Supplementary Data

Structure-Activity Relationship and Pharmacokinetic Studies of 3-*O*-Substitutedflavonols as Anti-Prostate Cancer Agents

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[b]Department of Chemistry and [c]RCMI Cancer Research Center, Xavier University of Louisiana, 1 Drexel Drive, New Orleans, LA 70125, USA

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Corresponding author.

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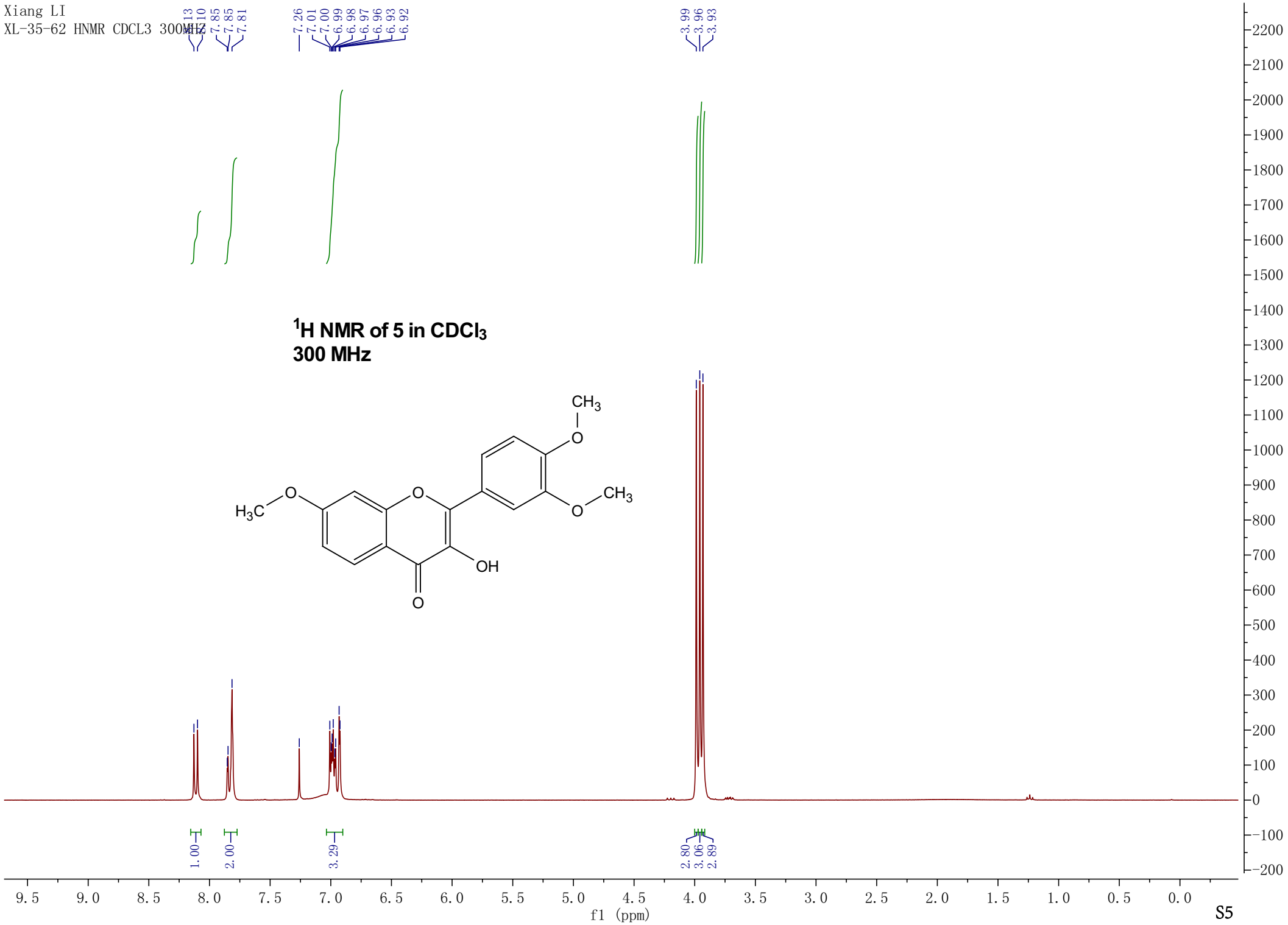
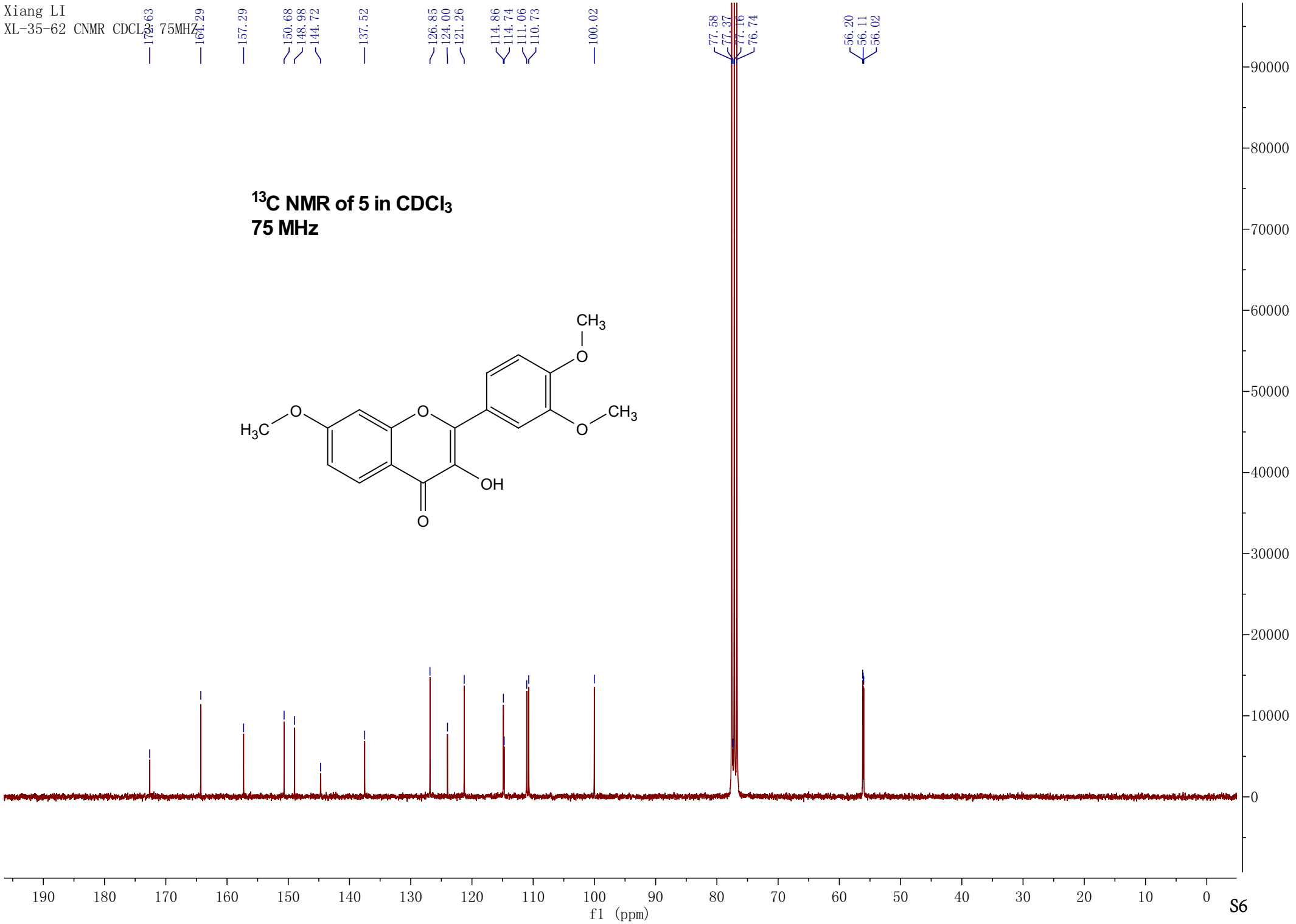
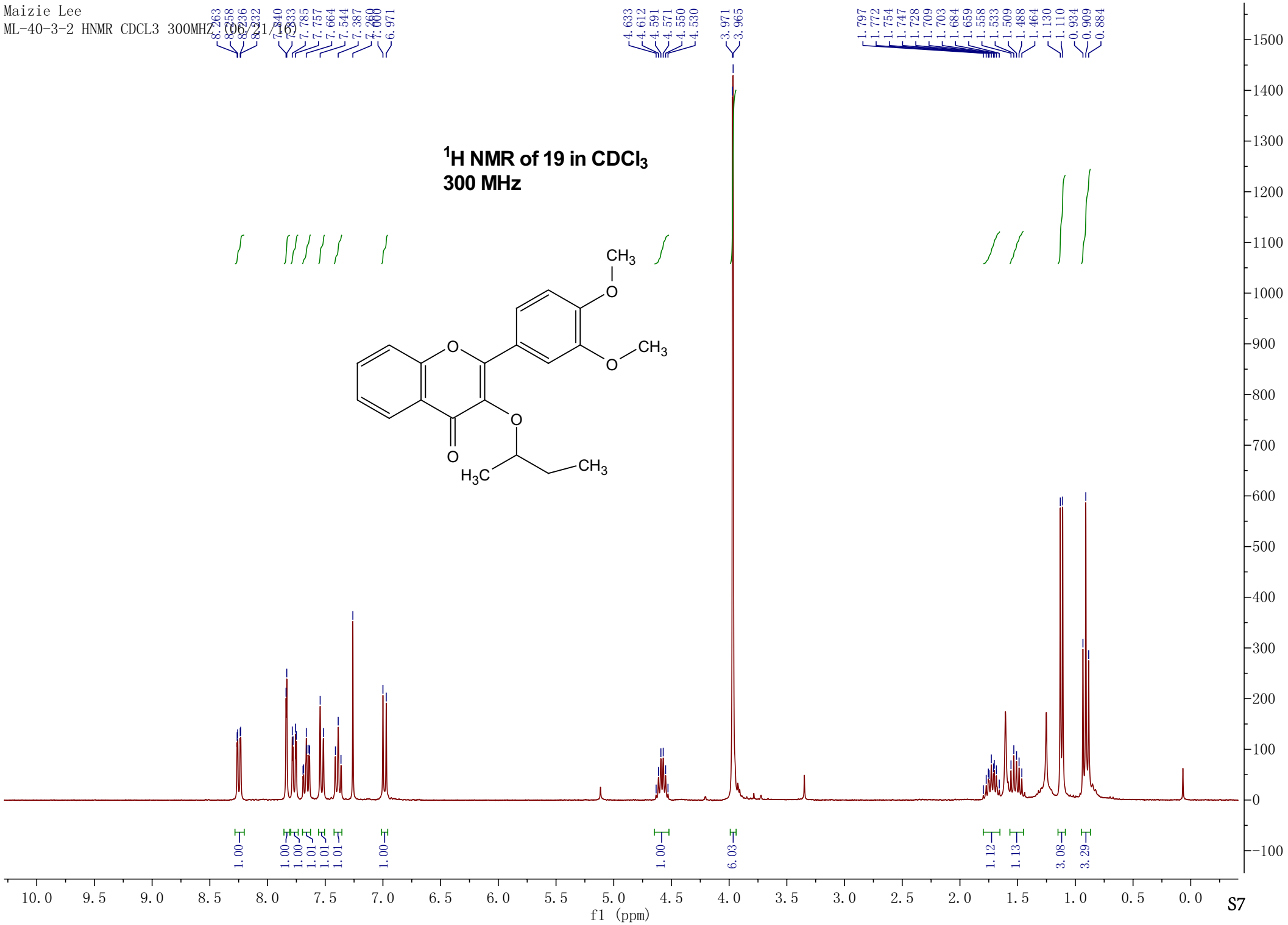
Xiang LI
XL-35-62 HNMR CDCL3 300MHZ



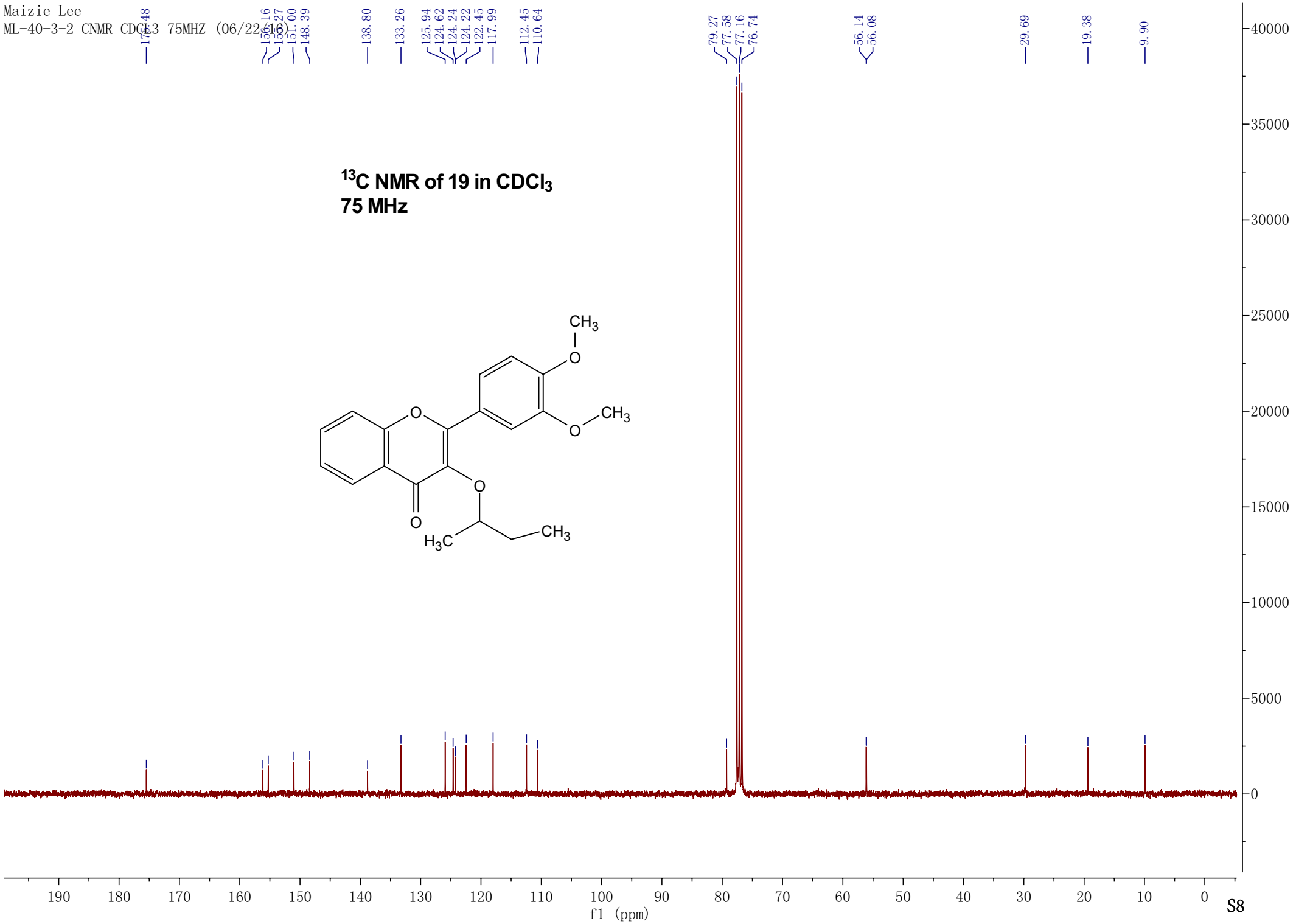

Xiang LI
XL-35-62 CNMR CDCL3 75MHZ
179.63
164.29
157.29
150.68
148.98
144.72
137.52
126.85
124.00
121.26
114.86
114.74
111.06
110.73
100.02
77.58
77.37
77.16
76.74
56.20
56.11
56.02
13C NMR of 5 in CDCl3
75 MHz
CH3
O
O
CH3
H3C
O
O
OH
O
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

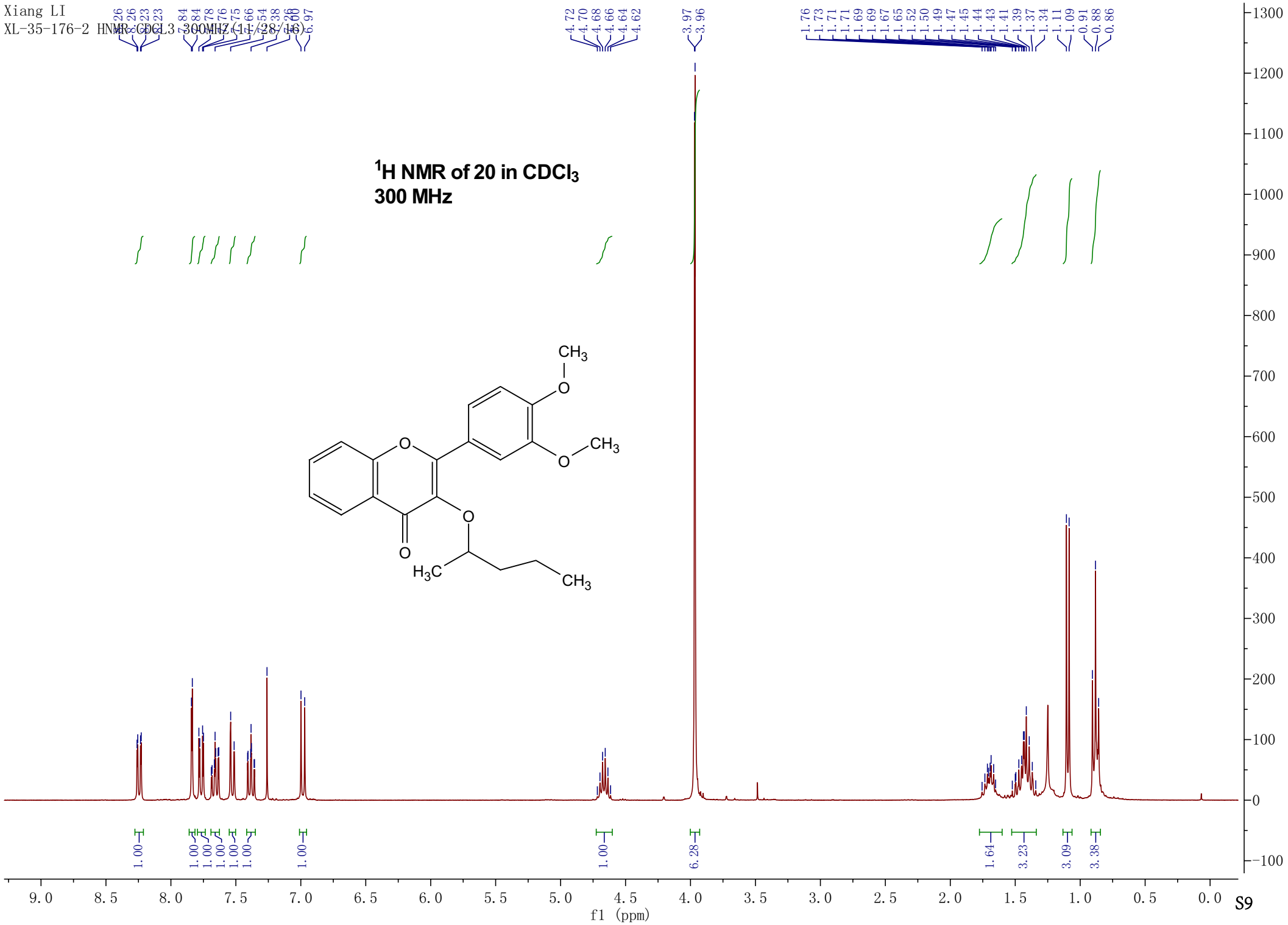
Maizie Lee
ML-40-3-2 HNMR CDCL3 300MHZ (06/21/16)



