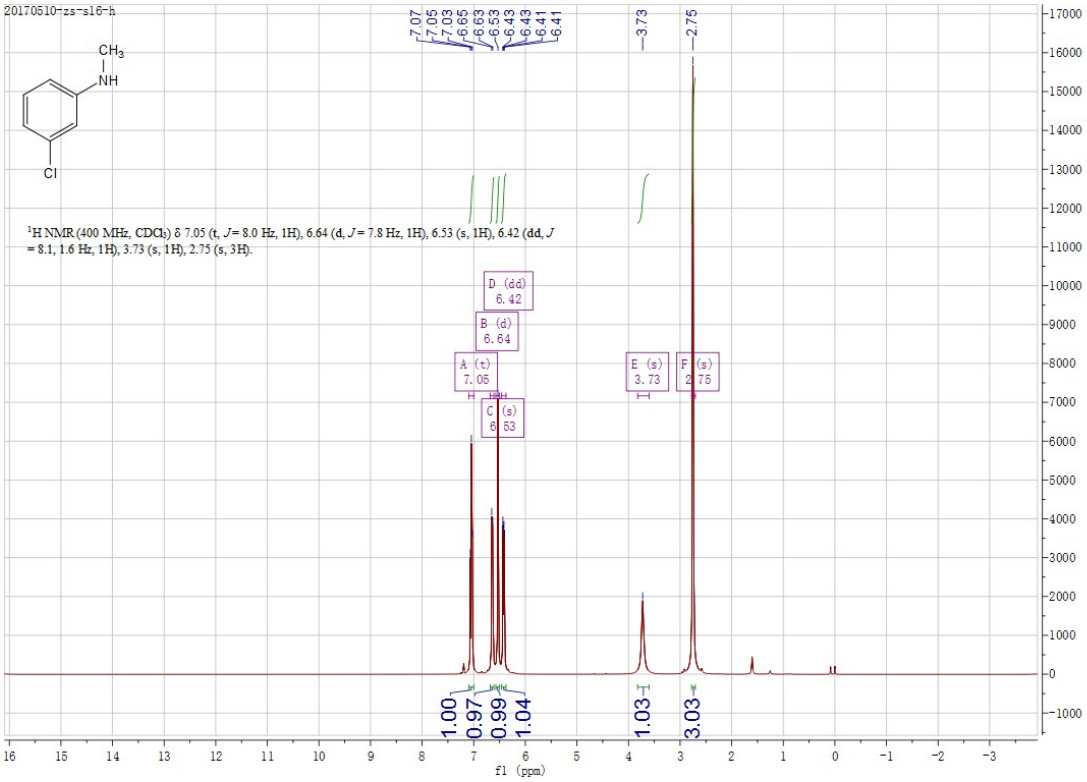

20170504-zs-s15-c
CH3
NH
CH3
149.48
139.01
129.13
118.26
113.25
109.70
30.82
21.69
13C NMR (101 MHz, CDCl3) δ 149.48 (s), 139.01 (s), 129.13 (s), 118.26 (s), 113.25 (s), 109.70 (s), 30.82 (s), 21.69 (s).
J (s) 139.01
K (s) 149.48
I (s) 129.13
G (s) 113.25
F (s) 109.70
H (s) 118.26
B (s) 30.82
A (s) 21.69
f1 (ppm)

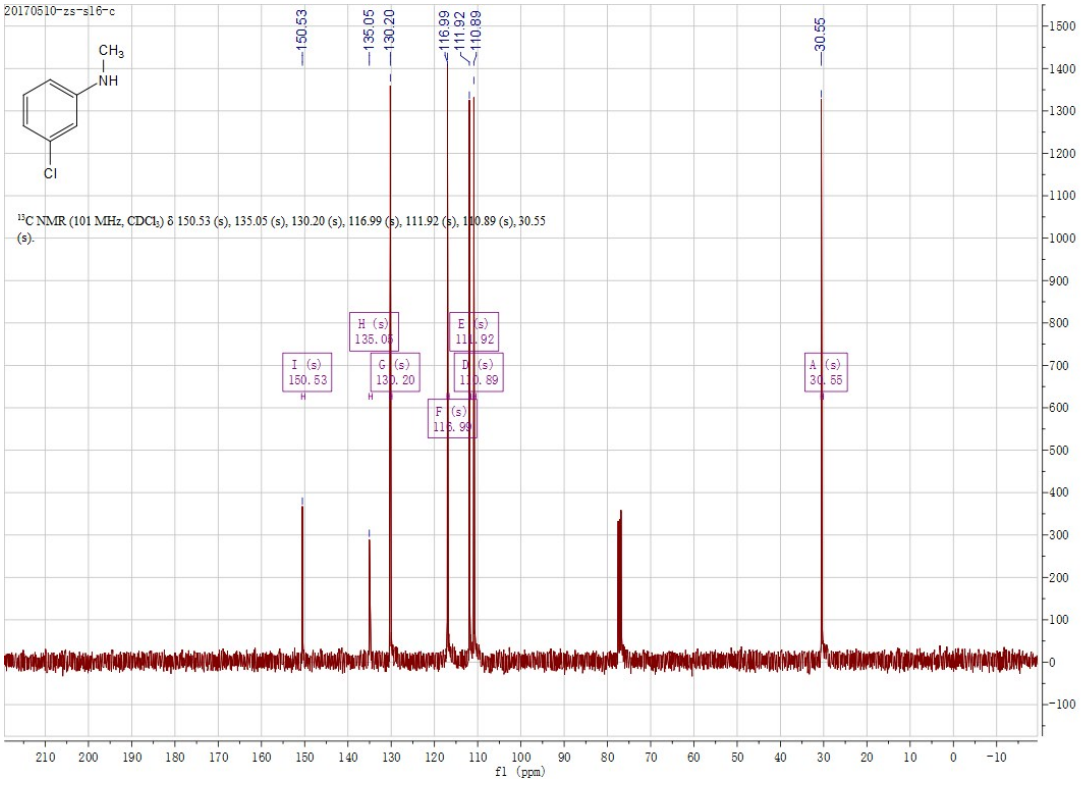
2c


20170606-zs-s17-h
CH3
NH
F
7.10
7.08
7.07
7.05
6.37
6.36
6.34
6.34
6.32
6.32
6.28
6.27
3.75
2.77
1H NMR (400 MHz, CDCl3) δ 7.07 (dd, J = 14.9, 8.1 Hz, 1H), 6.35 (ddd, J = 10.1, 8.5, 2.6 Hz, 2H), 6.26 (dt, J = 11.7, 2.3 Hz, 1H), 3.75 (s, 1H), 2.77 (s, 3H).
B (ddd) 6.35
A (dd) 7.07
C (dt) 6.26
D (s) 3.75
E (s) 2.77
1.00
1.95
0.99
0.94
3.06
f1 (ppm)

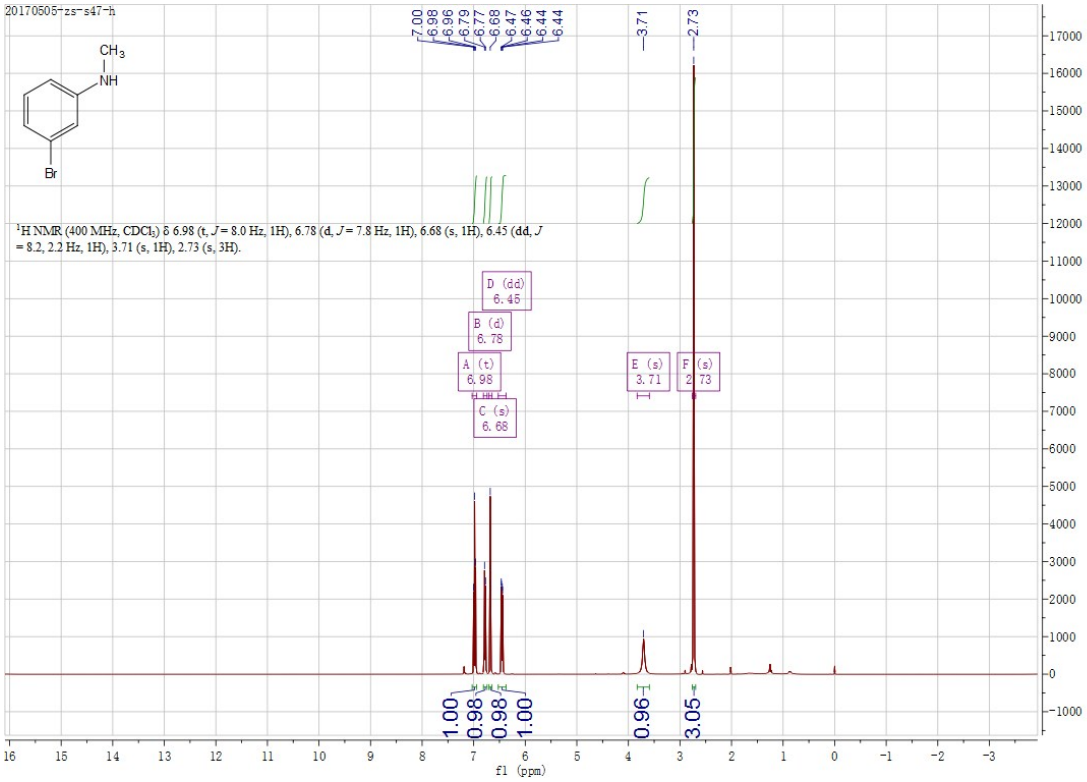

20170606-zs-s17-c
CH3
NH
F
165.47
163.06
151.27
151.16
130.29
130.19
108.40
108.38
103.61
103.40
99.04
98.79
30.57
13C NMR (101 MHz, CDCl3) δ 164.27 (d, J = 242.3 Hz), 151.22 (d, J = 10.7 Hz), 130.24 (d, J = 10.3 Hz), 108.39 (d, J = 2.2 Hz), 103.51 (d, J = 21.6 Hz), 98.92 (d, J = 25.3 Hz), 30.57 (s).
B (d) 164.27
K (d) 151.22
J (d) 130.24
I (d) 108.39
C (d) 103.51
D (d) 98.92
A (s) 30.57
f1 (ppm)

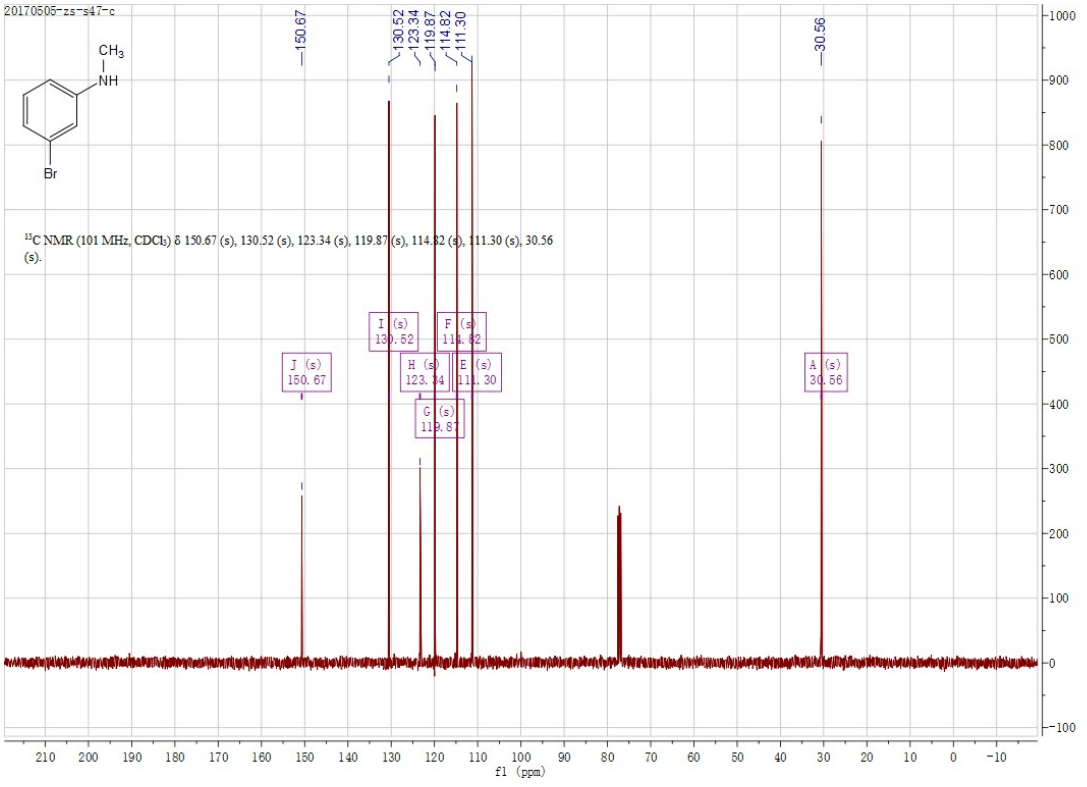
2d


20170510-zs-s16-h
CH3
NH
Cl
7.07
7.05
7.03
6.66
6.63
6.53
6.43
6.41
6.41
3.73
2.75
1H NMR (400 MHz, CDCl3) δ 7.05 (t, J = 8.0 Hz, 1H), 6.64 (d, J = 7.8 Hz, 1H), 6.53 (s, 1H), 6.42 (dd, J = 8.1, 1.6 Hz, 1H), 3.73 (s, 1H), 2.75 (s, 3H).
D (dd) 6.42
B (d) 6.64
A (t) 7.05
C (s) 6.53
E (s) 3.73
F (s) 2.75
1.00
0.97
0.99
1.04
1.03
3.03
f1 (ppm)

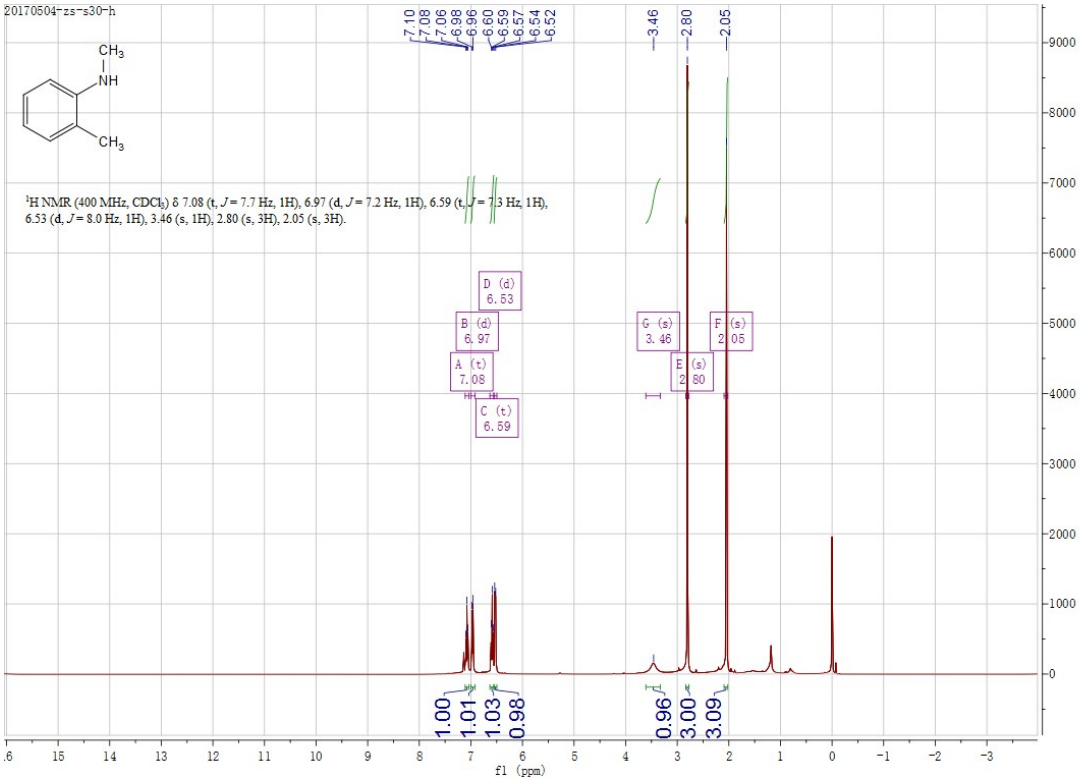

20170510-zs-s16-c
CH3
NH
Cl
150.53
135.05
130.20
116.99
111.92
110.89
30.55
13C NMR (101 MHz, CDCl3) δ 150.53 (s), 135.05 (s), 130.20 (s), 116.99 (s), 111.92 (s), 110.89 (s), 30.55 (s).
I (s) 150.53
H (s) 135.05
G (s) 130.20
F (s) 116.99
E (s) 111.92
D (s) 110.89
A (s) 30.55
f1 (ppm)

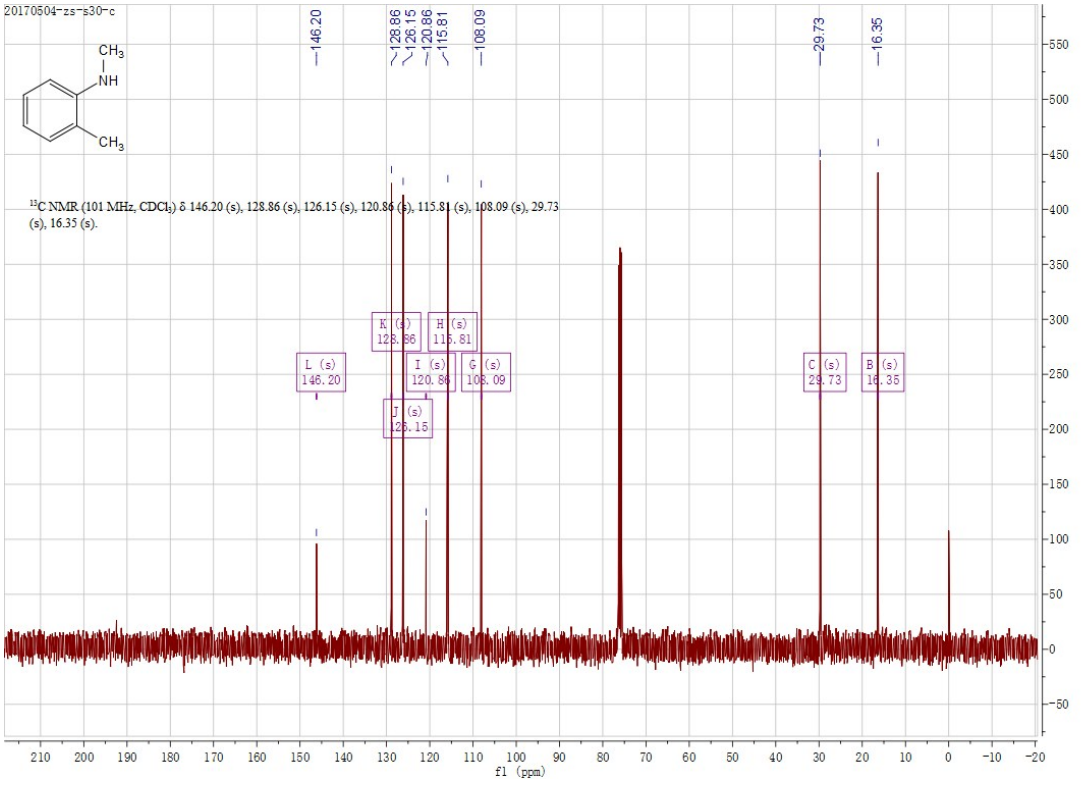
2e


20170506-zs-s47-h
CH3
NH
Br
7.00
6.98
6.96
6.79
6.77
6.68
6.47
6.46
6.44
6.44
3.71
2.73
1H NMR (400 MHz, CDCl3) δ 6.98 (t, J = 8.0 Hz, 1H), 6.78 (d, J = 7.8 Hz, 1H), 6.68 (s, 1H), 6.45 (dd, J = 8.2, 2.2 Hz, 1H), 3.71 (s, 1H), 2.73 (s, 3H).
D (dd) 6.45
B (d) 6.78
A (t) 6.98
C (s) 6.68
E (s) 3.71
F (s) 2.73
1.00
0.98
0.98
1.00
0.96
3.05
f1 (ppm)

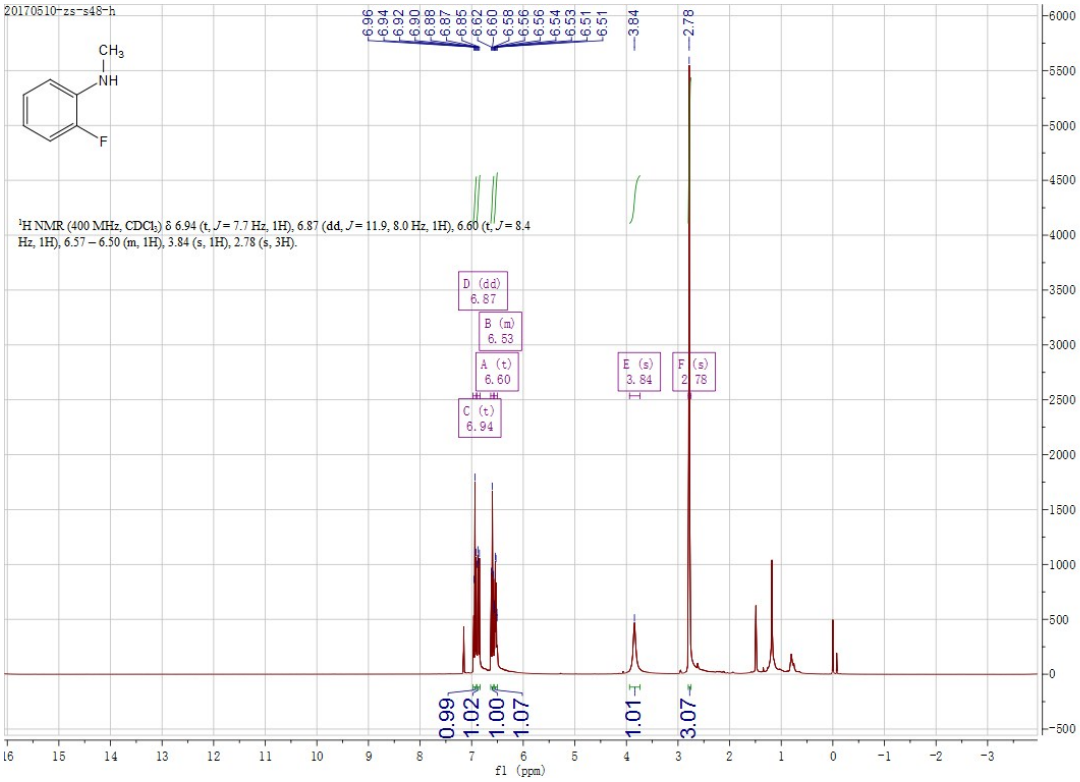

20170506-zs-s47-c
CH3
NH
Br
150.67
130.52
123.34
119.87
114.82
111.30
30.56
13C NMR (101 MHz, CDCl3) δ 150.67 (s), 130.52 (s), 123.34 (s), 119.87 (s), 114.82 (s), 111.30 (s), 30.56 (s).
I (s) 130.52
F (s) 114.82
J (s) 150.67
H (s) 123.34
E (s) 111.30
G (s) 119.87
A (s) 30.56
f1 (ppm)

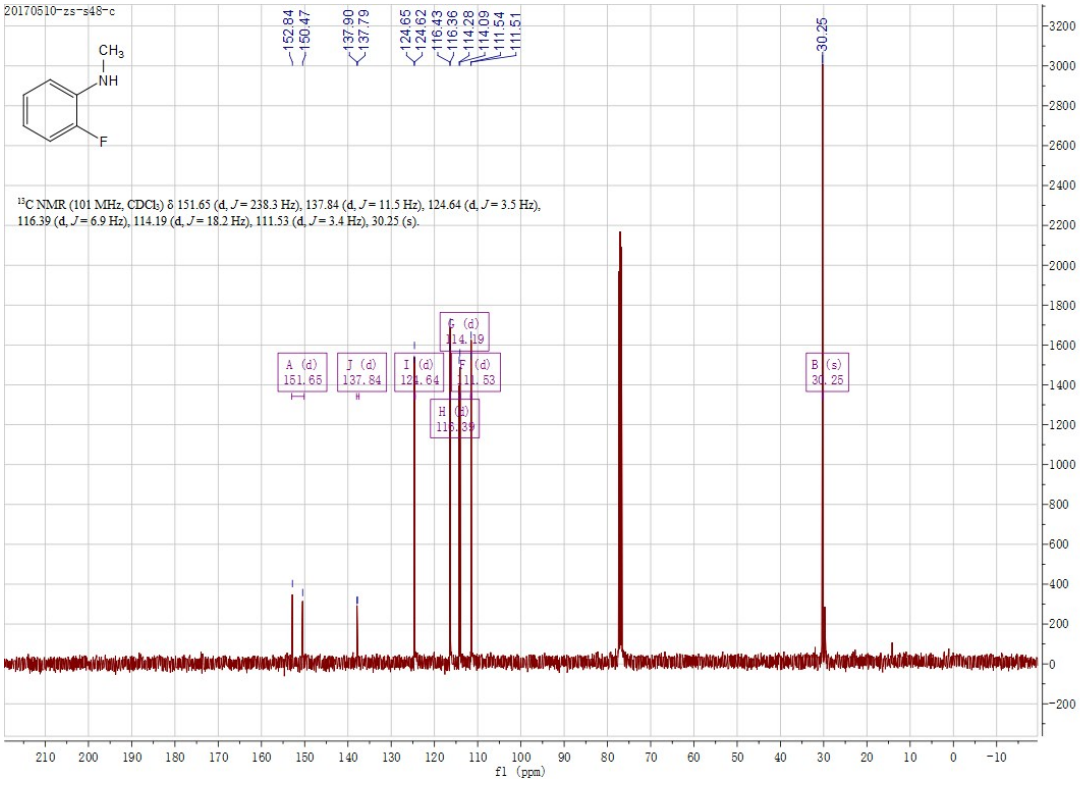
2f


20170504-zs-s30-h
CH3
NH
CH3
7.10
7.08
7.06
6.98
6.96
6.60
6.59
6.57
6.54
6.52
3.46
2.80
2.05
1H NMR (400 MHz, CDCl3) δ 7.08 (t, J = 7.7 Hz, 1H), 6.97 (d, J = 7.2 Hz, 1H), 6.59 (t, J = 7.3 Hz, 1H), 6.53 (d, J = 8.0 Hz, 1H), 3.46 (s, 1H), 2.80 (s, 3H), 2.05 (s, 3H).
D (d) 6.53
B (d) 6.97
A (t) 7.08
C (t) 6.59
G (s) 3.46
F (s) 2.05
E (s) 2.80
1.00
1.01
1.03
0.98
0.96
3.00
3.09
f1 (ppm)

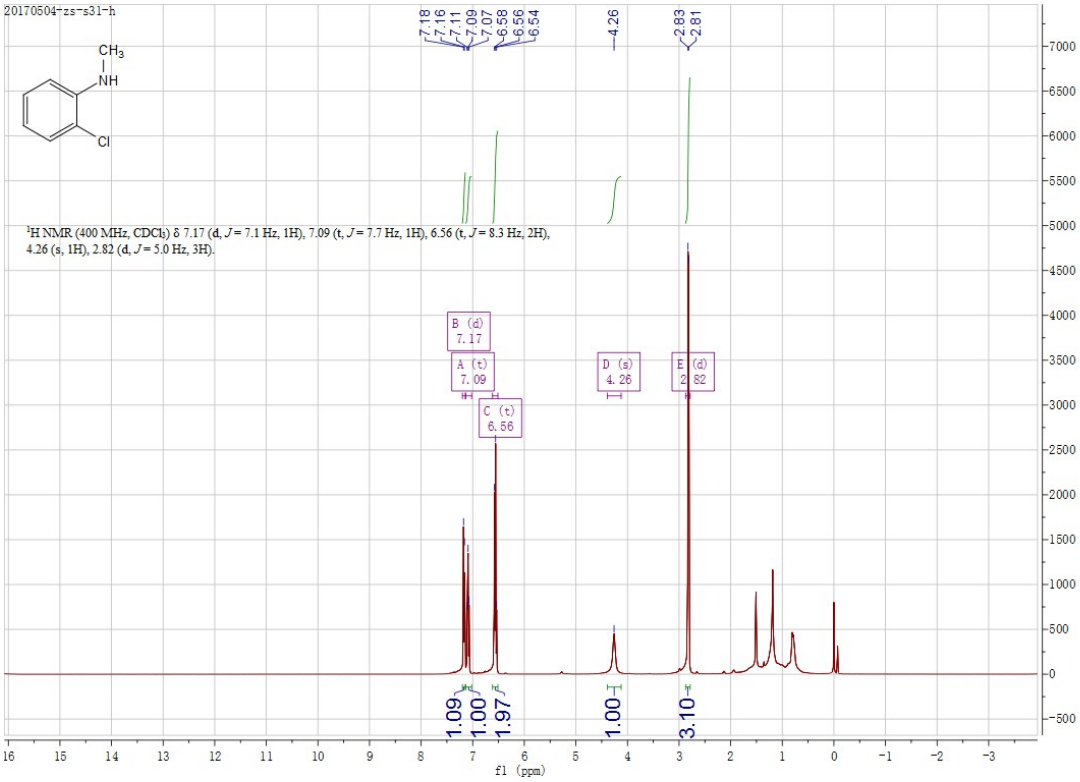

20170504-zs-s30-c
CH3
NH
CH3
146.20
128.86
126.15
120.86
115.81
108.09
29.73
16.35
13C NMR (101 MHz, CDCl3) δ 146.20 (s), 128.86 (s), 126.15 (s), 120.86 (s), 115.81 (s), 108.09 (s), 29.73 (s), 16.35 (s).
K (s) 128.86
H (s) 115.81
L (s) 146.20
I (s) 120.86
G (s) 108.09
J (s) 126.15
C (s) 29.73
B (s) 16.35
f1 (ppm)

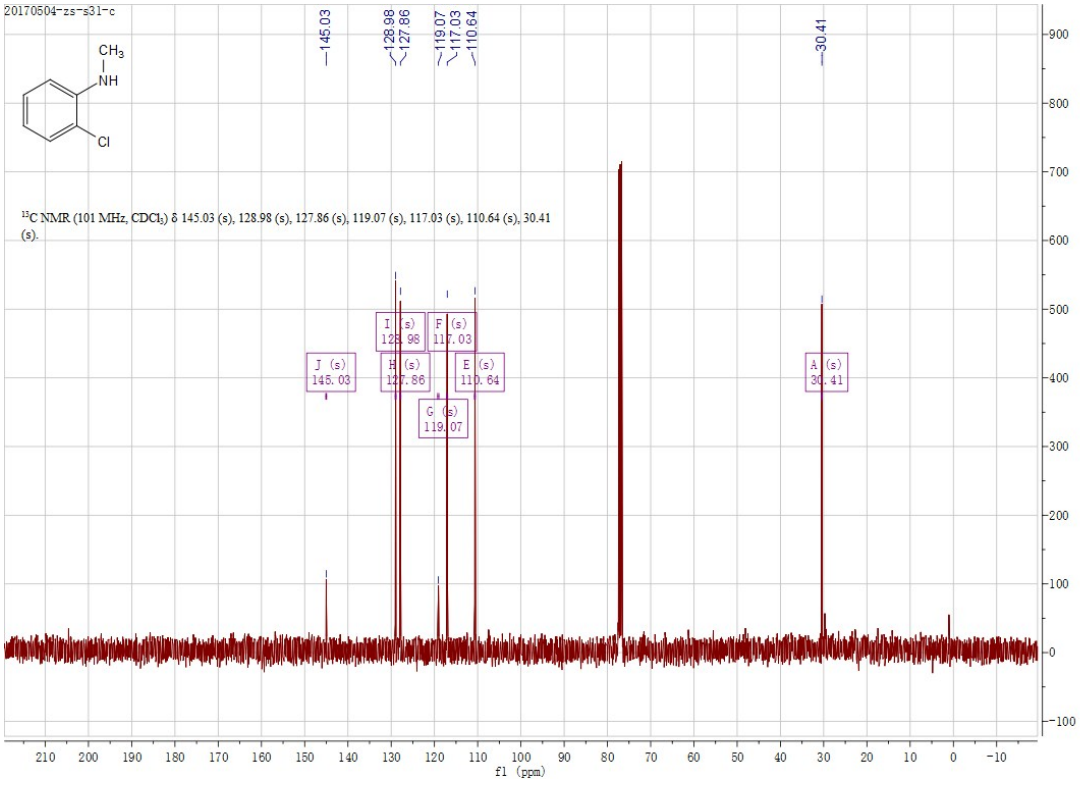
2g


20170510-zs-s48-h
CH3
NH
F
6.96
6.94
6.92
6.90
6.88
6.87
6.85
6.62
6.60
6.58
6.56
6.56
6.54
6.53
6.51
6.51
3.84
2.78
1H NMR (400 MHz, CDCl3) δ 6.94 (t, J = 7.7 Hz, 1H), 6.87 (dd, J = 11.9, 8.0 Hz, 1H), 6.60 (t, J = 8.4 Hz, 1H), 6.57 – 6.50 (m, 1H), 3.84 (s, 1H), 2.78 (s, 3H).
D (dd) 6.87
B (m) 6.53
A (t) 6.60
C (t) 6.94
E (s) 3.84
F (s) 2.78
0.99
1.02
1.00
1.07
1.01
3.07
f1 (ppm)