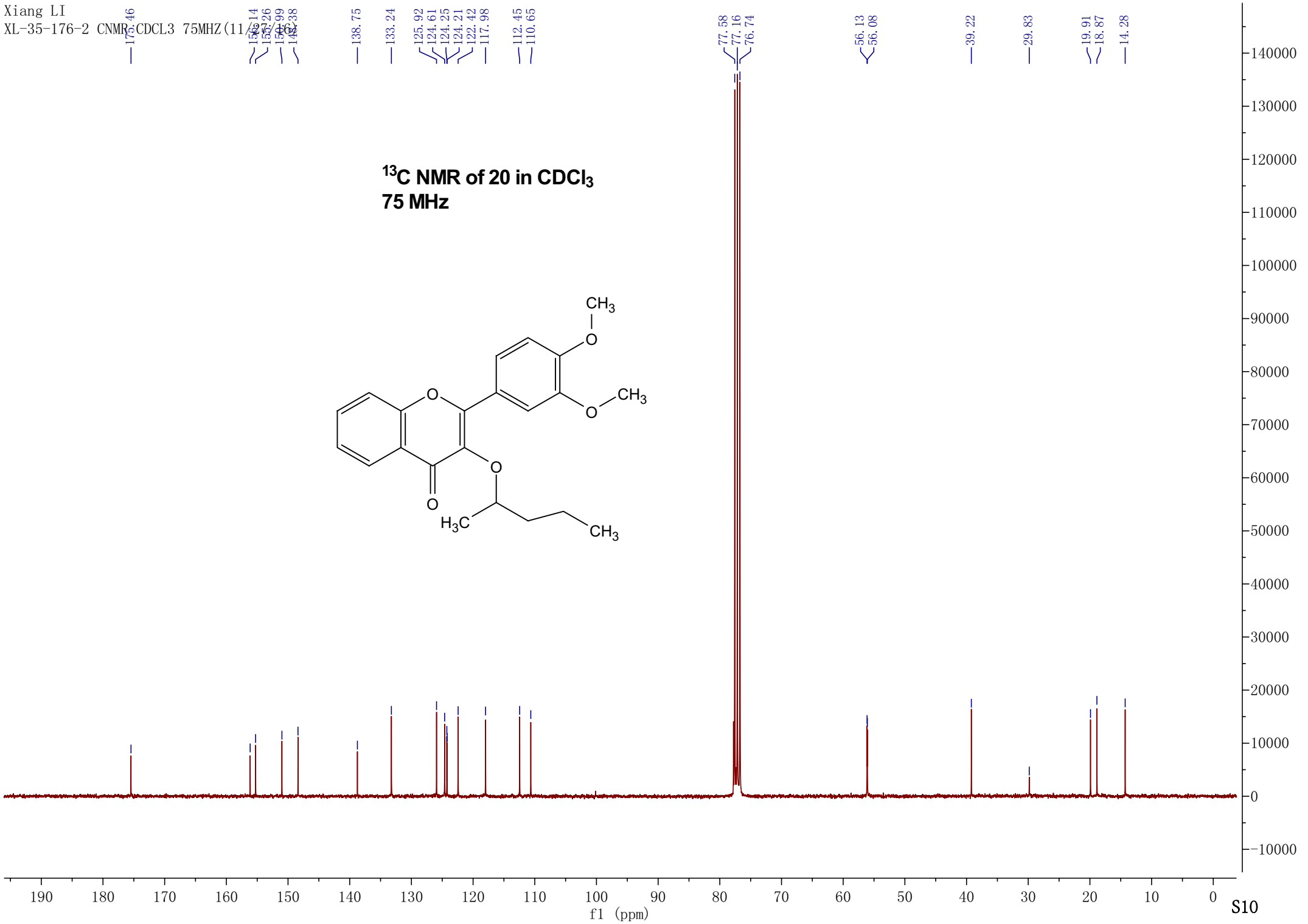
^{1}H NMR of 19 in $CDCl_3$
300 MHz

Maizie Lee
ML-40-3-2 CNMR CDCl3 75MHZ (06/22/16)

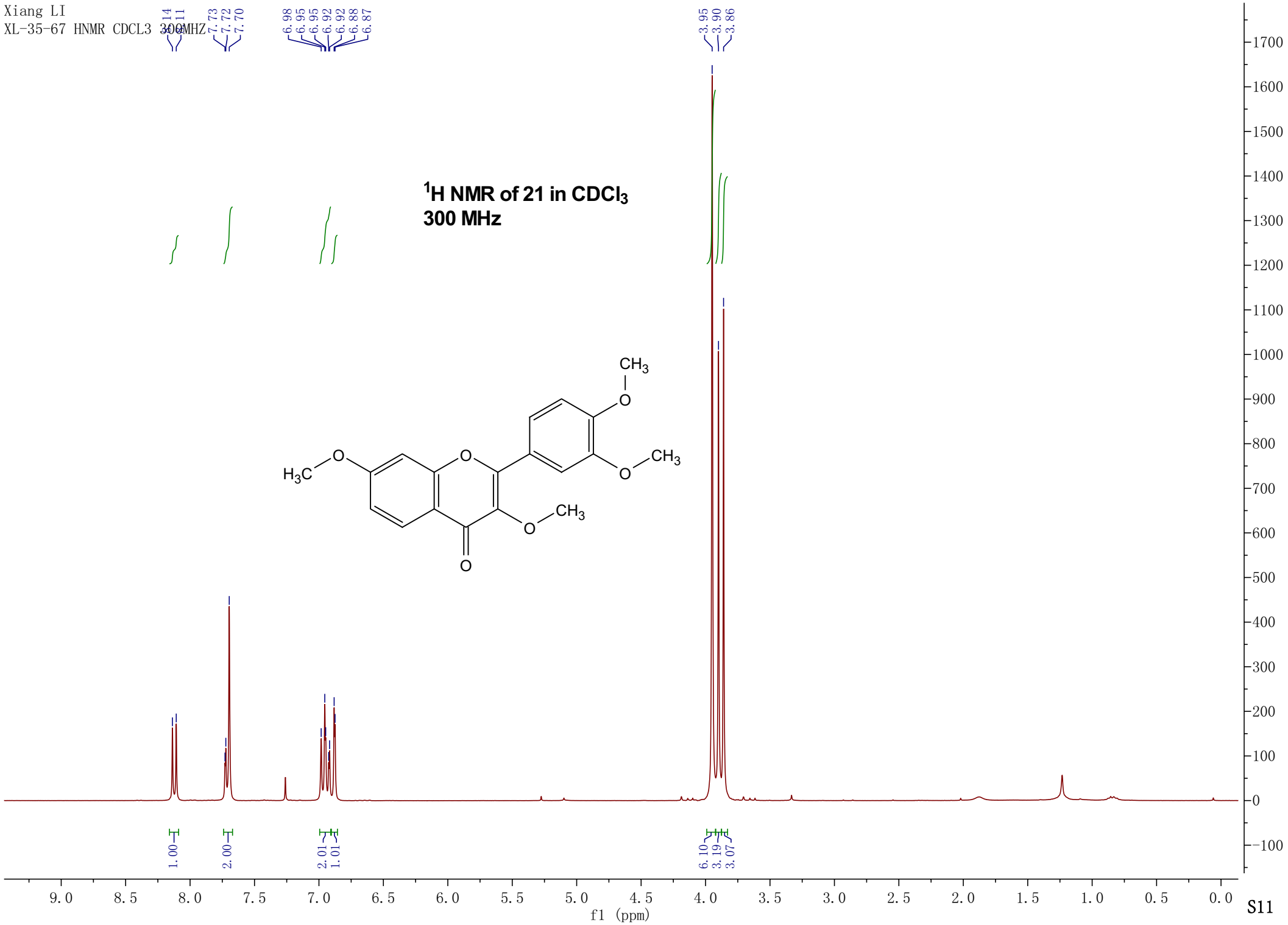



Xiang LI
XL-35-176-2 HNMR CDCL3 300MHZ (11/28/16)
^{1}H NMR of 20 in CDCl$_3$
300 MHz
CH$_3$
O
O
CH$_3$
O
O
O
H$_3$C
CH$_3$
f1 (ppm)

Xiang LI
XL-35-176-2 CNMR:CDCL3 75MHZ(11/27/16)



Xiang LI
XL-35-67 HNMR CDCL3 300MHZ

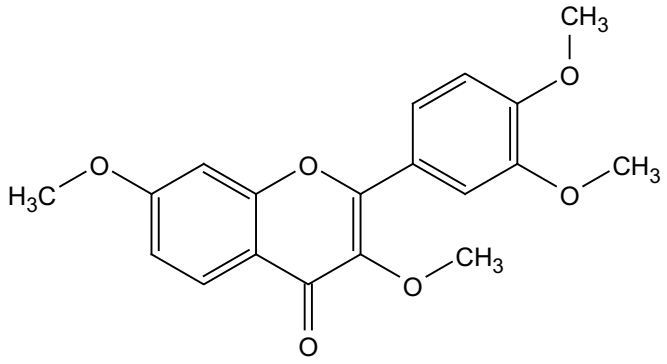


^{1}H NMR of 21 in $CDCl_3$
300 MHz

Xiang LI
XL-35-67 CNMR CDCl3 75MHZ

174.48
164.03
156.95
155.08
151.09
148.76
140.81
127.17
123.57
122.02
118.14
114.31
111.44
110.89
100.03
77.58
77.16
76.74
60.06
56.13
56.05
55.92

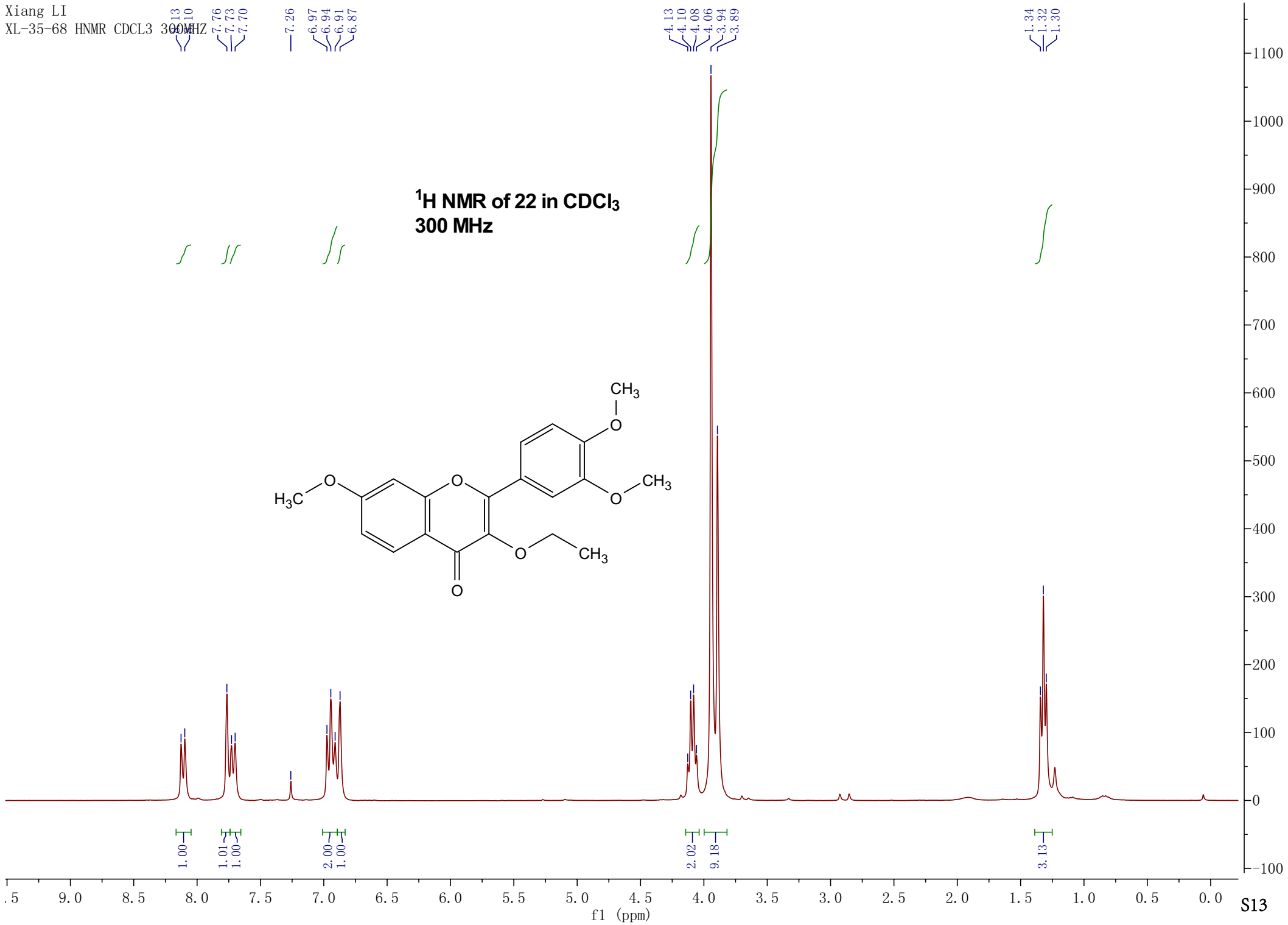
^{13}C NMR of 21 in $CDCl_3$
75 MHz



340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000

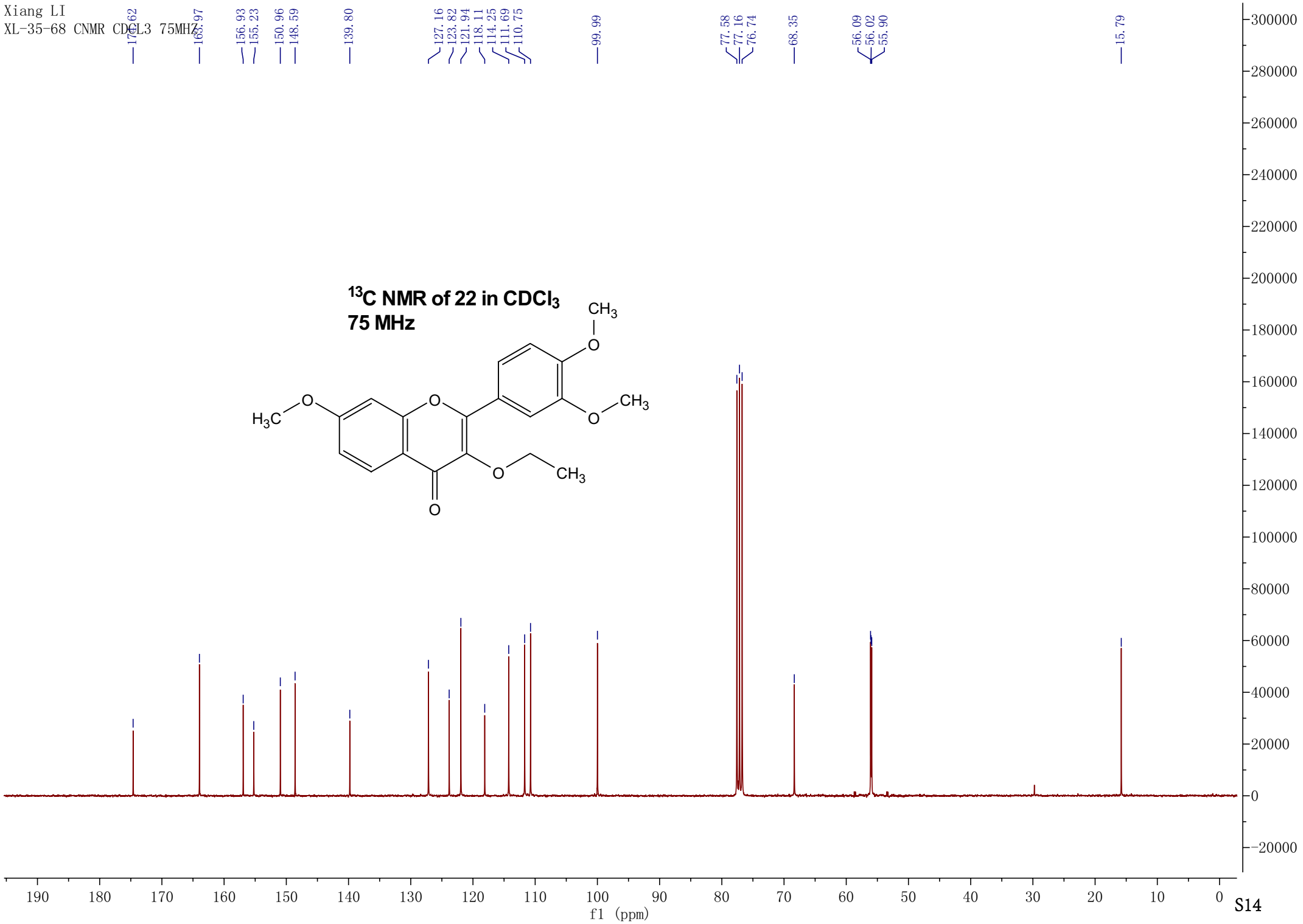
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Xiang LI
XL-35-68 HNMR CDCL3 300MHZ