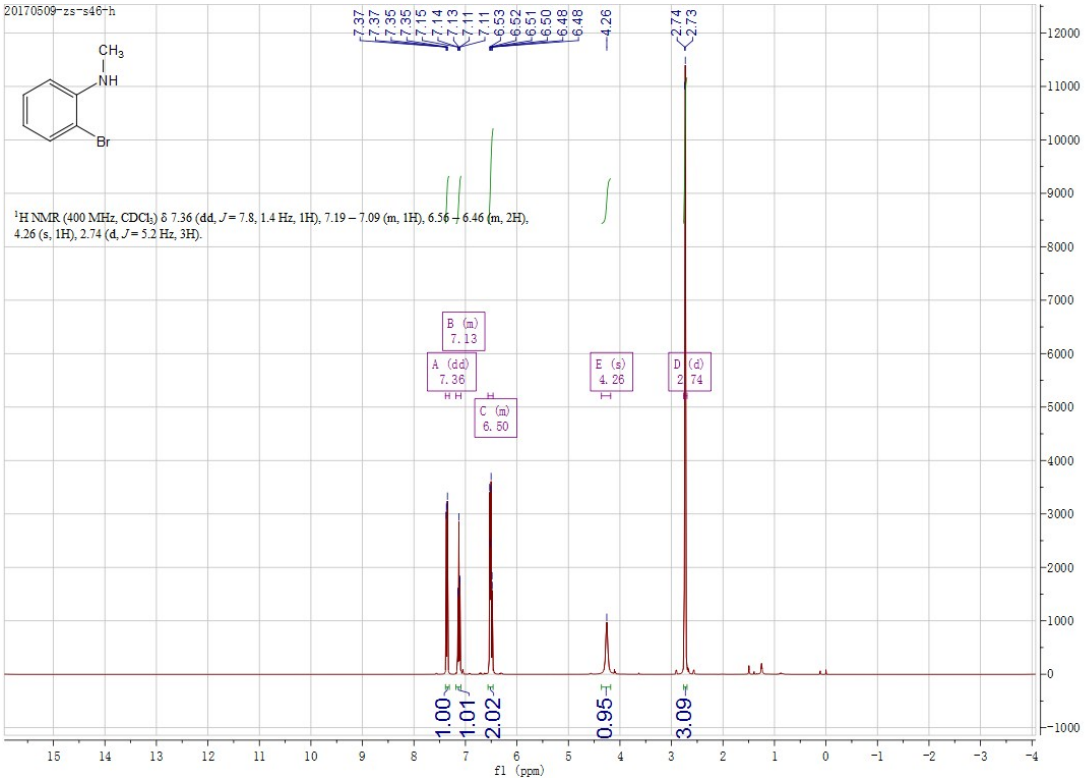

20170510-zs-s48-c
CH3
NH
F
152.84
150.47
137.90
137.79
124.65
124.62
116.43
116.36
114.28
114.09
111.54
111.51
30.25
13C NMR (101 MHz, CDCl3) δ 151.65 (d, J = 238.3 Hz), 137.84 (d, J = 11.5 Hz), 124.64 (d, J = 3.5 Hz), 116.39 (d, J = 6.9 Hz), 114.19 (d, J = 18.2 Hz), 111.53 (d, J = 3.4 Hz), 30.25 (s).
A (d) 151.65
J (d) 137.84
I (d) 124.64
G (d) 114.19
F (d) 111.53
H (d) 116.39
B (s) 30.25
f1 (ppm)

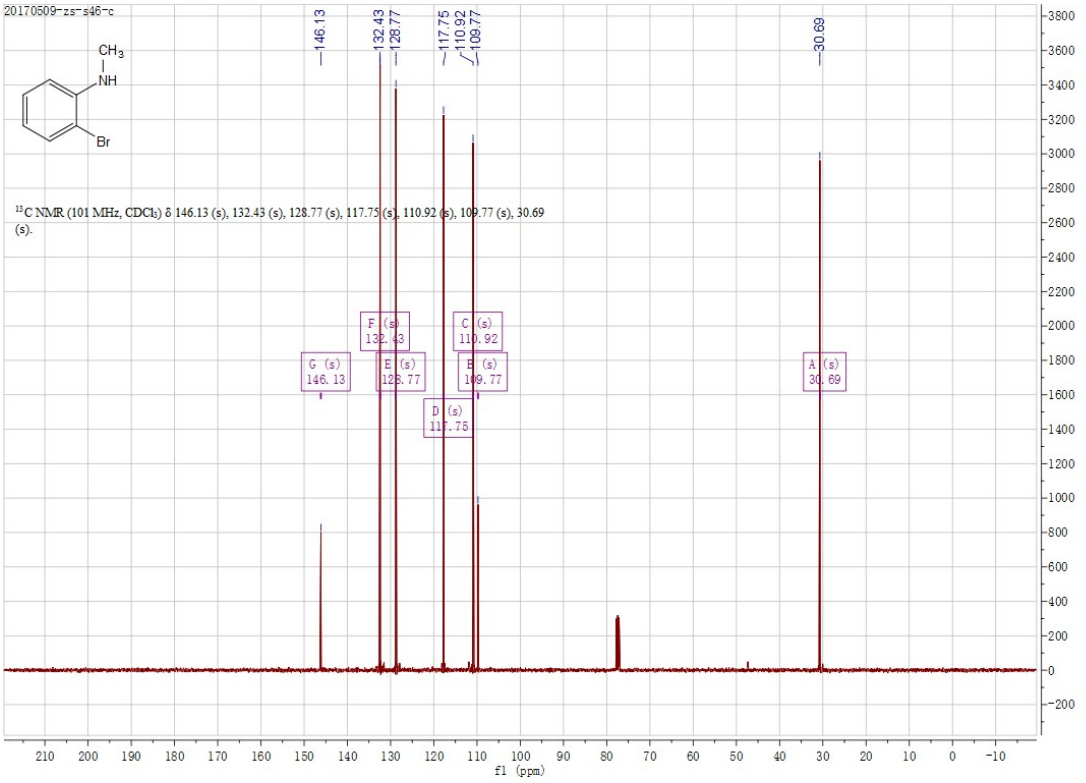
2h


20170504-zs-s31-h
CH3
NH
Cl
7.18
7.16
7.11
7.09
7.07
6.58
6.56
6.54
4.26
2.83
2.81
1H NMR (400 MHz, CDCl3) δ 7.17 (d, J = 7.1 Hz, 1H), 7.09 (t, J = 7.7 Hz, 1H), 6.56 (t, J = 8.3 Hz, 2H), 4.26 (s, 1H), 2.82 (d, J = 5.0 Hz, 3H).
B (d) 7.17
A (t) 7.09
C (t) 6.56
D (s) 4.26
E (d) 2.82
1.09
1.00
1.97
1.00
3.10
f1 (ppm)

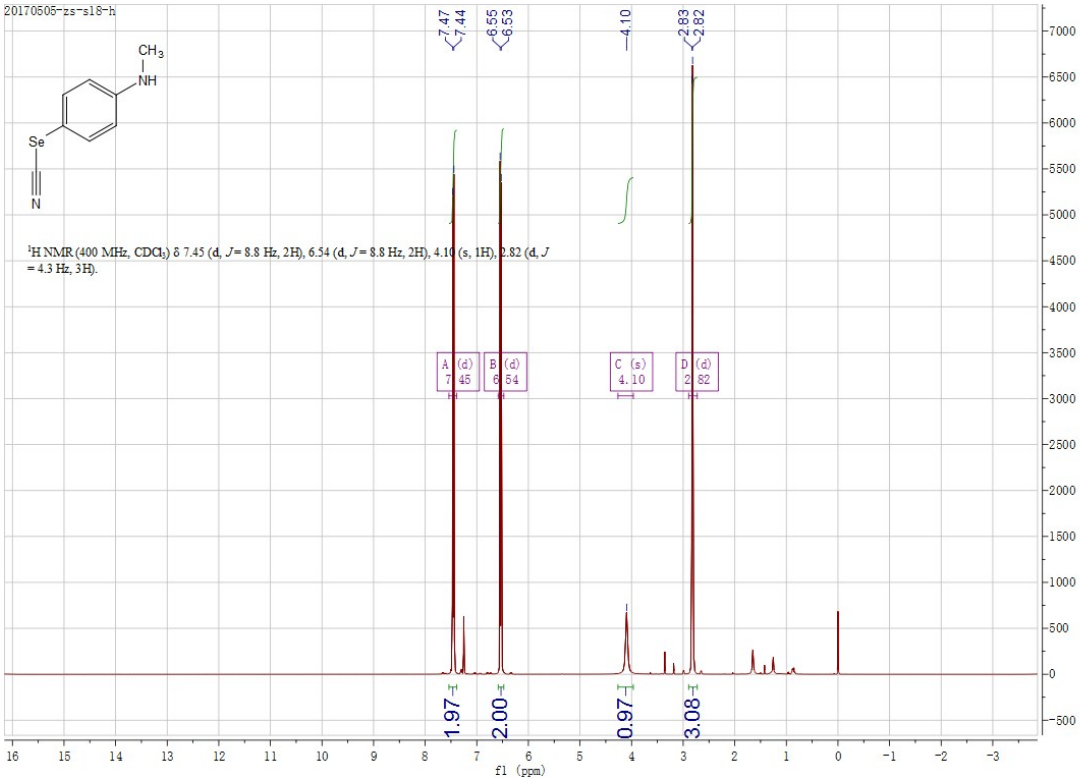

20170504-zs-s31-c
CH3
NH
Cl
145.03
128.98
127.86
119.07
117.03
110.64
30.41
13C NMR (101 MHz, CDCl3) δ 145.03 (s), 128.98 (s), 127.86 (s), 119.07 (s), 117.03 (s), 110.64 (s), 30.41 (s).
I (s) 128.98
F (s) 117.03
J (s) 145.03
H (s) 127.86
E (s) 110.64
G (s) 119.07
A (s) 30.41
f1 (ppm)

2i

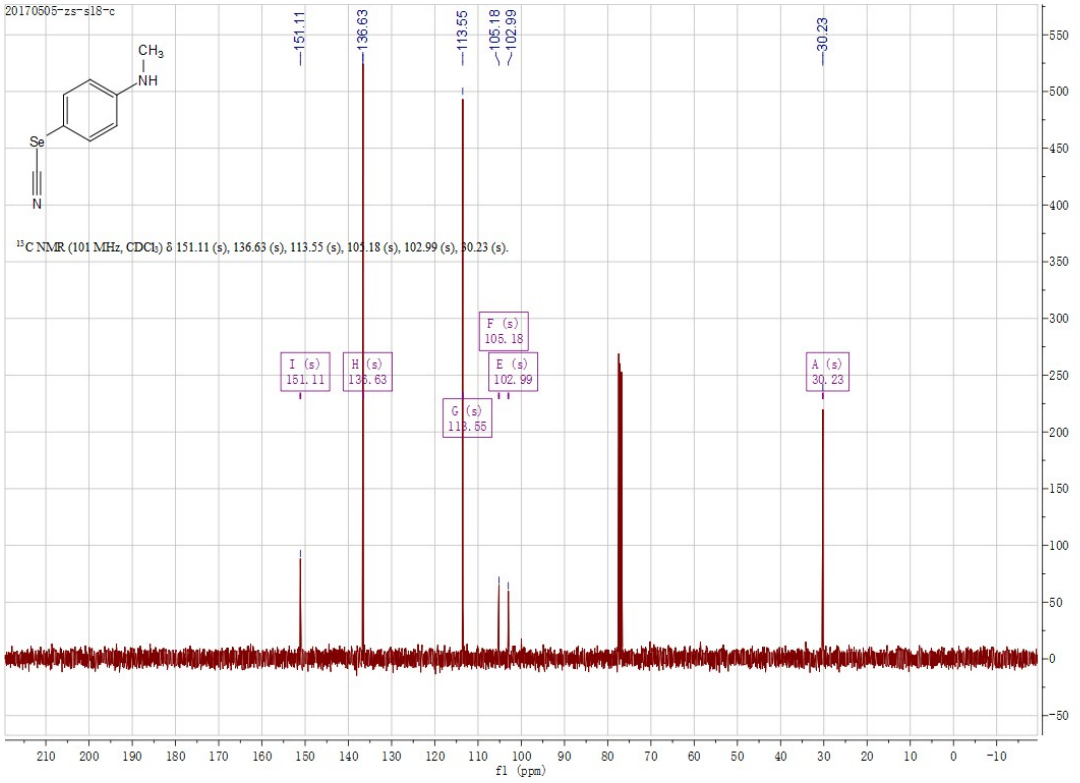

20170509-zs-s46-h
CH3
NH
Br
7.37
7.37
7.36
7.35
7.15
7.14
7.13
7.11
7.11
6.53
6.52
6.51
6.50
6.48
6.48
4.26
2.74
2.73
1H NMR (400 MHz, CDCl3) δ 7.36 (dd, J = 7.8, 1.4 Hz, 1H), 7.19 – 7.09 (m, 1H), 6.56 – 6.46 (m, 2H), 4.26 (s, 1H), 2.74 (d, J = 5.2 Hz, 3H).
B (m) 7.13
A (dd) 7.36
C (m) 6.50
E (s) 4.26
D (d) 2.74
1.00
1.01
2.02
0.95
3.09
f1 (ppm)


20170509-zs-s46-c
CH3
NH
Br
146.13
132.43
128.77
117.75
110.92
109.77
30.69
13C NMR (101 MHz, CDCl3) δ 146.13 (s), 132.43 (s), 128.77 (s), 117.75 (s), 110.92 (s), 109.77 (s), 30.69 (s).
F (s) 132.43
C (s) 110.92
G (s) 146.13
E (s) 128.77
B (s) 109.77
D (s) 117.75
A (s) 30.69
f1 (ppm)

3a

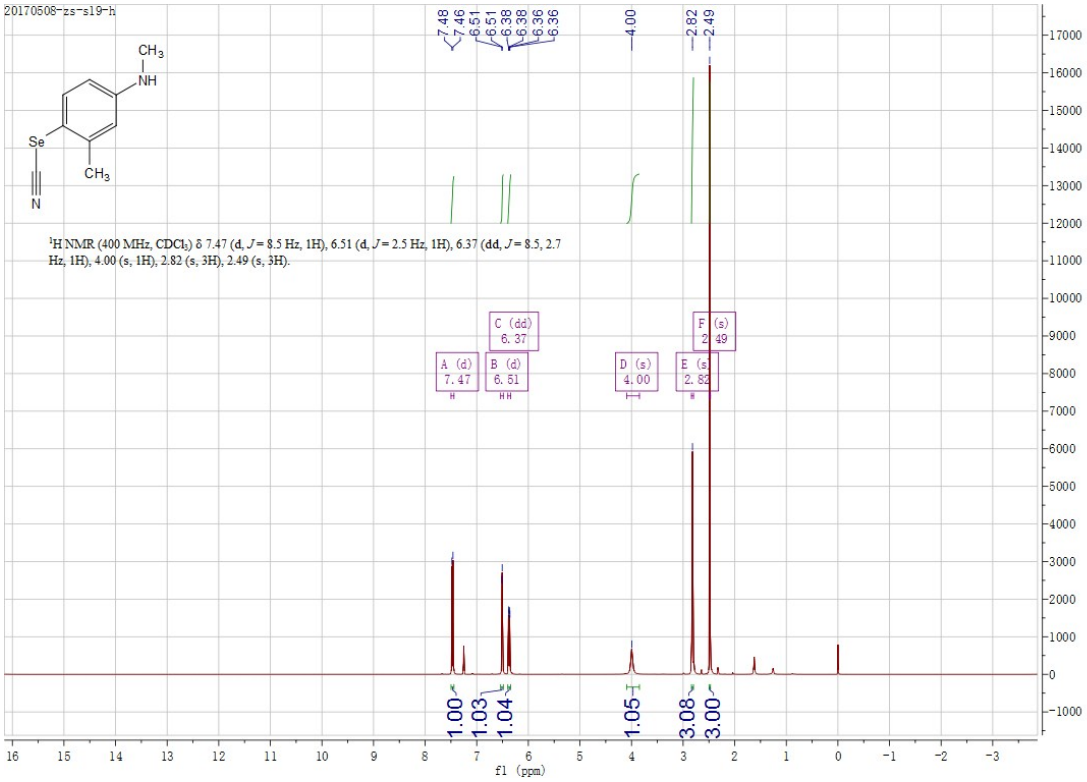


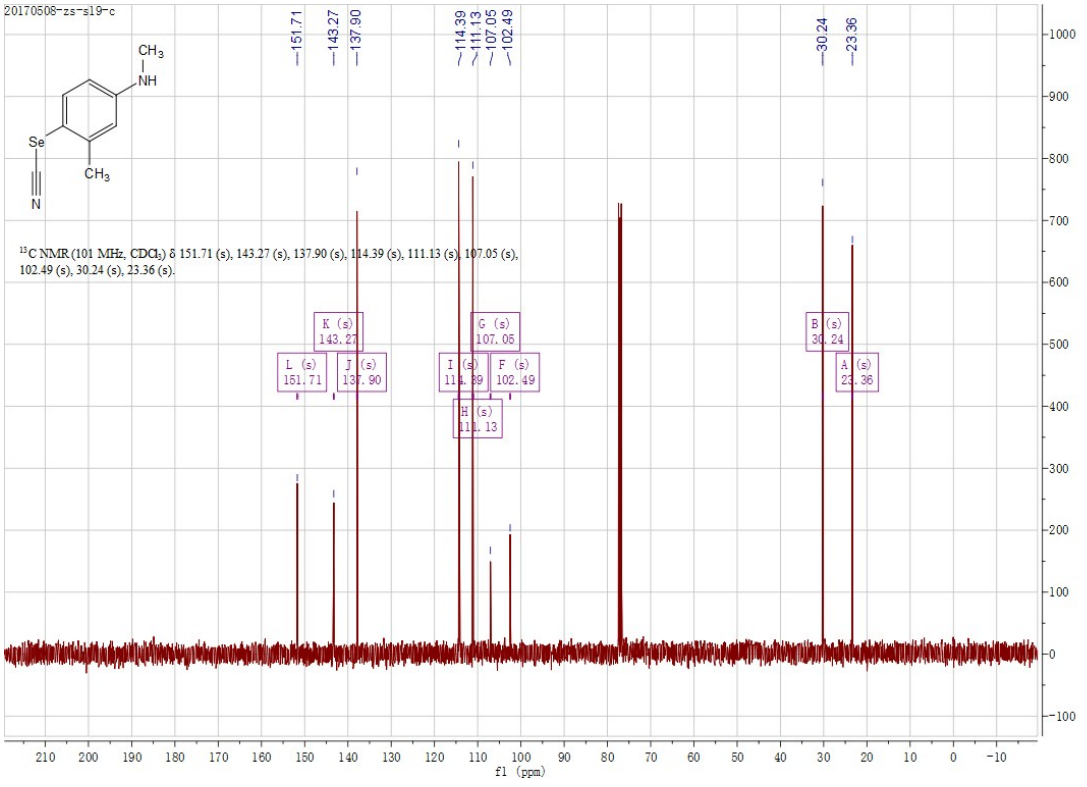
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 8.8 Hz, 2H), 6.54 (d, J = 8.8 Hz, 2H), 4.10 (s, 1H), 2.82 (d, J = 4.3 Hz, 3H).



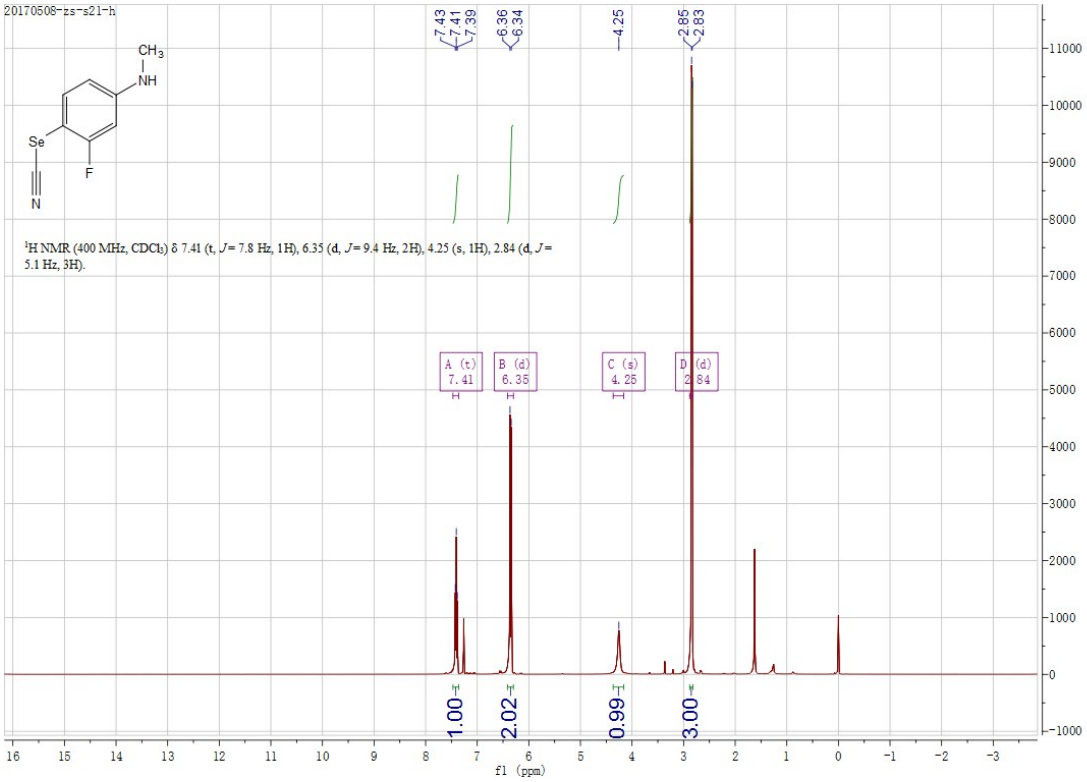
^{13}C NMR (101 MHz, $CDCl_3$) δ 151.11 (s), 136.63 (s), 113.55 (s), 105.18 (s), 102.99 (s), 30.23 (s).

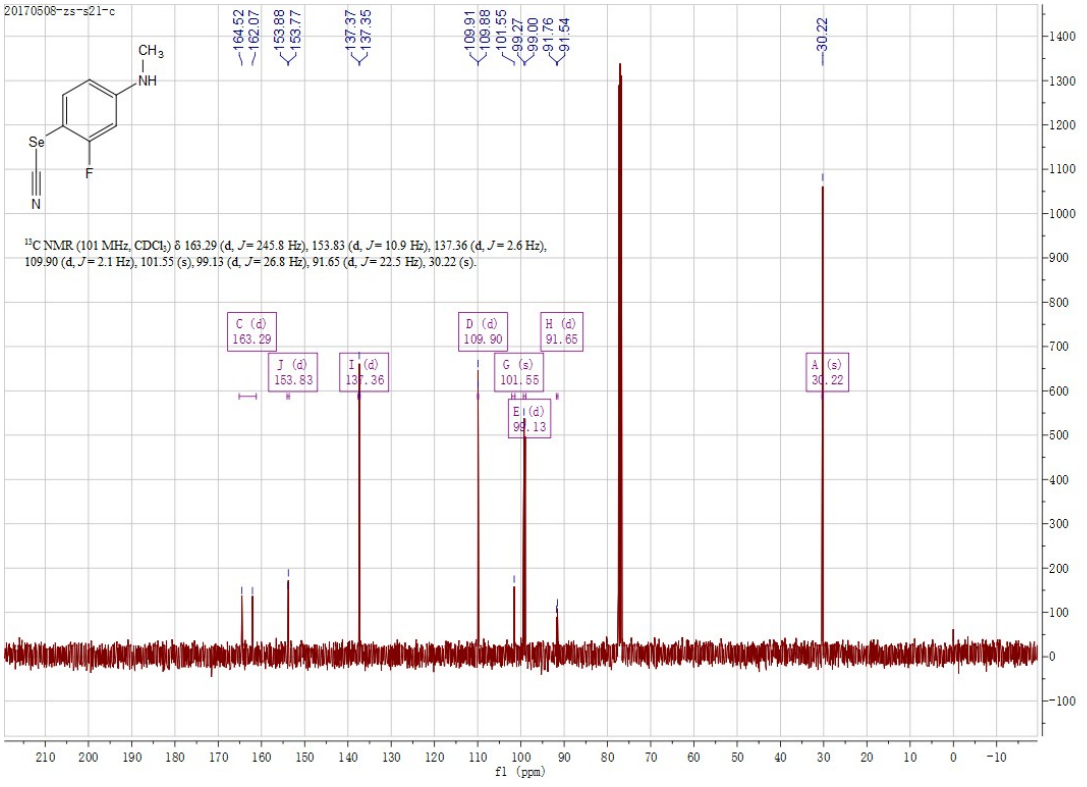
3b


20170508-zs-s19-h
CH3
NH
Se
CH3
N
7.48
7.46
6.51
6.51
6.38
6.38
6.36
6.36
4.00
2.82
2.49
1H NMR (400 MHz, CDCl3) δ 7.47 (d, J = 8.5 Hz, 1H), 6.51 (d, J = 2.5 Hz, 1H), 6.37 (dd, J = 8.5, 2.7 Hz, 1H), 4.00 (s, 1H), 2.82 (s, 3H), 2.49 (s, 3H).
A (d) 7.47
B (d) 6.51
C (dd) 6.37
D (s) 4.00
E (s) 2.82
F (s) 2.49
1.00
1.03
1.04
1.05
3.08
3.00
f1 (ppm)

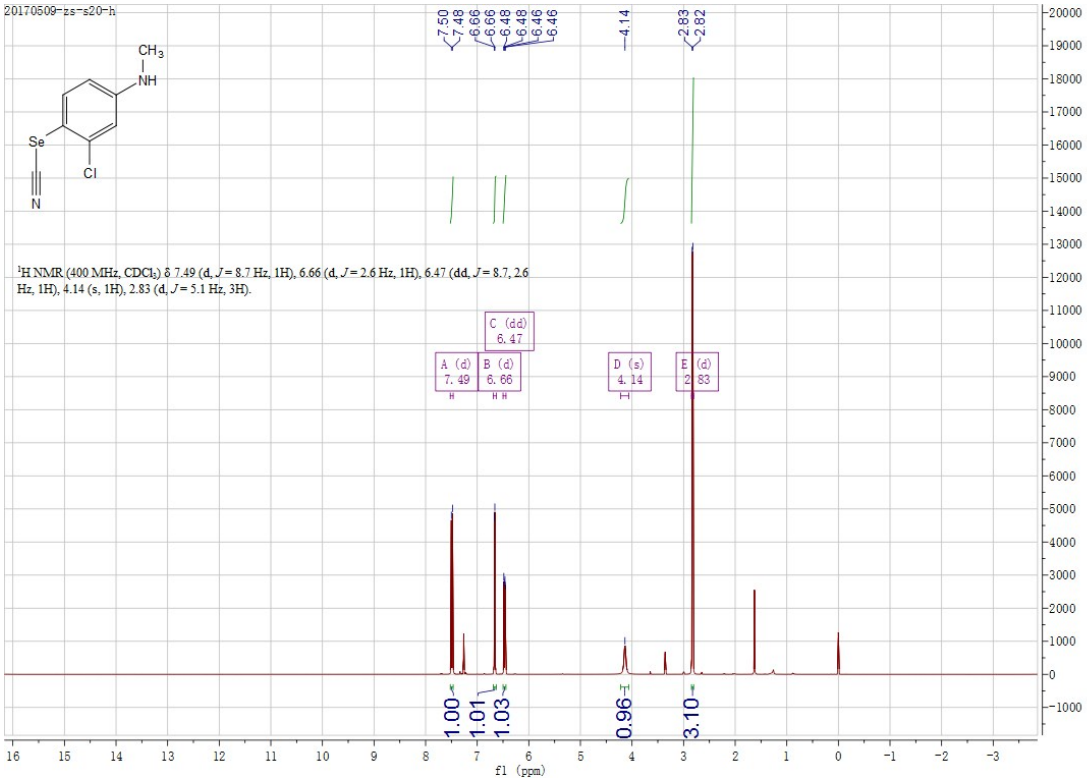

20170508-zs-s19-c
CH3
NH
Se
CH3
N
151.71
143.27
137.90
114.39
111.13
107.05
102.49
30.24
23.36
13C NMR (101 MHz, CDCl3) δ 151.71 (s), 143.27 (s), 137.90 (s), 114.39 (s), 111.13 (s), 107.05 (s), 102.49 (s), 30.24 (s), 23.36 (s).
K (s) 143.27
L (s) 151.71
J (s) 137.90
G (s) 107.05
I (s) 114.39
F (s) 102.49
H (s) 111.13
B (s) 30.24
A (s) 23.36
f1 (ppm)

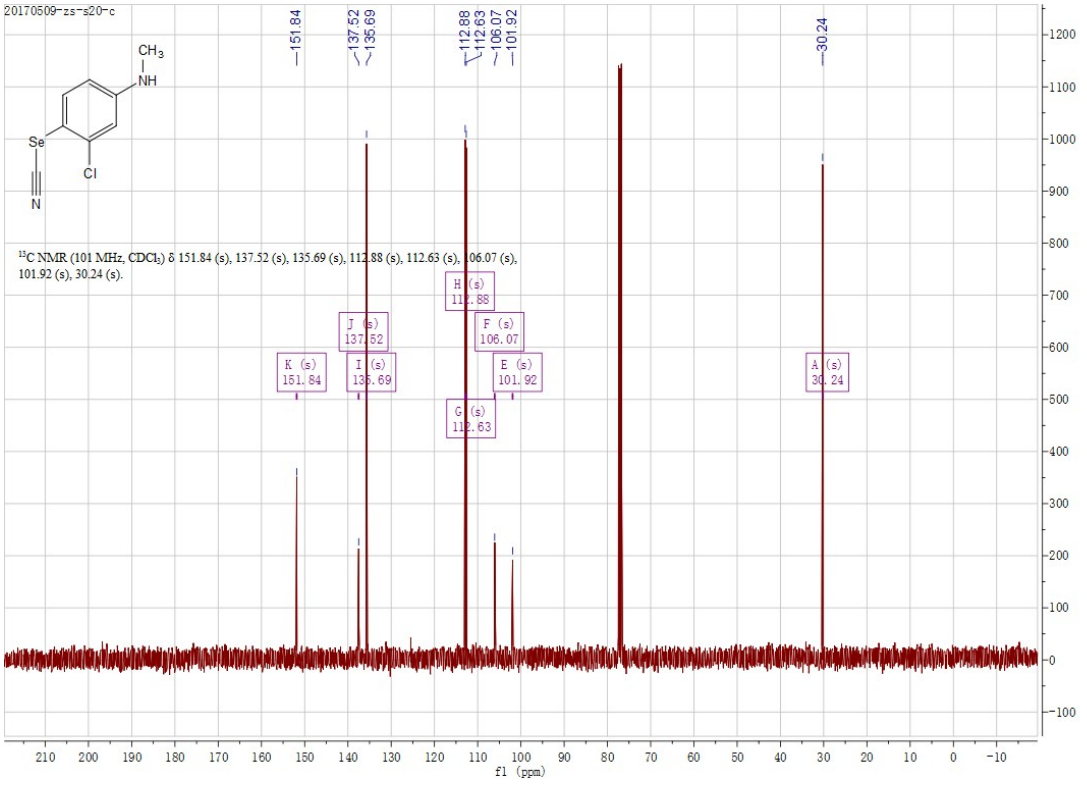
3c


20170508-zs-s21-h
CH3
NH
Se
F
N
7.43
7.41
7.39
6.36
6.34
4.25
2.85
2.83
1H NMR (400 MHz, CDCl3) δ 7.41 (t, J = 7.8 Hz, 1H), 6.35 (d, J = 9.4 Hz, 2H), 4.25 (s, 1H), 2.84 (d, J = 5.1 Hz, 3H).
A (t) 7.41
B (d) 6.35
C (s) 4.25
D (d) 2.84
1.00
2.02
0.99
3.00
f1 (ppm)

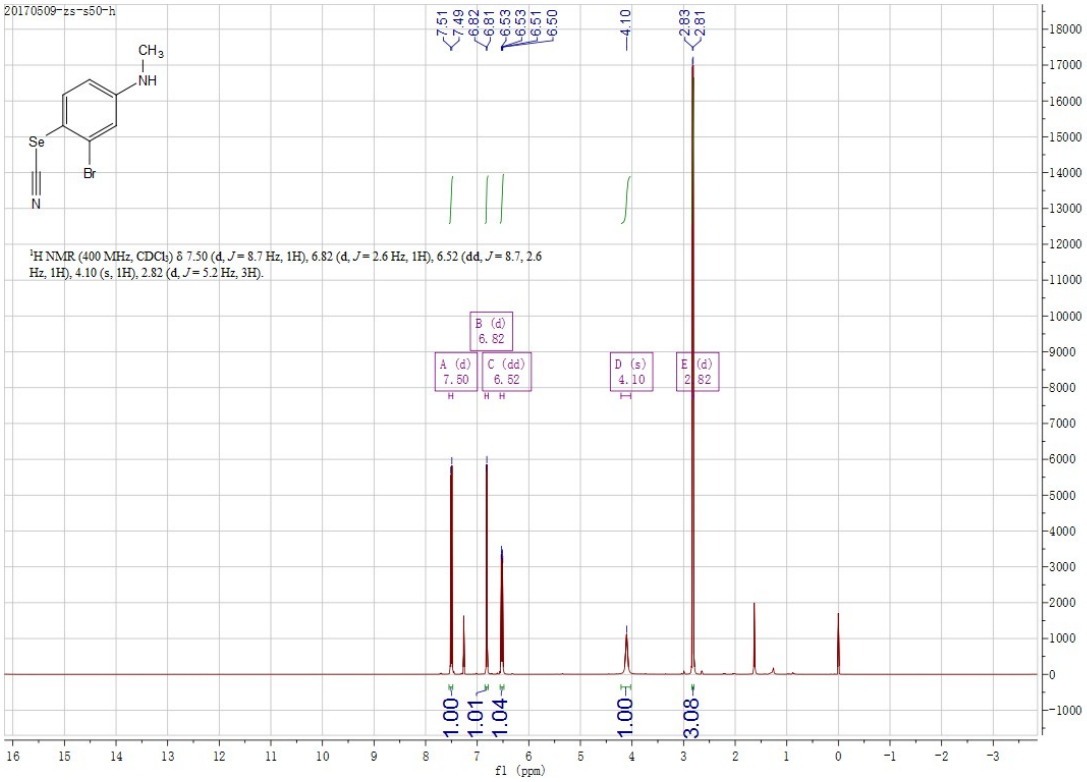

20170508-zs-s21-c
CH3
NH
Se
F
N
164.52
162.07
153.88
153.77
137.37
137.35
109.91
109.88
101.55
99.27
99.00
91.76
91.54
30.22
13C NMR (101 MHz, CDCl3) δ 163.29 (d, J = 245.8 Hz), 153.83 (d, J = 10.9 Hz), 137.36 (d, J = 2.6 Hz), 109.90 (d, J = 2.1 Hz), 101.55 (s), 99.13 (d, J = 26.8 Hz), 91.65 (d, J = 22.5 Hz), 30.22 (s).
C (d) 163.29
J (d) 153.83
I (d) 137.36
D (d) 109.90
H (d) 91.65
G (s) 101.55
E (d) 99.13
A (s) 30.22
f1 (ppm)

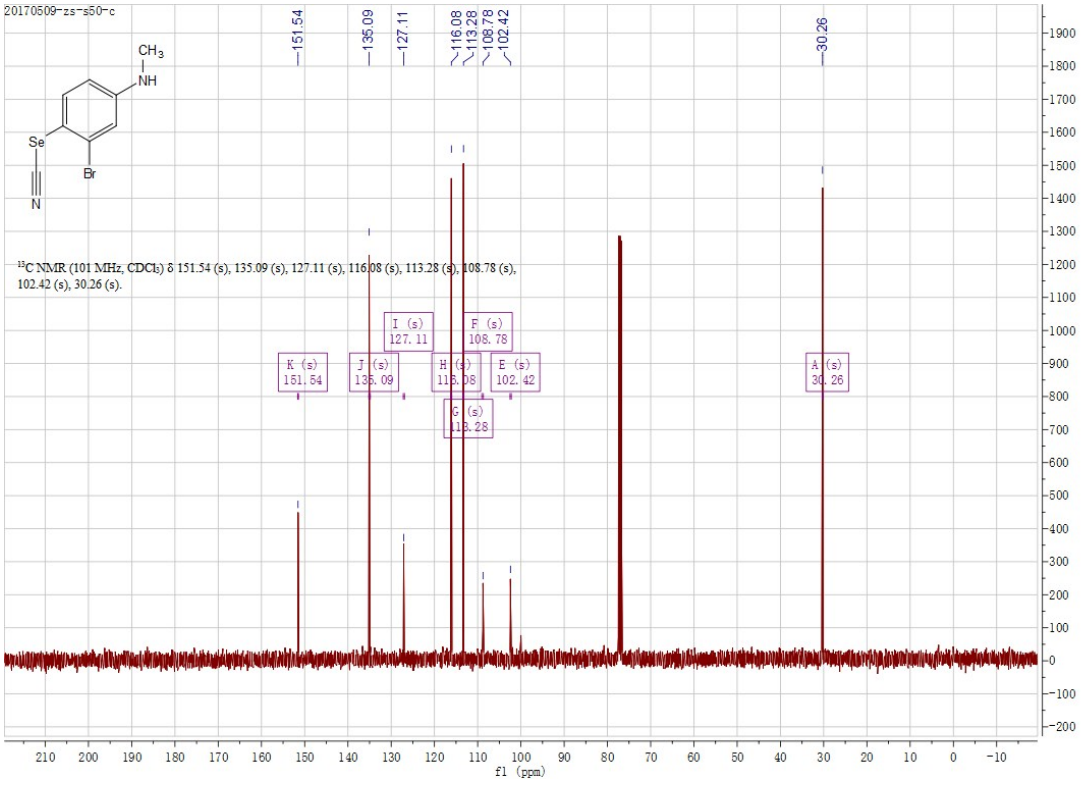
3d


20170509-zs-s20-h
CH3
NH
Se
Cl
N
7.50
7.48
6.66
6.66
6.48
6.48
6.46
6.46
4.14
2.83
2.82
1H NMR (400 MHz, CDCl3) δ 7.49 (d, J = 8.7 Hz, 1H), 6.66 (d, J = 2.6 Hz, 1H), 6.47 (dd, J = 8.7, 2.6 Hz, 1H), 4.14 (s, 1H), 2.83 (d, J = 5.1 Hz, 3H).
C (dd) 6.47
A (d) 7.49
B (d) 6.66
D (s) 4.14
E (d) 2.83
1.00
1.01
1.03
0.96
3.10
f1 (ppm)

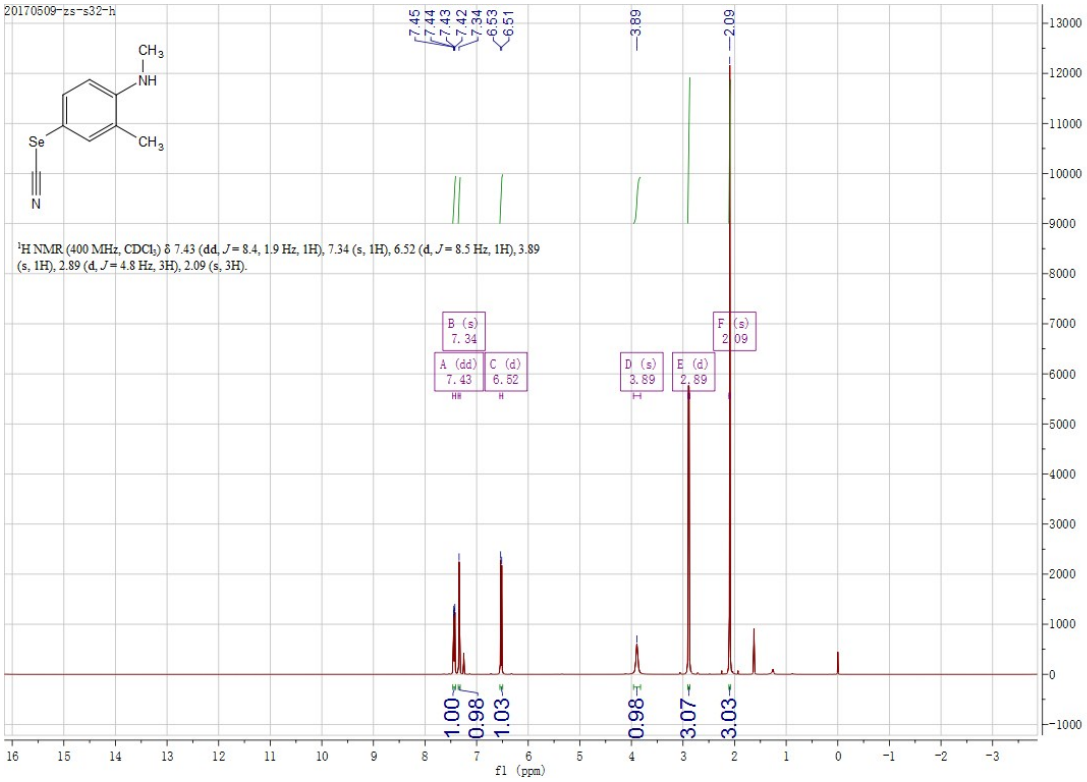

20170509-zs-s20-c
CH3
NH
Se
Cl
N
151.84
137.52
135.69
112.88
112.63
106.07
101.92
30.24
13C NMR (101 MHz, CDCl3) δ 151.84 (s), 137.52 (s), 135.69 (s), 112.88 (s), 112.63 (s), 106.07 (s), 101.92 (s), 30.24 (s).
H (s) 112.88
J (s) 137.52
F (s) 106.07
K (s) 151.84
I (s) 135.69
E (s) 101.92
G (s) 112.63
A (s) 30.24
f1 (ppm)

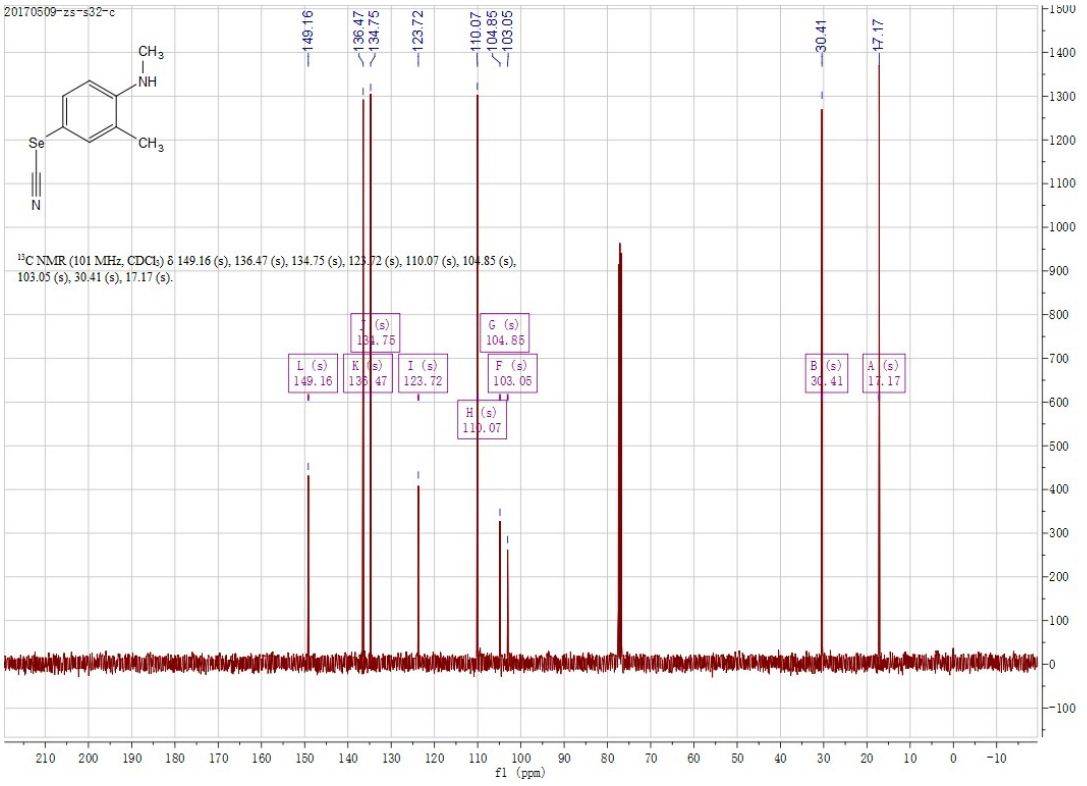
3e


20170509-zs-s50-h
CH3
NH
Se
Br
N
7.51
7.49
6.82
6.81
6.53
6.51
6.50
4.10
2.83
2.81
1H NMR (400 MHz, CDCl3) δ 7.50 (d, J = 8.7 Hz, 1H), 6.82 (d, J = 2.6 Hz, 1H), 6.52 (dd, J = 8.7, 2.6 Hz, 1H), 4.10 (s, 1H), 2.82 (d, J = 5.2 Hz, 3H).
B (d) 6.82
A (d) 7.50
C (dd) 6.52
D (s) 4.10
E (d) 2.82
1.00
1.01
1.04
1.00
3.08
f1 (ppm)

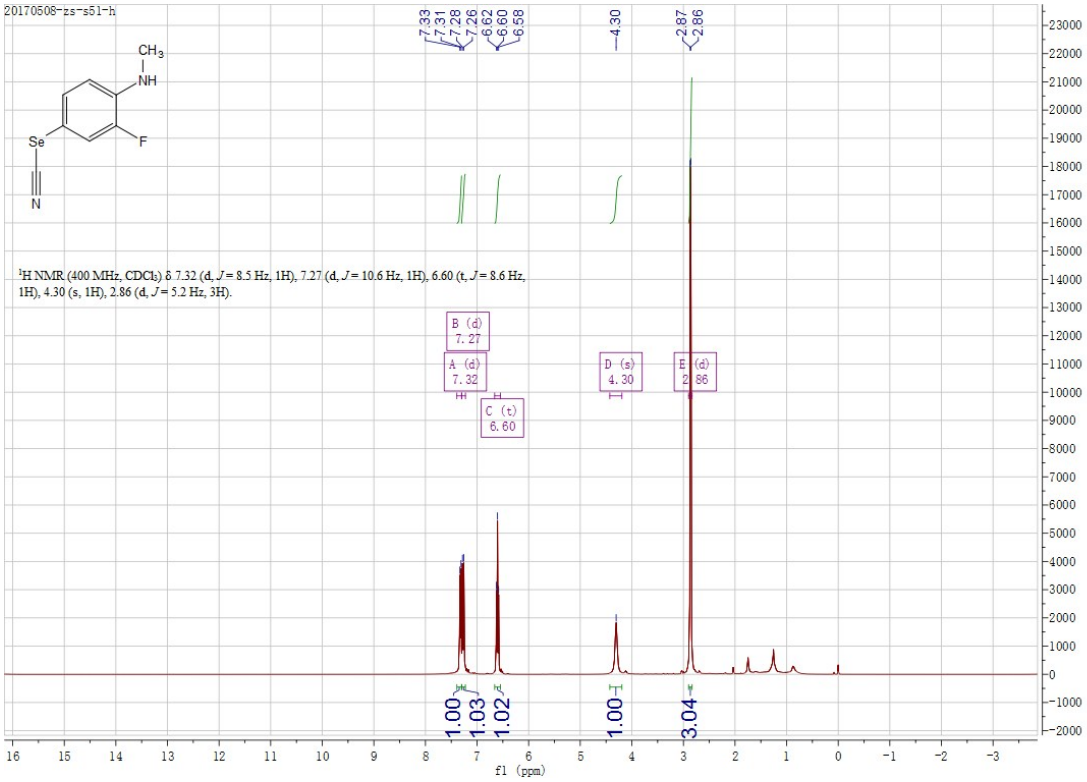

20170509-zs-s50-c
CH3
NH
Se
Br
N
151.54
135.09
127.11
116.08
113.28
108.78
102.42
30.26
13C NMR (101 MHz, CDCl3) δ 151.54 (s), 135.09 (s), 127.11 (s), 116.08 (s), 113.28 (s), 108.78 (s), 102.42 (s), 30.26 (s).
I (s) 127.11
F (s) 108.78
K (s) 151.54
J (s) 135.09
H (s) 116.08
E (s) 102.42
G (s) 113.28
A (s) 30.26
f1 (ppm)

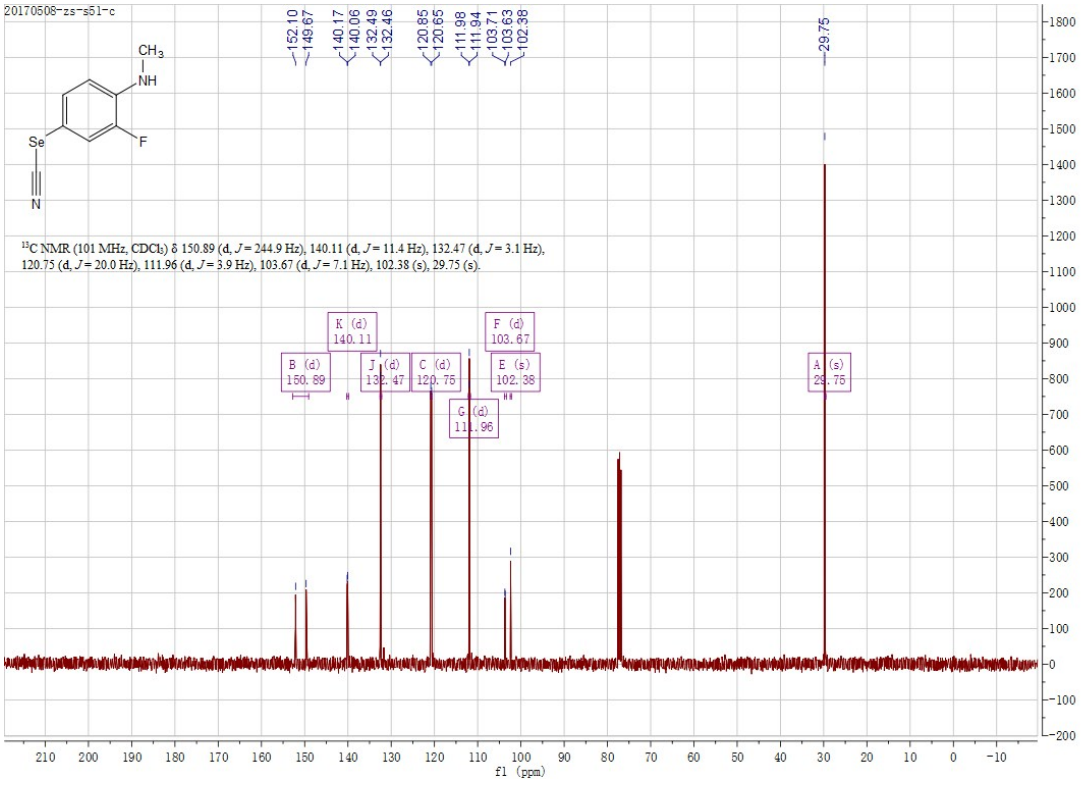
3f


20170509-zs-s32-h
CH3
NH
Se
CH3
N
7.45
7.44
7.43
7.42
7.34
6.53
6.51
3.89
2.09
¹H NMR (400 MHz, CDCl₃) δ 7.43 (dd, J = 8.4, 1.9 Hz, 1H), 7.34 (s, 1H), 6.52 (d, J = 8.5 Hz, 1H), 3.89 (s, 1H), 2.89 (d, J = 4.8 Hz, 3H), 2.09 (s, 3H).
B (s) 7.34
A (dd) 7.43
C (d) 6.52
D (s) 3.89
E (d) 2.89
F (s) 2.09
1.00
0.98
1.03
0.98
3.07
3.03
f1 (ppm)

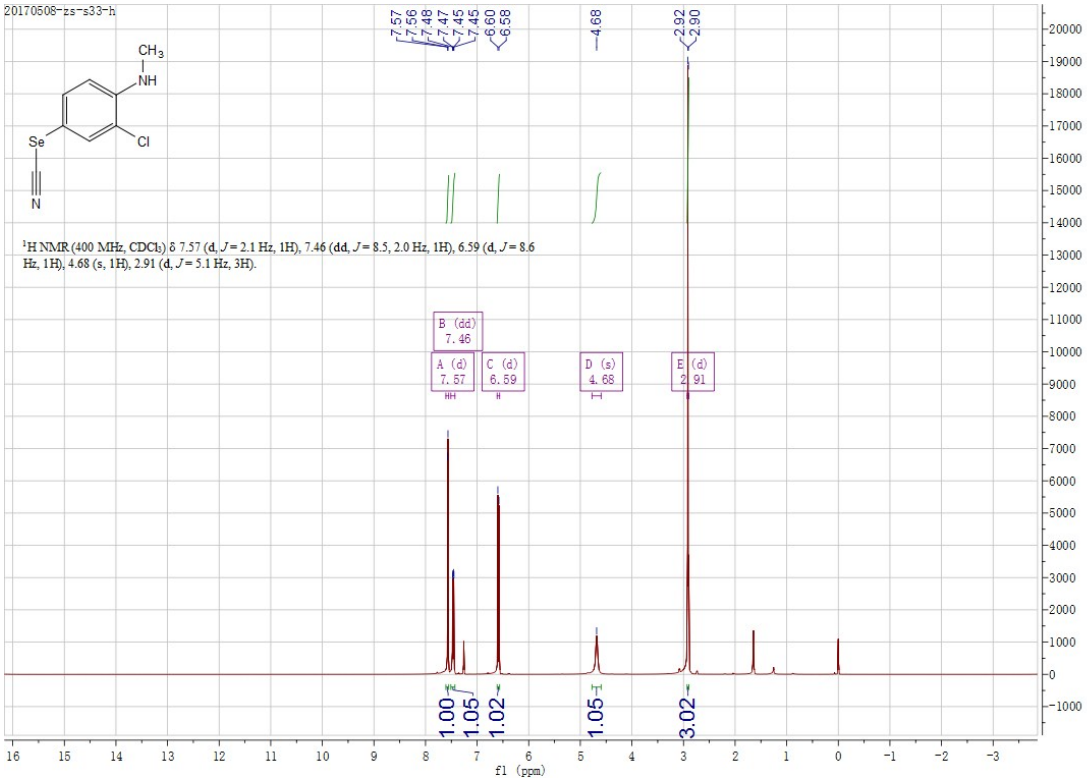

20170509-zs-s32-c
CH3
NH
Se
CH3
N
149.16
136.47
134.75
123.72
110.07
104.85
103.05
30.41
17.17
¹³C NMR (101 MHz, CDCl₃) δ 149.16 (s), 136.47 (s), 134.75 (s), 123.72 (s), 110.07 (s), 104.85 (s), 103.05 (s), 30.41 (s), 17.17 (s).
L (s) 149.16
K (s) 136.47
J (s) 134.75
I (s) 123.72
H (s) 110.07
G (s) 104.85
F (s) 103.05
B (s) 30.41
A (s) 17.17
f1 (ppm)

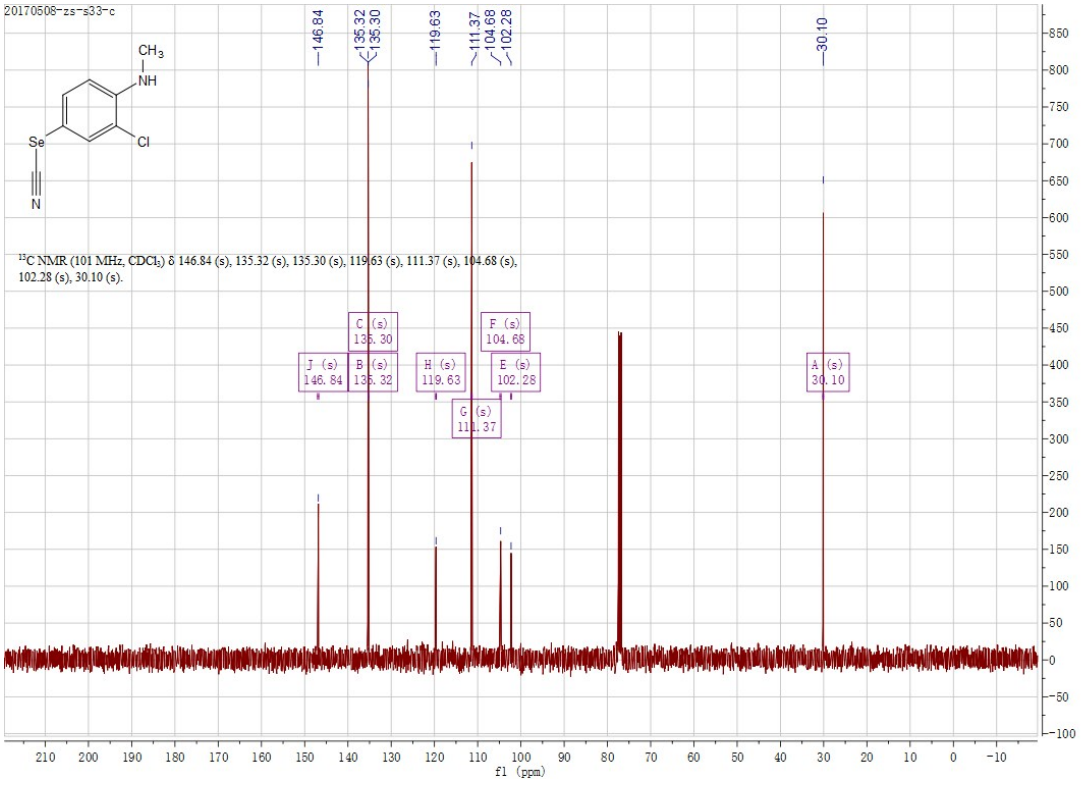
3g


20170508-zs-s51-h
CH3
NH
Se
F
N
7.33
7.31
7.28
7.26
6.62
6.60
6.58
4.30
2.87
2.86
1H NMR (400 MHz, CDCl3) δ 7.32 (d, J = 8.5 Hz, 1H), 7.27 (d, J = 10.6 Hz, 1H), 6.60 (t, J = 8.6 Hz, 1H), 4.30 (s, 1H), 2.86 (d, J = 5.2 Hz, 3H).
B (d) 7.27
A (d) 7.32
C (t) 6.60
D (s) 4.30
E (d) 2.86
1.00
1.03
1.02
1.00
3.04
f1 (ppm)

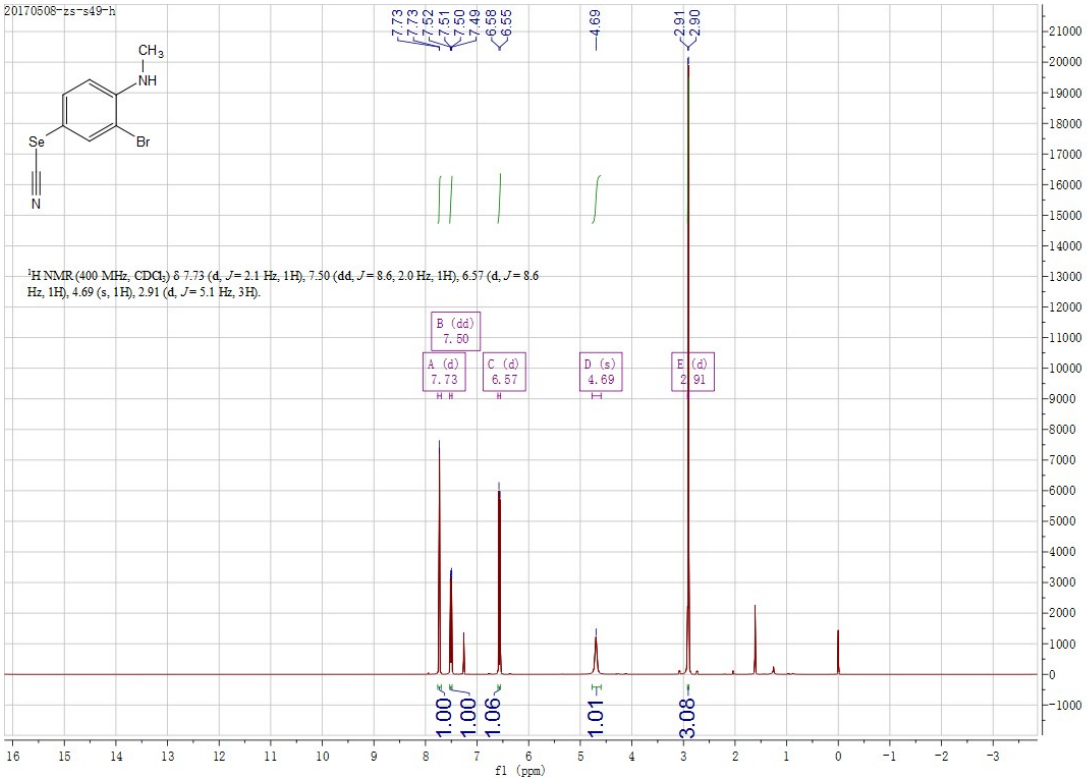

20170508-zs-s51-c
CH3
NH
Se
F
N
152.10
149.67
140.17
140.06
132.49
132.46
120.85
120.65
111.98
111.94
103.71
103.63
102.38
29.75
13C NMR (101 MHz, CDCl3) δ 150.89 (d, J = 244.9 Hz), 140.11 (d, J = 11.4 Hz), 132.47 (d, J = 3.1 Hz), 120.75 (d, J = 20.0 Hz), 111.96 (d, J = 3.9 Hz), 103.67 (d, J = 7.1 Hz), 102.38 (s), 29.75 (s).
K (d) 140.11
F (d) 103.67
B (d) 150.89
J (d) 132.47
C (d) 120.75
E (s) 102.38
G (d) 111.96
A (s) 29.75
f1 (ppm)

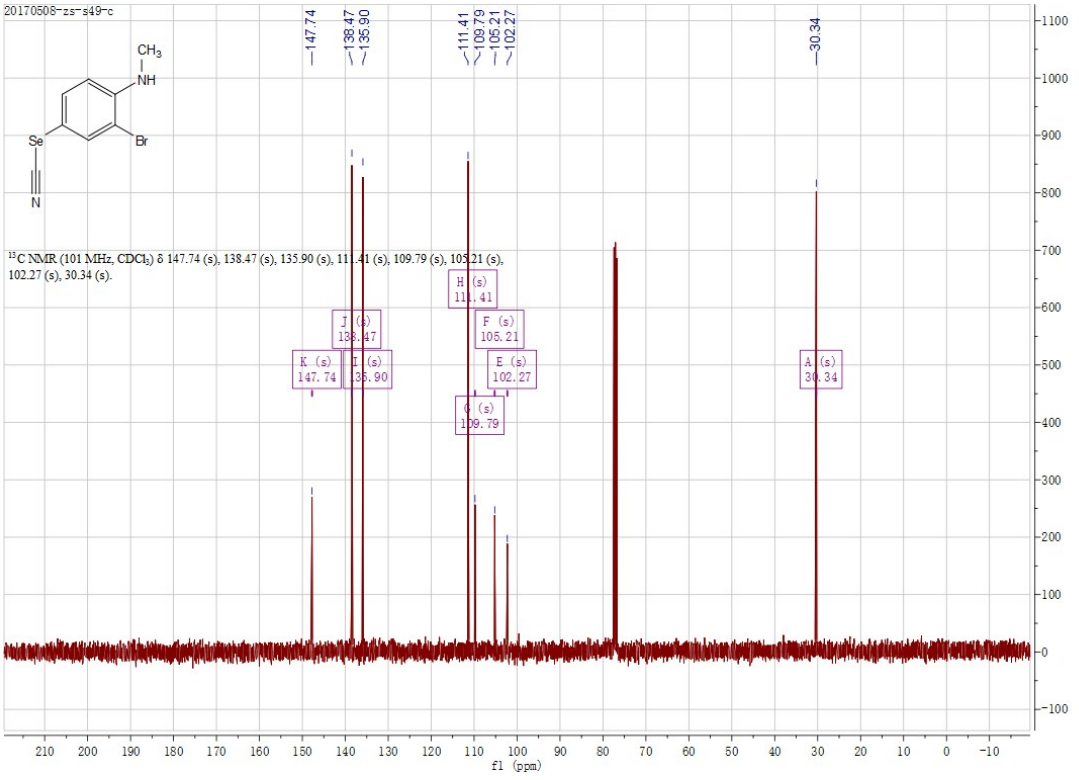
3h


20170508-zs-s33-h
CH3
NH
Se
Cl
N
7.57
7.56
7.48
7.47
7.45
7.45
6.60
6.58
4.68
2.92
2.90
1H NMR (400 MHz, CDCl3) δ 7.57 (d, J = 2.1 Hz, 1H), 7.46 (dd, J = 8.5, 2.0 Hz, 1H), 6.59 (d, J = 8.6 Hz, 1H), 4.68 (s, 1H), 2.91 (d, J = 5.1 Hz, 3H).
B (dd) 7.46
A (d) 7.57
C (d) 6.59
D (s) 4.68
E (d) 2.91
1.00
1.05
1.02
1.05
3.02
f1 (ppm)

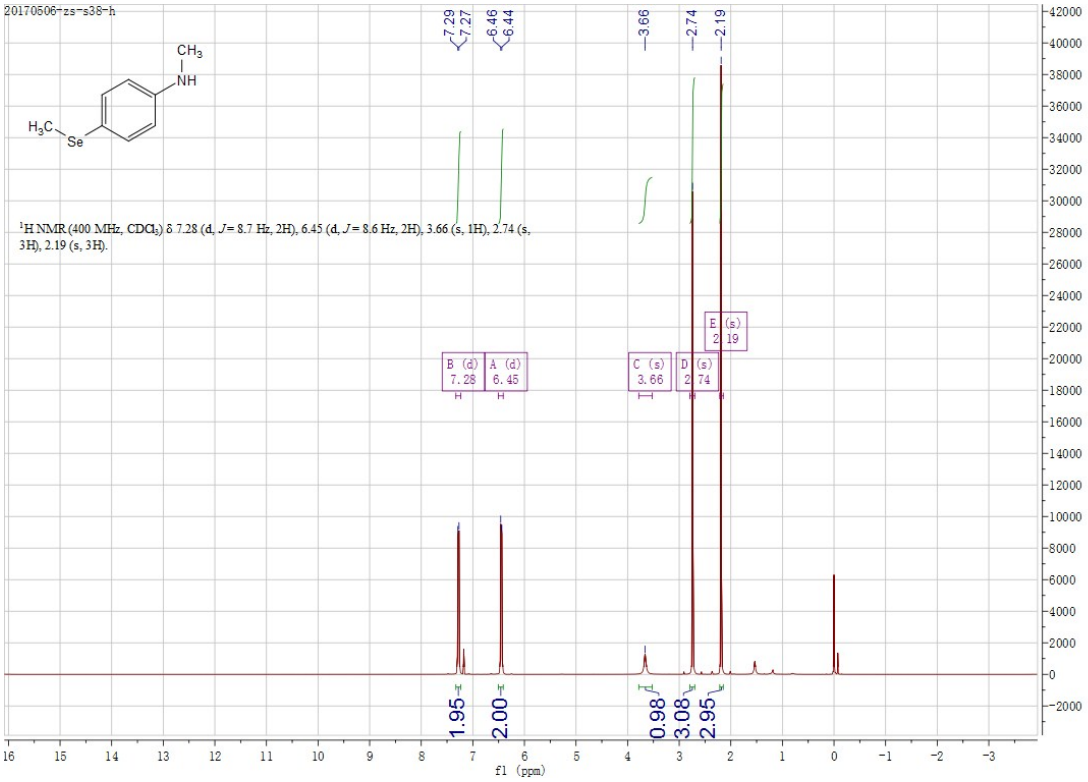

20170508-zs-s33-c
CH3
NH
Se
Cl
N
146.84
135.32
135.30
119.63
111.37
104.68
102.28
30.10
13C NMR (101 MHz, CDCl3) δ 146.84 (s), 135.32 (s), 135.30 (s), 119.63 (s), 111.37 (s), 104.68 (s), 102.28 (s), 30.10 (s).
C (s) 135.30
F (s) 104.68
J (s) 146.84
B (s) 135.32
H (s) 119.63
E (s) 102.28
G (s) 111.37
A (s) 30.10
f1 (ppm)