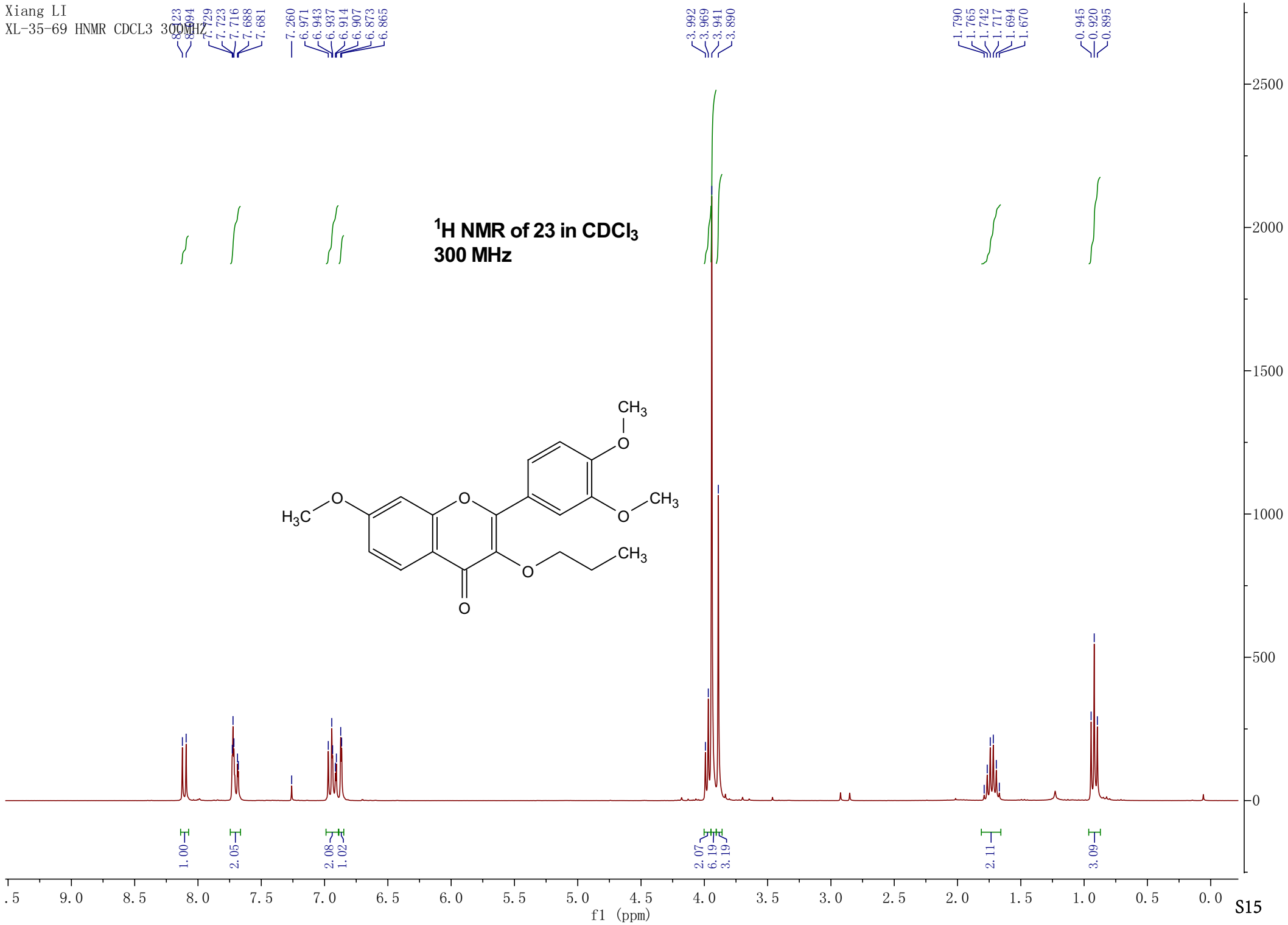


^{1}H NMR of 22 in $CDCl_3$
300 MHz

Xiang LI
XL-35-68 CNMR CDCL3 75MHZ

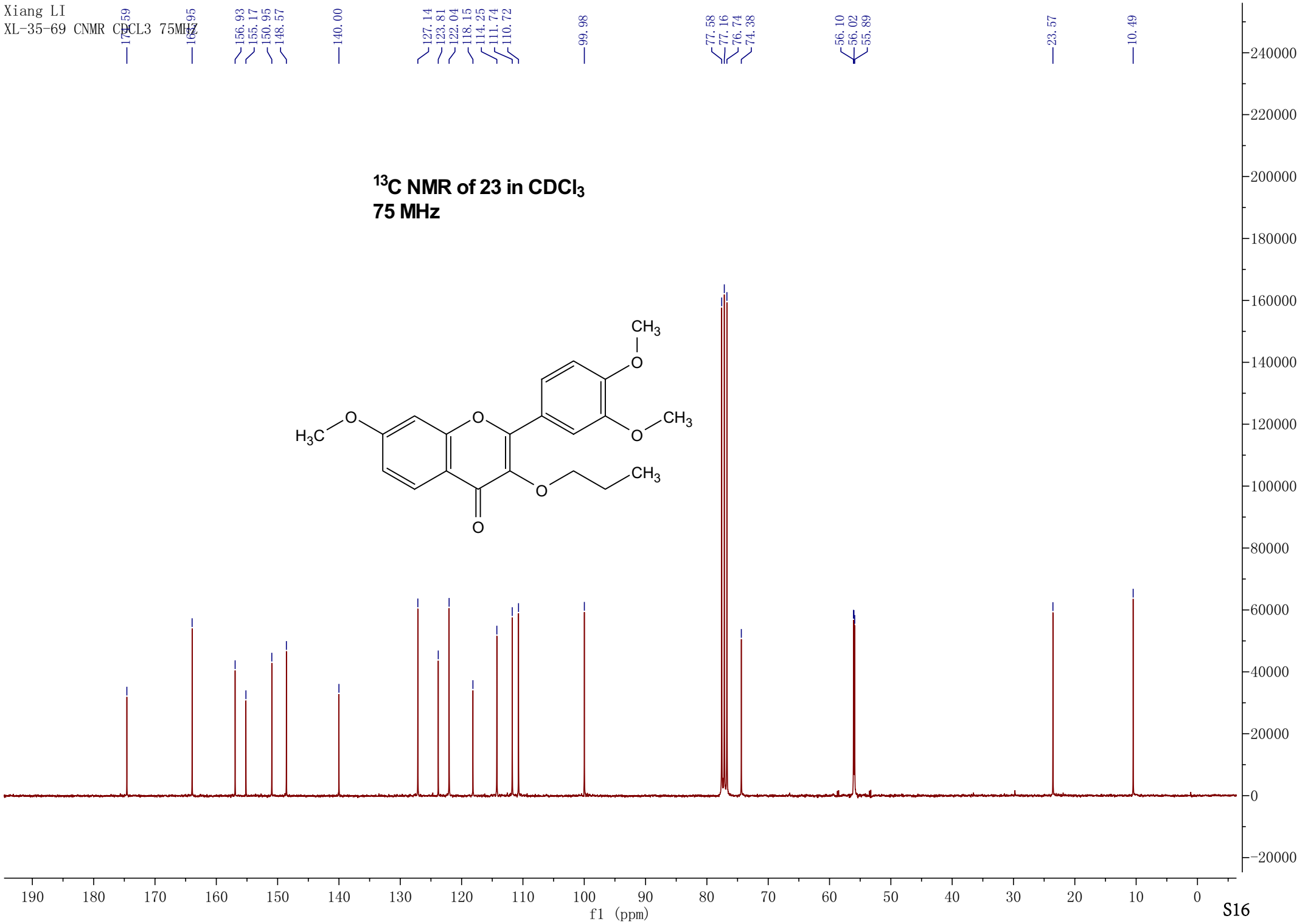


Xiang LI
XL-35-69 HNMR CDCL3 300MHZ

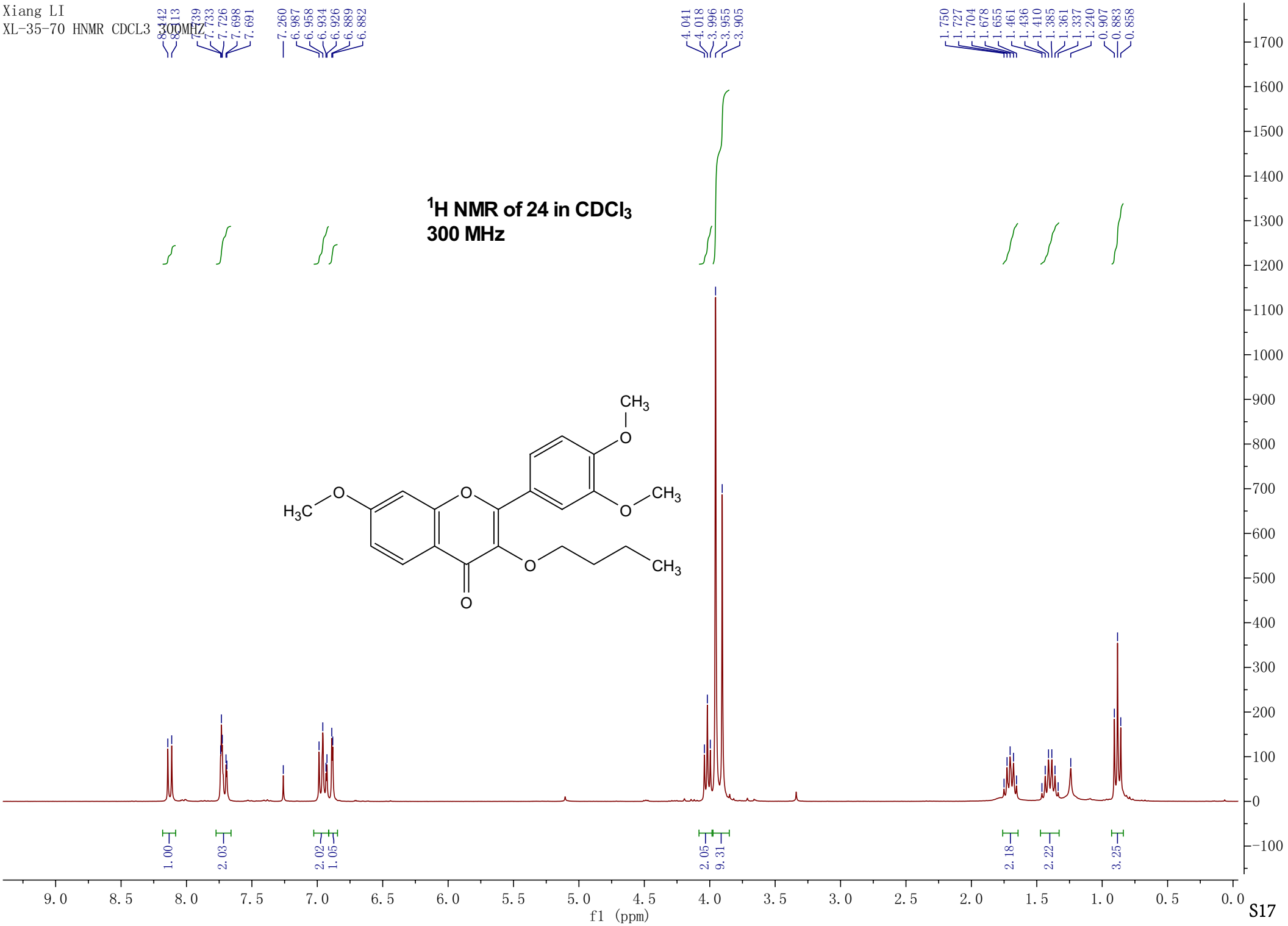


^{1}H NMR of 23 in $CDCl_3$
300 MHz

Xiang LI
XL-35-69 CNMR CDCL3 75MHZ



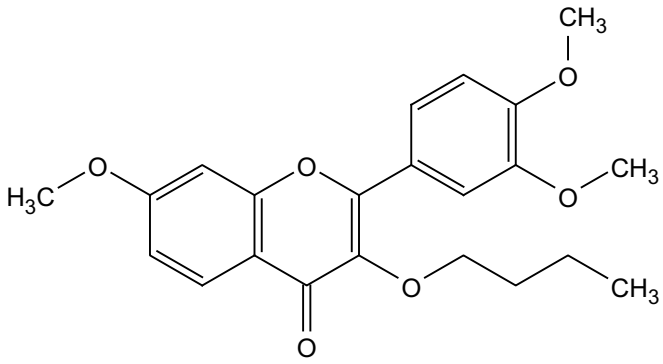
Xiang LI
XL-35-70 HNMR CDCL3 300MHZ



Xiang LI
XL-35-70 CNMR CDCL3 75MHZ

174.54
163.88
158.88
155.15
150.88
148.51
139.97
127.11
123.76
121.95
118.11
114.18
111.68
110.66
99.93
72.48
56.02
55.97
55.83
32.28
19.13
13.82

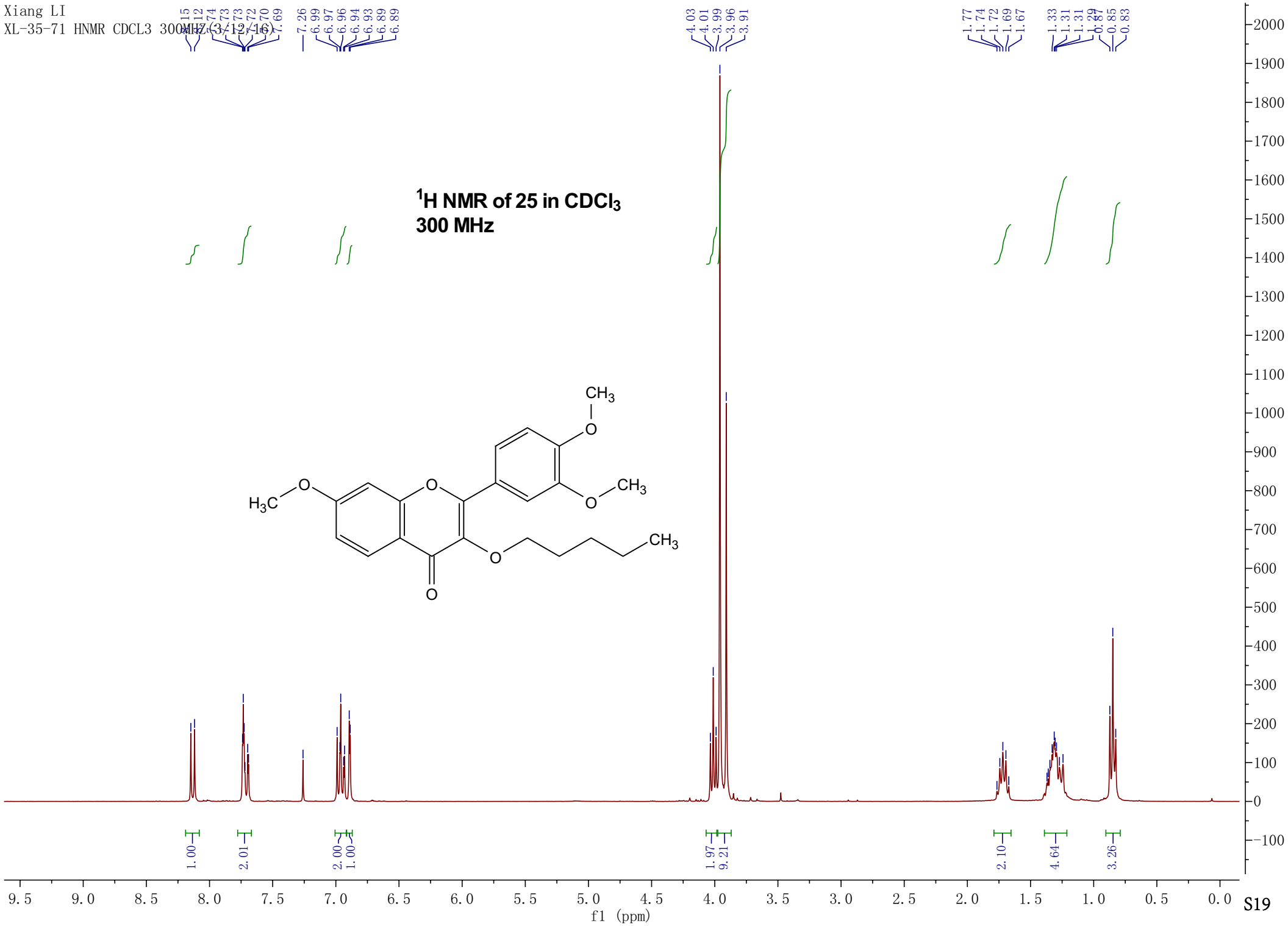
^{13}C NMR of 24 in $CDCl_3$
75 MHz



600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000

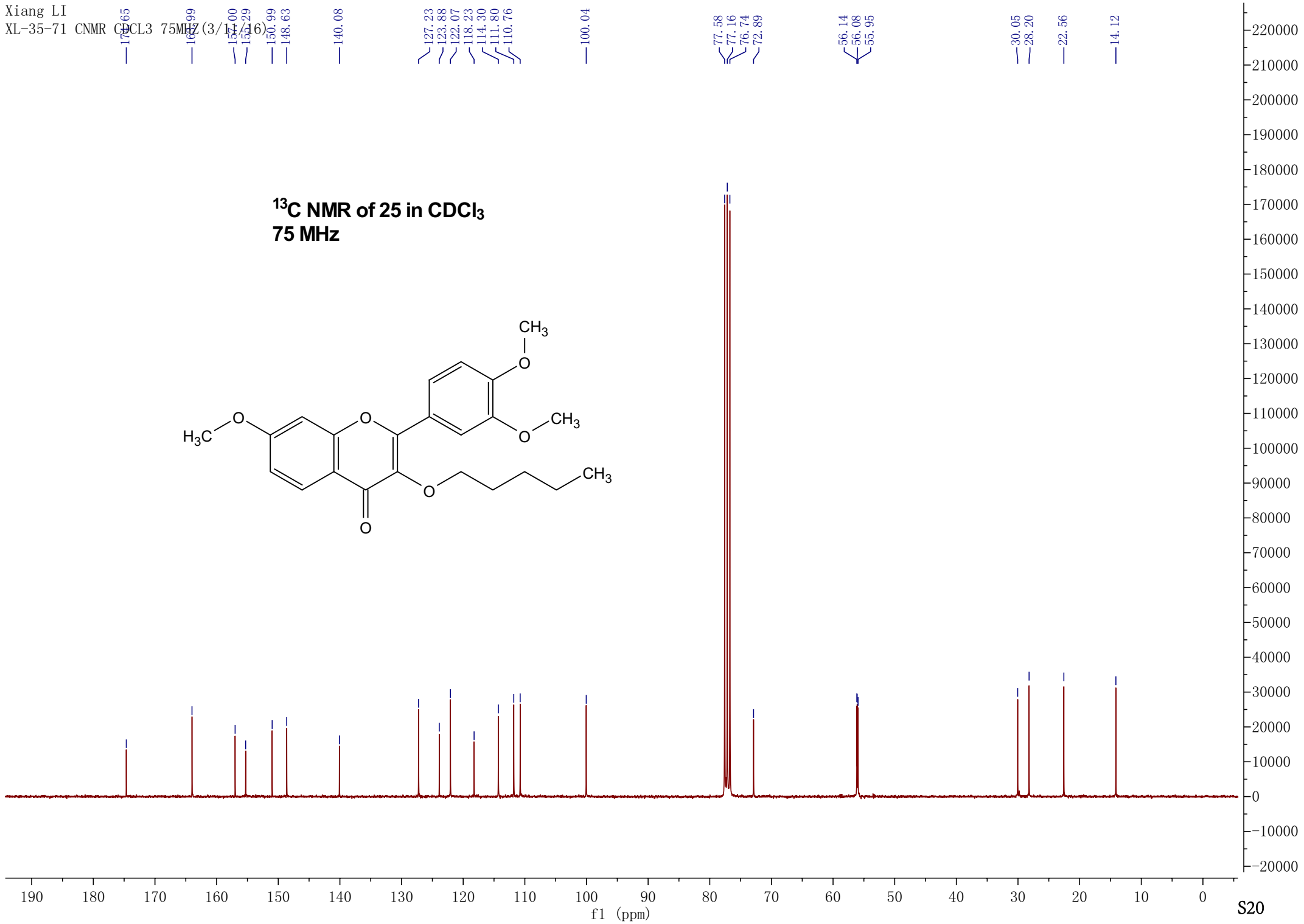
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