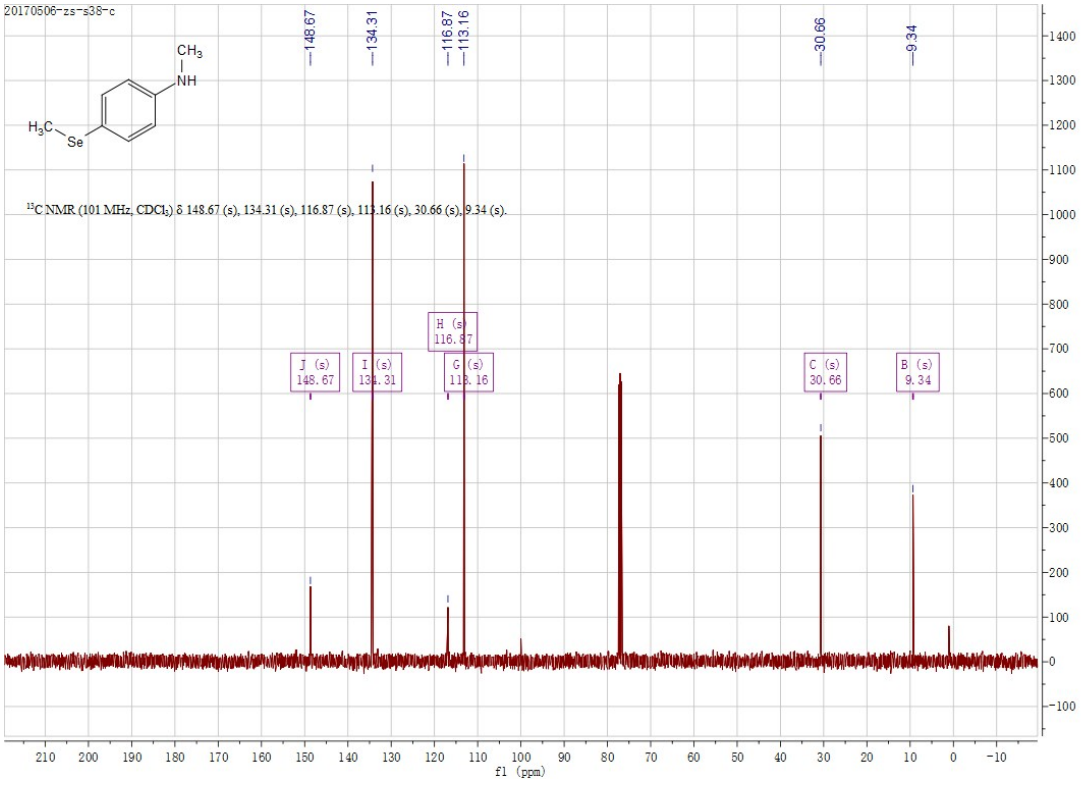
3i


20170508-zs-s49-h
CH3
NH
Se
Br
N
7.73
7.73
7.52
7.51
7.50
7.49
6.58
6.55
4.69
2.91
2.90
1H NMR (400 MHz, CDCl3) δ 7.73 (d, J = 2.1 Hz, 1H), 7.50 (dd, J = 8.6, 2.0 Hz, 1H), 6.57 (d, J = 8.6 Hz, 1H), 4.69 (s, 1H), 2.91 (d, J = 5.1 Hz, 3H).
B (dd) 7.50
A (d) 7.73
C (d) 6.57
D (s) 4.69
E (d) 2.91
1.00
1.00
1.06
1.01
3.08
f1 (ppm)

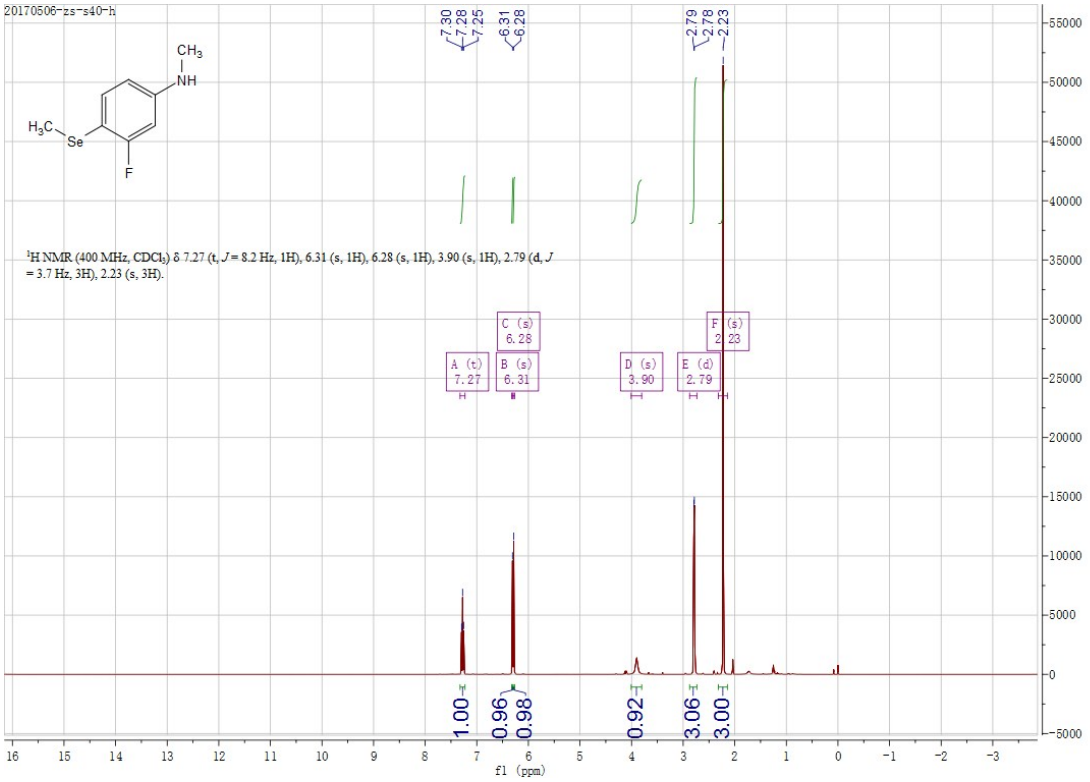

20170508-zs-s49-c
CH3
NH
Se
Br
N
147.74
138.47
135.90
111.41
109.79
105.21
102.27
30.34
13C NMR (101 MHz, CDCl3) δ 147.74 (s), 138.47 (s), 135.90 (s), 111.41 (s), 109.79 (s), 105.21 (s), 102.27 (s), 30.34 (s).
H (s) 111.41
J (s) 138.47
F (s) 105.21
K (s) 147.74
I (s) 135.90
E (s) 102.27
G (s) 109.79
A (s) 30.34
f1 (ppm)

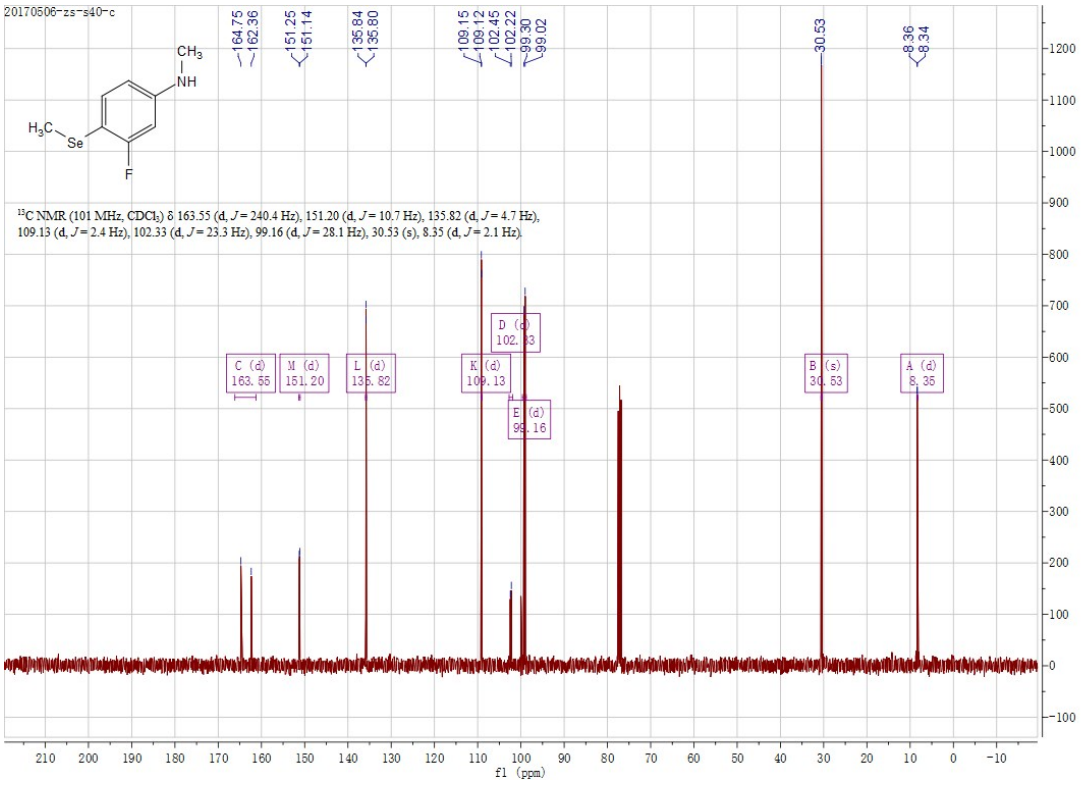
4a


20170506-zs-s38-h
CH3
NH
H3C
Se
7.29
7.27
6.46
6.44
3.66
2.74
2.19
1H NMR (400 MHz, CDCl3) δ 7.28 (d, J= 8.7 Hz, 2H), 6.45 (d, J= 8.6 Hz, 2H), 3.66 (s, 1H), 2.74 (s, 3H), 2.19 (s, 3H).
B (d) 7.28
A (d) 6.45
C (s) 3.66
D (s) 2.74
E (s) 2.19
1.95
2.00
0.98
3.08
2.95
f1 (ppm)

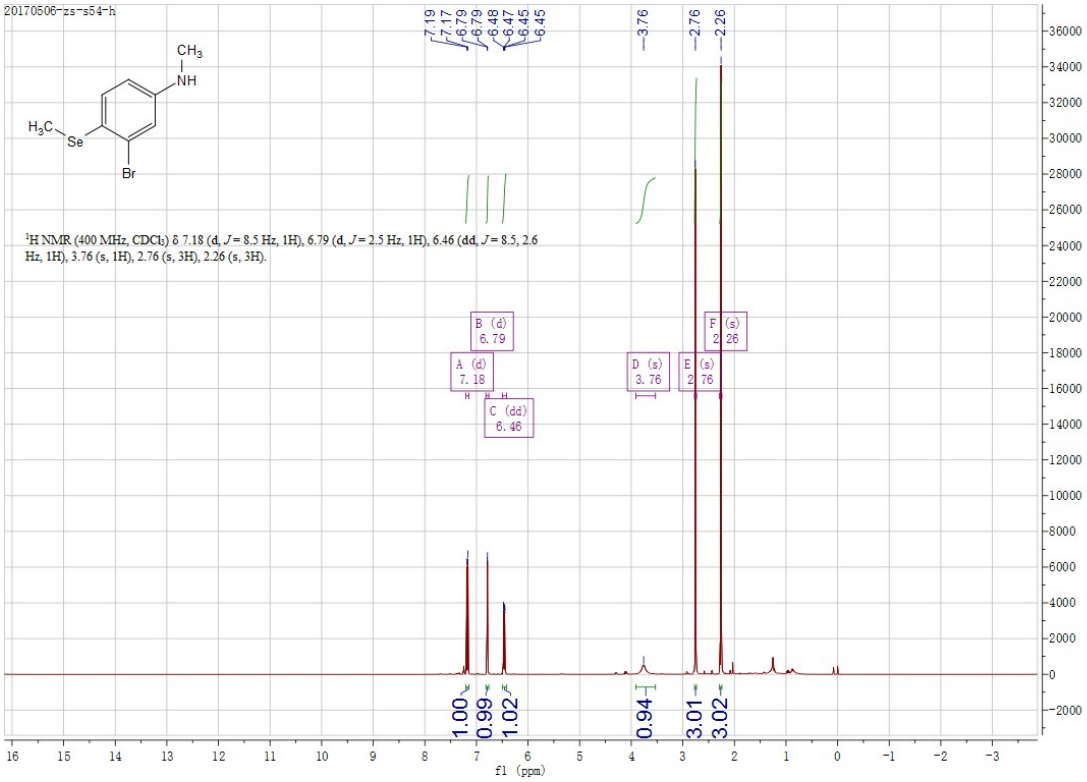

20170506-zs-s38-c
CH3
NH
H3C
Se
148.67
134.31
116.87
113.16
30.66
9.34
13C NMR (101 MHz, CDCl3) δ 148.67 (s), 134.31 (s), 116.87 (s), 113.16 (s), 30.66 (s), 9.34 (s).
J (s) 148.67
I (s) 134.31
H (s) 116.87
G (s) 113.16
C (s) 30.66
B (s) 9.34
f1 (ppm)

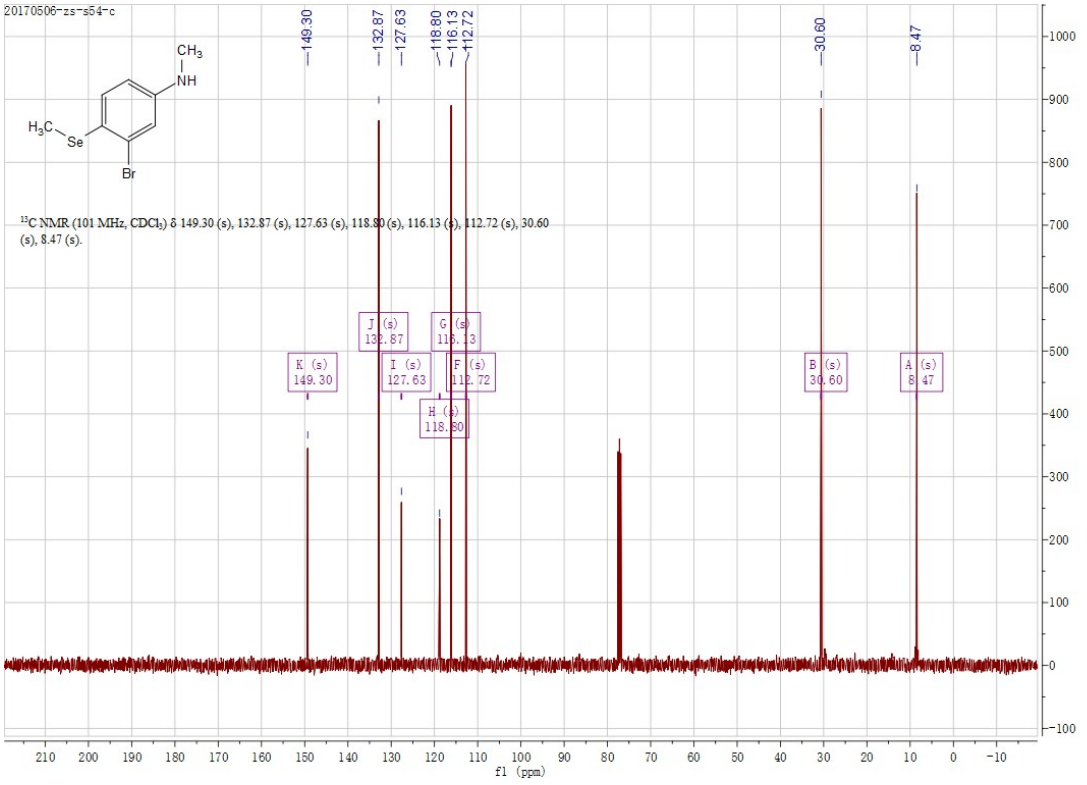
4c


20170506-zs-s40-h
CH3
NH
H3C
Se
F
7.30
7.28
7.25
6.31
6.28
2.79
2.78
2.23
1H NMR (400 MHz, CDCl3) δ 7.27 (t, J = 8.2 Hz, 1H), 6.31 (s, 1H), 6.28 (s, 1H), 3.90 (s, 1H), 2.79 (d, J = 3.7 Hz, 3H), 2.23 (s, 3H).
C (s) 6.28
F (s) 2.23
A (t) 7.27
B (s) 6.31
D (s) 3.90
E (d) 2.79
1.00
0.96
0.98
0.92
3.06
3.00
f1 (ppm)

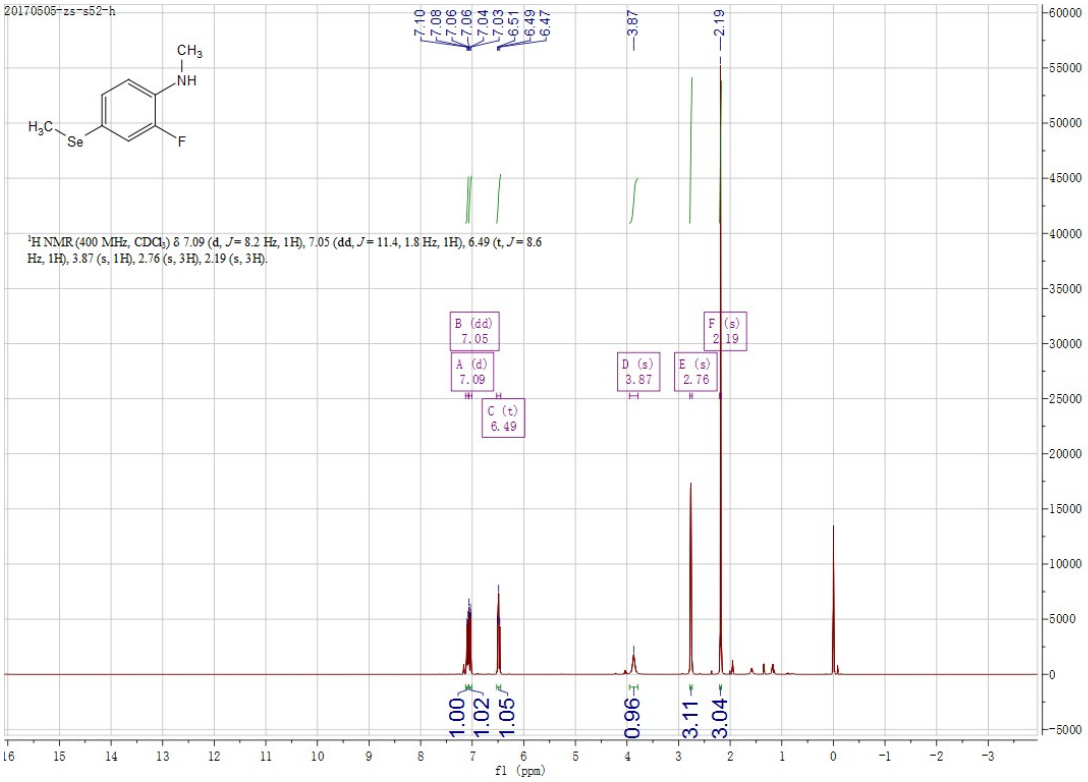

20170506-zs-s40-c
CH3
NH
H3C
Se
F
164.75
162.36
151.25
151.14
135.84
135.80
109.15
109.12
102.45
102.22
99.30
99.02
30.53
8.36
8.34
13C NMR (101 MHz, CDCl3) δ 163.55 (d, J = 240.4 Hz), 151.20 (d, J = 10.7 Hz), 135.82 (d, J = 4.7 Hz), 109.13 (d, J = 2.4 Hz), 102.33 (d, J = 23.3 Hz), 99.16 (d, J = 28.1 Hz), 30.53 (s), 8.35 (d, J = 2.1 Hz).
C (d) 163.55
M (d) 151.20
L (d) 135.82
K (d) 109.13
D (d) 102.33
E (d) 99.16
B (s) 30.53
A (d) 8.35
f1 (ppm)

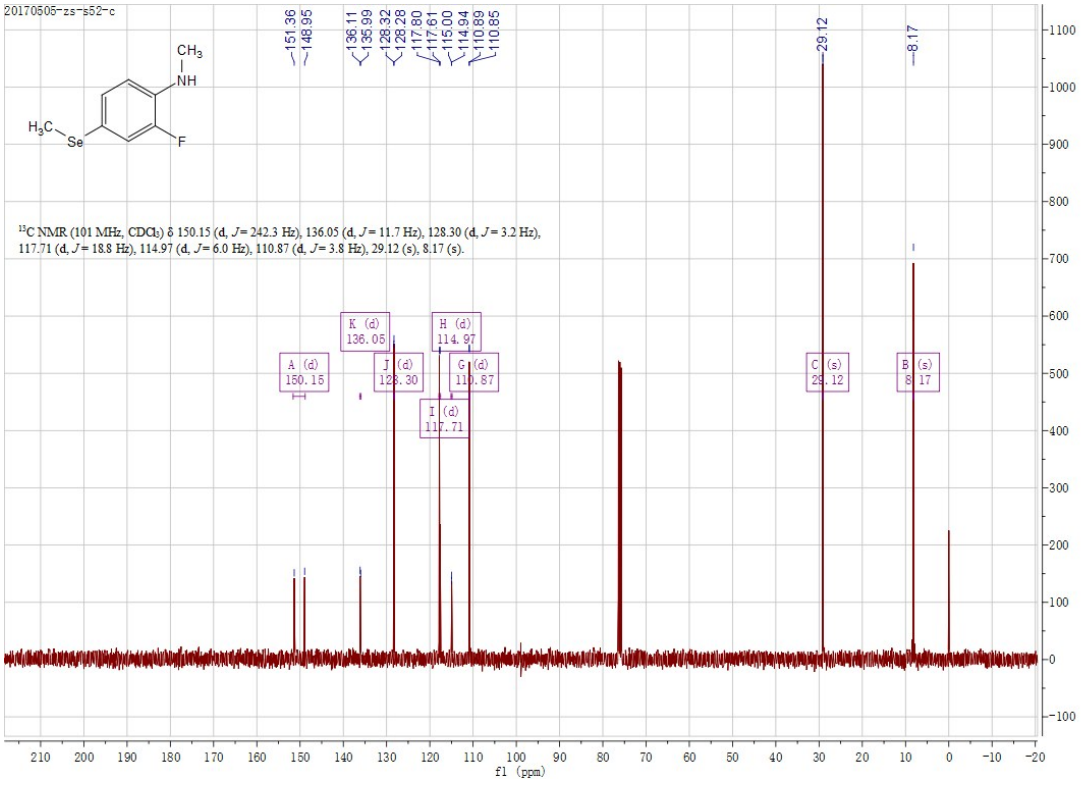
4e


20170506-zs-s54-h
7.19
7.17
6.79
6.79
6.48
6.47
6.45
6.45
3.76
2.76
2.26
CH3
NH
H3C
Se
Br
1H NMR (400 MHz, CDCl3) δ 7.18 (d, J = 8.5 Hz, 1H), 6.79 (d, J = 2.5 Hz, 1H), 6.46 (dd, J = 8.5, 2.6 Hz, 1H), 3.76 (s, 1H), 2.76 (s, 3H), 2.26 (s, 3H).
B (d) 6.79
A (d) 7.18
C (dd) 6.46
D (s) 3.76
E (s) 2.76
F (s) 2.26
1.00
0.99
1.02
0.94
3.01
3.02
f1 (ppm)

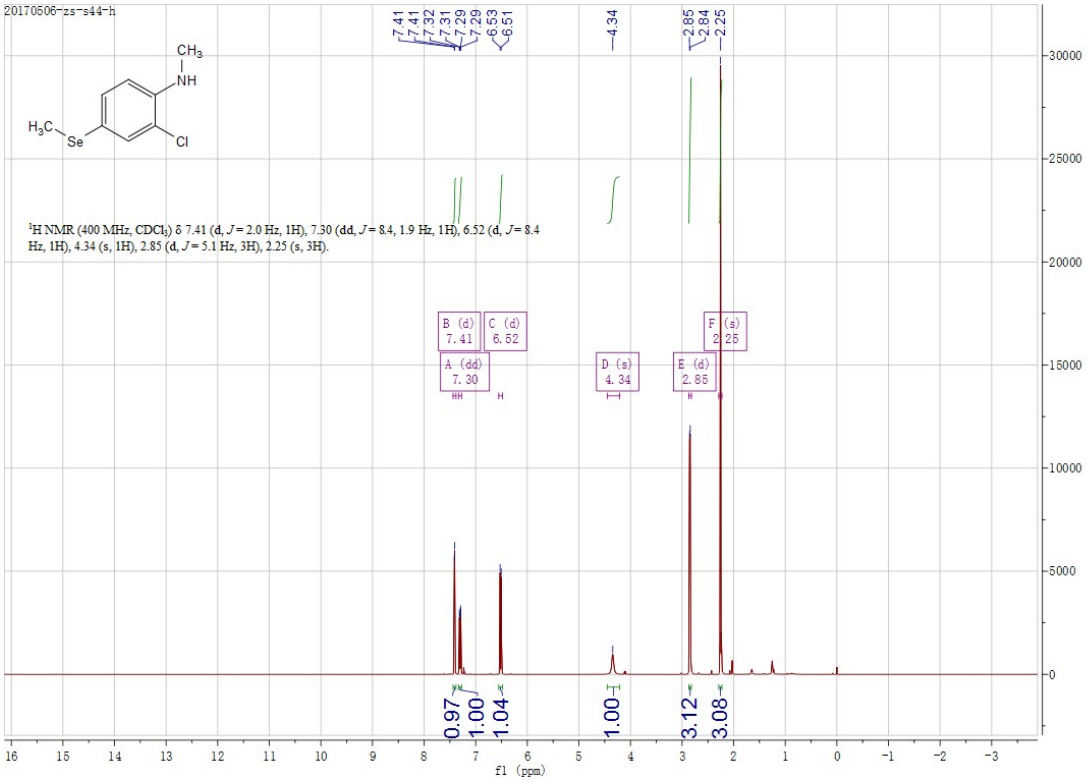

20170506-zs-s54-c
149.30
132.87
127.63
118.80
116.13
112.72
30.60
8.47
CH3
NH
H3C
Se
Br
13C NMR (101 MHz, CDCl3) δ 149.30 (s), 132.87 (s), 127.63 (s), 118.80 (s), 116.13 (s), 112.72 (s), 30.60 (s), 8.47 (s).
J (s) 132.87
G (s) 116.13
K (s) 149.30
I (s) 127.63
F (s) 112.72
H (s) 118.80
B (s) 30.60
A (s) 8.47
f1 (ppm)

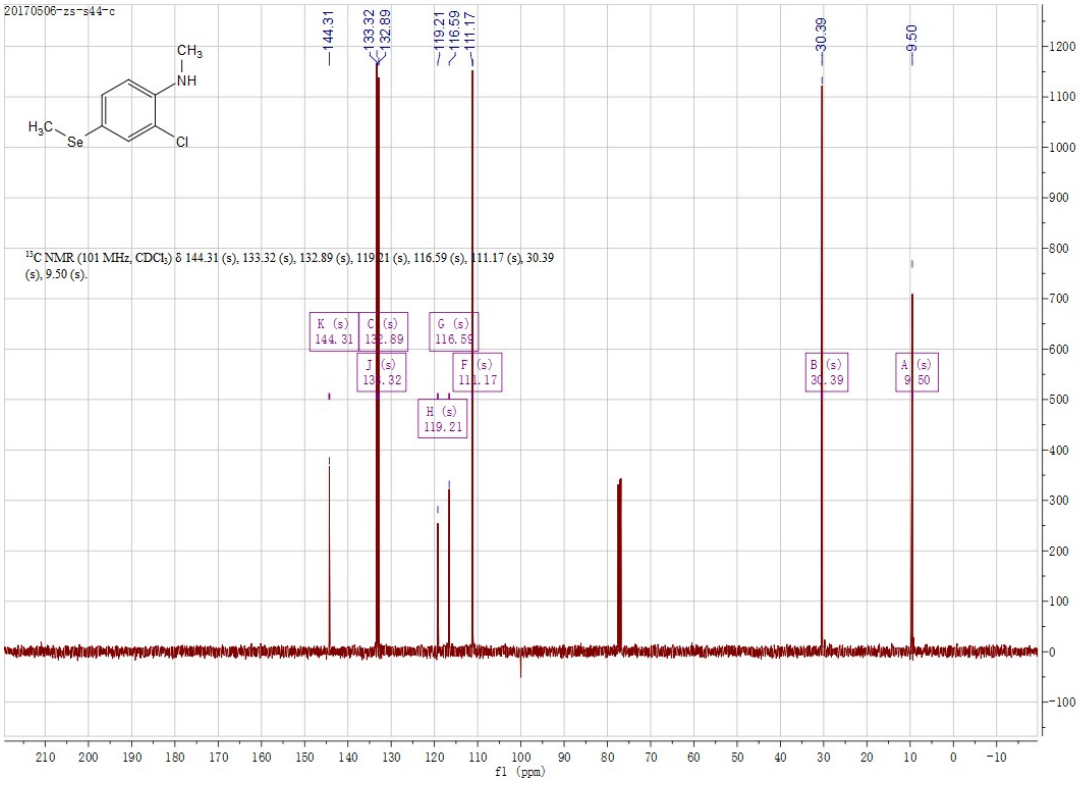
4g


20170506-zs-s52-h
CH3
NH
H3C
Se
F
7.10
7.08
7.06
7.06
7.04
7.03
6.51
6.49
6.47
3.87
2.19
1H NMR (400 MHz, CDCl3) δ 7.09 (d, J = 8.2 Hz, 1H), 7.05 (dd, J = 11.4, 1.8 Hz, 1H), 6.49 (t, J = 8.6 Hz, 1H), 3.87 (s, 1H), 2.76 (s, 3H), 2.19 (s, 3H).
B (dd) 7.05
A (d) 7.09
C (t) 6.49
D (s) 3.87
E (s) 2.76
F (s) 2.19
1.00
1.02
1.05
0.96
3.11
3.04
f1 (ppm)

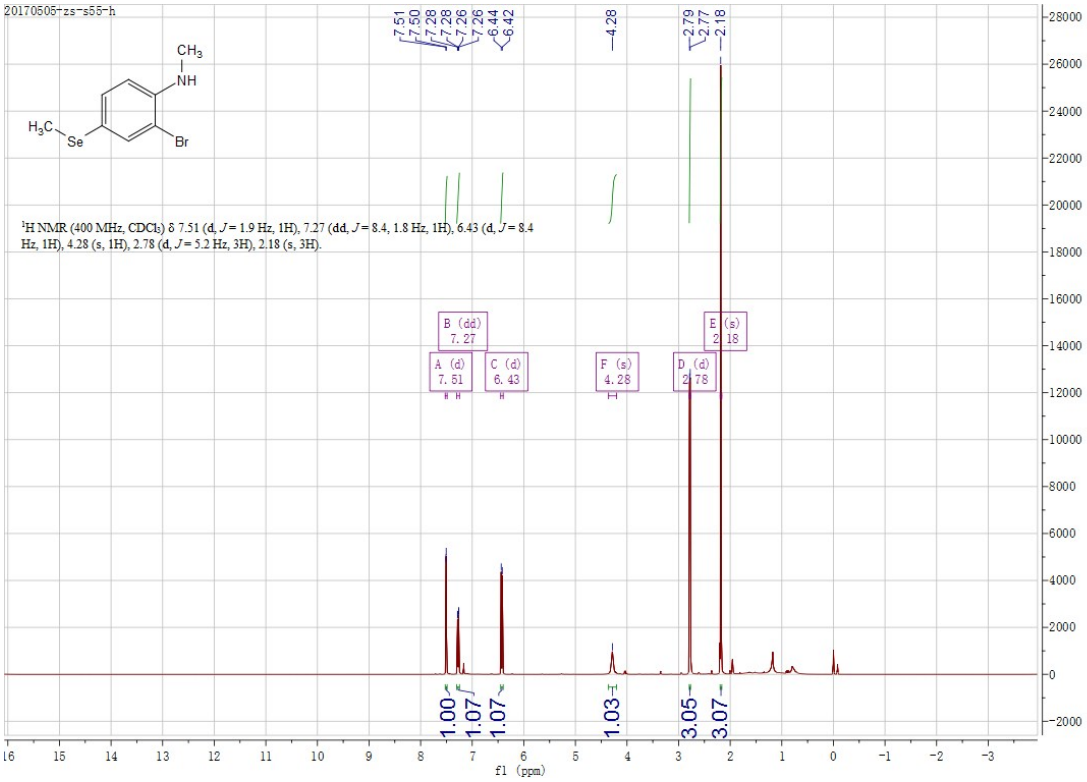

20170506-zs-s52-c
CH3
NH
H3C
Se
F
151.36
148.95
136.11
135.99
128.32
128.28
117.80
117.61
115.00
114.94
110.89
110.85
29.12
8.17
13C NMR (101 MHz, CDCl3) δ 150.15 (d, J = 242.3 Hz), 136.05 (d, J = 11.7 Hz), 128.30 (d, J = 3.2 Hz), 117.71 (d, J = 18.8 Hz), 114.97 (d, J = 6.0 Hz), 110.87 (d, J = 3.8 Hz), 29.12 (s), 8.17 (s).
K (d) 136.05
H (d) 114.97
A (d) 150.15
J (d) 128.30
G (d) 110.87
I (d) 117.71
C (s) 29.12
B (s) 8.17
f1 (ppm)

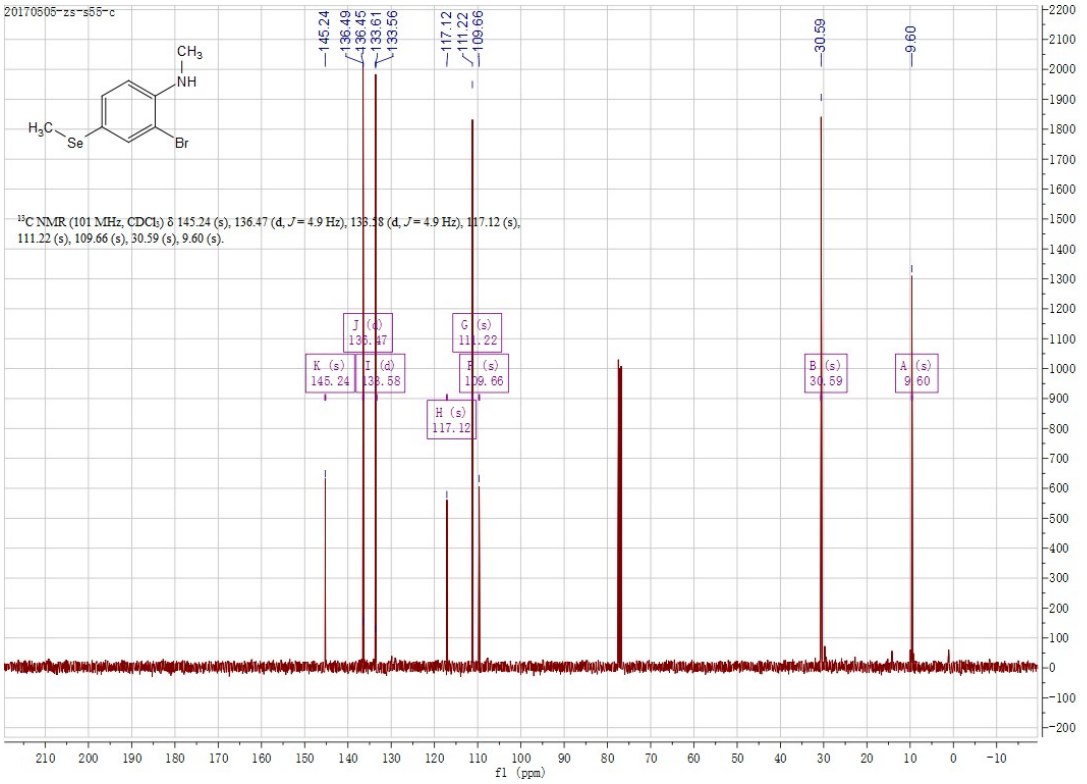
4h


20170506-zs-s44-h
CH3
NH
H3C
Se
Cl
7.41
7.41
7.32
7.31
7.29
7.29
6.53
6.51
4.34
2.85
2.84
2.25
1H NMR (400 MHz, CDCl3) δ 7.41 (d, J = 2.0 Hz, 1H), 7.30 (dd, J = 8.4, 1.9 Hz, 1H), 6.52 (d, J = 8.4 Hz, 1H), 4.34 (s, 1H), 2.85 (d, J = 5.1 Hz, 3H), 2.25 (s, 3H).
B (d) 7.41
C (d) 6.52
A (dd) 7.30
D (s) 4.34
E (d) 2.85
F (s) 2.25
0.97
1.00
1.04
1.00
3.12
3.08
f1 (ppm)

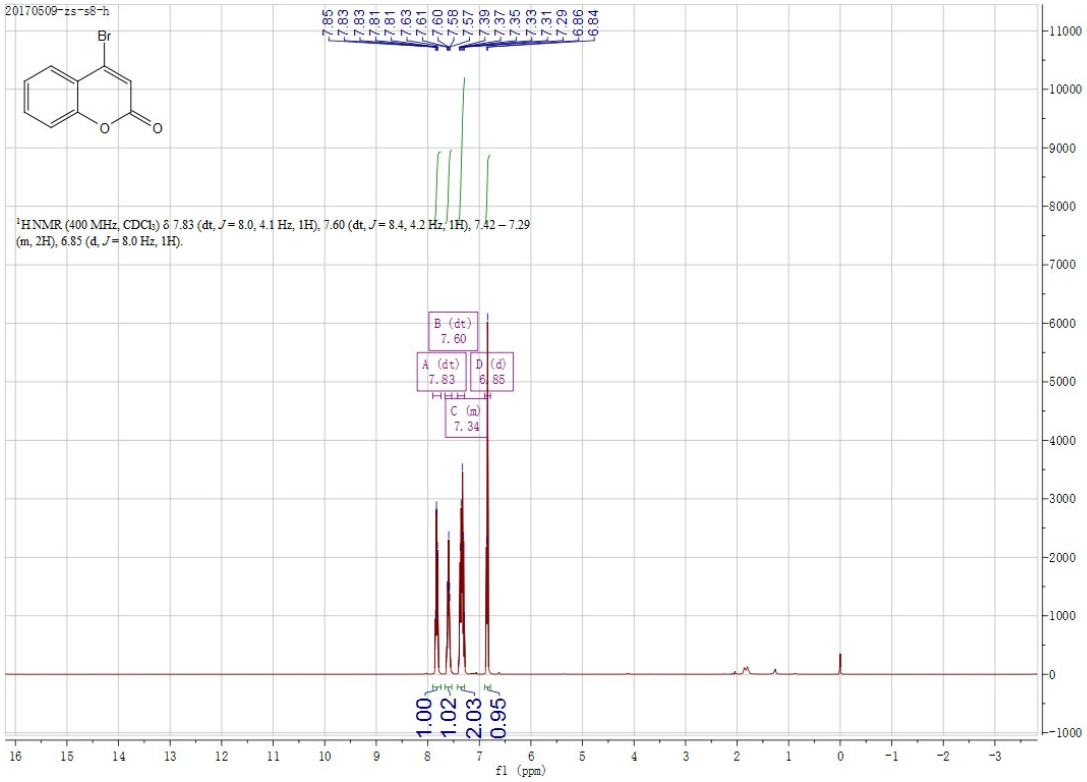

20170506-zs-s44-c
CH3
NH
H3C
Se
Cl
144.31
133.32
132.89
119.21
116.59
111.17
30.39
9.50
13C NMR (101 MHz, CDCl3) δ 144.31 (s), 133.32 (s), 132.89 (s), 119.21 (s), 116.59 (s), 111.17 (s), 30.39 (s), 9.50 (s).
K (s) 144.31
C (s) 132.89
J (s) 133.32
G (s) 116.59
F (s) 111.17
H (s) 119.21
B (s) 30.39
A (s) 9.50
f1 (ppm)

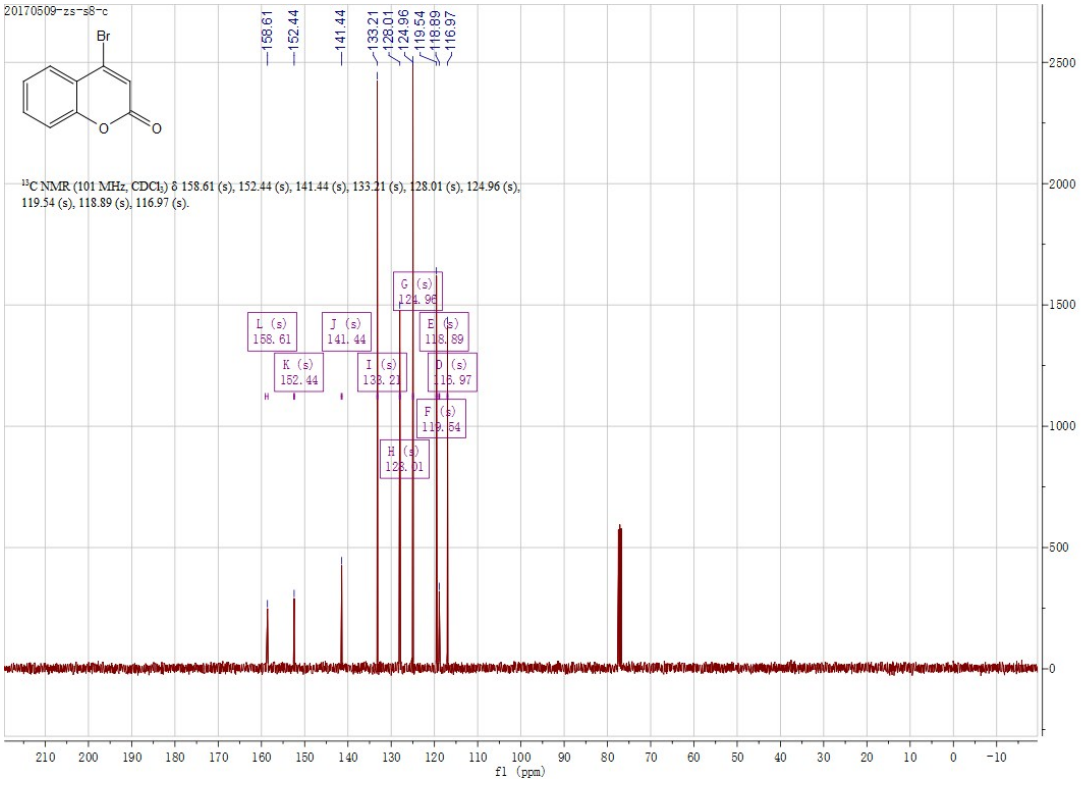
4i


20170506-zs-s55-h
CH3
NH
H3C
Se
Br
7.51
7.50
7.28
7.28
7.26
7.26
6.44
6.42
4.28
2.79
2.77
2.18
1H NMR (400 MHz, CDCl3) δ 7.51 (d, J = 1.9 Hz, 1H), 7.27 (dd, J = 8.4, 1.8 Hz, 1H), 6.43 (d, J = 8.4 Hz, 1H), 4.28 (s, 1H), 2.78 (d, J = 5.2 Hz, 3H), 2.18 (s, 3H).
B (dd) 7.27
A (d) 7.51
C (d) 6.43
F (s) 4.28
D (d) 2.78
E (s) 2.18
1.00
1.07
1.07
1.03
3.05
3.07
f1 (ppm)


20170506-zs-s55-c
CH3
NH
H3C
Se
Br
145.24
136.49
136.45
133.61
133.56
117.12
111.22
109.66
30.59
9.60
13C NMR (101 MHz, CDCl3) δ 145.24 (s), 136.47 (d, J = 4.9 Hz), 133.58 (d, J = 4.9 Hz), 117.12 (s), 111.22 (s), 109.66 (s), 30.59 (s), 9.60 (s).
J (d) 136.47
K (s) 145.24
I (d) 133.58
G (s) 111.22
F (s) 109.66
H (s) 117.12
B (s) 30.59
A (s) 9.60
f1 (ppm)

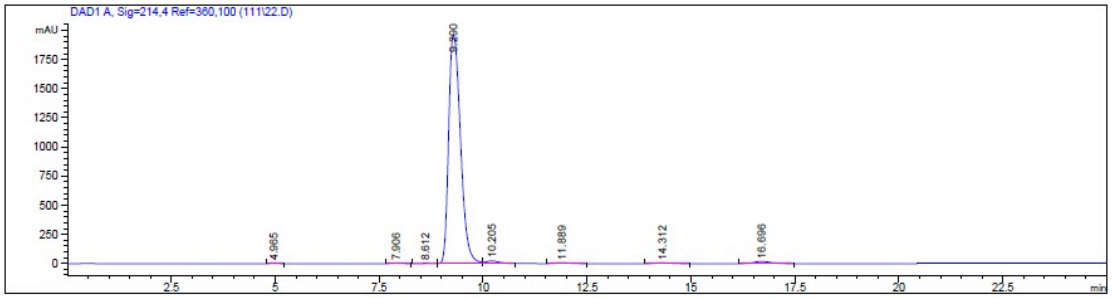
9


20170509-zs-s8-h
Br
O
O
7.85
7.83
7.83
7.81
7.81
7.63
7.61
7.60
7.58
7.57
7.39
7.37
7.35
7.33
7.31
7.29
6.86
6.84
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.83 (dt, J = 8.0, 4.1 Hz, 1H), 7.60 (dt, J = 8.4, 4.2 Hz, 1H), 7.42 – 7.29 (m, 2H), 6.85 (d, J = 8.0 Hz, 1H).
B (dt) 7.60
A (dt) 7.83
D (d) 6.85
C (m) 7.34
1.00
1.02
2.03
0.95
f1 (ppm)


20170509-zs-s8-c
Br
O
O
158.61
152.44
141.44
133.21
128.01
124.96
119.54
118.89
116.97
^{13}C NMR (101 MHz, CDCl$_3$) δ 158.61 (s), 152.44 (s), 141.44 (s), 133.21 (s), 128.01 (s), 124.96 (s), 119.54 (s), 118.89 (s), 116.97 (s).
G (s) 124.96
L (s) 158.61
J (s) 141.44
E (s) 118.89
K (s) 152.44
I (s) 133.21
D (s) 116.97
F (s) 119.54
H (s) 128.01
f1 (ppm)

SI3. HPLC chromatograms of target compounds.

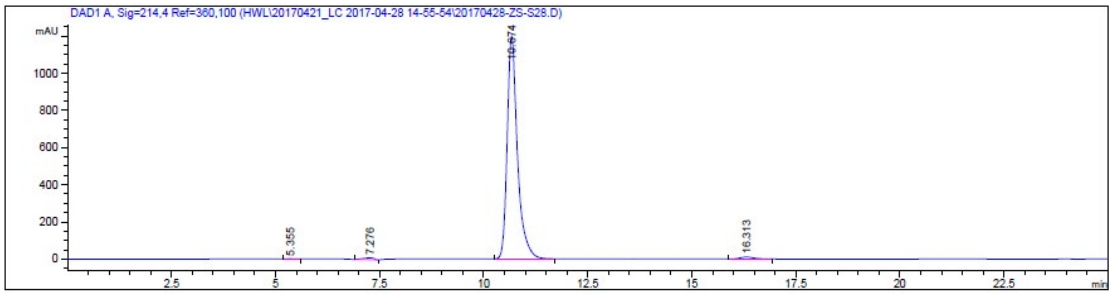
5a



信号 1: DAD1 A, Sig=214,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	4.965	BB	0.1538	29.80213	2.95197	0.0738
2	7.906	BB	0.2085	53.32410	3.97602	0.1320
3	8.612	BV	0.2781	63.23665	3.47899	0.1565
4	9.290	VV	0.3115	3.88544e4	1958.47876	96.1545
5	10.205	VB	0.3176	484.04605	22.62786	1.1979
6	11.889	BB	0.3377	184.81200	8.23838	0.4574
7	14.312	BB	0.3929	182.29555	7.06848	0.4511
8	16.696	BB	0.4551	556.37531	18.80707	1.3769
总量：				4.04083e4	2025.62753	

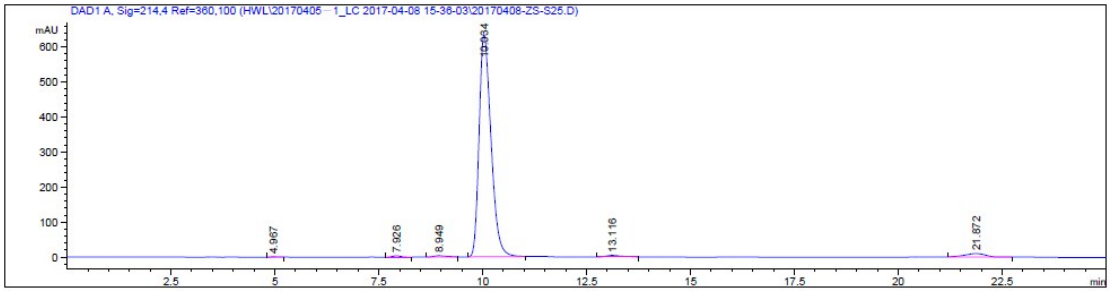
5b



信号 1: DAD1 A, Sig=214,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.355	BB	0.1535	18.26600	1.75384	0.0871
2	7.276	BV	0.2367	170.42955	10.42422	0.8124
3	10.674	BB	0.2540	2.05357e4	1198.21057	97.8836
4	16.313	BB	0.3768	255.32059	10.45871	1.2170
总量 :				2.09797e4	1220.84735	

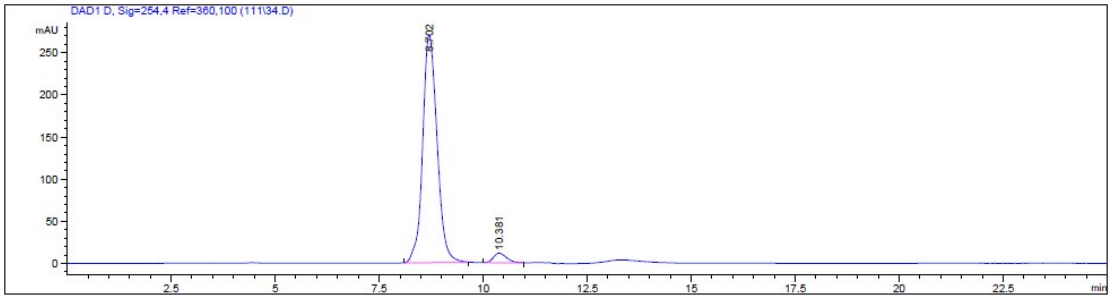
5d



信号 1: DAD1 A, Sig=214,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	4.967	BB	0.1516	14.44799	1.45860	0.1091
2	7.926	BB	0.2028	51.83836	3.95888	0.3915
3	8.949	BB	0.3051	70.61434	3.44612	0.5333
4	10.034	BB	0.3087	1.26550e4	634.58673	95.5707
5	13.116	BB	0.3888	118.89474	4.49250	0.8979
6	21.872	BB	0.5109	330.70428	9.76955	2.4975
总量 :				1.32415e4	657.71239	

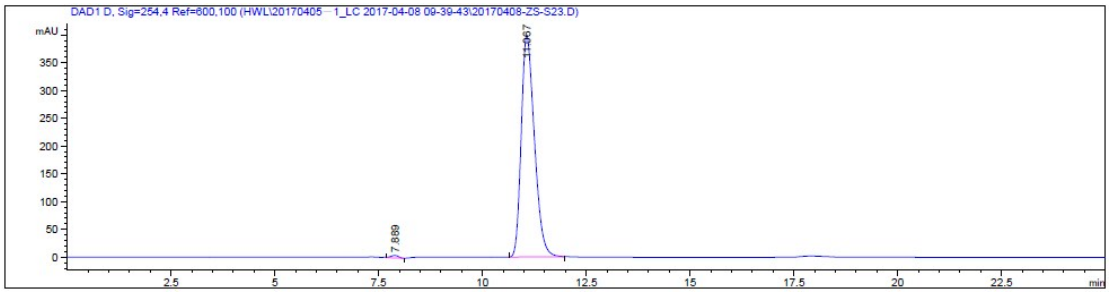
5f



信号 1: DAD1 D, Sig=254,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.702	BB	0.3792	6517.57129	270.41797	96.3678
2	10.381	BB	0.3403	245.65152	11.35811	3.6322
总量 :				6763.22281	281.77608	

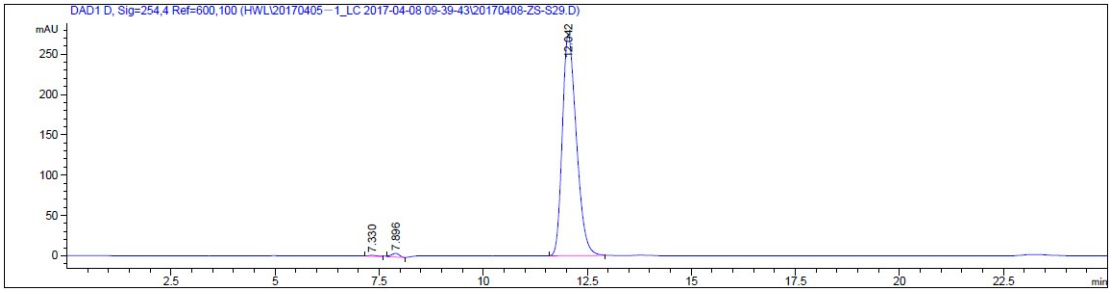
6a



信号 1: DAD1 D, Sig=254,4 Ref=600,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.889	BV	0.2001	60.21667	4.62014	0.6797
2	11.067	BB	0.3414	8798.48047	398.75320	99.3203
总量：				8858.69714	403.37335	

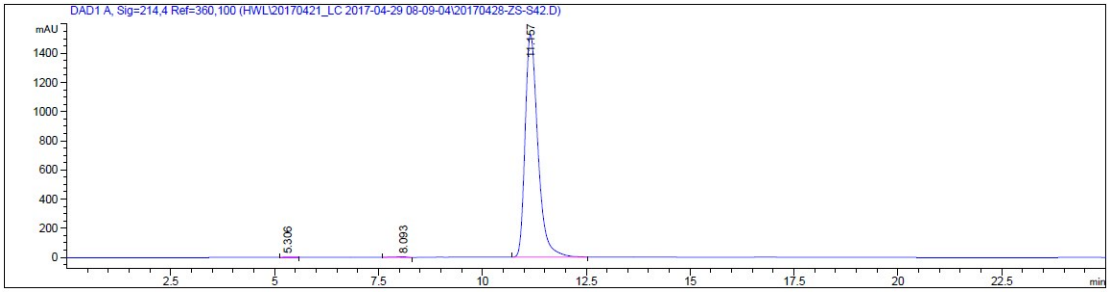
6b



信号 1: DAD1 D, Sig=254,4 Ref=600,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.330	BB	0.2318	16.97533	1.03235	0.2610
2	7.896	BV	0.2020	61.11156	4.69059	0.9395
3	12.042	BB	0.3635	6426.50830	274.16095	98.7995
总量：				6504.59519	279.88389	

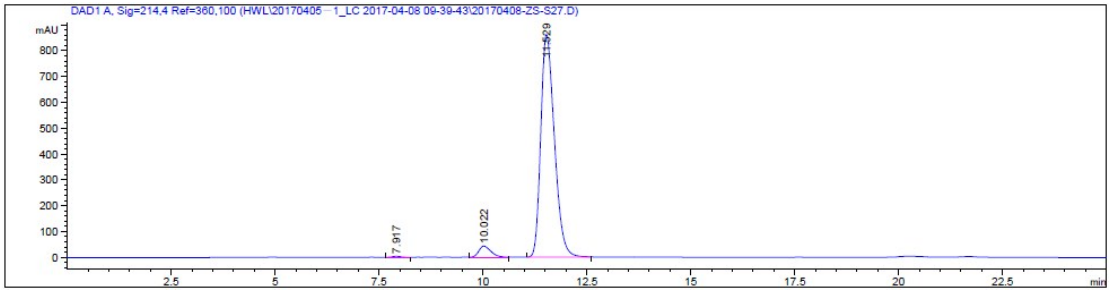
6c



信号 1: DAD1 A, Sig=214,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.306	BB	0.1654	27.09065	2.44238	0.0828
2	8.093	BV	0.2889	102.87139	4.94067	0.3143
3	11.157	BB	0.3271	3.25973e4	1526.43457	99.6029
总量 :				3.27273e4	1533.81762	

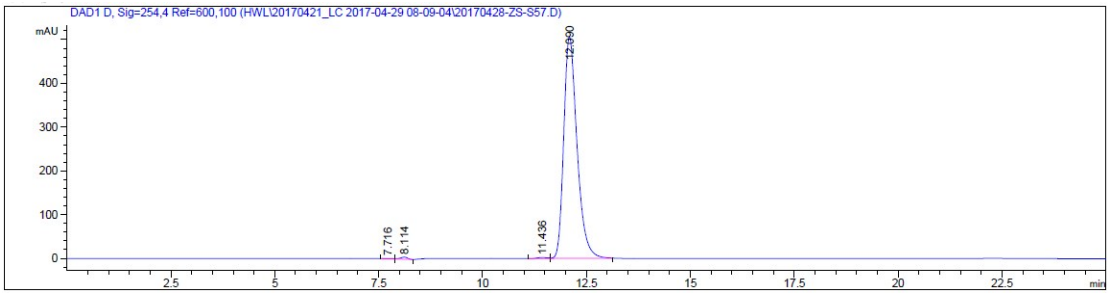
6d



信号 1: DAD1 A, Sig=214,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.917	BB	0.2046	51.47862	3.93598	0.2511
2	10.022	BB	0.3094	860.54681	43.01915	4.1983
3	11.529	BB	0.3492	1.95857e4	861.59259	95.5506
总量 :				2.04977e4	908.54772	

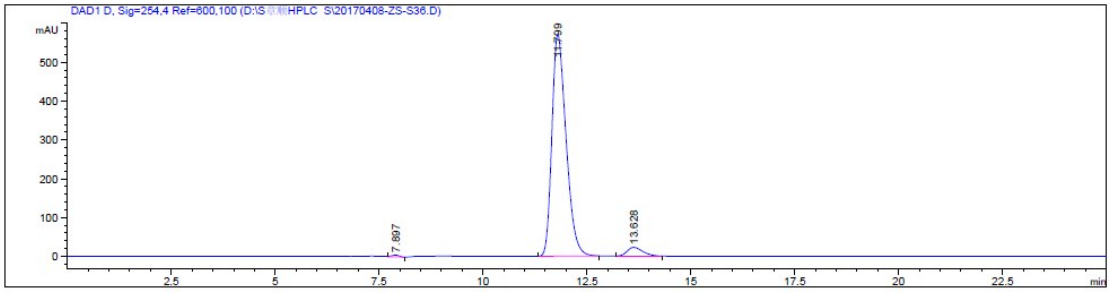
6e



信号 1: DAD1 D, Sig=254,4 Ref=600,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.716	BV	0.1983	14.07667	1.06463	0.1240
2	8.114	VV	0.1829	57.74492	4.85137	0.5088
3	11.436	BV	0.2744	39.93086	2.27907	0.3518
4	12.090	VB	0.3387	1.12375e4	506.78720	99.0153
总量：				1.13493e4	514.98227	

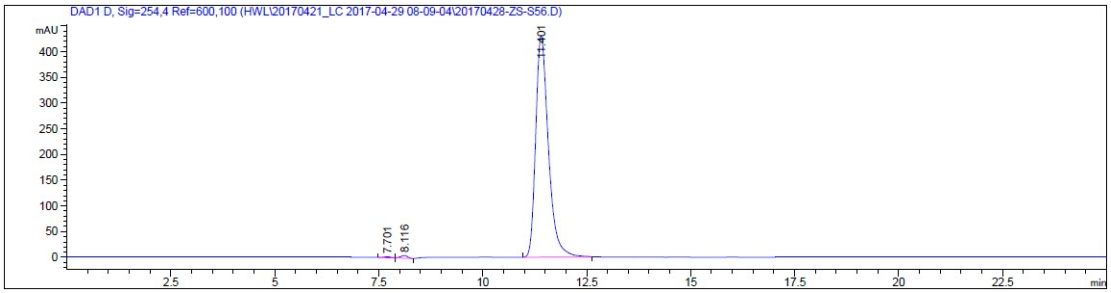
6f



信号 1: DAD1 D, Sig=254,4 Ref=600,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.897	BV	0.1952	60.15074	4.70264	0.4242
2	11.799	BB	0.3602	1.35255e4	571.24225	95.3969
3	13.628	BB	0.3951	592.47699	22.65251	4.1788
总量：				1.41781e4	598.59740	

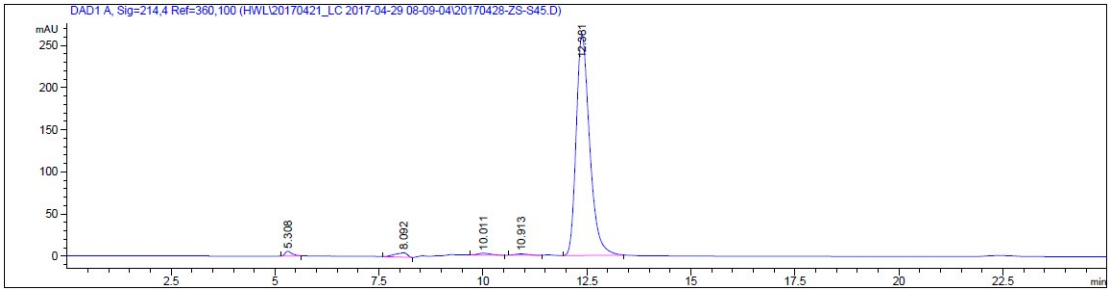
6g



信号 1: DAD1 D, Sig=254,4 Ref=600,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.701	BV	0.2077	20.95818	1.55090	0.2271
2	8.116	VV	0.1811	61.46288	5.22865	0.6659
3	11.401	BB	0.3217	9147.55371	430.86957	99.1070
总量 :				9229.97476	437.64912	

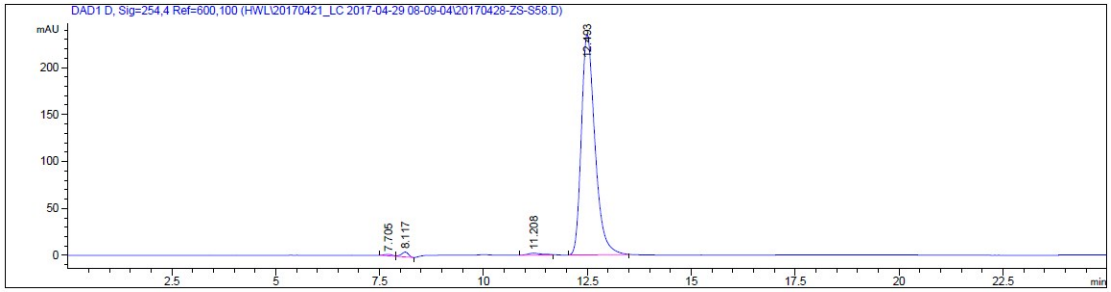
6h



信号 1: DAD1 A, Sig=214,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.308	BB	0.1728	68.31203	5.74381	1.1105
2	8.092	BV	0.2804	106.79716	5.27124	1.7361
3	10.011	BB	0.3001	44.63189	2.18732	0.7255
4	10.913	BB	0.3001	30.56148	1.53609	0.4968
5	12.381	BB	0.3428	5901.18018	261.99106	95.9310
总量 :				6151.48274	276.72952	

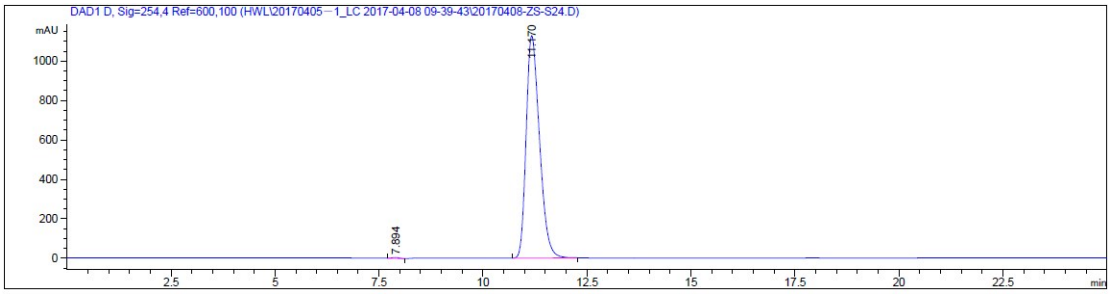
6i



信号 1: DAD1 D, Sig=254,4 Ref=600,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.705	BV	0.2116	22.20893	1.60383	0.4046
2	8.117	VV	0.1824	60.58751	5.18405	1.1037
3	11.208	BB	0.3410	48.75994	2.03881	0.8883
4	12.493	BB	0.3463	5357.77637	234.68335	97.6034
总量 :				5489.33276	243.51004	

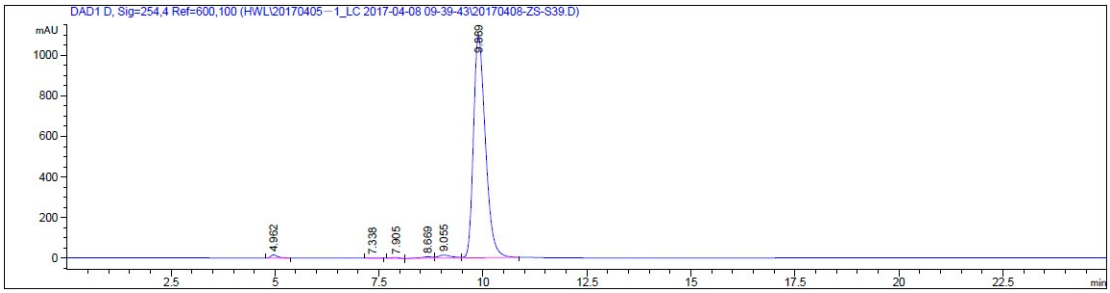
7a



信号 1: DAD1 D, Sig=254,4 Ref=600,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.894	BV	0.1981	59.68352	4.63887	0.2365
2	11.170	BB	0.3482	2.51814e4	1128.98633	99.7635
总量 :				2.52411e4	1133.62520	

10

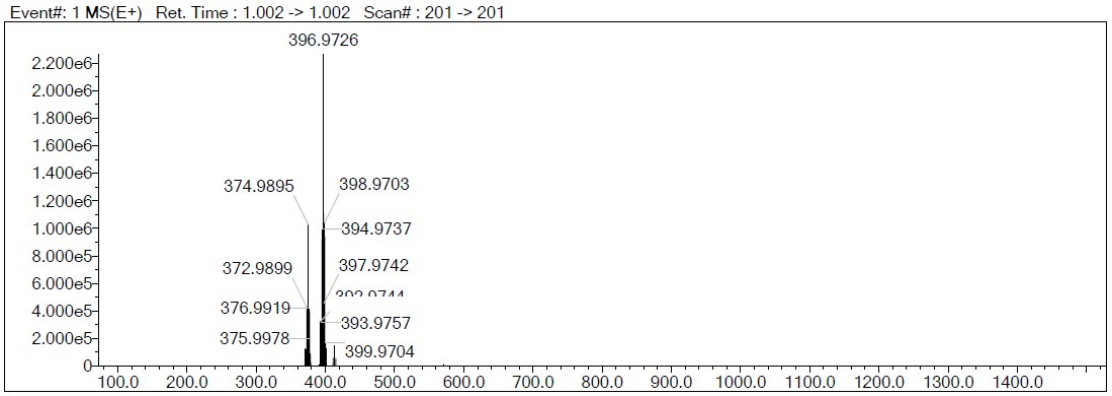


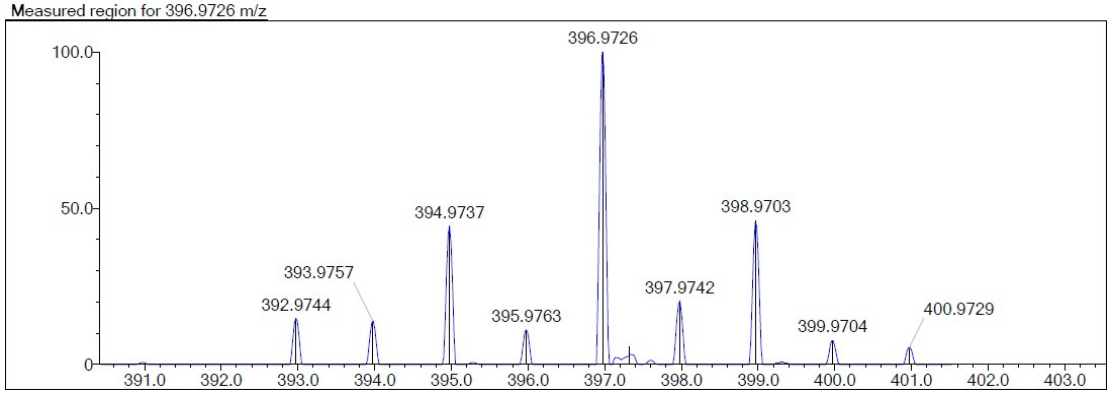
信号 1: DAD1 D, Sig=254,4 Ref=600,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	4.962	BB	0.1815	190.74367	15.72653	0.8459
2	7.338	BB	0.2295	16.36448	1.00730	0.0726
3	7.905	BV	0.1999	60.68776	4.66197	0.2691
4	8.669	VV	0.3080	141.36298	6.65067	0.6269
5	9.055	VV	0.3259	330.32471	14.94251	1.4649
6	9.889	VB	0.3064	2.18092e4	1095.00293	96.7205
总量：				2.25487e4	1137.99190	