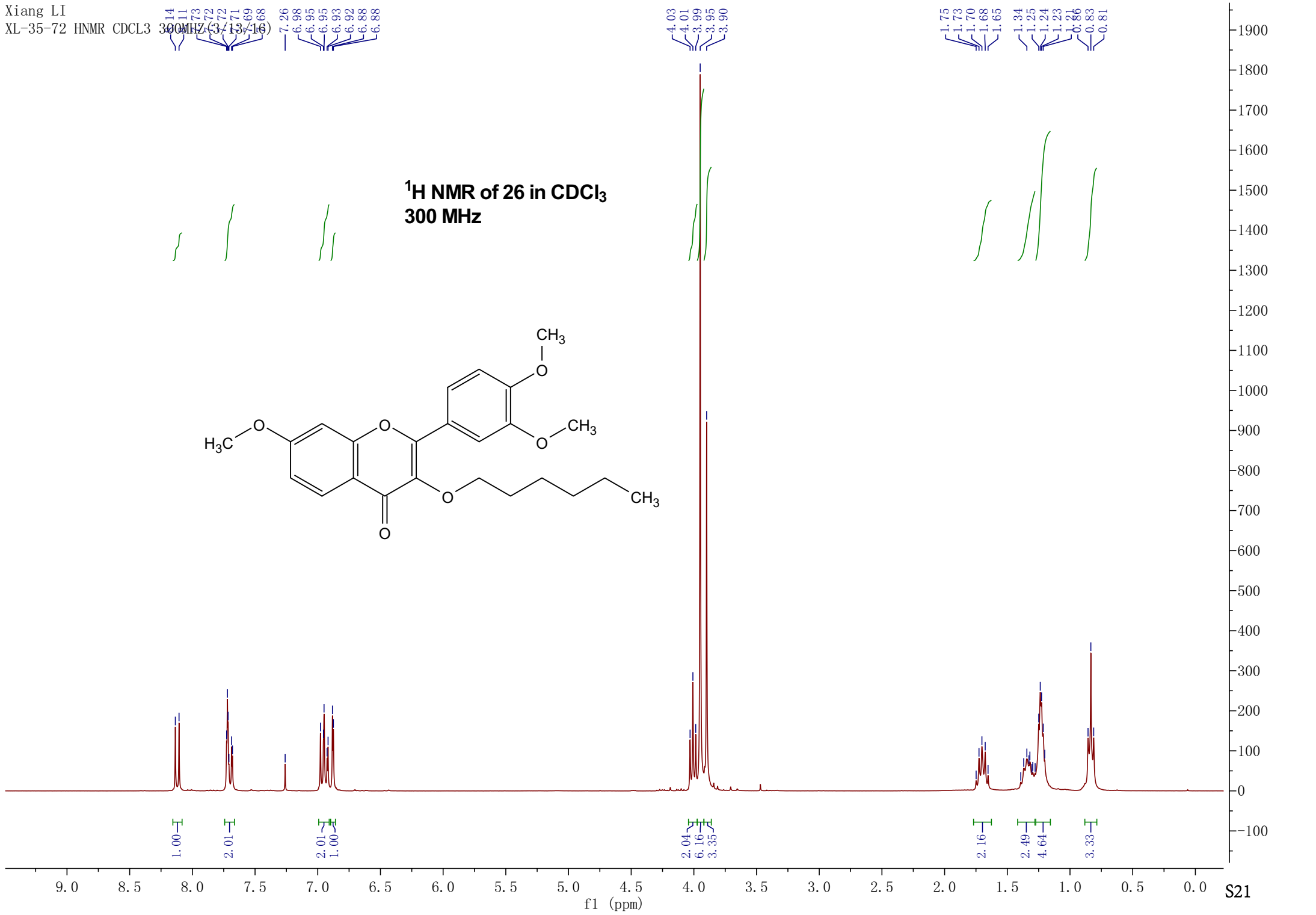
Xiang LI
XL-35-71 HNMR CDCL3 300MHZ (3/12/16)



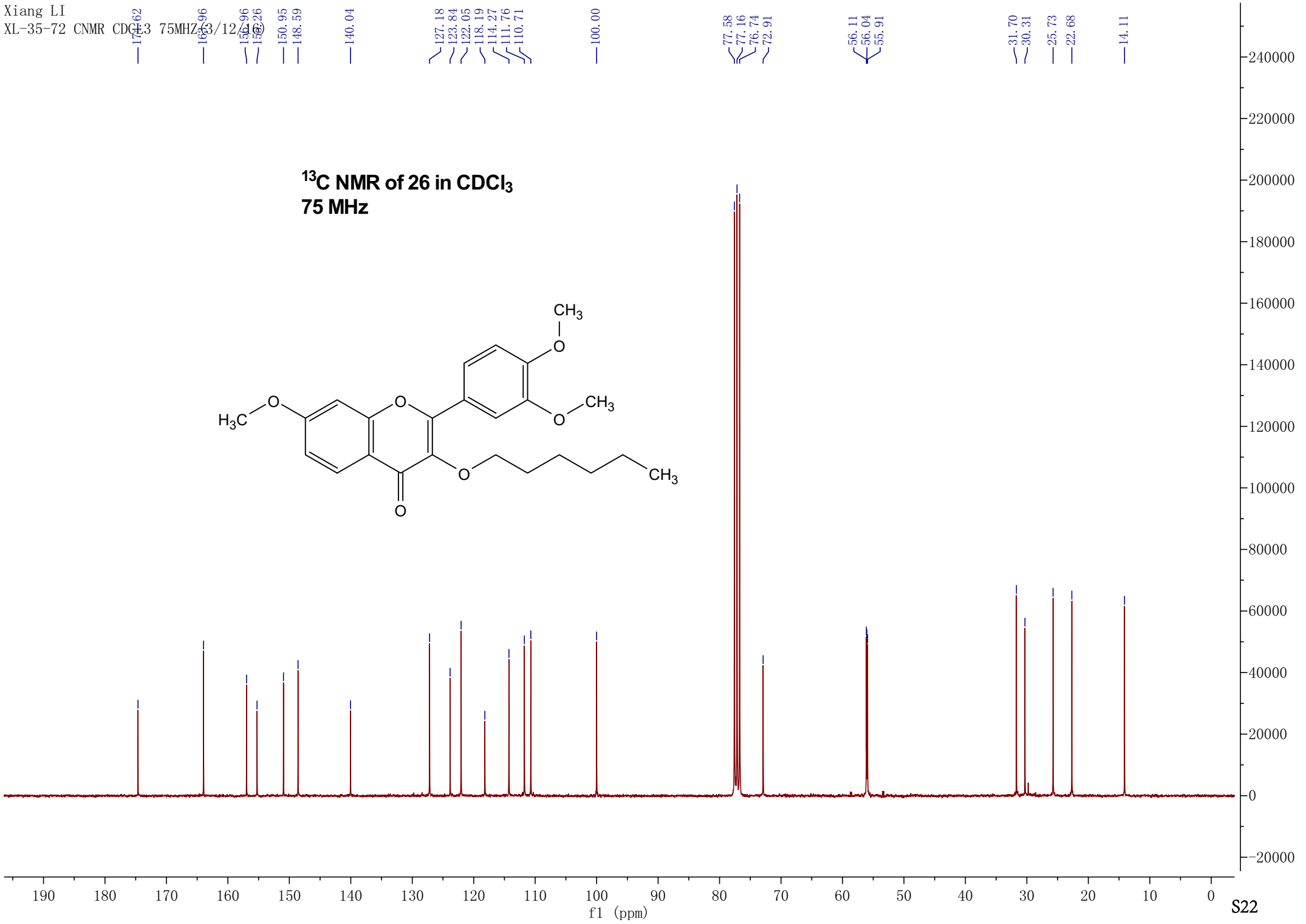
^{1}H NMR of 25 in $CDCl_3$
300 MHz

Xiang LI
XL-35-71 CNMR CDCL3 75MHZ(3/11/16)

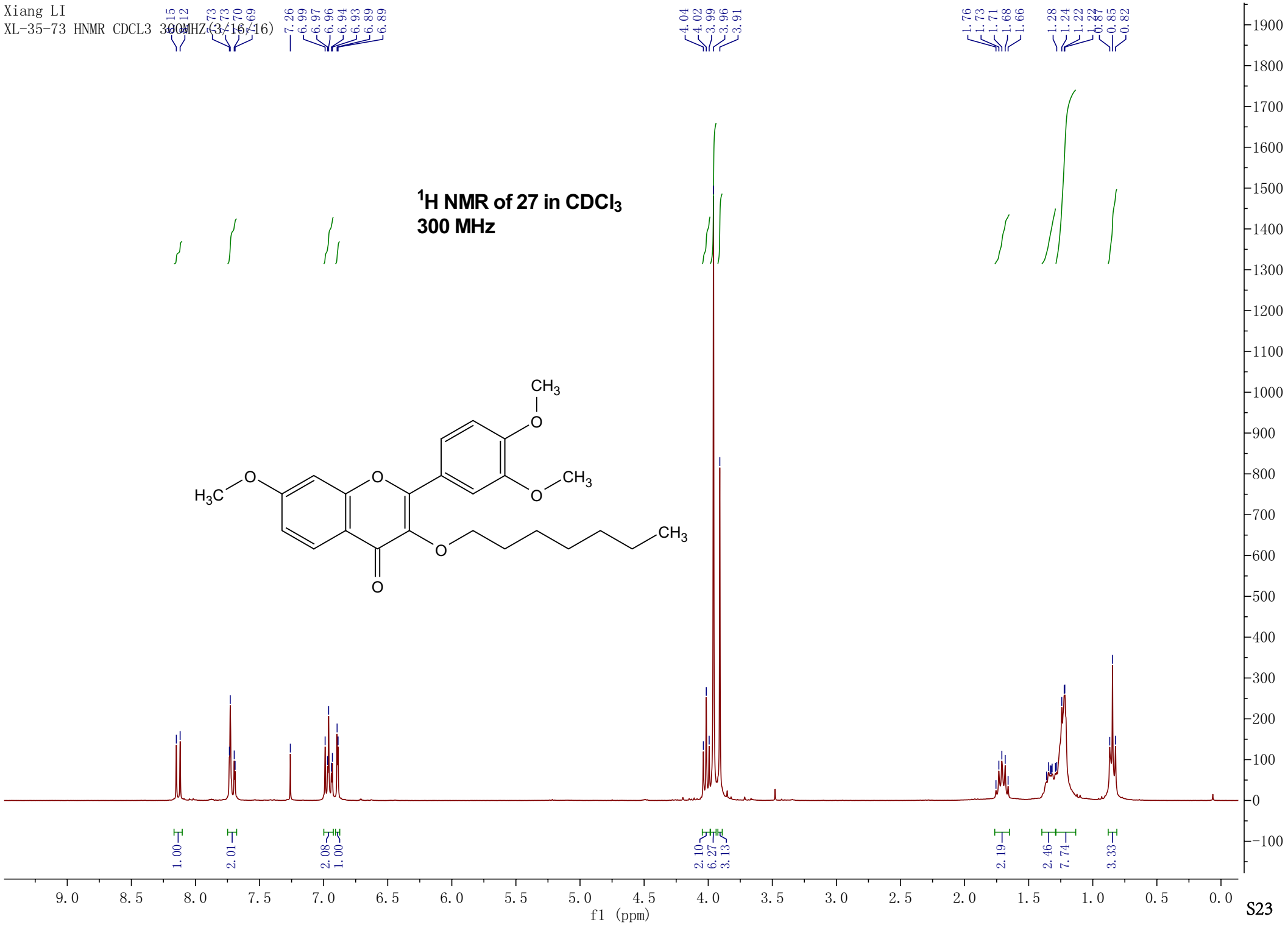



Xiang LI
XL-35-72 HNMR CDCL3 300MHZ(3/13/16)
7.26
6.98
6.95
6.95
6.93
6.92
6.88
6.88
4.03
4.01
3.99
3.95
3.90
1.75
1.73
1.70
1.68
1.65
1.34
1.25
1.24
1.23
0.86
0.83
0.81
1H NMR of 26 in CDCl3
300 MHz
CH3
O
O
CH3
H3C
O
O
O
CH3
O
1.00
2.01
2.01
1.00
2.04
6.16
3.35
2.16
2.49
4.64
3.33
f1 (ppm)
S21

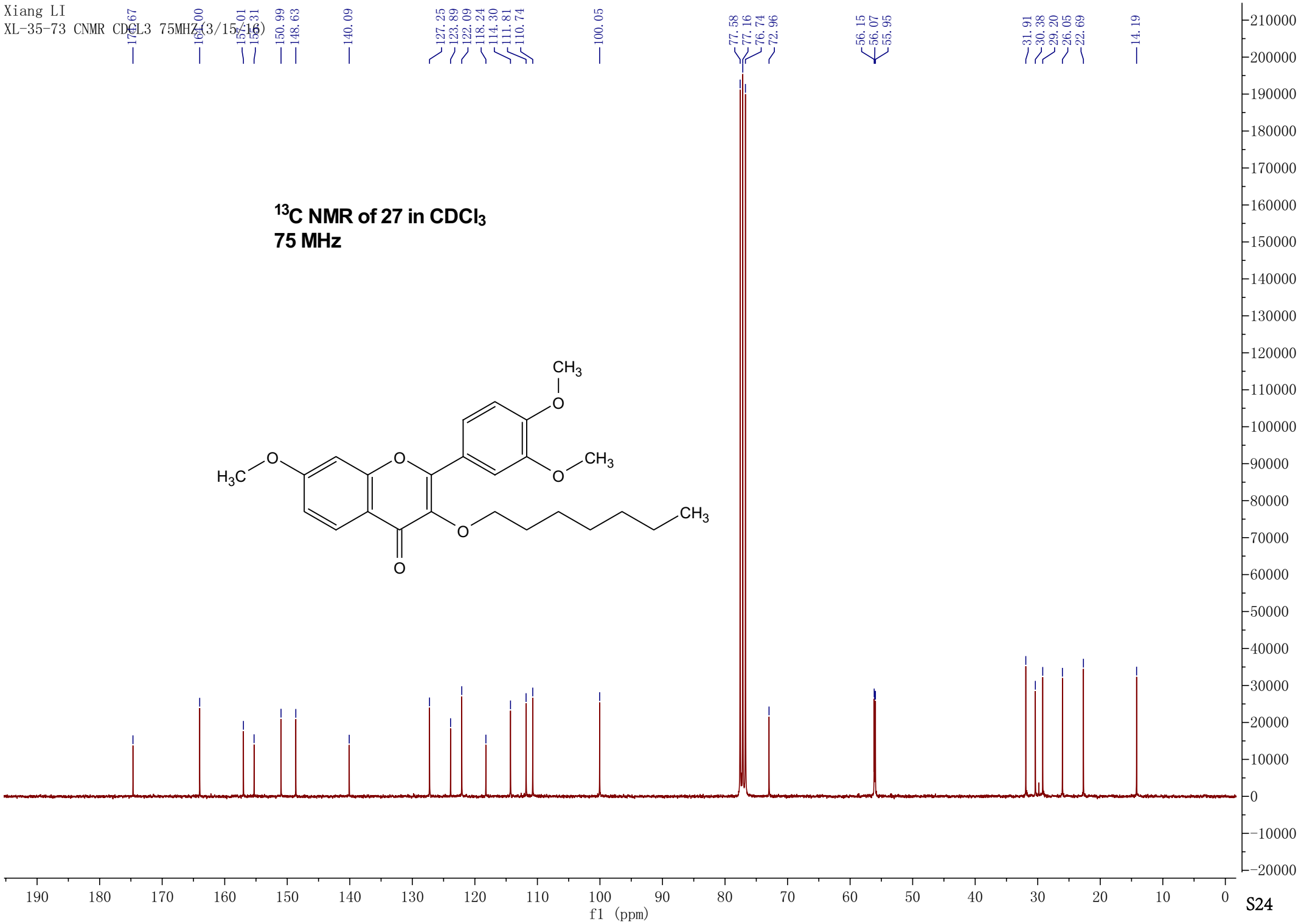
Xiang LI
XL-35-72 CNMR CDCL3 75MHZ(3/12/16)