SI4. HR-MS of target compounds

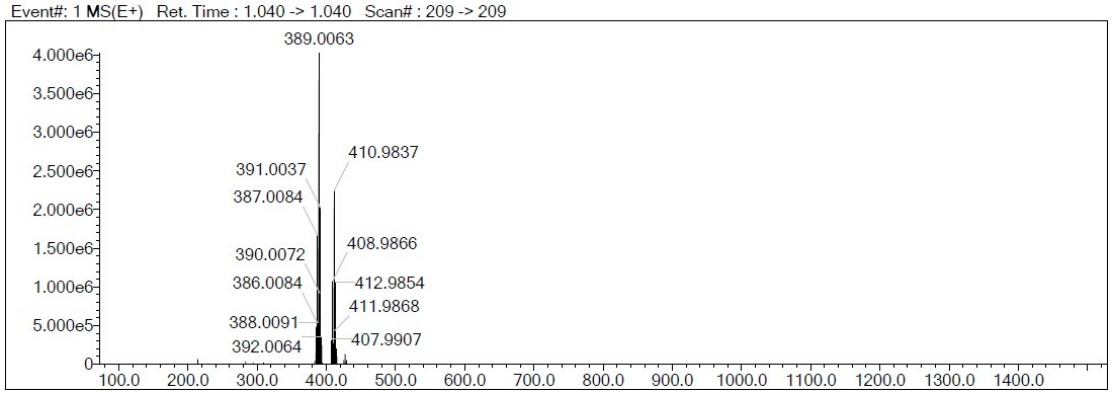
5a



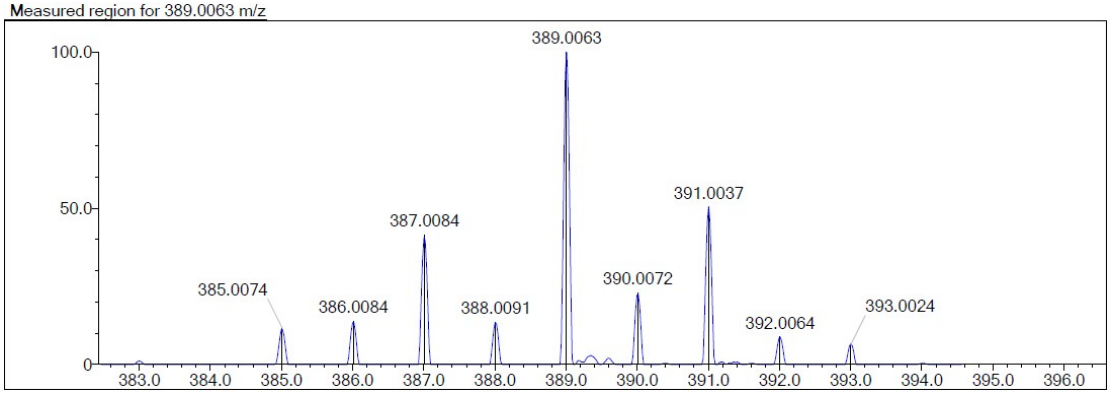


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	100.00	C16 H11 N4 Cl Se	[M+Na]+	396.9726	396.9728	-0.2	-0.50	100.00	13.0

5b



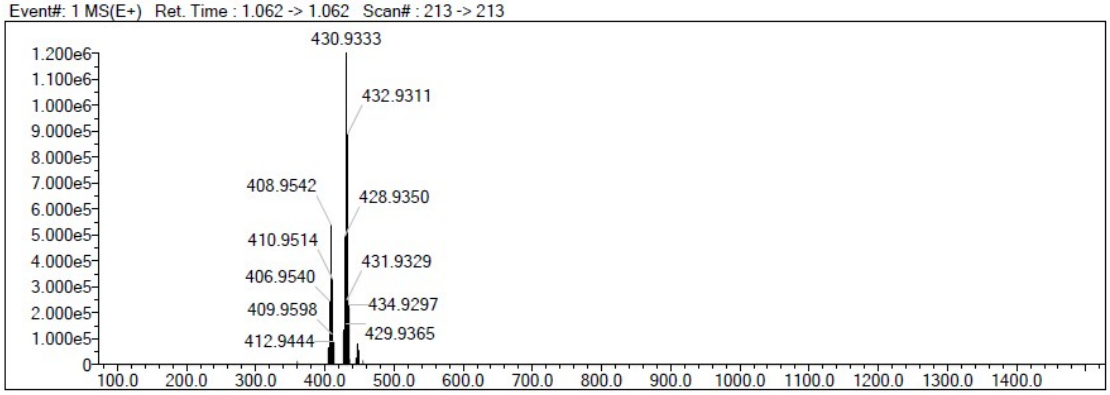
Measured region for 389.0063 m/z



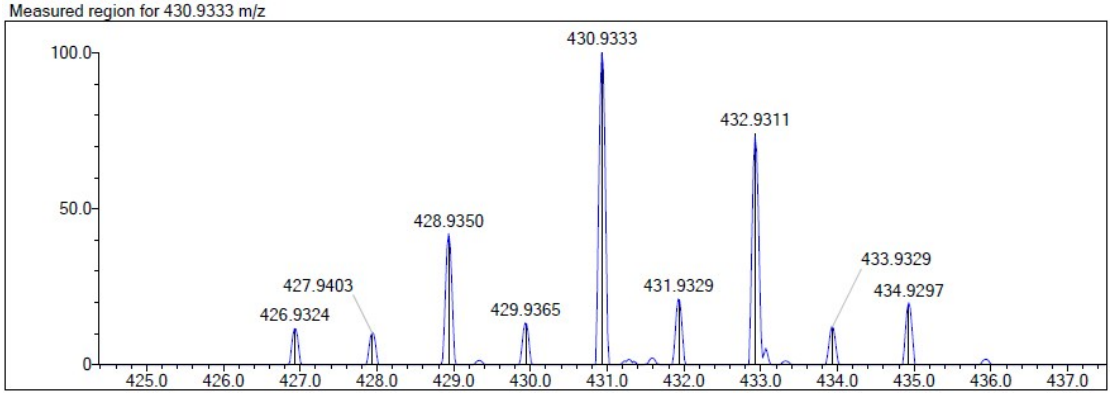
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.47	C17 H13 N4 Cl Se	[M+H]+	389.0063	389.0065	-0.2	-0.51	87.47	13.0

5d

Event#: 1 MS(E+) Ret. Time : 1.062 -> 1.062 Scan# : 213 -> 213

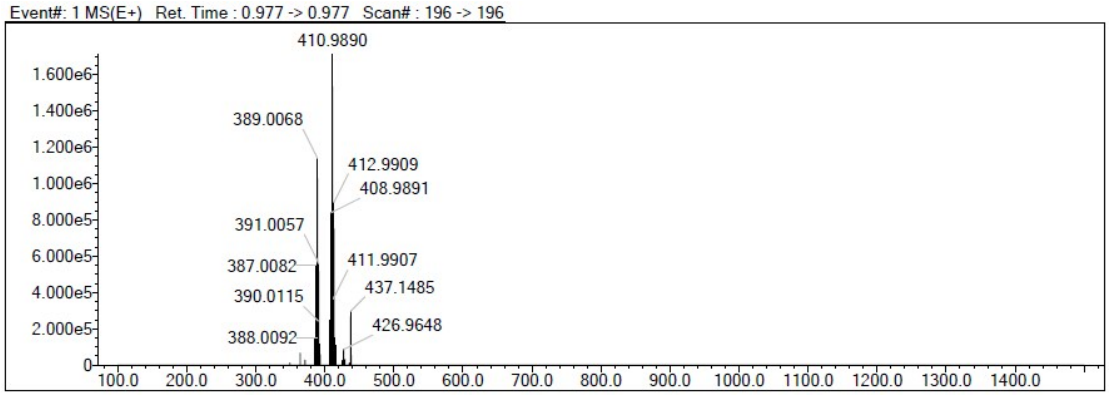


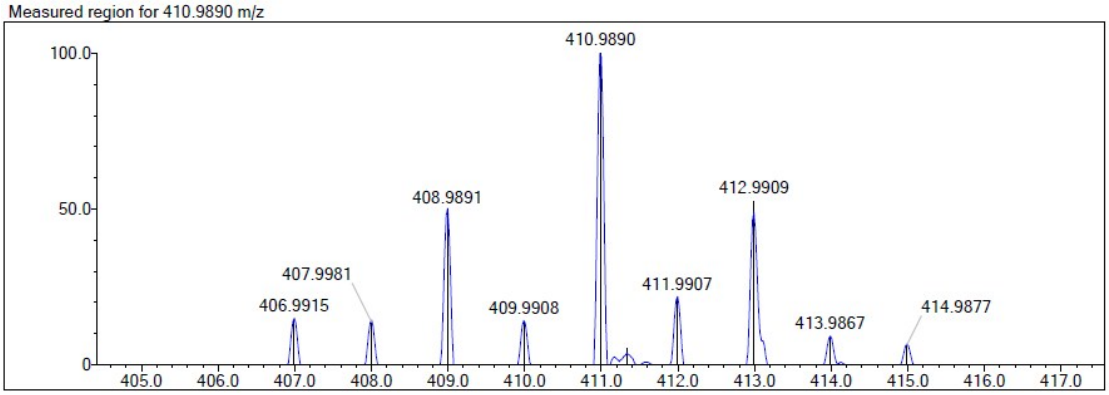
Measured region for 430.9333 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	89.62	C16 H10 N4 Cl2 Se	[M+Na]+	430.9333	430.9336	-0.3	-0.70	89.62	13.0

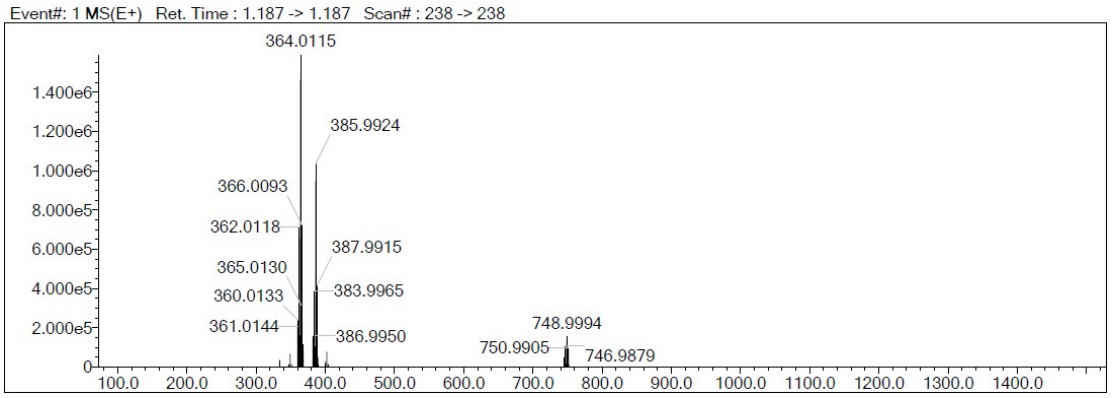
5f

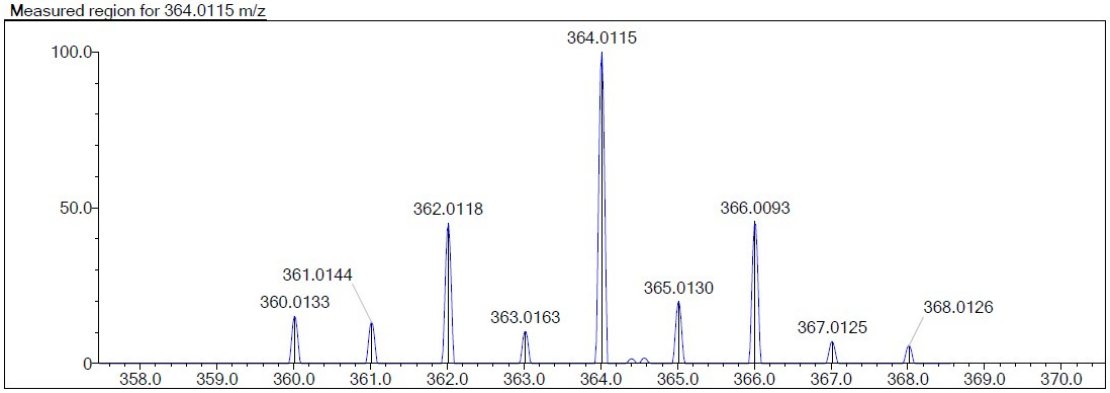




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	98.85	C17 H13 N4 Cl Se	[M+Na]+	410.9890	410.9884	0.6	1.46	100.00	13.0

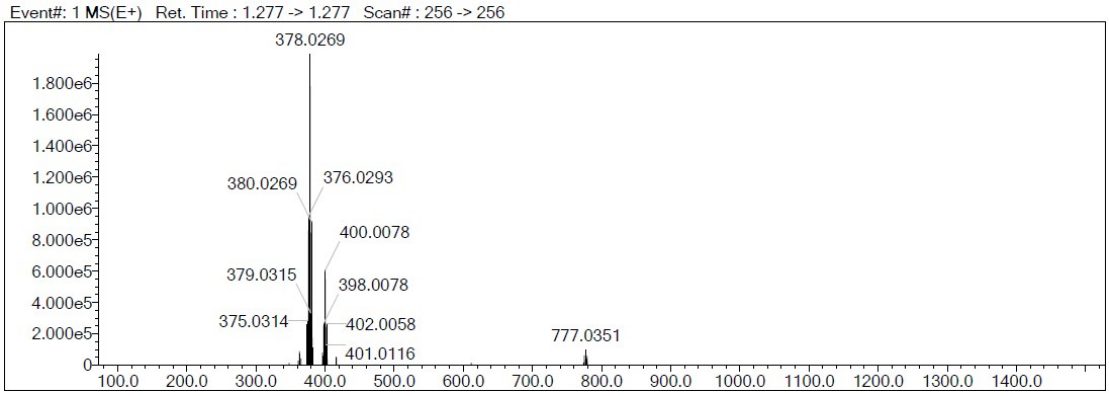
6a

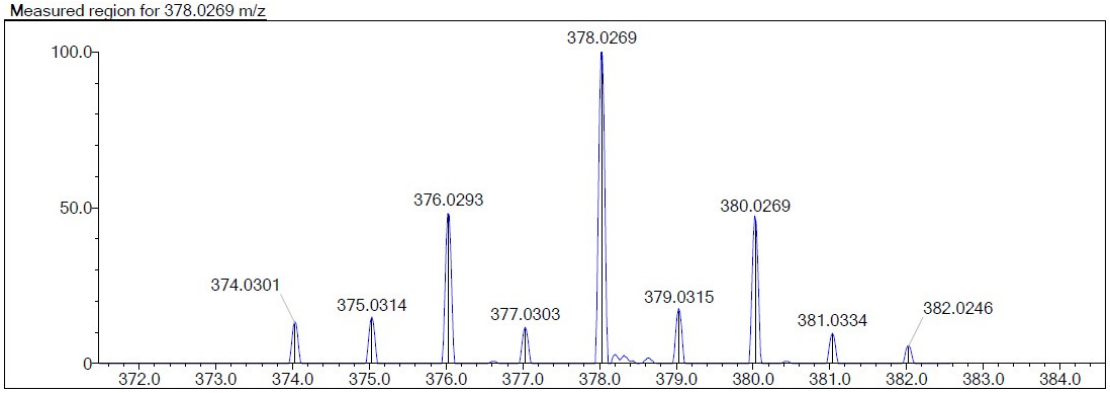




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	100.00	C16 H14 N3 Cl Se	[M+H]+	364.0115	364.0112	0.3	0.82	100.00	11.0

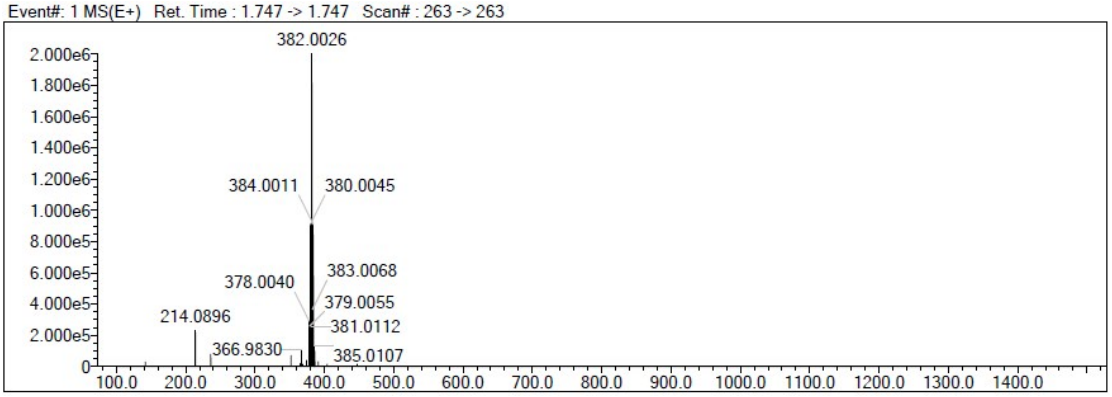
6b



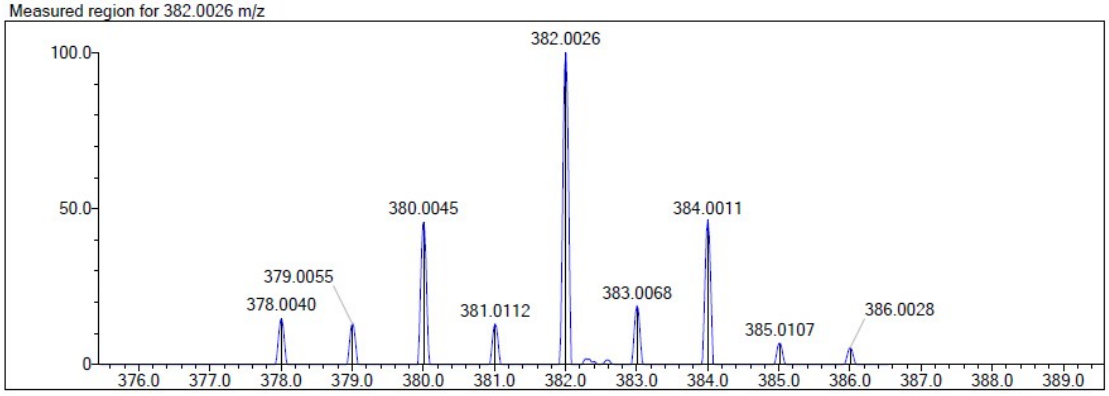


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	100.00	C17 H16 N3 Cl Se	[M+H]+	378.0269	378.0269	0.0	0.00	100.00	11.0

6c

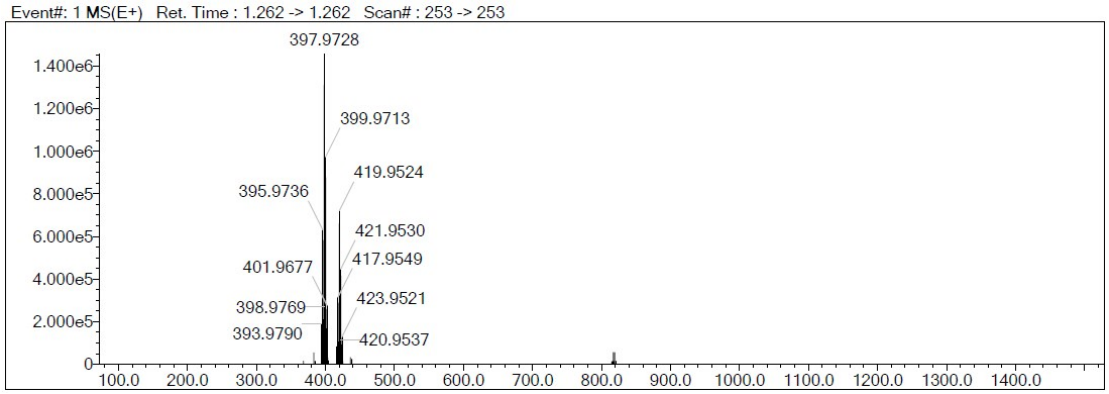


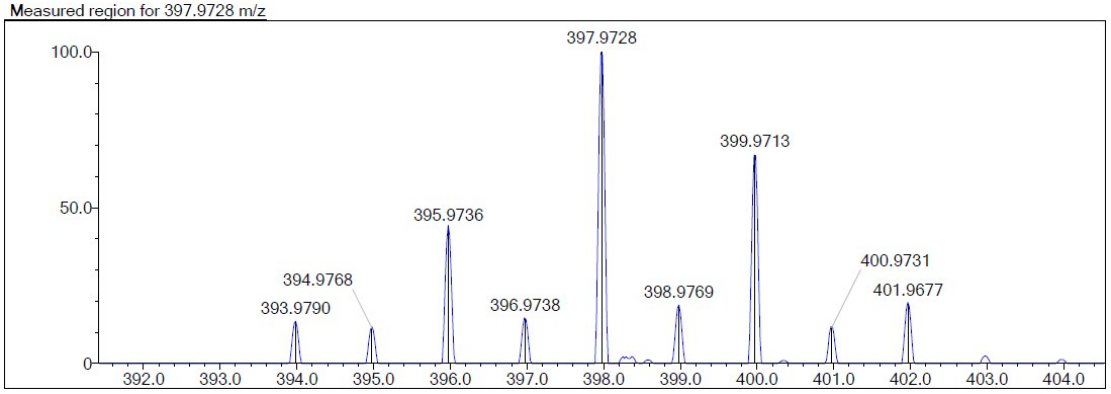
Measured region for 382.0026 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	97.28	C16 H13 N3 F Cl Se	[M+H]+	382.0026	382.0018	0.8	2.09	100.00	11.0

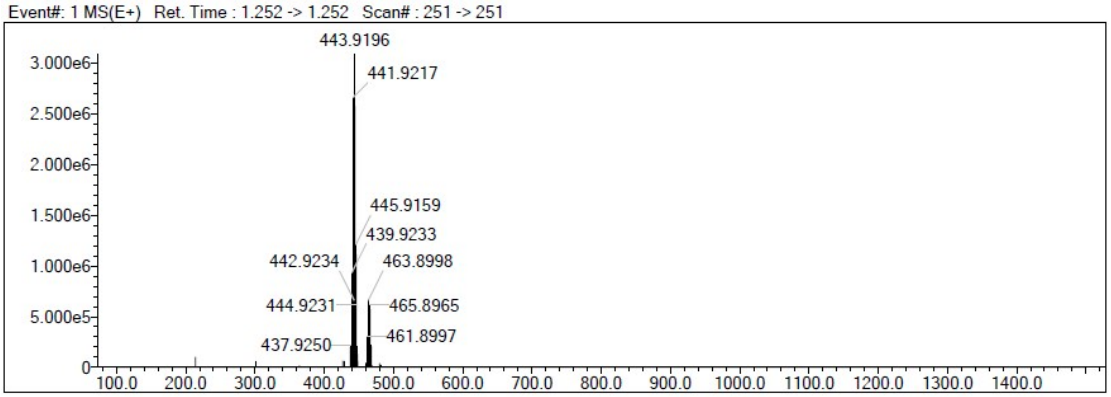
6d

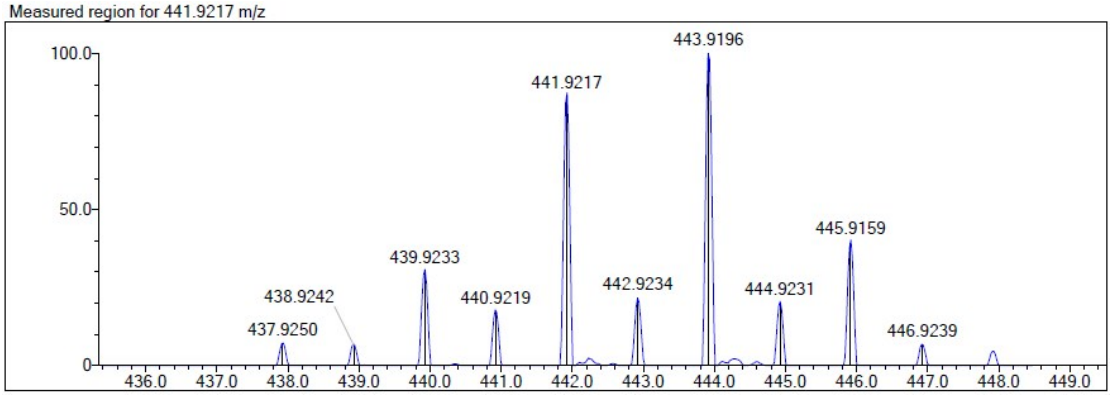




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	97.47	C16 H13 N3 Cl2 Se	[M+H]+	397.9728	397.9720	0.8	2.01	100.00	11.0

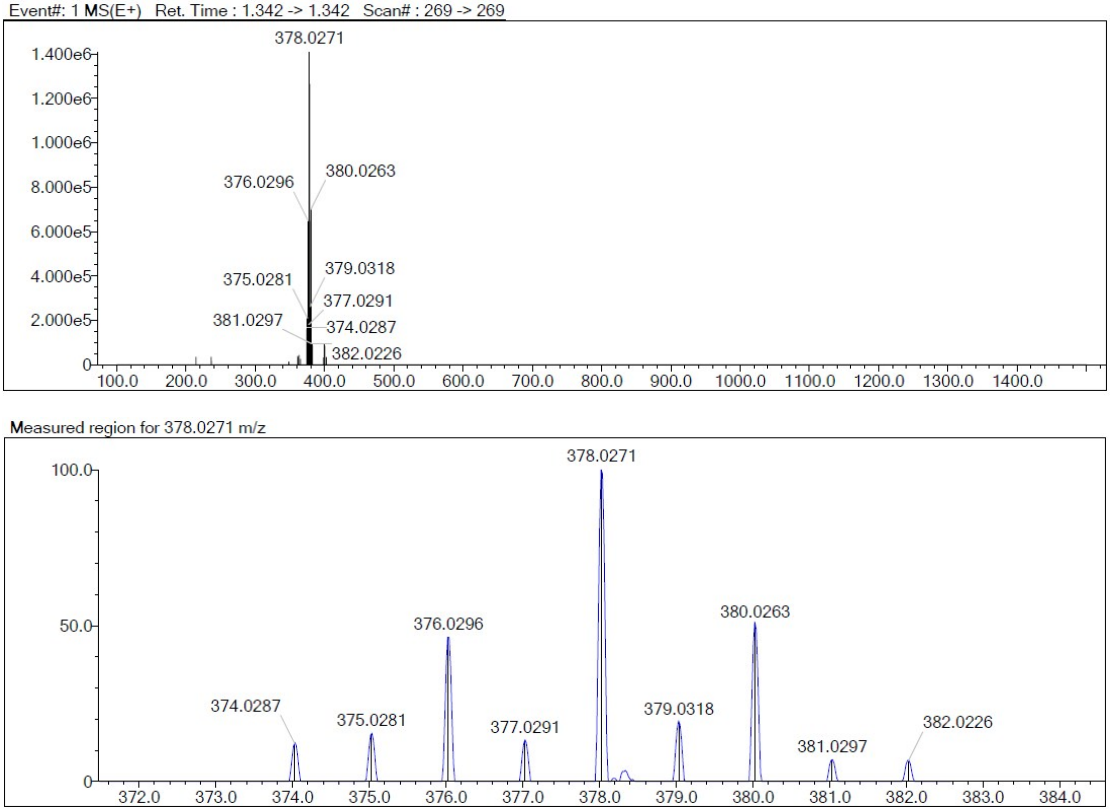
6e





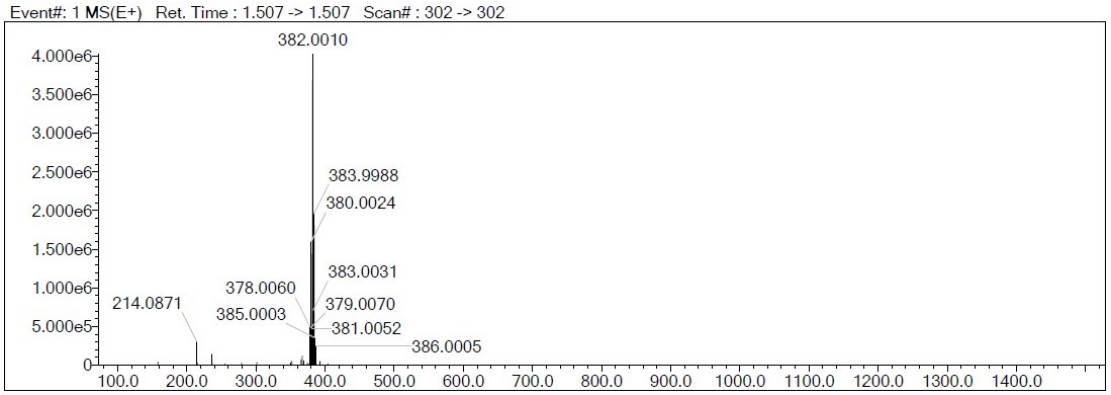
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
7	72.57	C16 H13 N3 Cl Se Br	[M+H]+	441.9217	441.9215	0.2	0.45	72.57	11.0

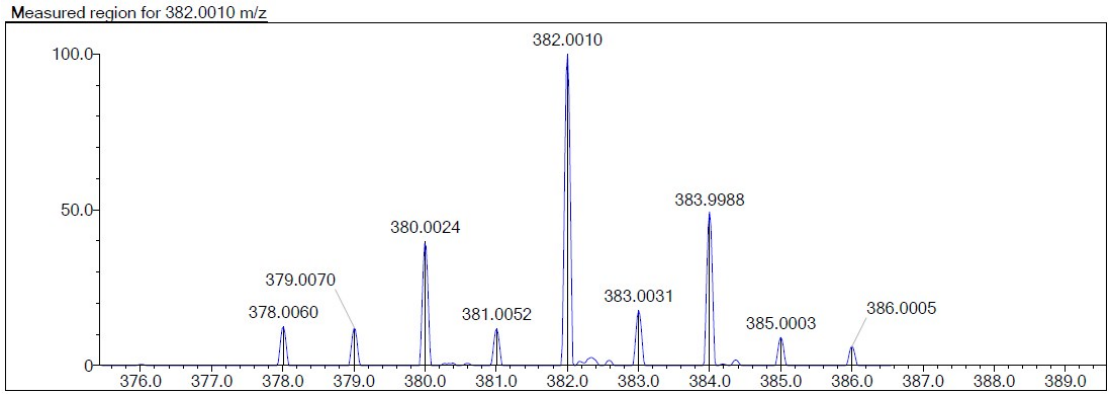
6f



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	94.09	C17 H16 N3 Cl Se	[M+H]+	378.0271	378.0269	0.2	0.53	94.09	11.0

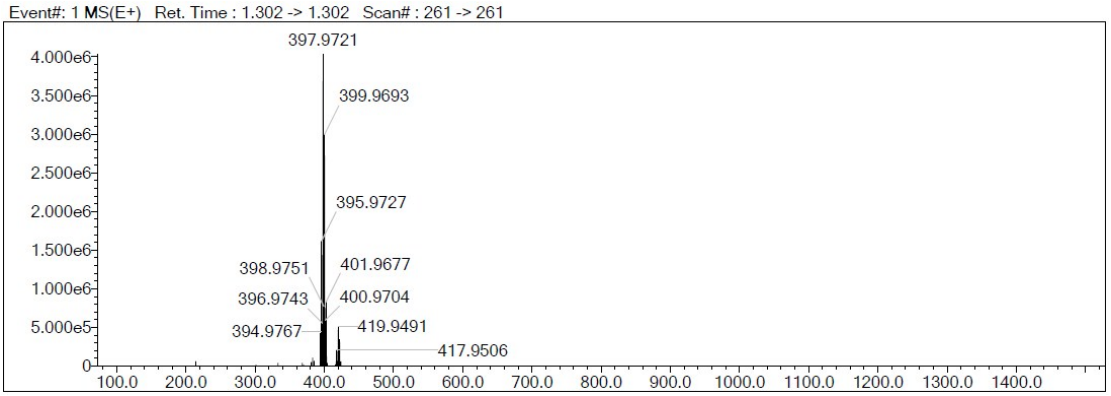
6g

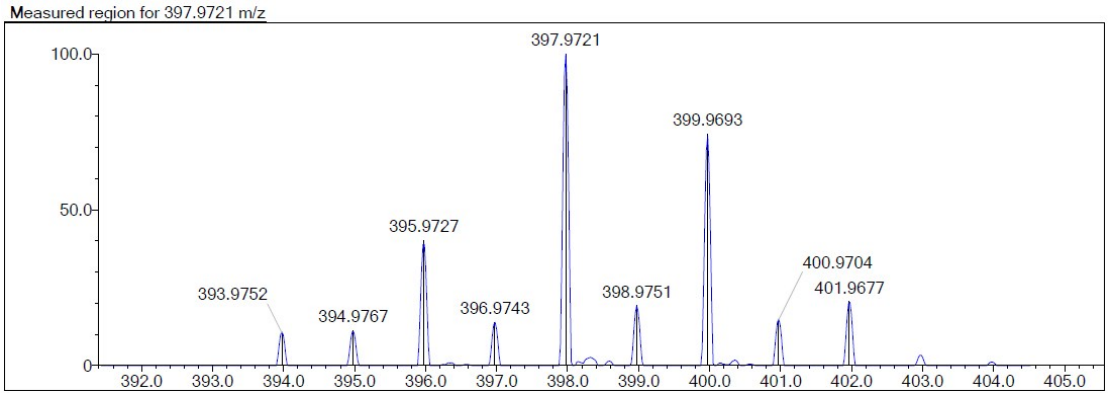




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	82.86	C16 H13 N3 F Cl Se	[M+H]+	382.0010	382.0018	-0.8	-2.09	85.18	11.0