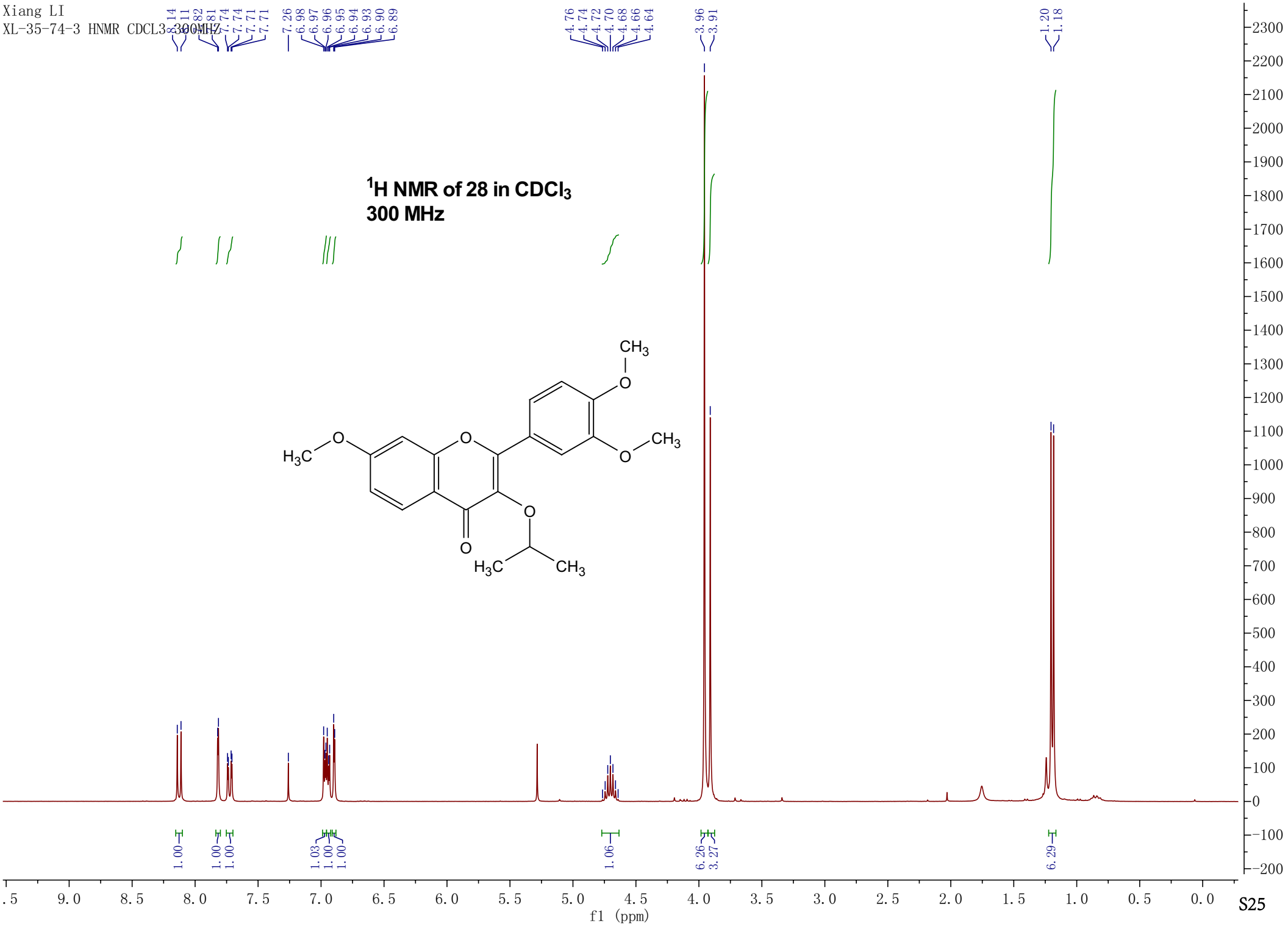
Xiang LI
XL-35-73 HNMR CDCL3 300MHZ(3/16/16)

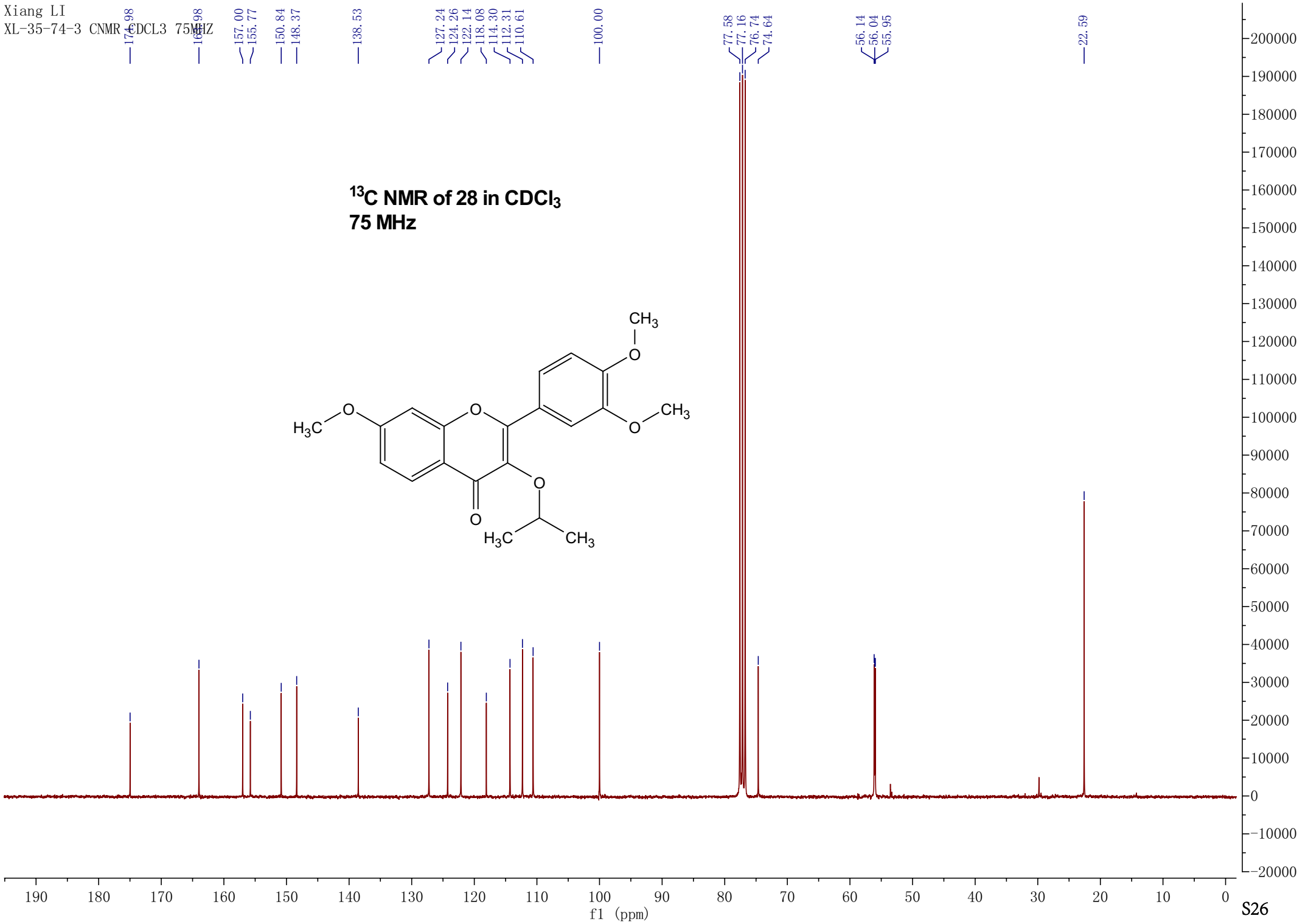


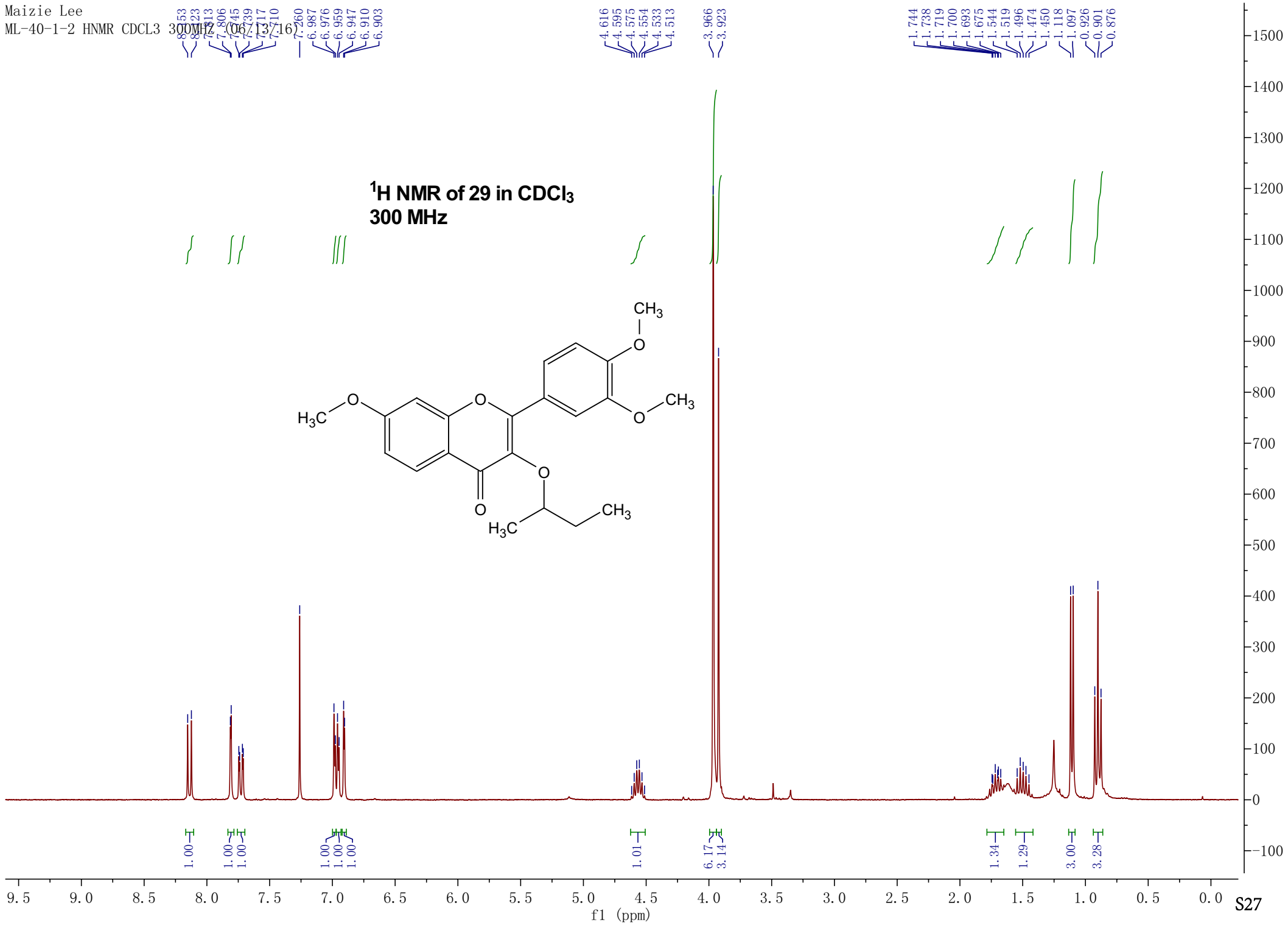
Xiang LI
XL-35-73 CNMR CDCL3 75MHZ(3/15/16)



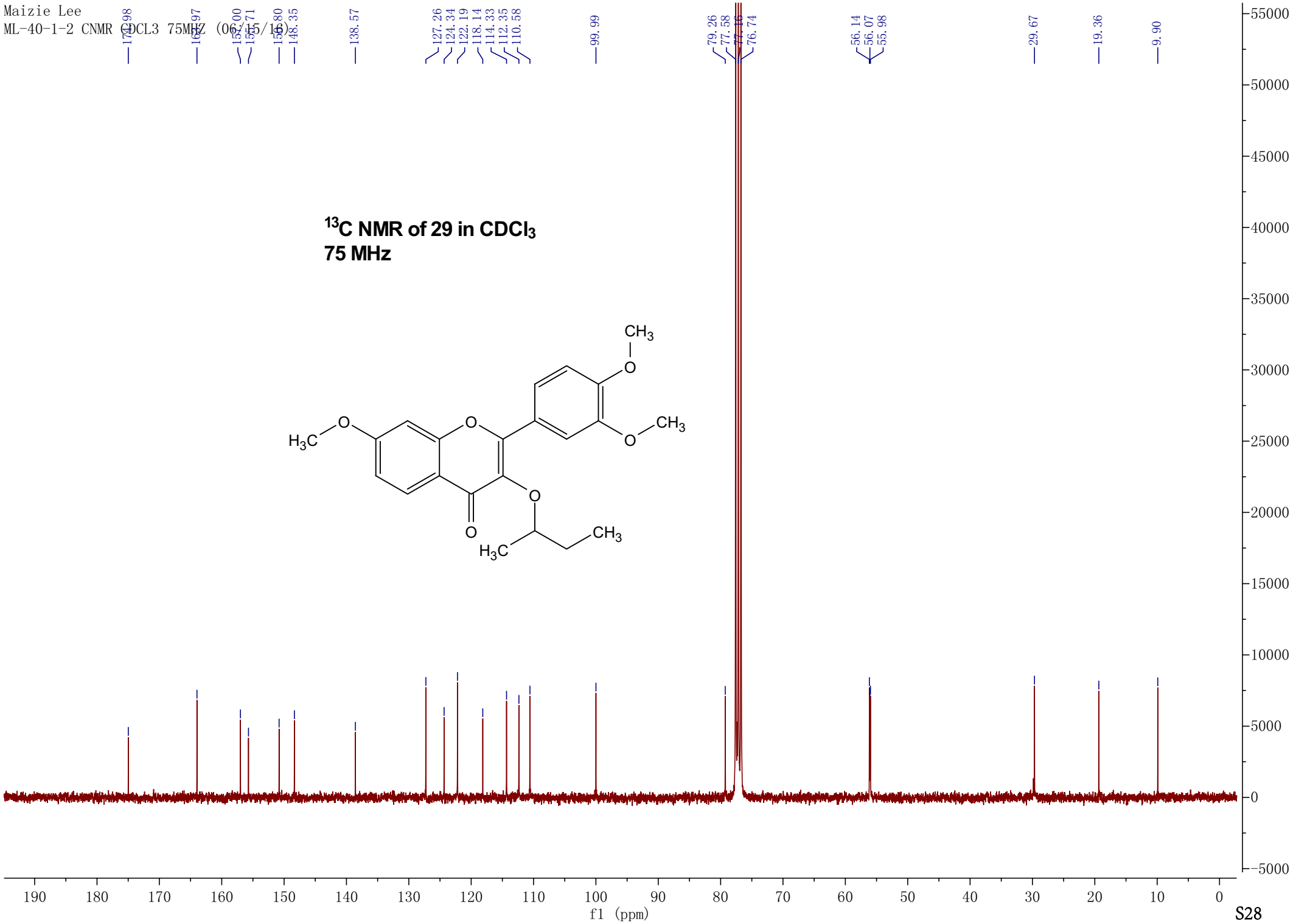
Xiang LI
XL-35-74-3 HNMR CDCL3 300MHZ



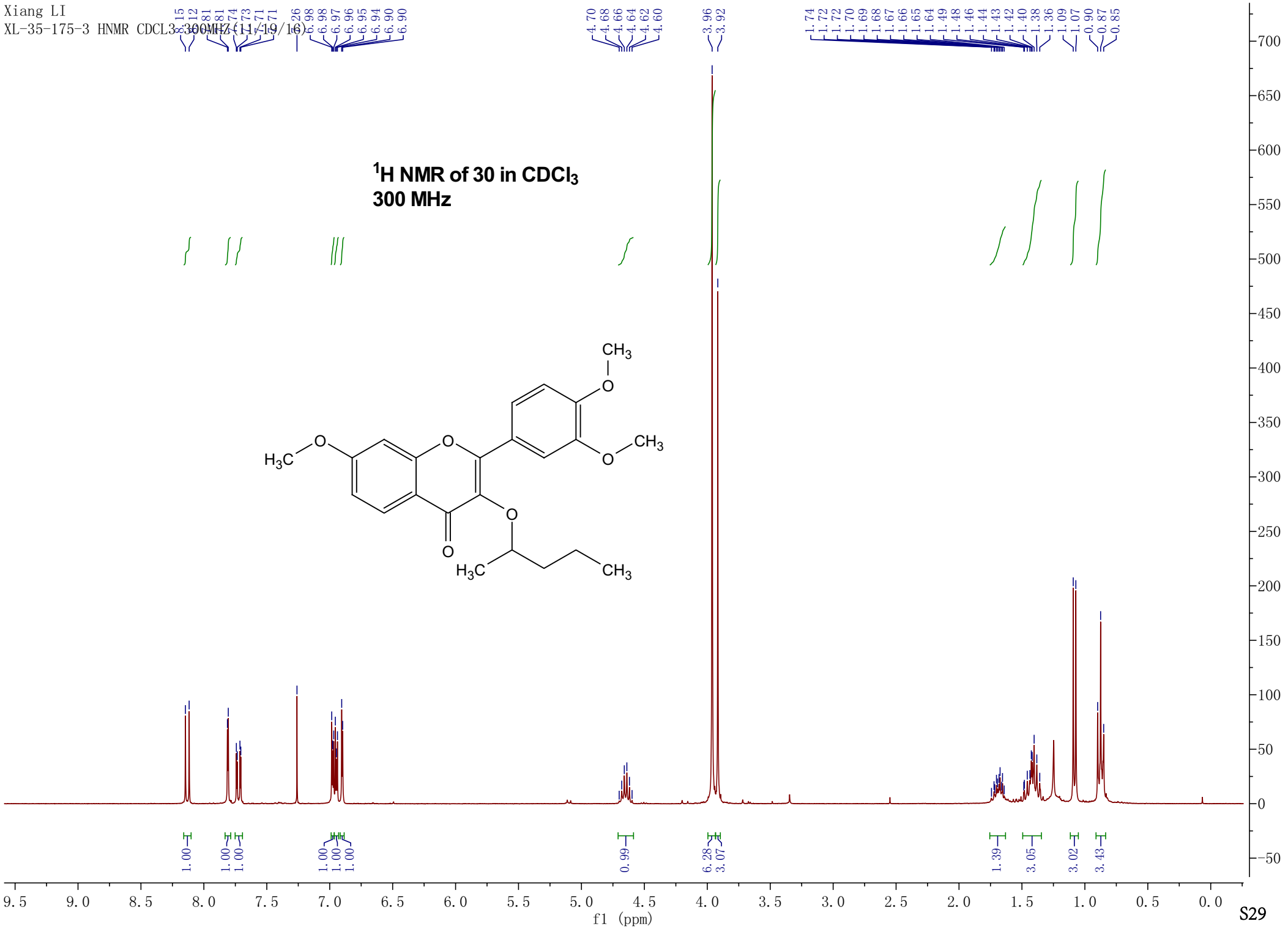

Xiang LI
XL-35-74-3 CNMR CDCL3 75MHZ
174.98
166.98
157.00
155.77
150.84
148.37
138.53
127.24
124.26
122.14
118.08
114.30
112.31
110.61
100.00
77.58
77.16
76.74
74.64
56.14
56.04
55.95
22.59
13C NMR of 28 in CDCl3
75 MHz
CH3
O
O
CH3
H3C
O
O
O
O
H3C
CH3
200000
190000
180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
-20000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Maizie Lee
ML-40-1-2 HNMR CDCL3 300MHZ (06/13/16)
^{1}H NMR of 29 in CDCl$_3$
300 MHz
f1 (ppm)

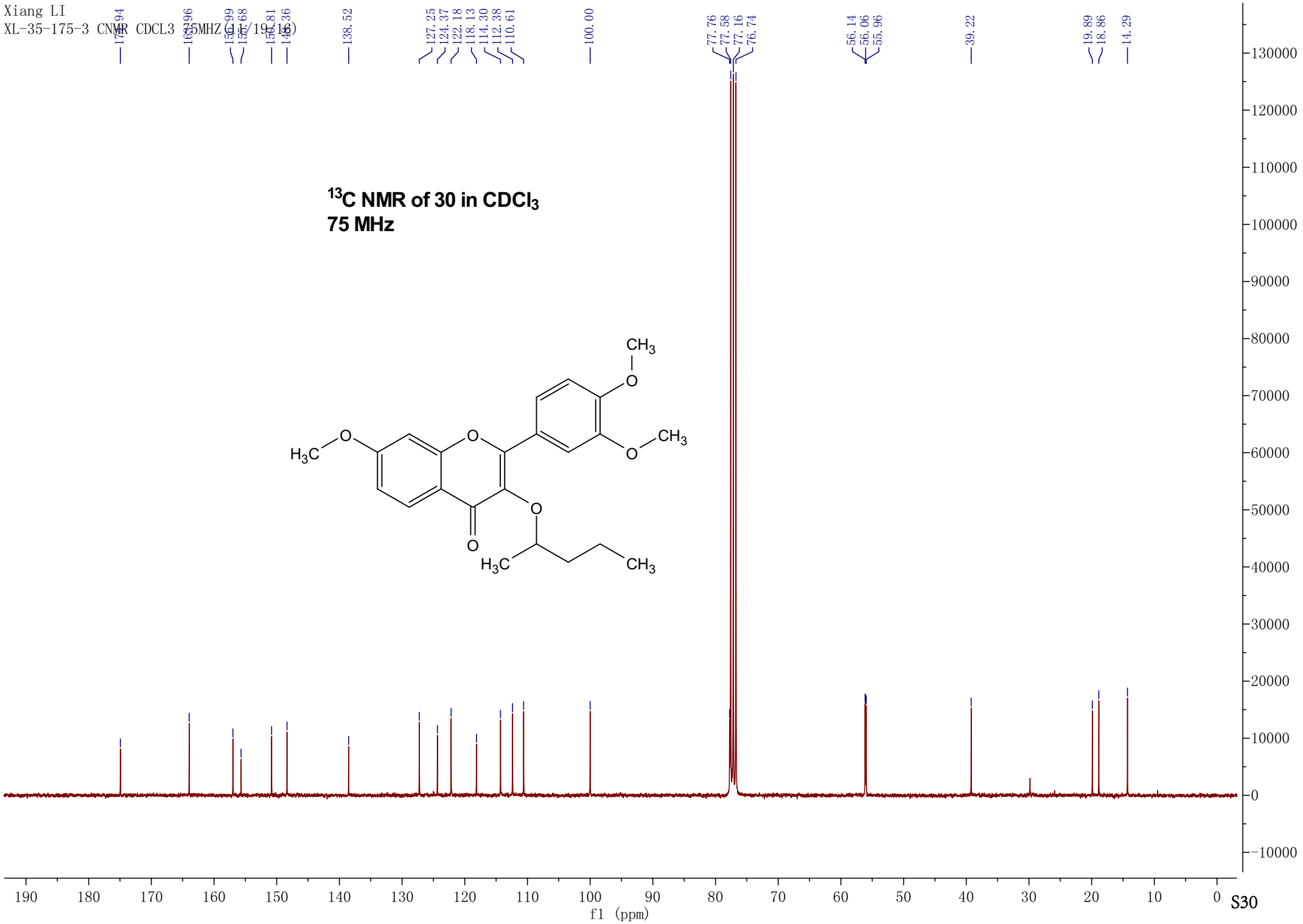
Maizie Lee
ML-40-1-2 CNMR CDCL3 75MHZ (06/15/16)

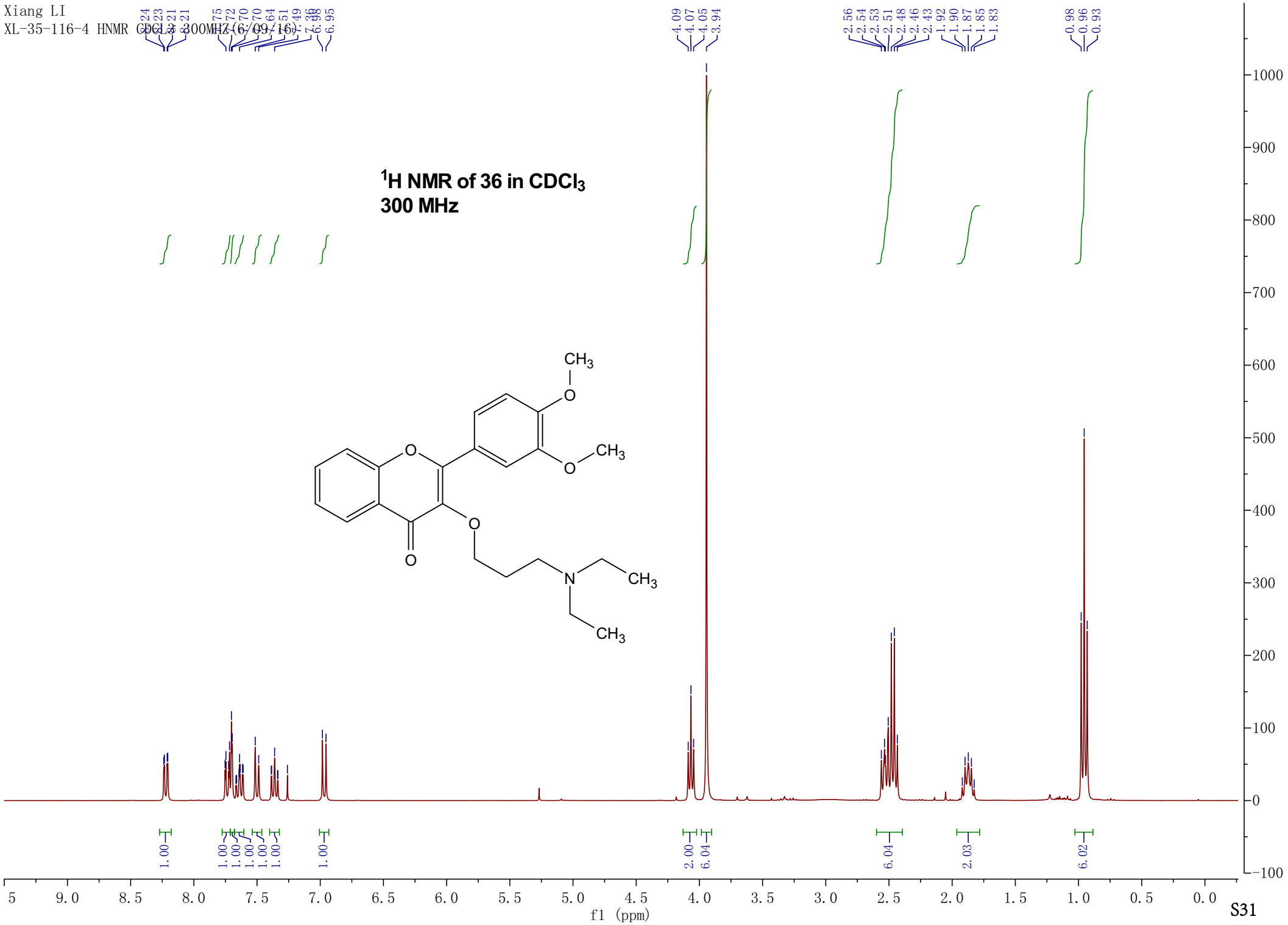


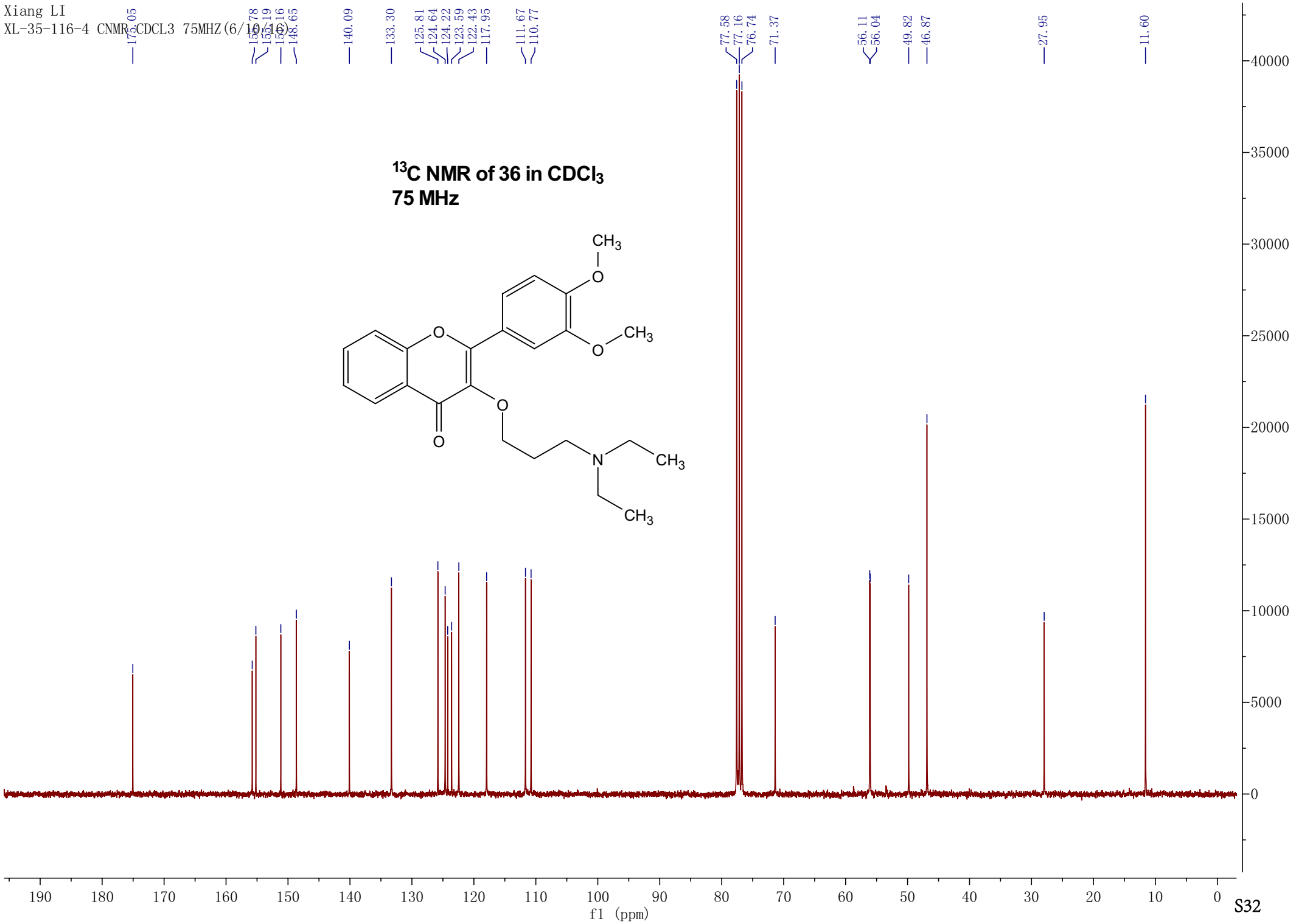
Xiang LI
XL-35-175-3 HNMR CDCL3 300MHZ (11/19/16)

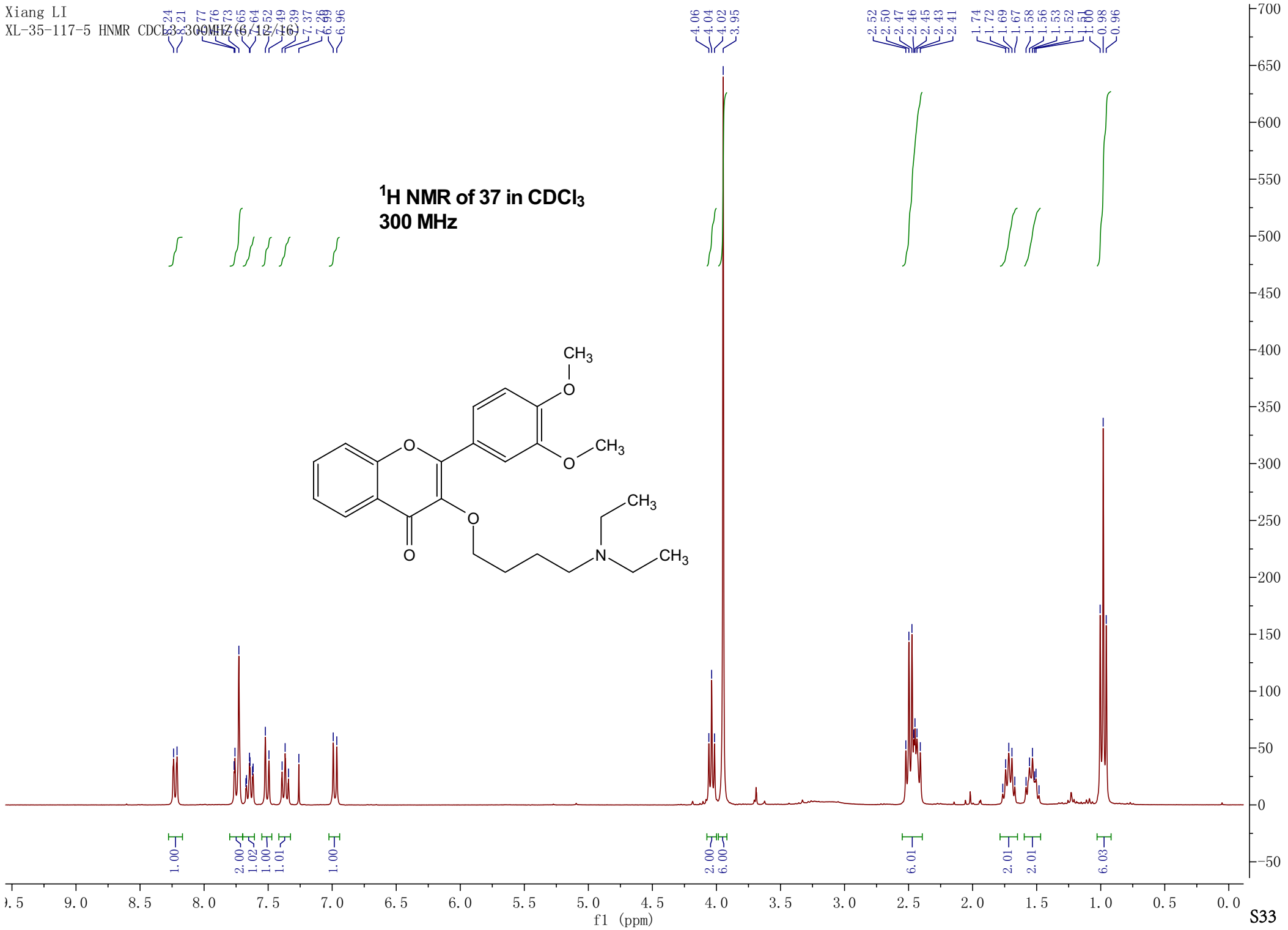


Xiang LI
XL-35-175-3 CNMR CDCL3 75MHZ(1:1/19.16)

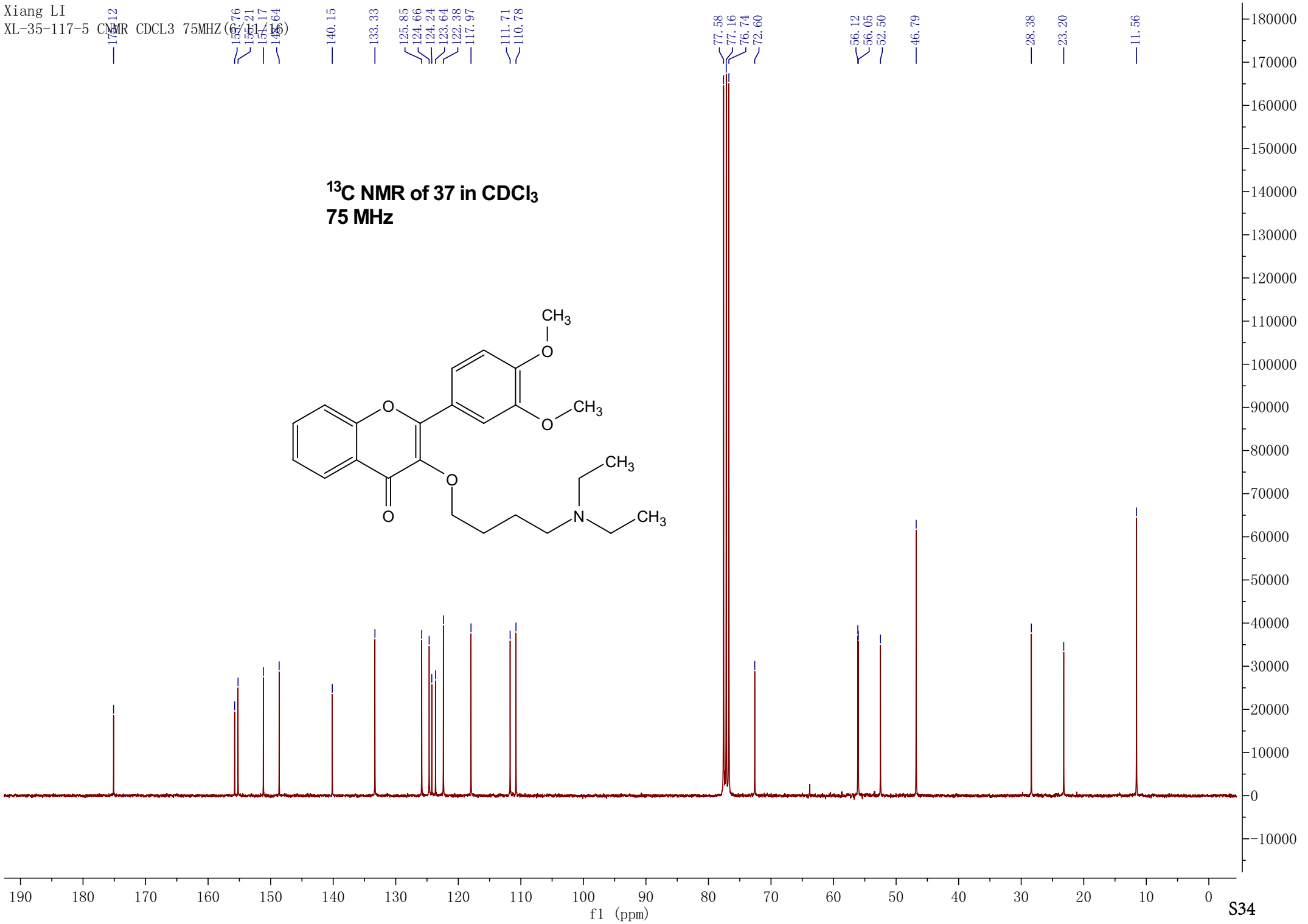



Xiang LI
XL-35-116-4 HNMR CDCL3 300MHZ(6/09/16)
^{1}H NMR of 36 in CDCl$_3$
300 MHz
f1 (ppm)