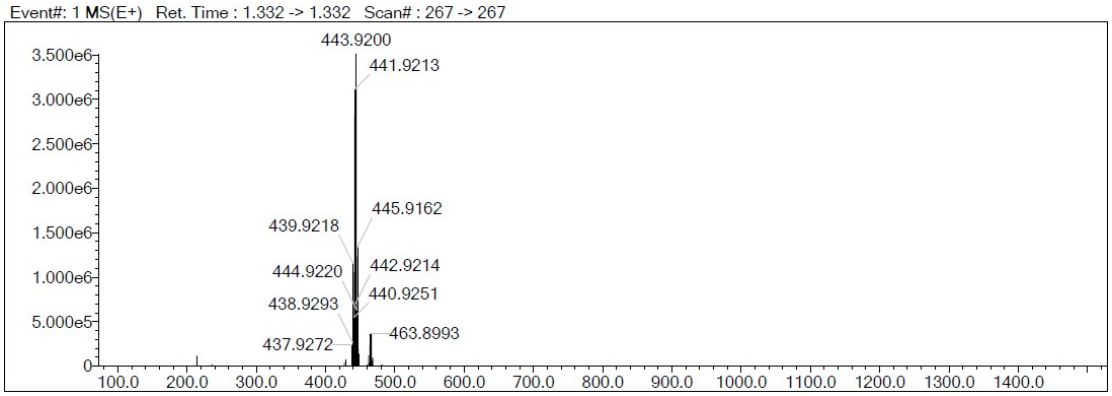
6h

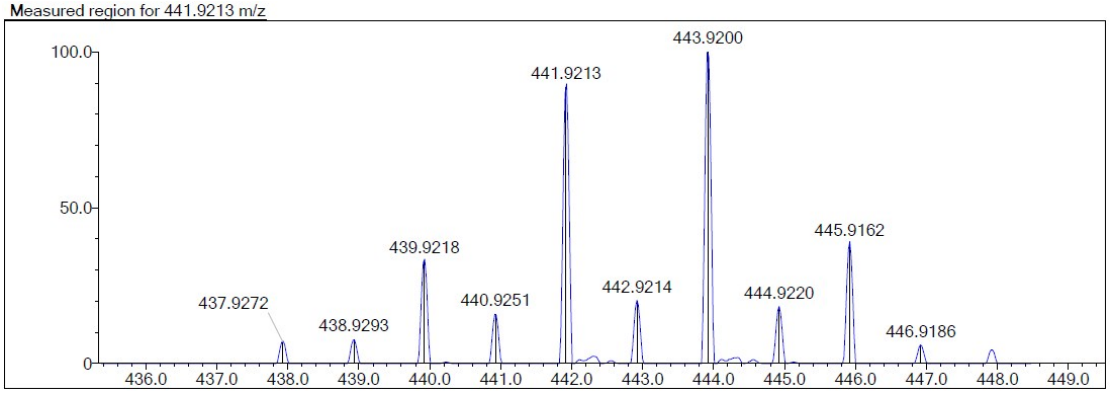




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	86.33	C16 H13 N3 Cl2 Se	[M+H]+	397.9721	397.9720	0.1	0.25	86.33	11.0

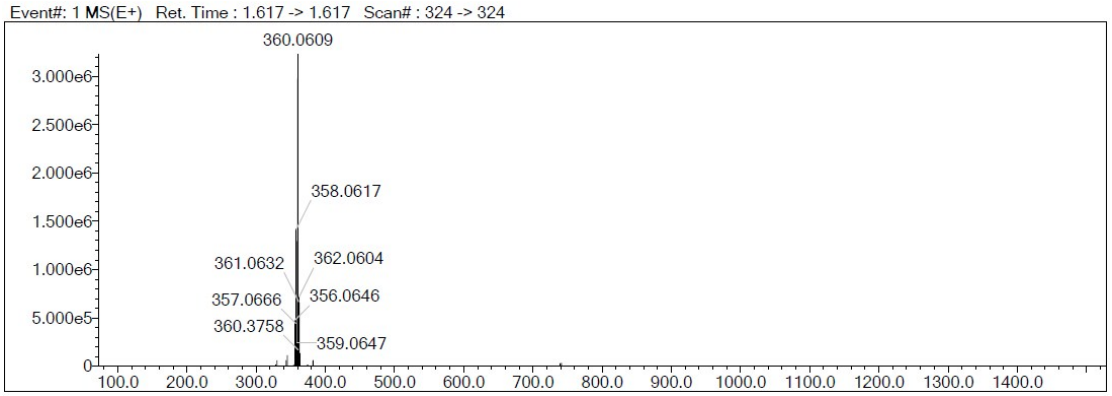
6i

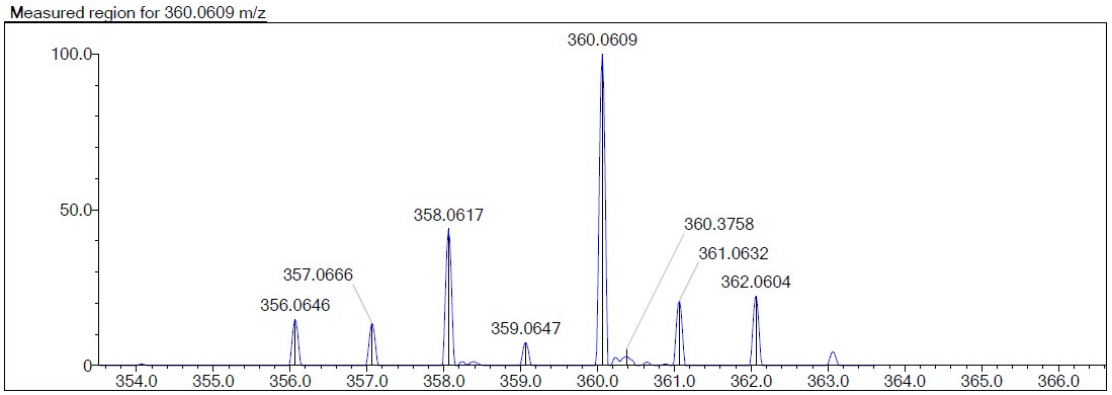




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
7	76.77	C16 H13 N3 Cl Se Br	[M+H]+	441.9213	441.9215	-0.2	-0.45	76.77	11.0

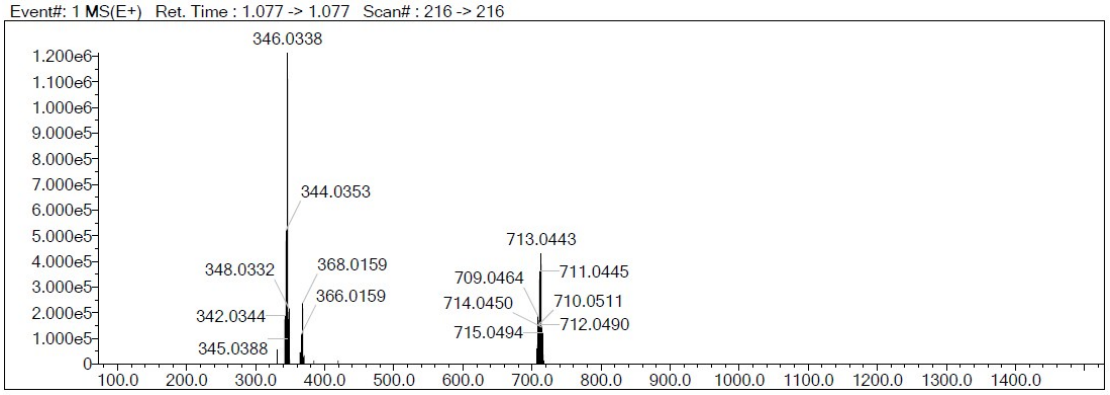
7a

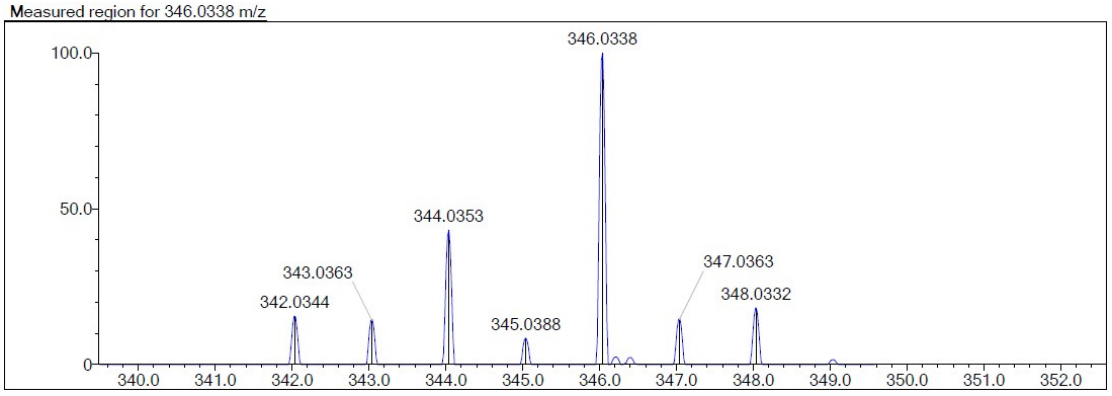




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	91.25	C17 H17 N3 O Se	[M+H]+	360.0609	360.0610	-0.1	-0.28	91.25	11.0

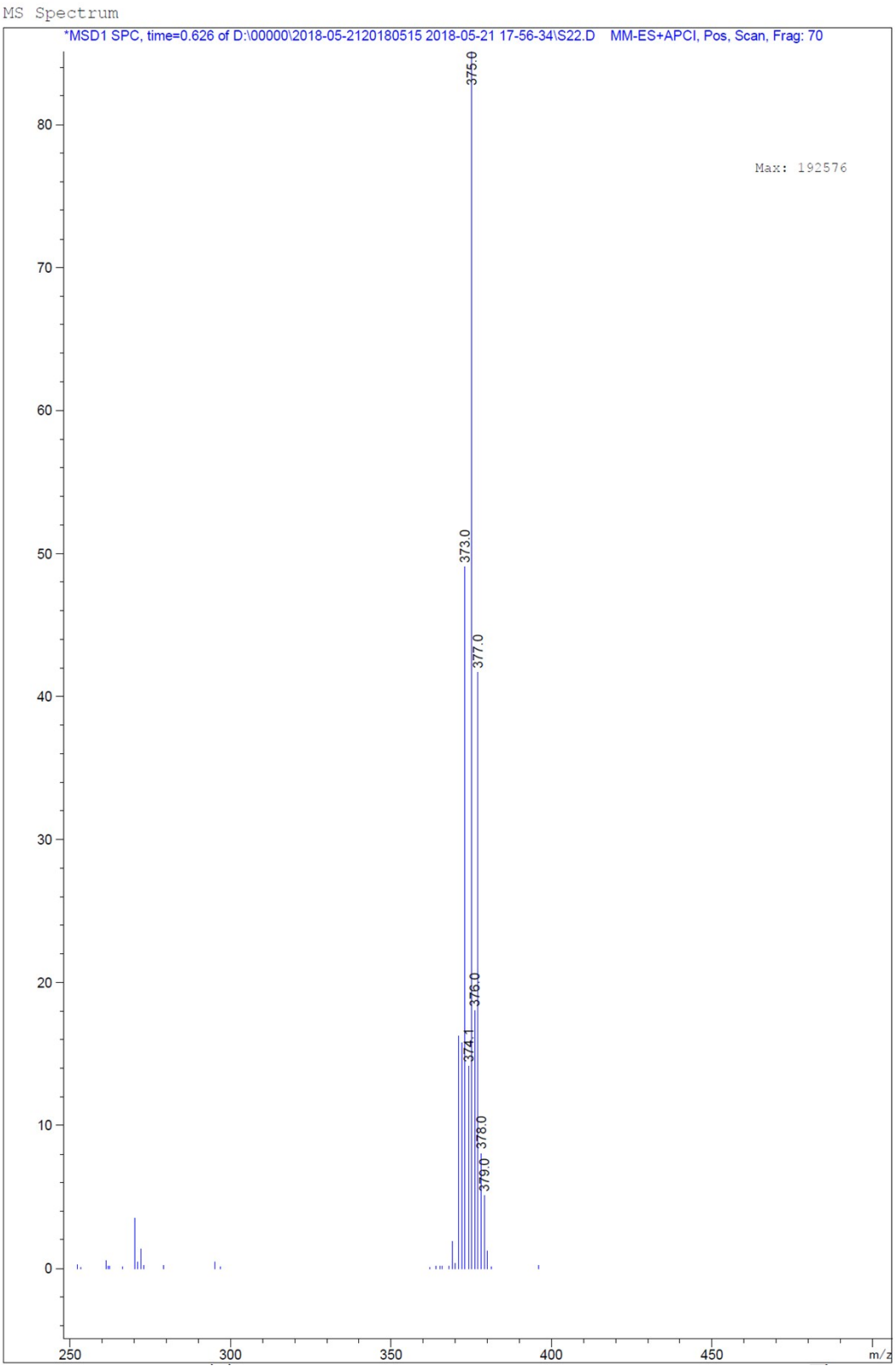
10



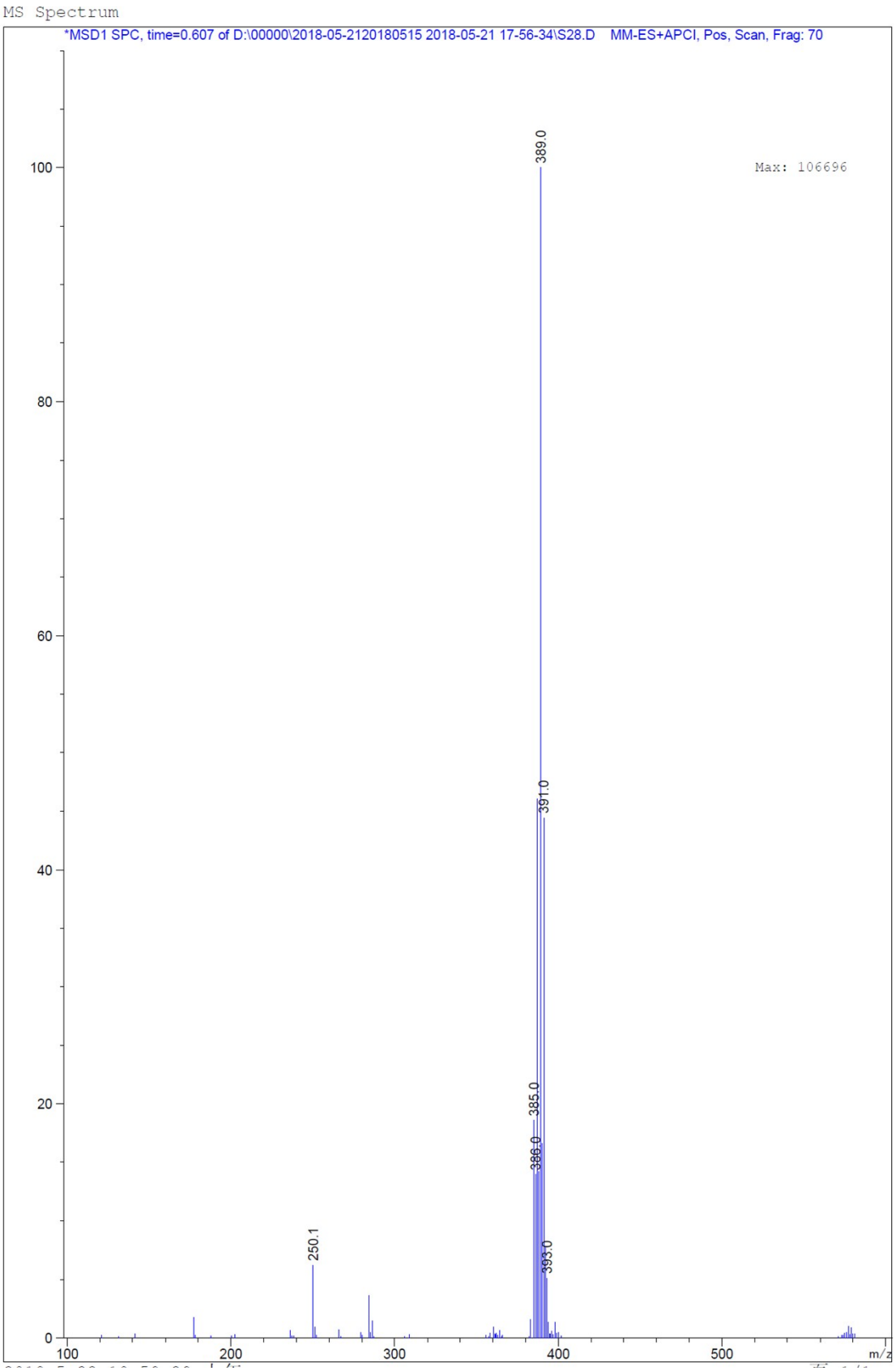


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	90.47	C17 H15 N O2 Se	[M+H]+	346.0338	346.0341	-0.3	-0.87	90.47	11.0