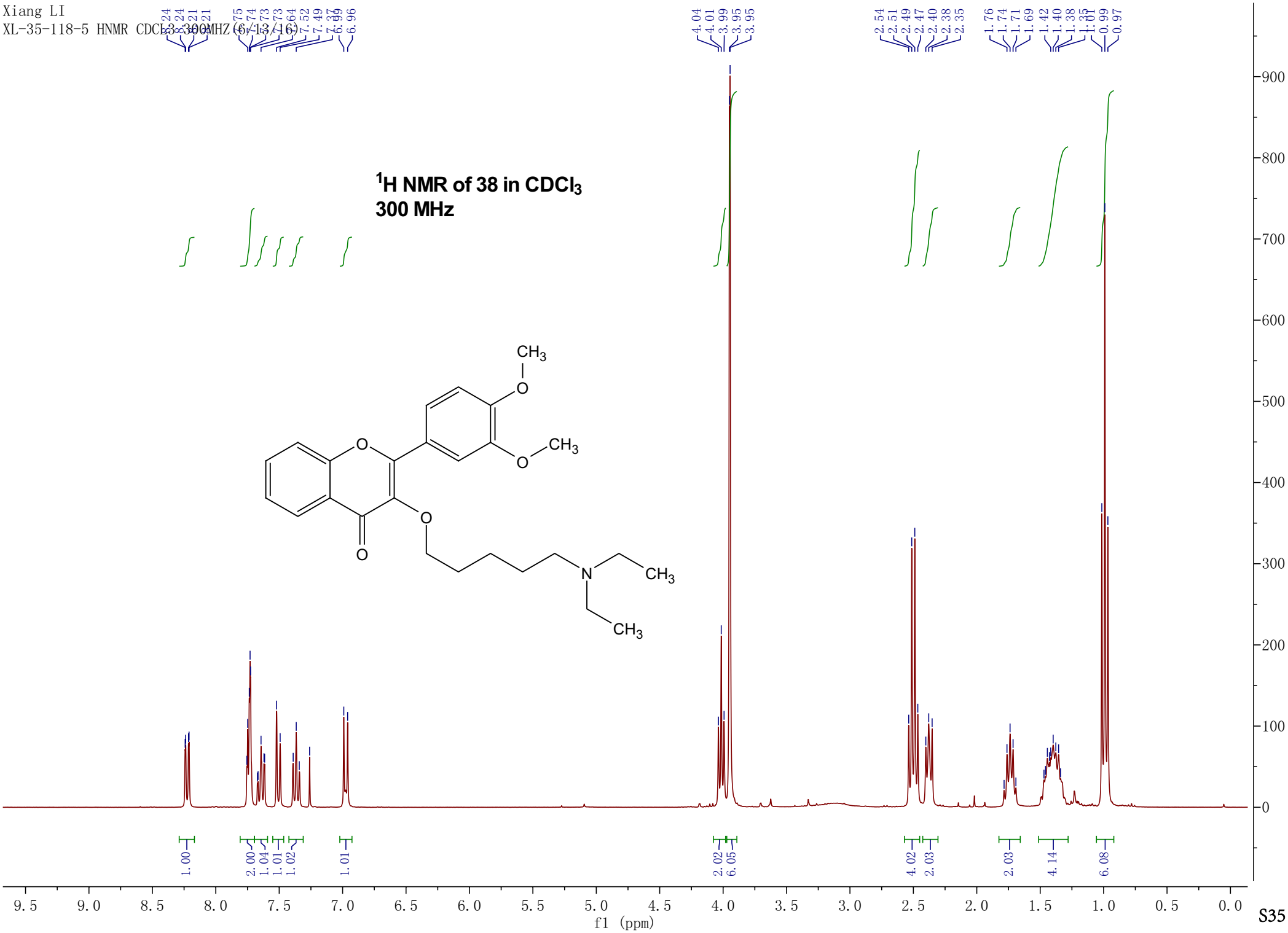

Xiang LI
XL-35-116-4 CNMR CDCL3 75MHZ(6/10/16)
175.05
155.78
155.19
155.16
148.65
140.09
133.30
125.81
124.64
124.22
123.59
122.43
117.95
111.67
110.77
77.58
77.16
76.74
71.37
56.11
56.04
49.82
46.87
27.95
11.60
13C NMR of 36 in CDCl3
75 MHz
CH3
O
CH3
O
O
O
O
N
CH3
CH3
40000
35000
30000
25000
20000
15000
10000
5000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Xiang LI
XL-35-117-5 HNMR CDCL3 300MHZ(6/12/16)
^{1}H NMR of 37 in $CDCl_3$
300 MHz
f1 (ppm)

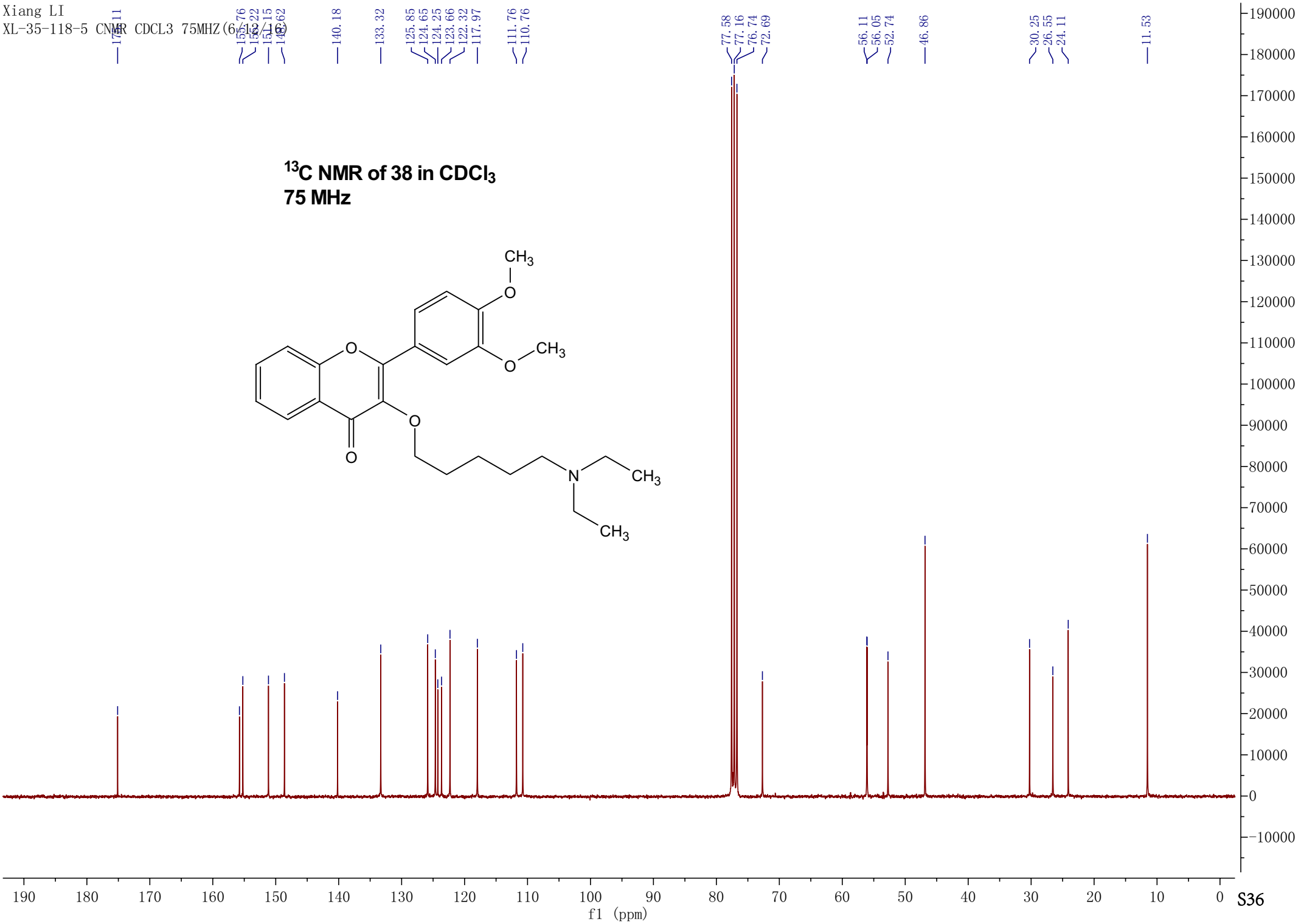
Xiang LI
XL-35-117-5 CNMR CDCL3 75MHZ(6/11/16)



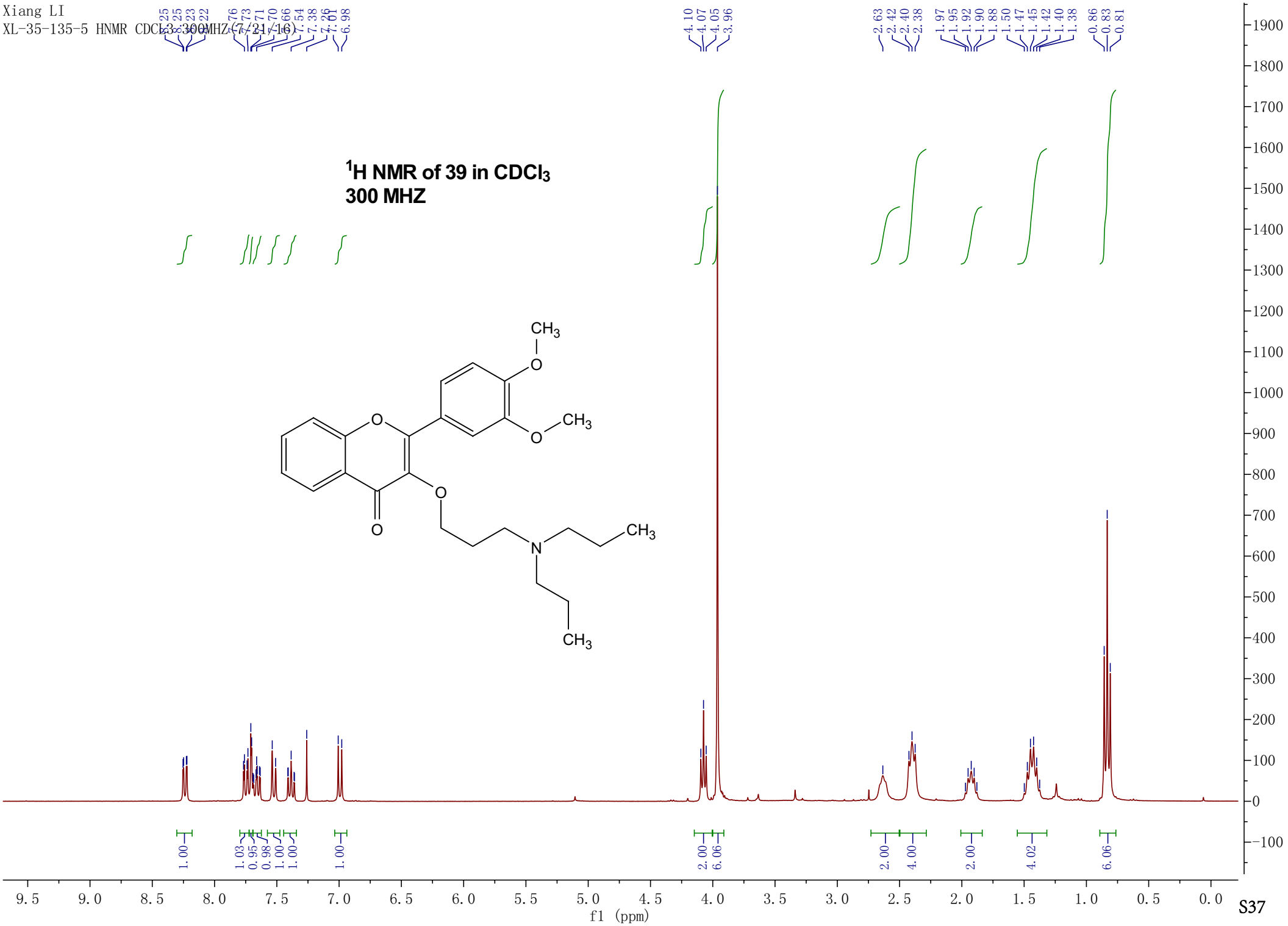
Xiang LI
XL-35-118-5 HNMR CDCL3 300MHZ (6/13/16)



Xiang LI
XL-35-118-5 CNMR CDCL3 75MHZ(6-12-16)