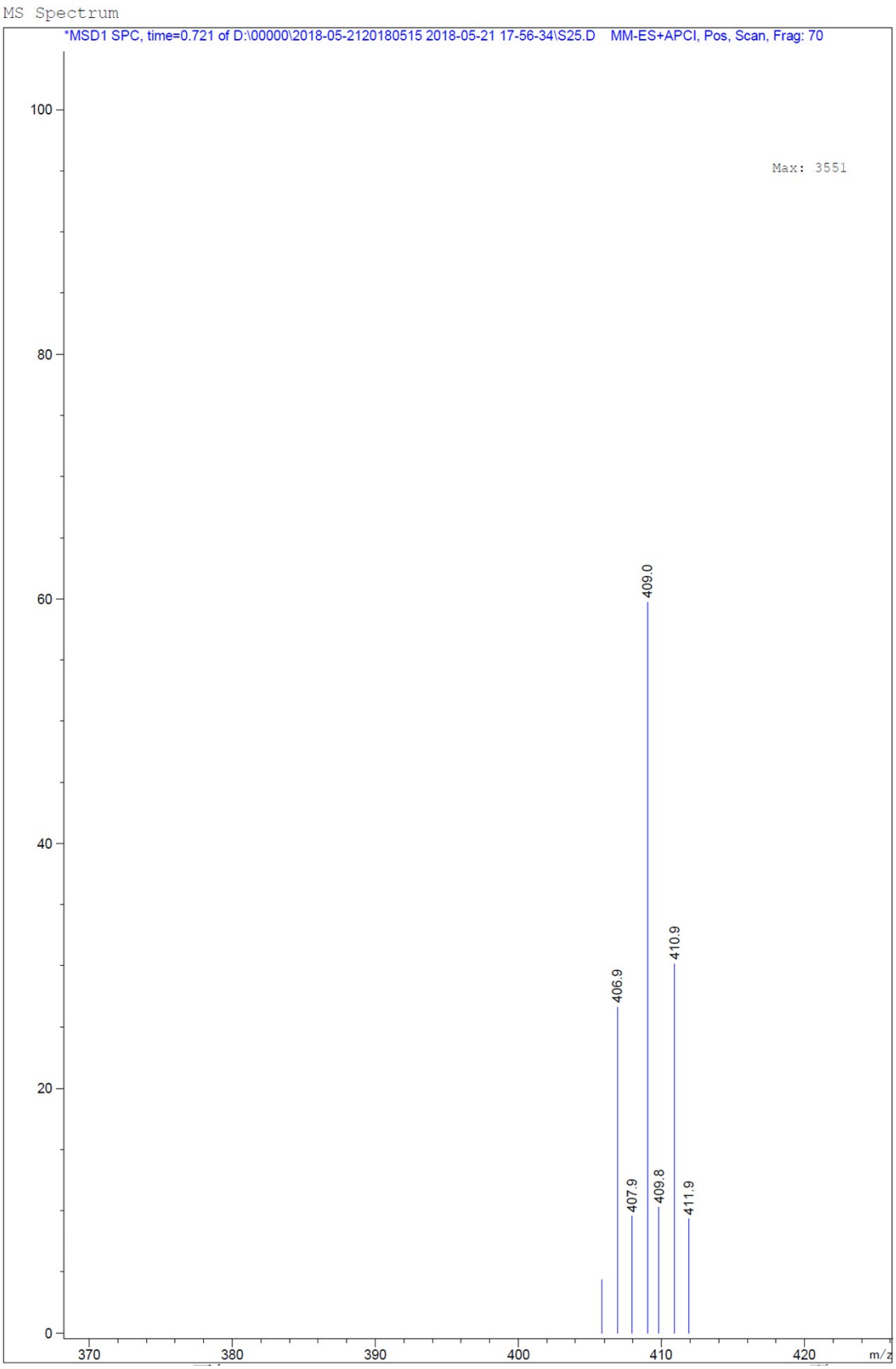
SI5. LR-MS of target compounds



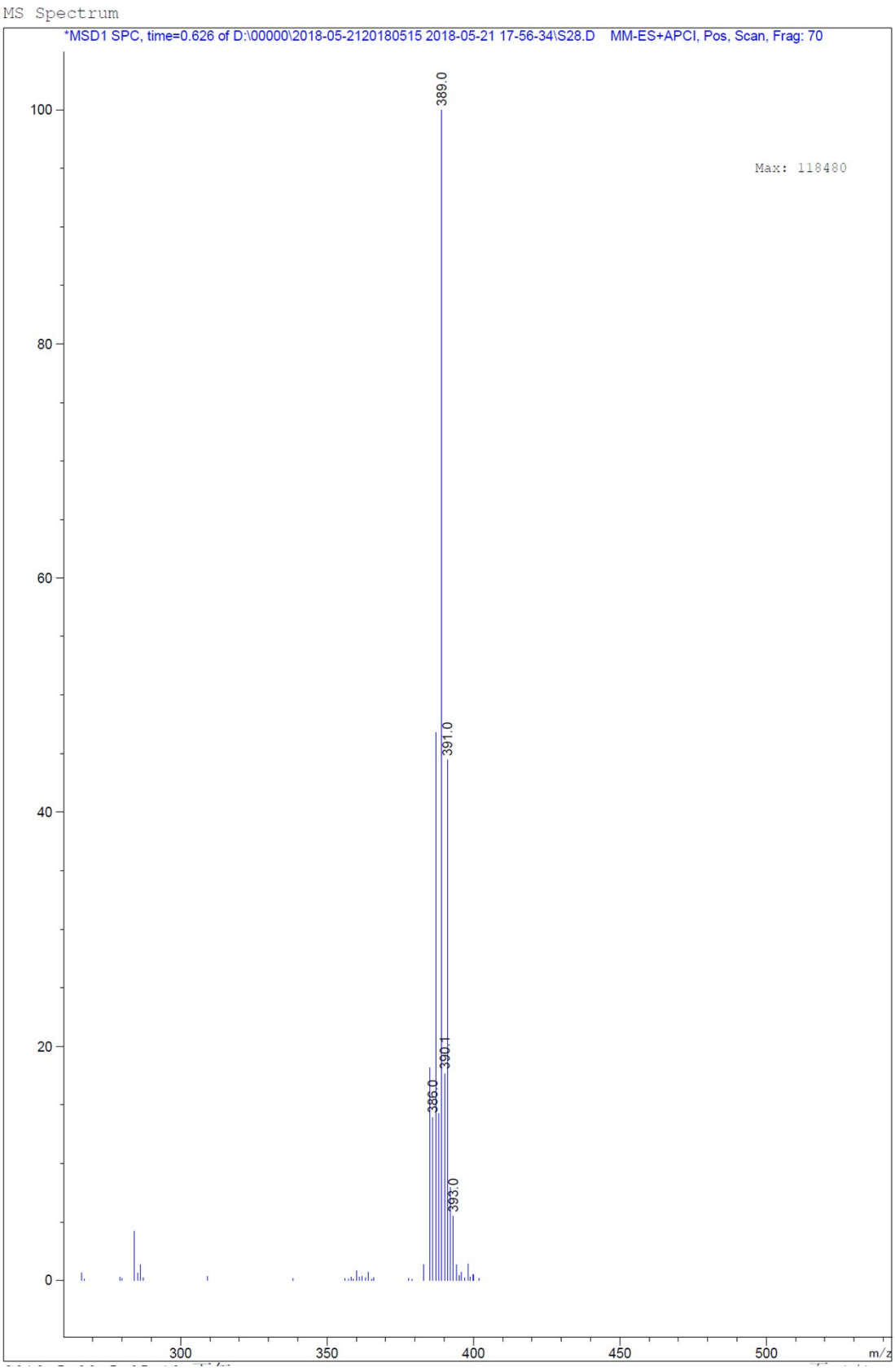
MS of compound **5a**



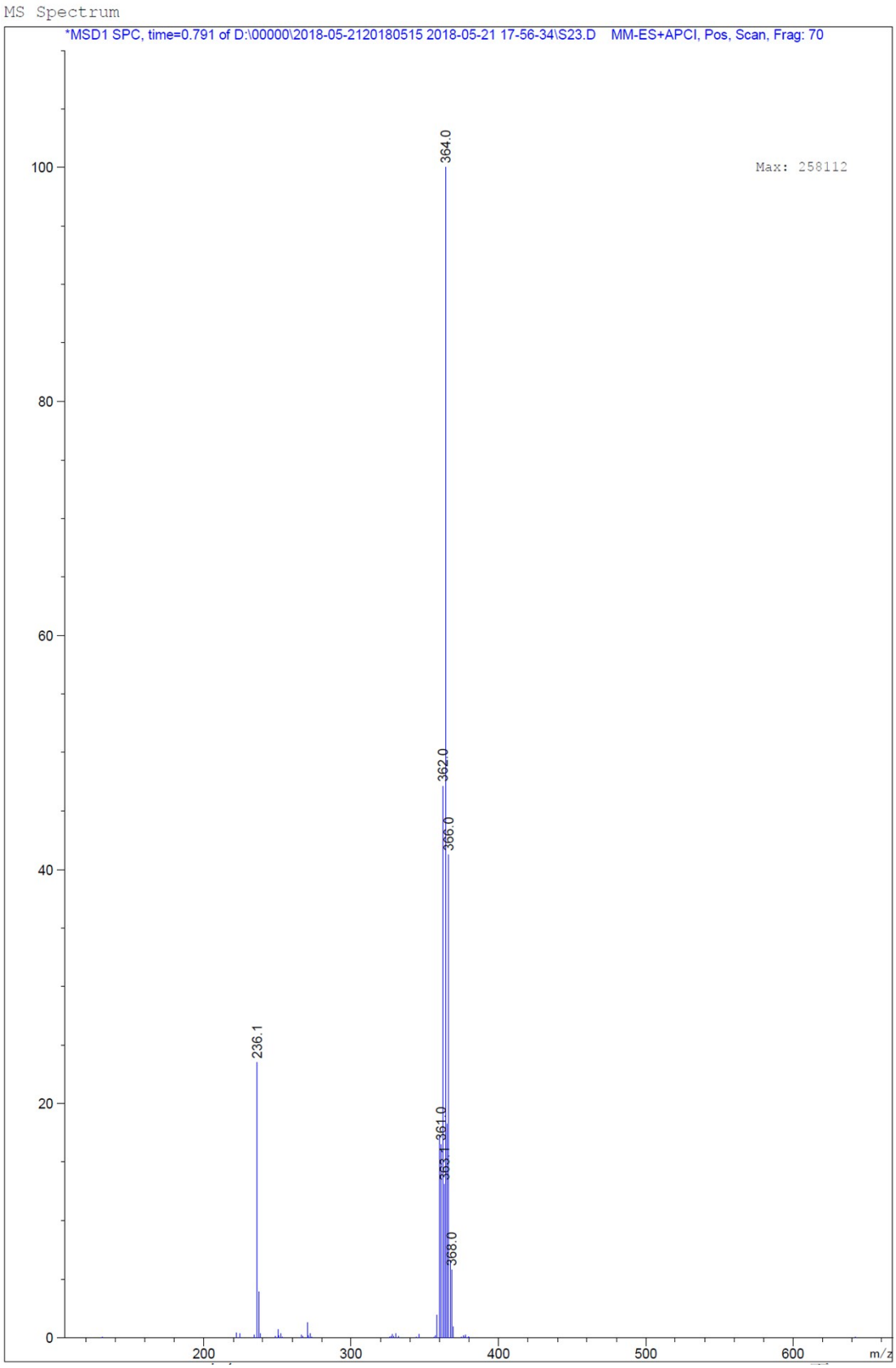
MS of compound **5b**



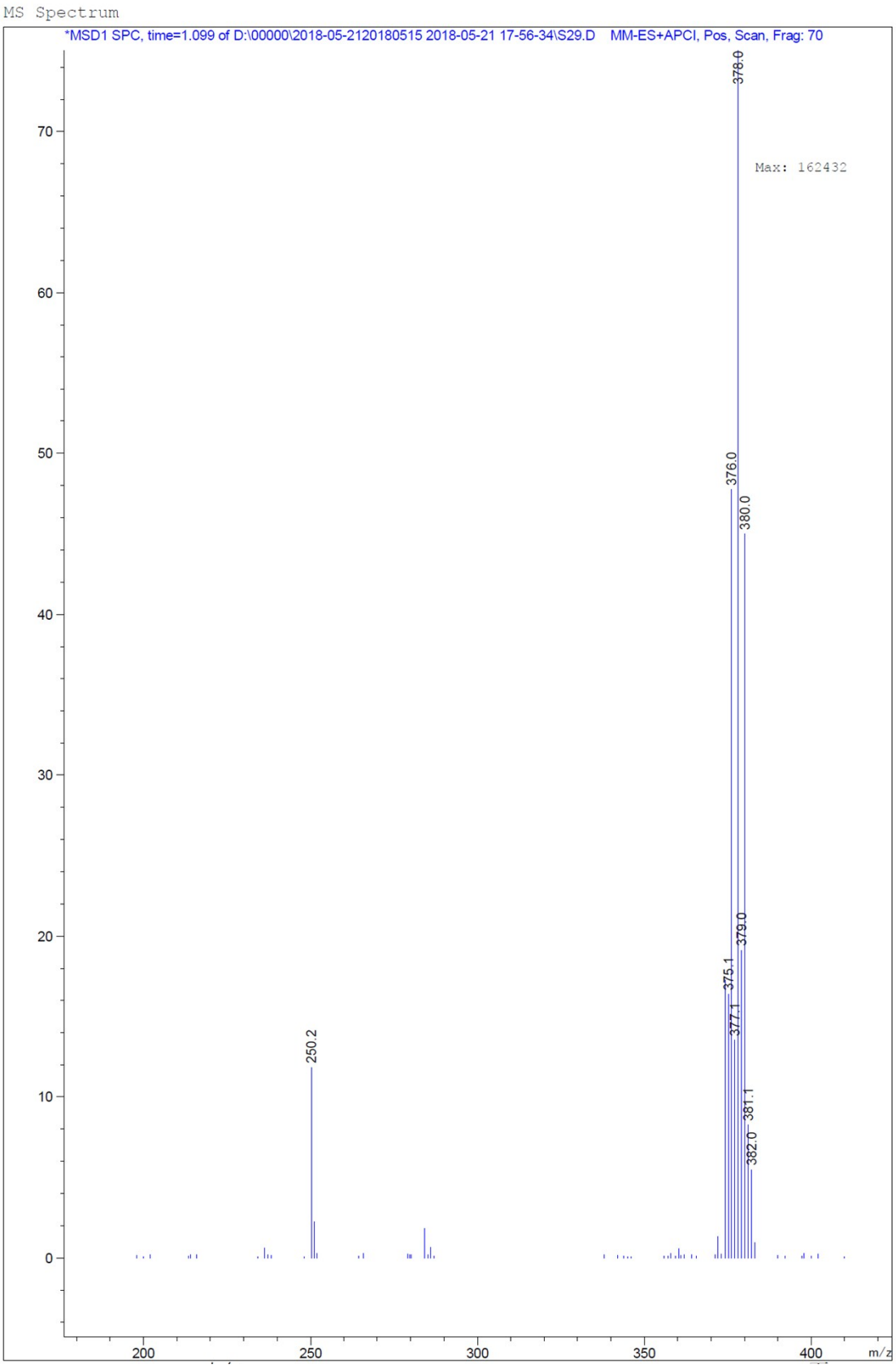
MS of compound **5d**



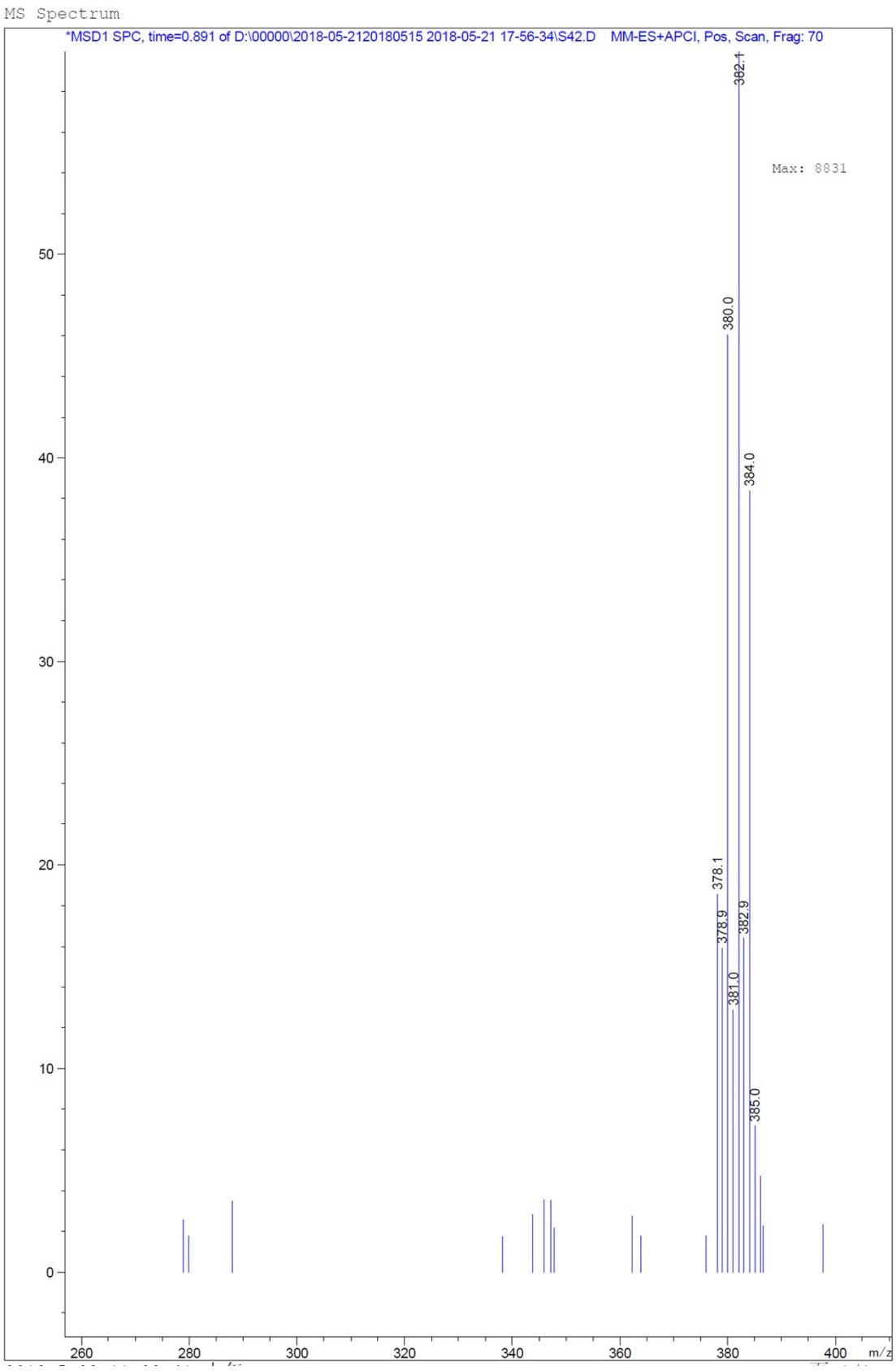
MS of compound **5f**



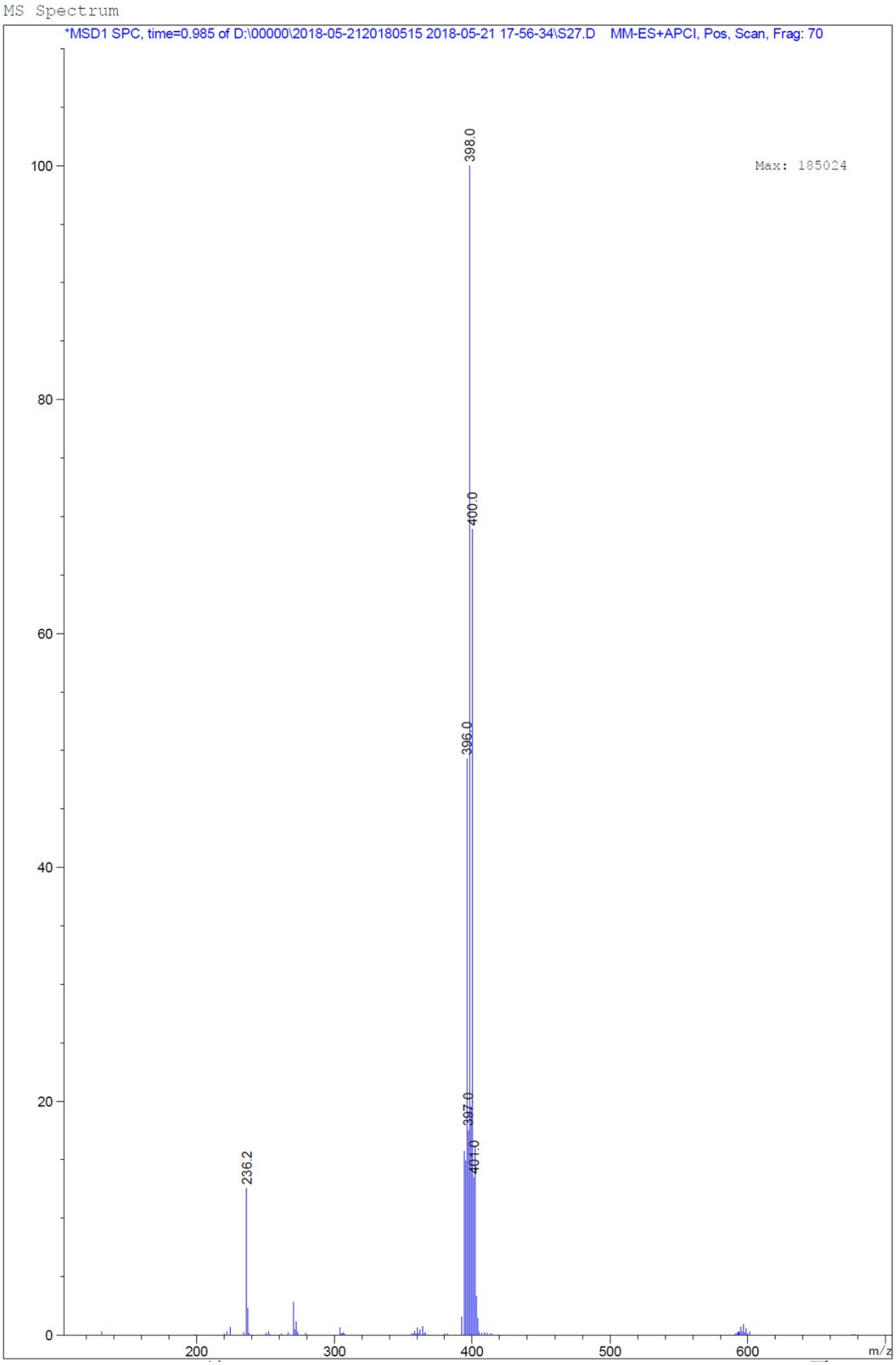
MS of compound **6a**



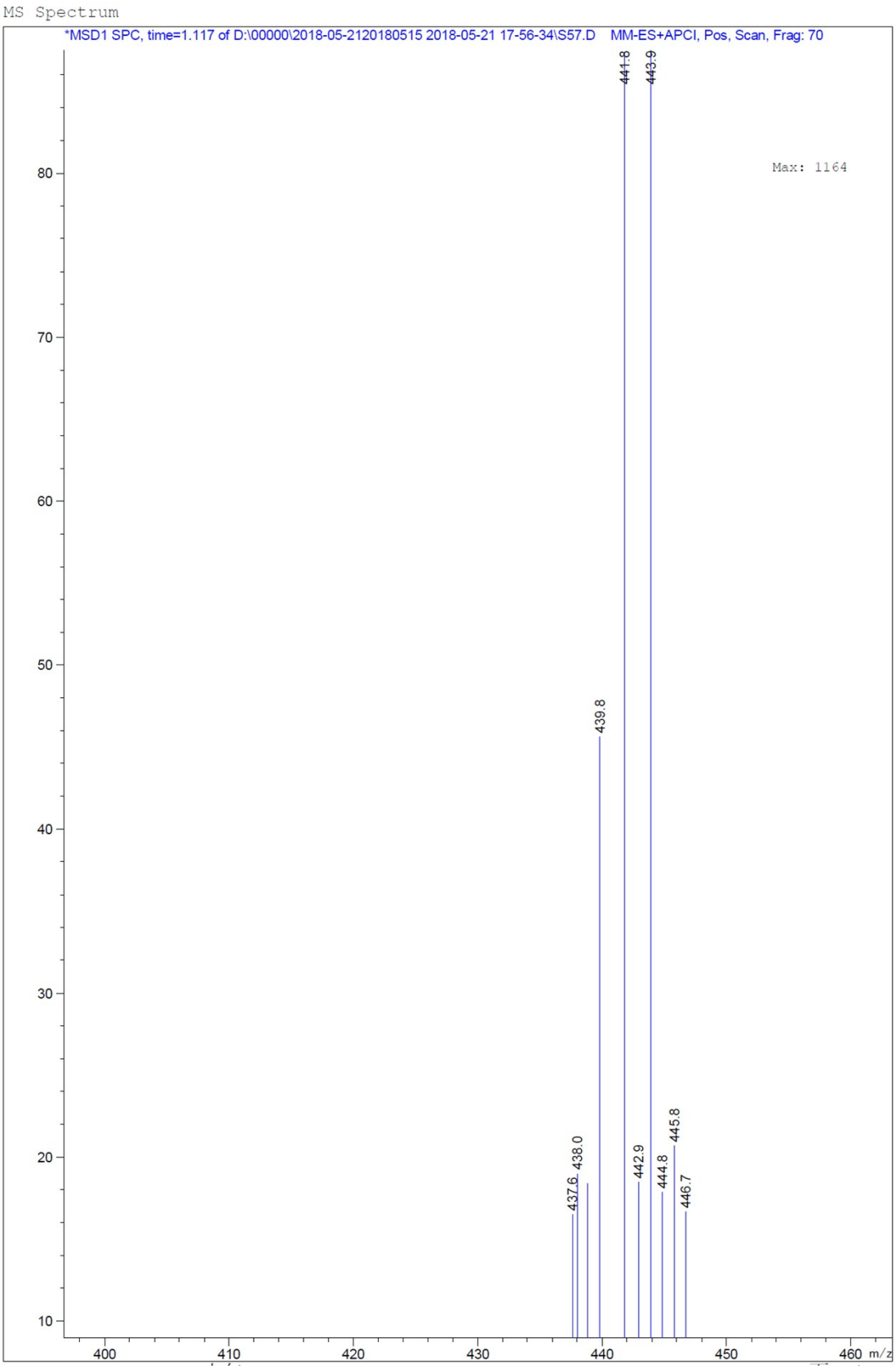
MS of compound **6b**



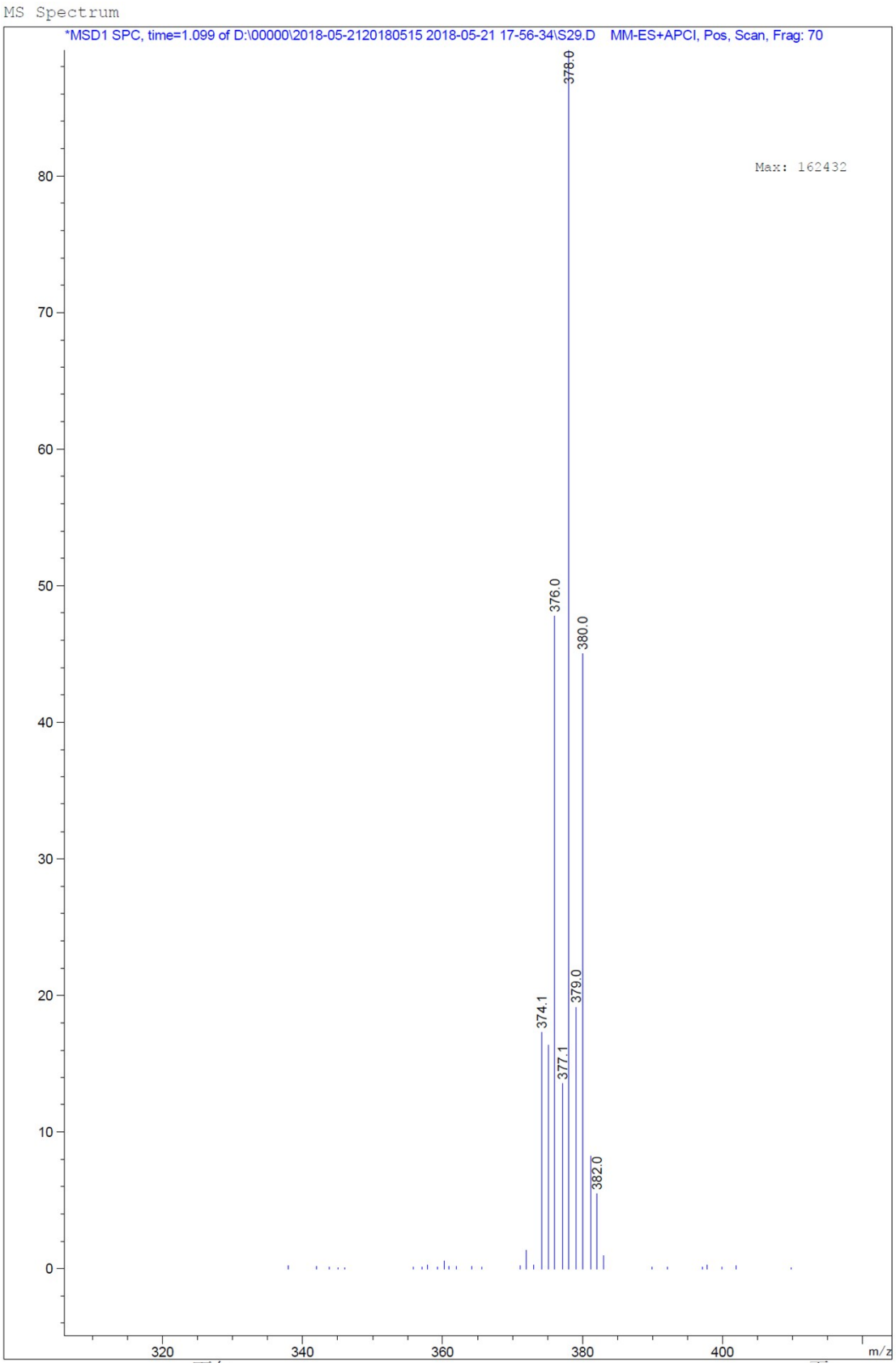
MS of compound **6c**



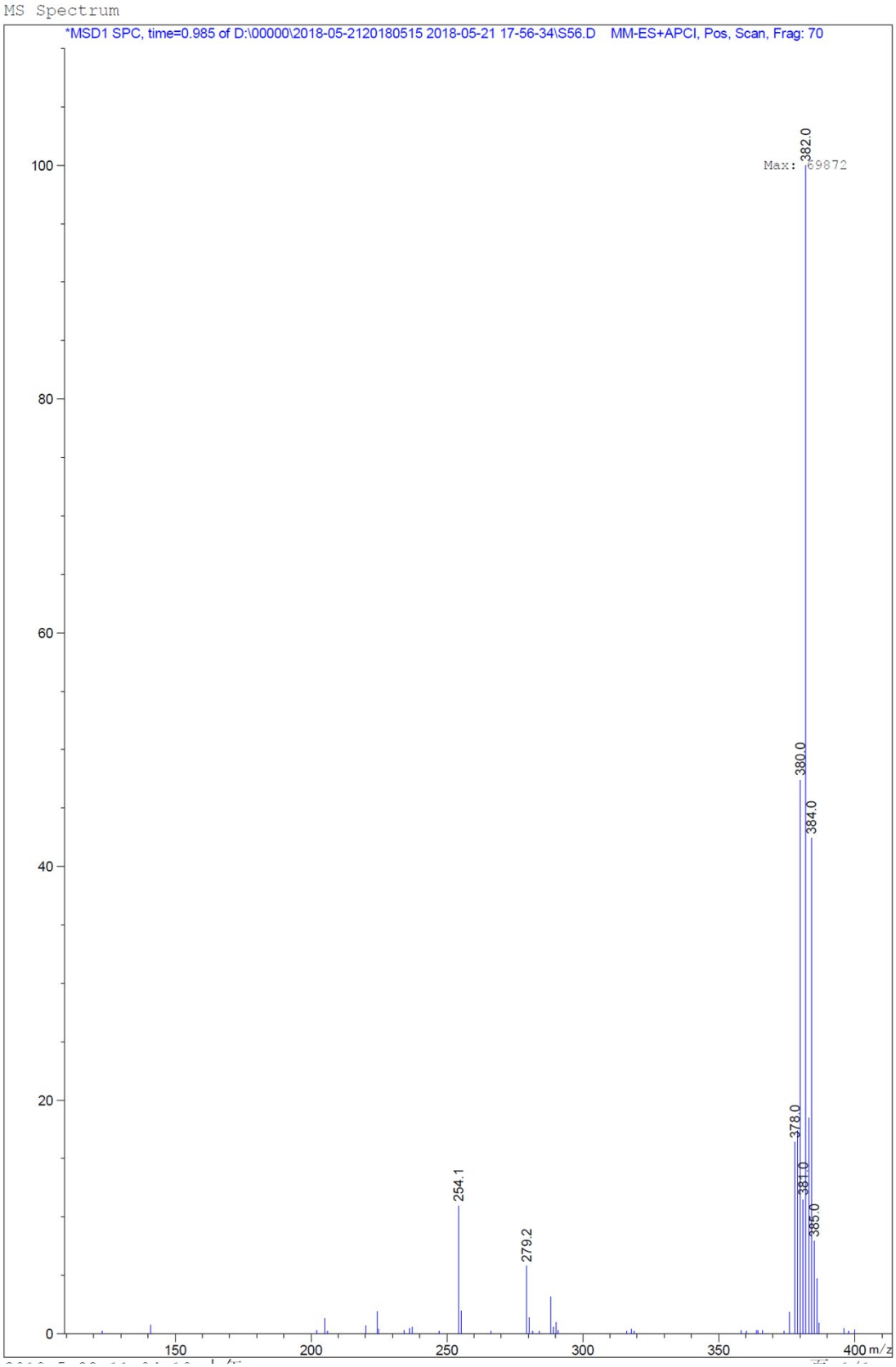
MS of compound **6d**



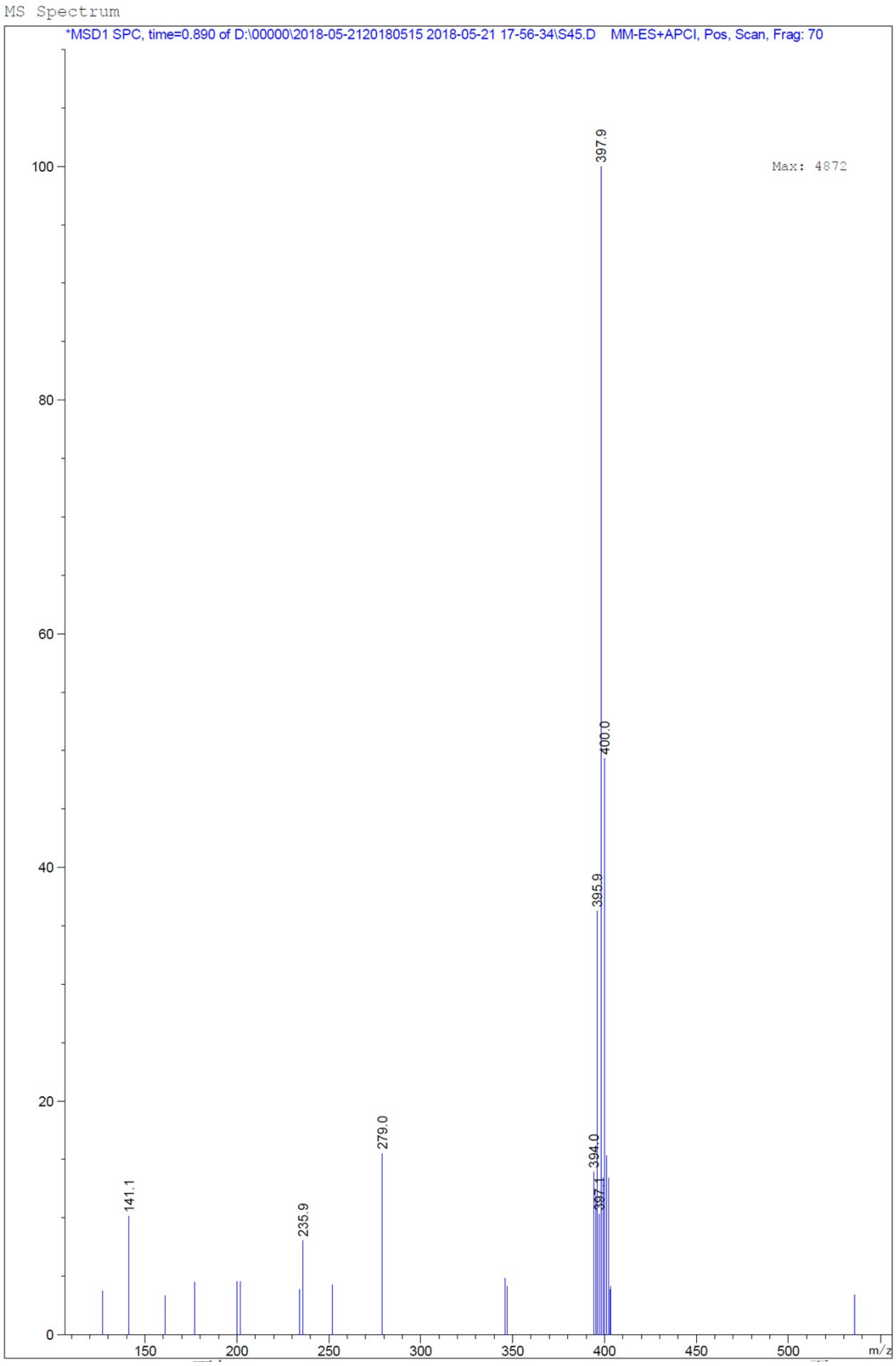
MS of compound **6e**



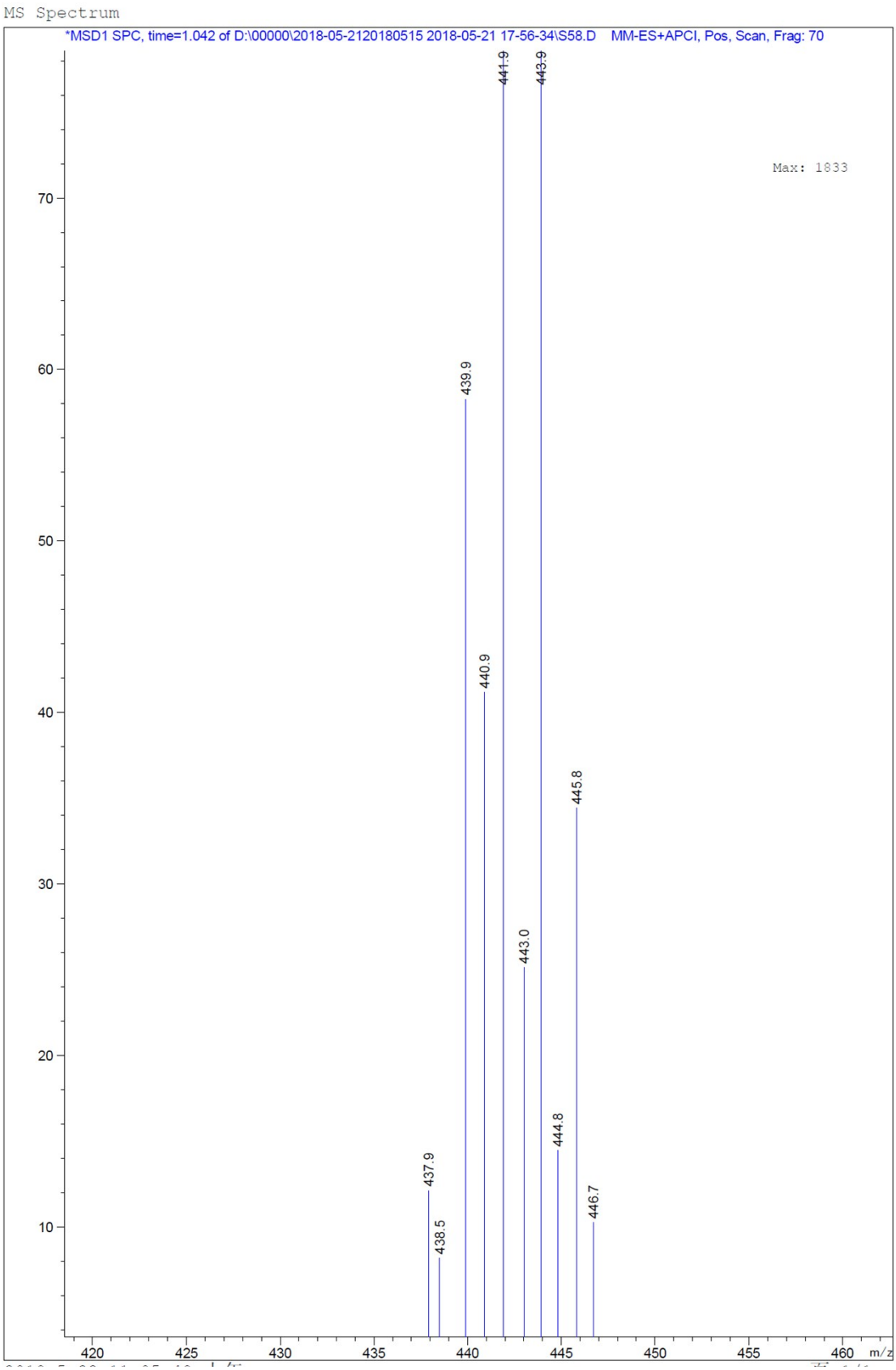
MS of compound **6f**



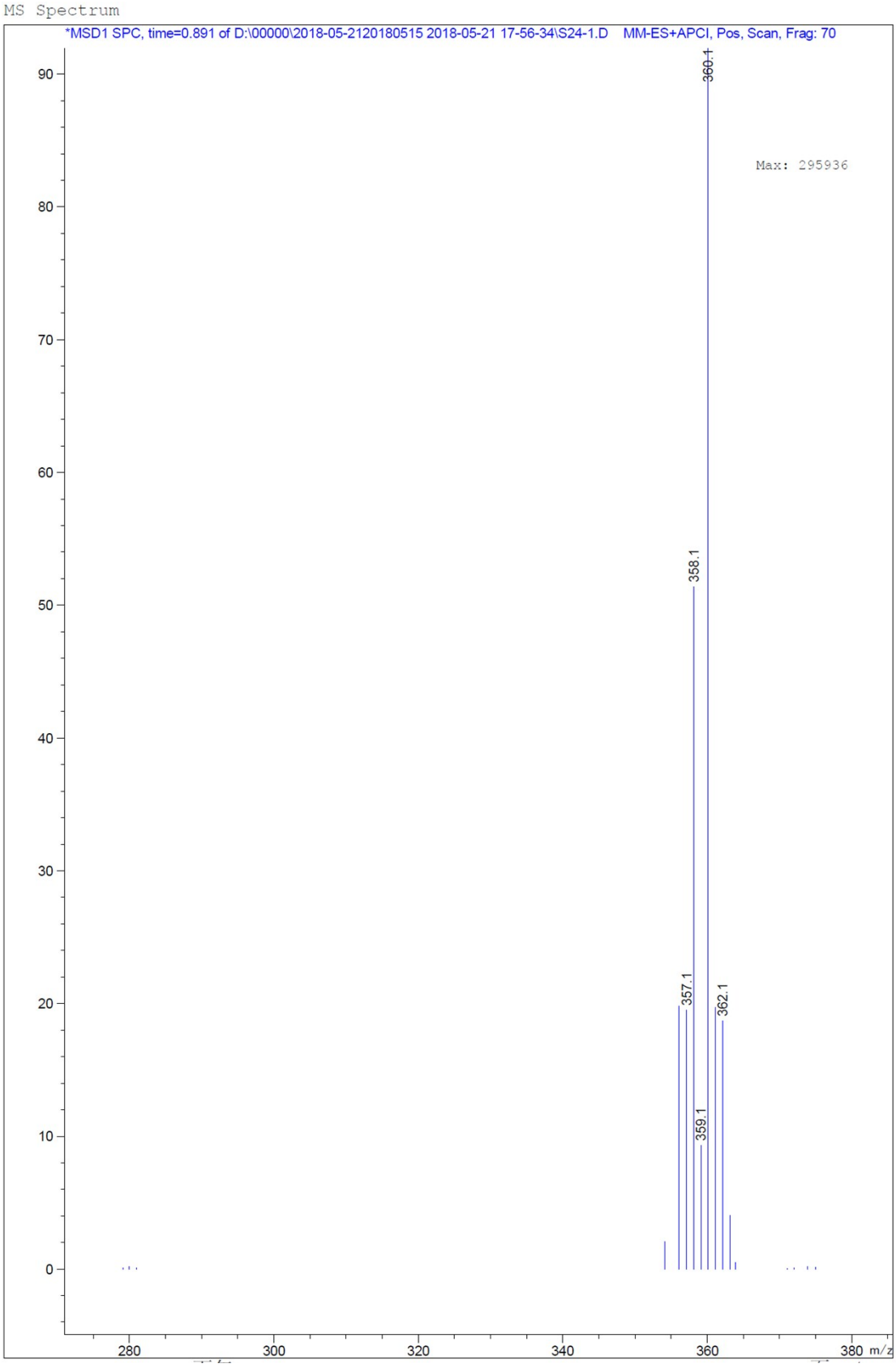
MS of compound **6g**



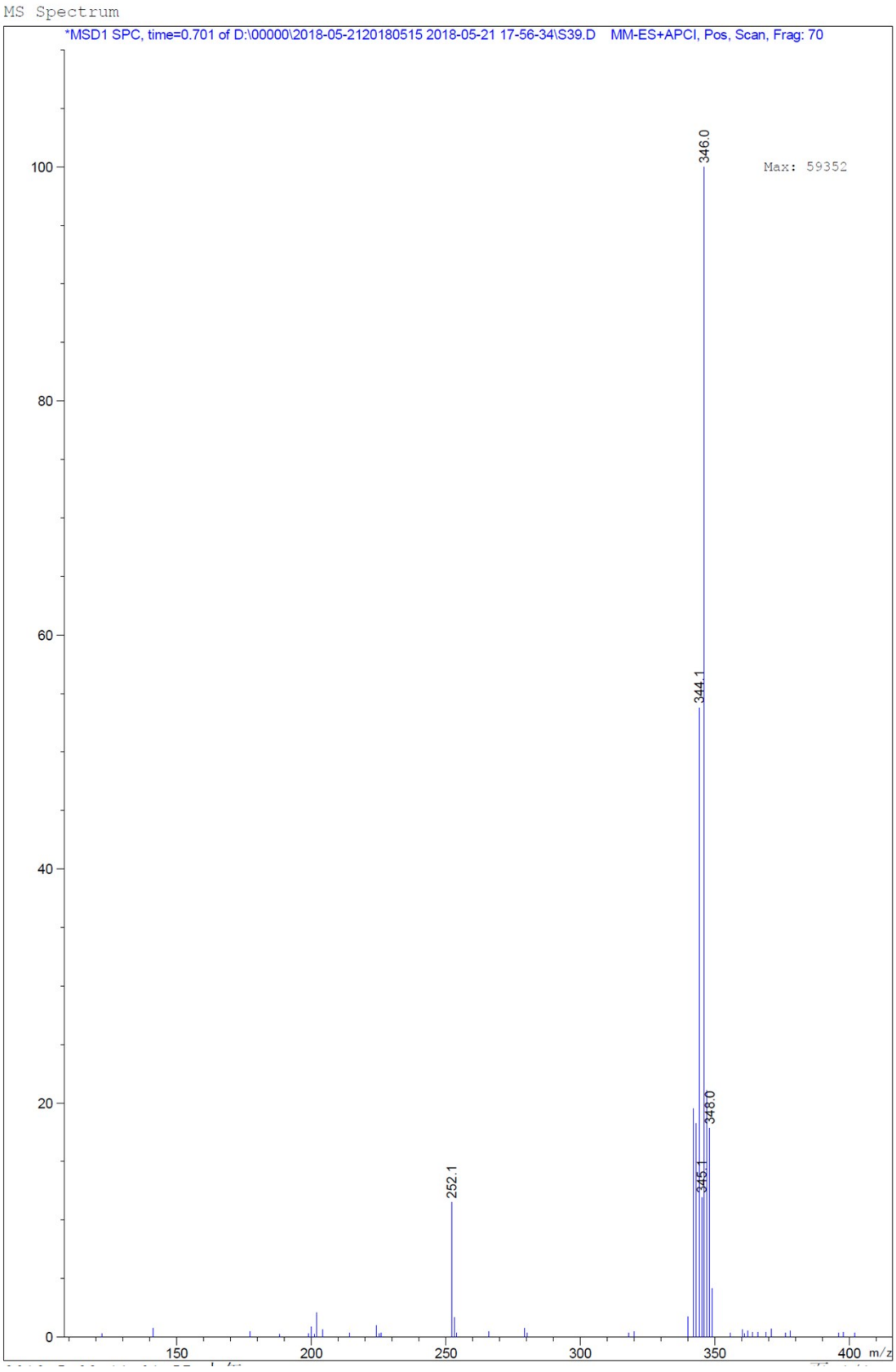
MS of compound **6h**



MS of compound **6i**



MS of compound **7a**



MS of compound **10**