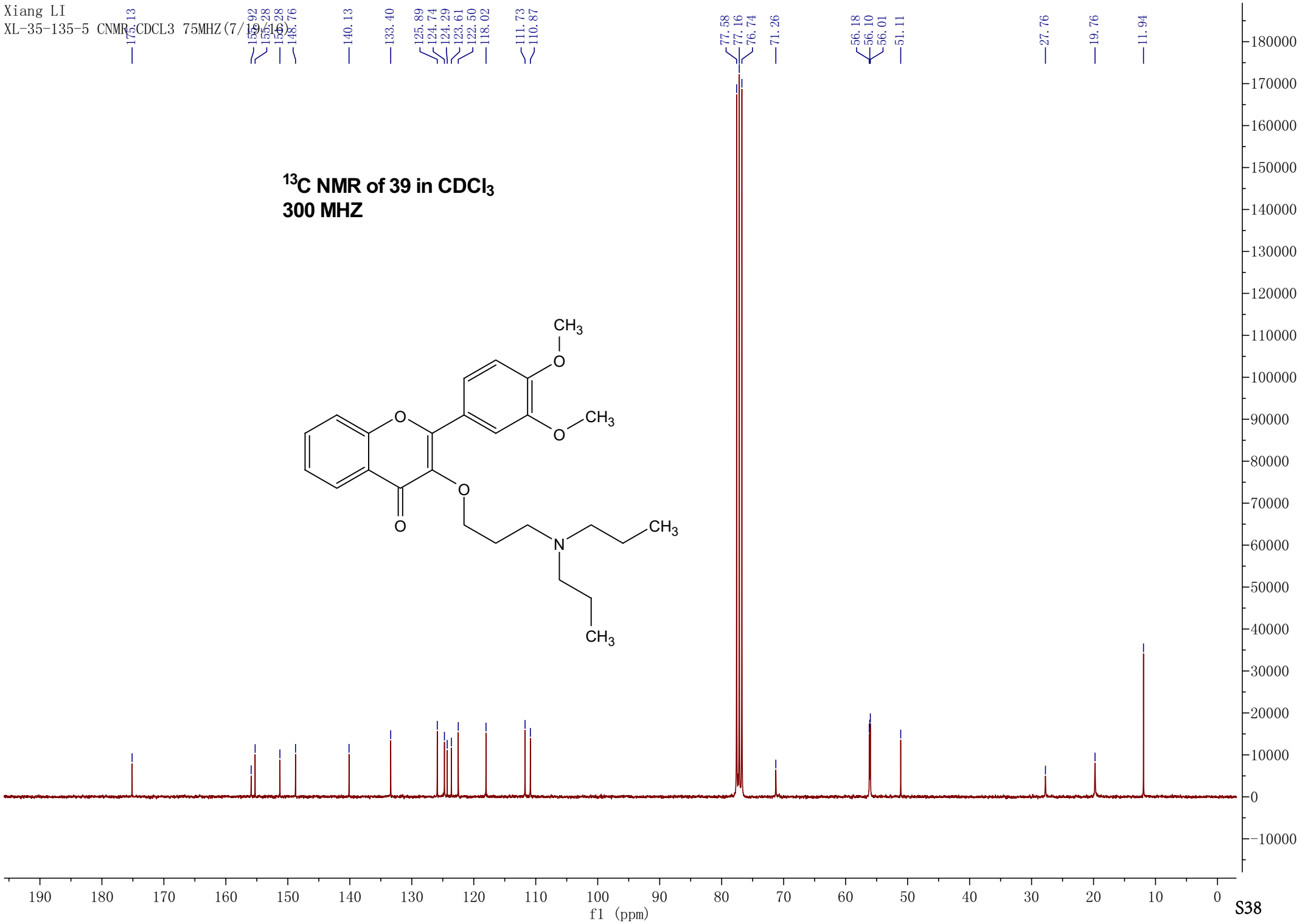


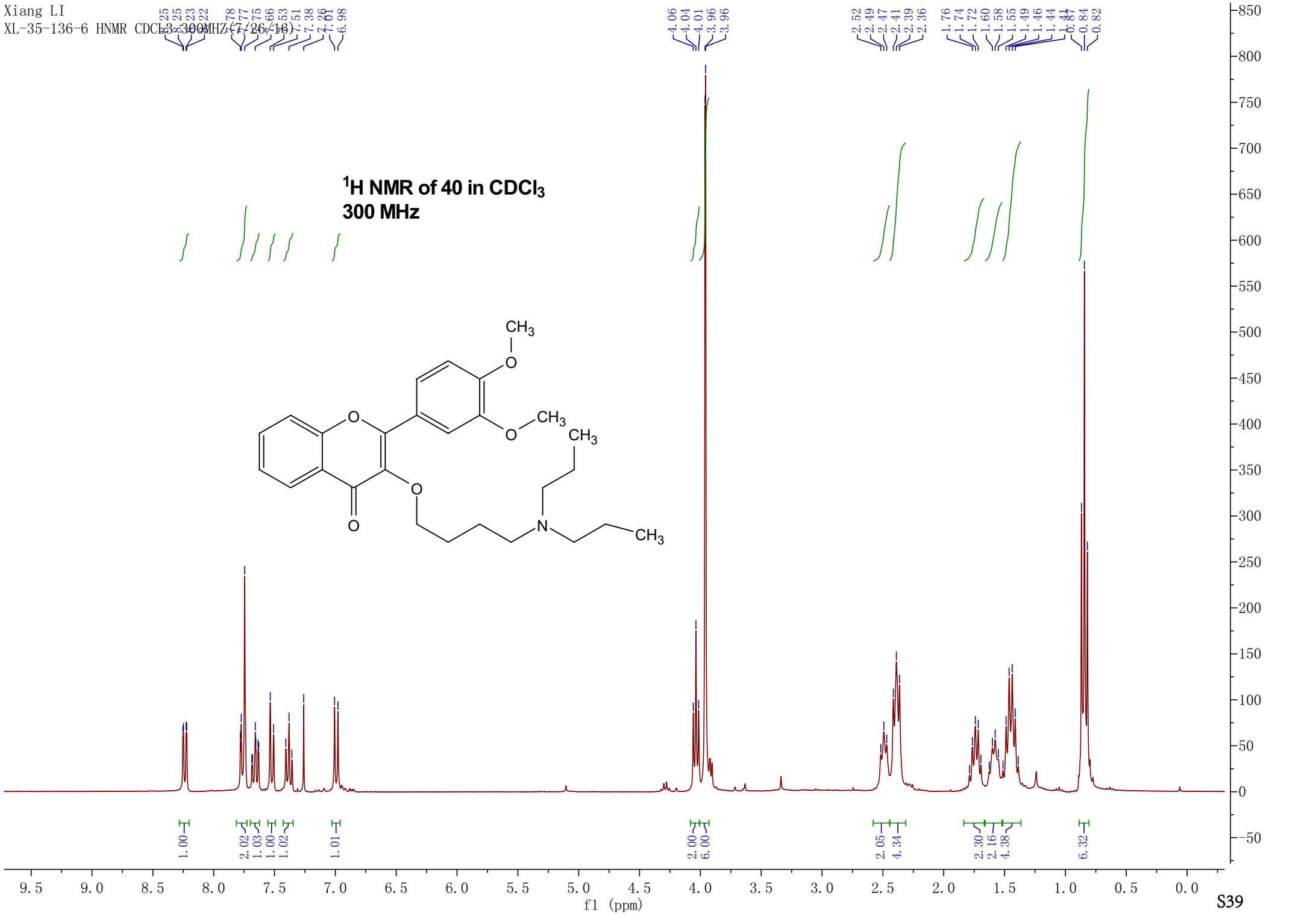
Xiang LI
XL-35-135-5 HNMR CDCl3 300MHZ (7-21-16)



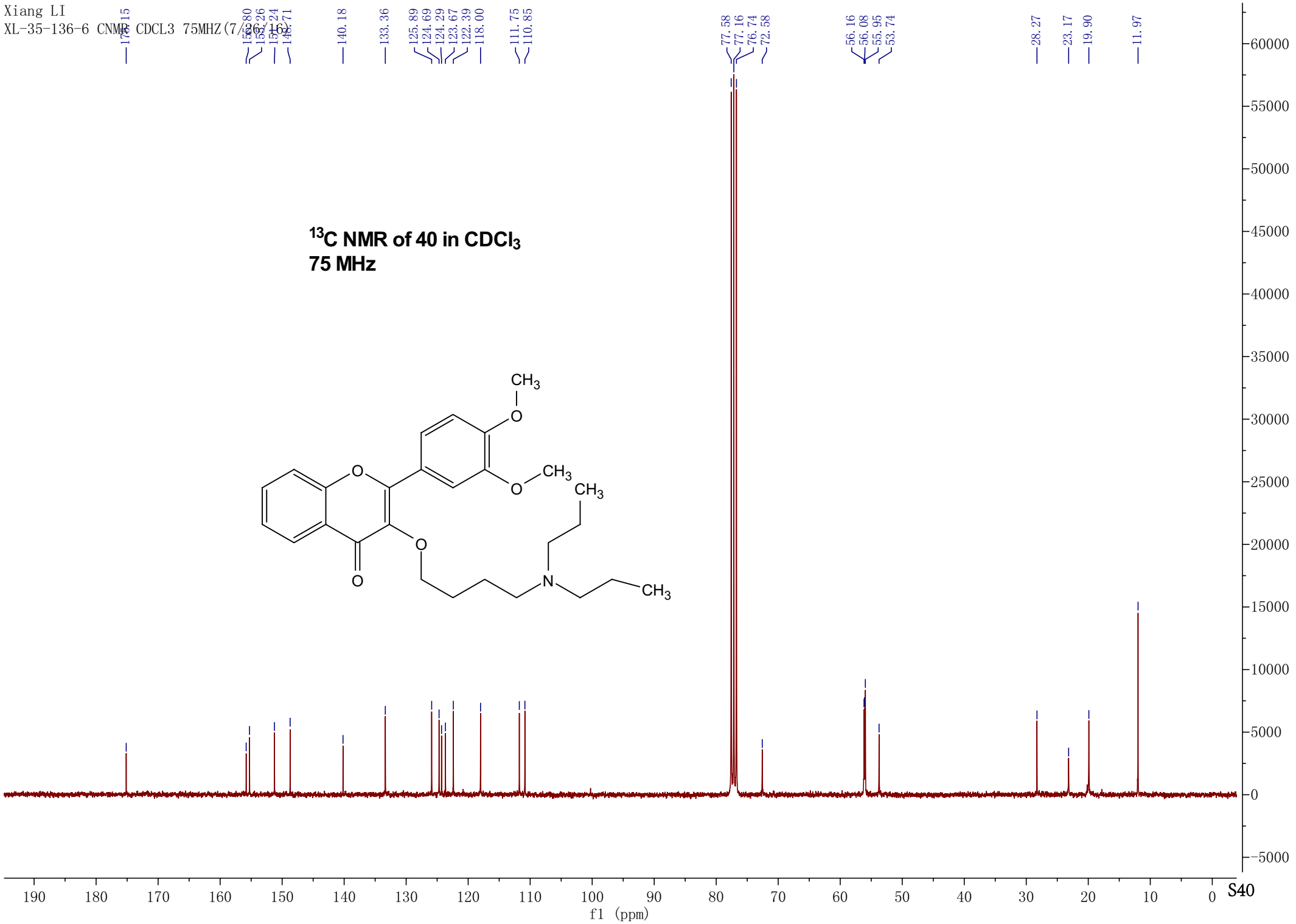
^{1}H NMR of 39 in $CDCl_3$
300 MHZ

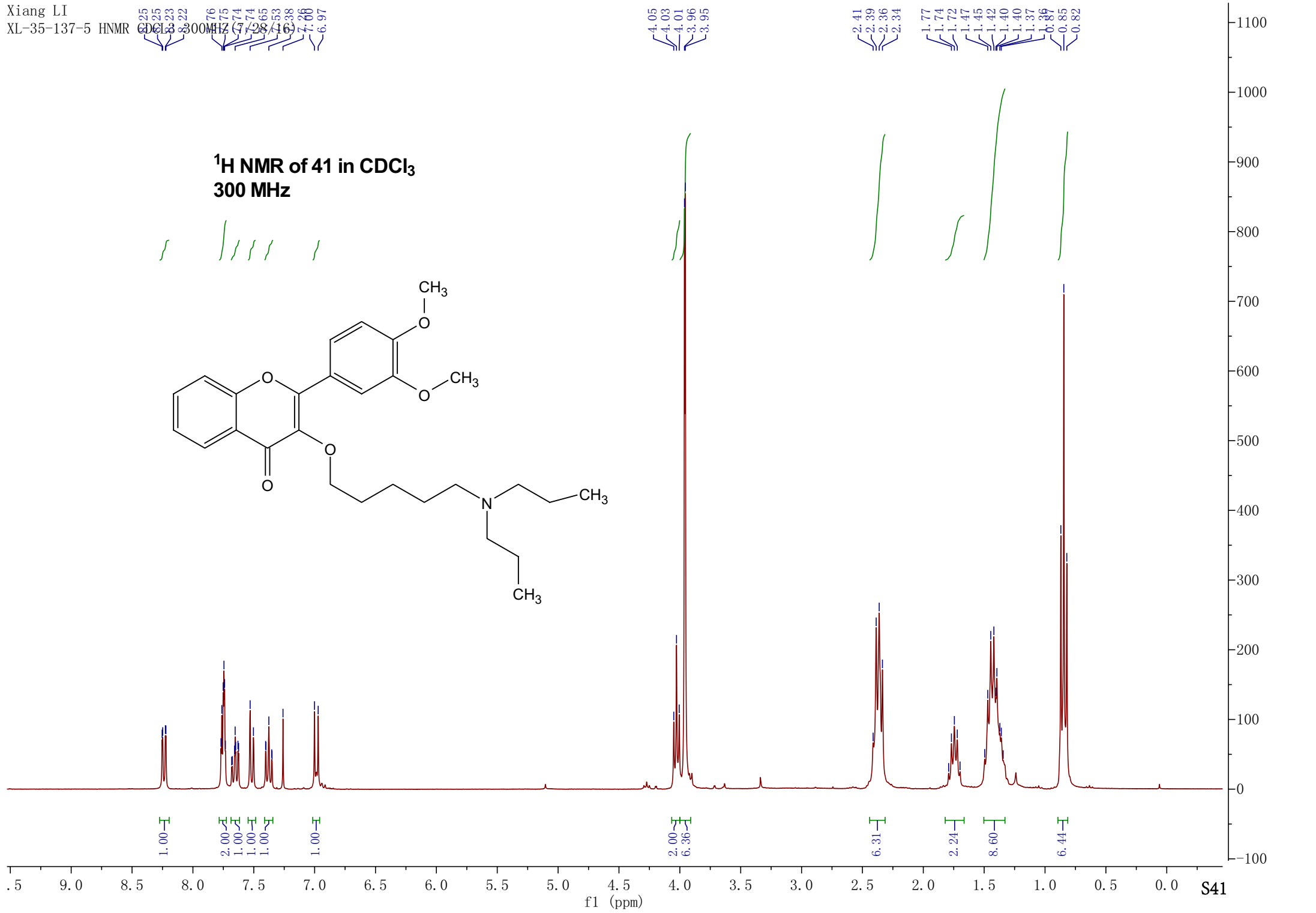
Xiang LI
XL-35-135-5 CNMR-CDCL3 75MHZ(7/19/16)



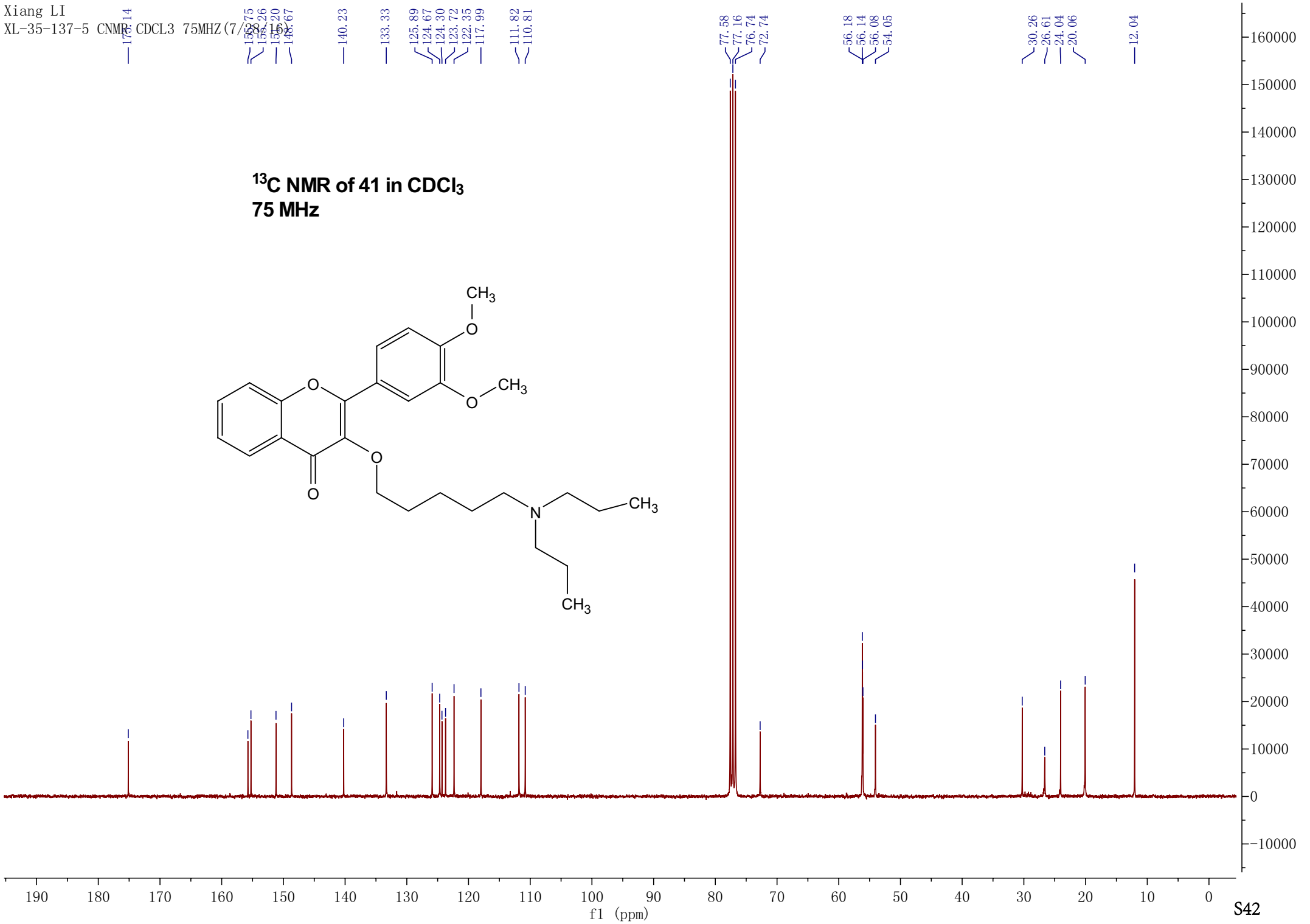

Xiang LI
XL-35-136-6 HNMR CDCL3 300MHZ(7/26/16)
^{1}H NMR of 40 in $CDCl_3$
300 MHz
f1 (ppm)

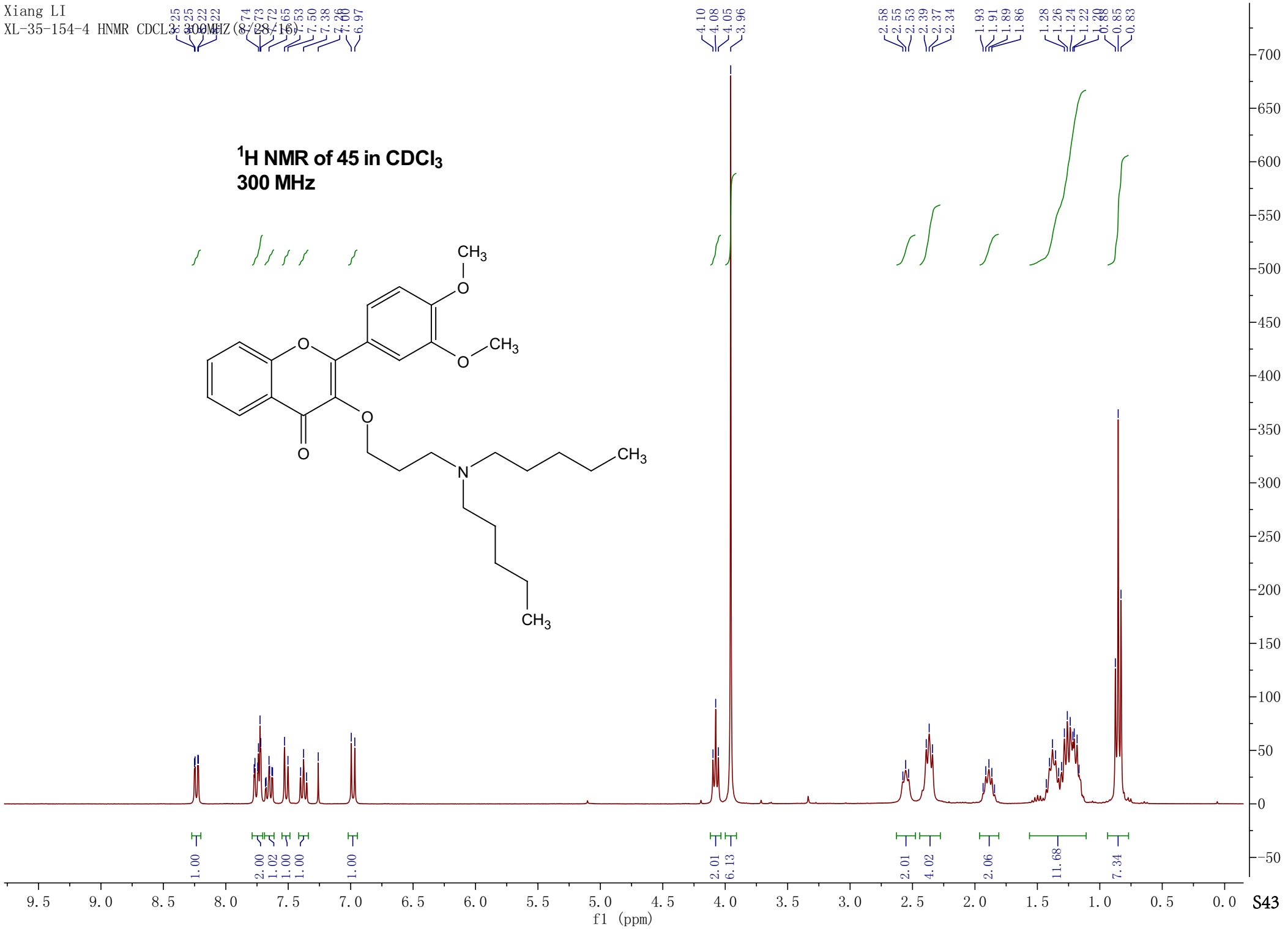
Xiang LI
XL-35-136-6 CNMR CDCL3 75MHZ(7/26/16)



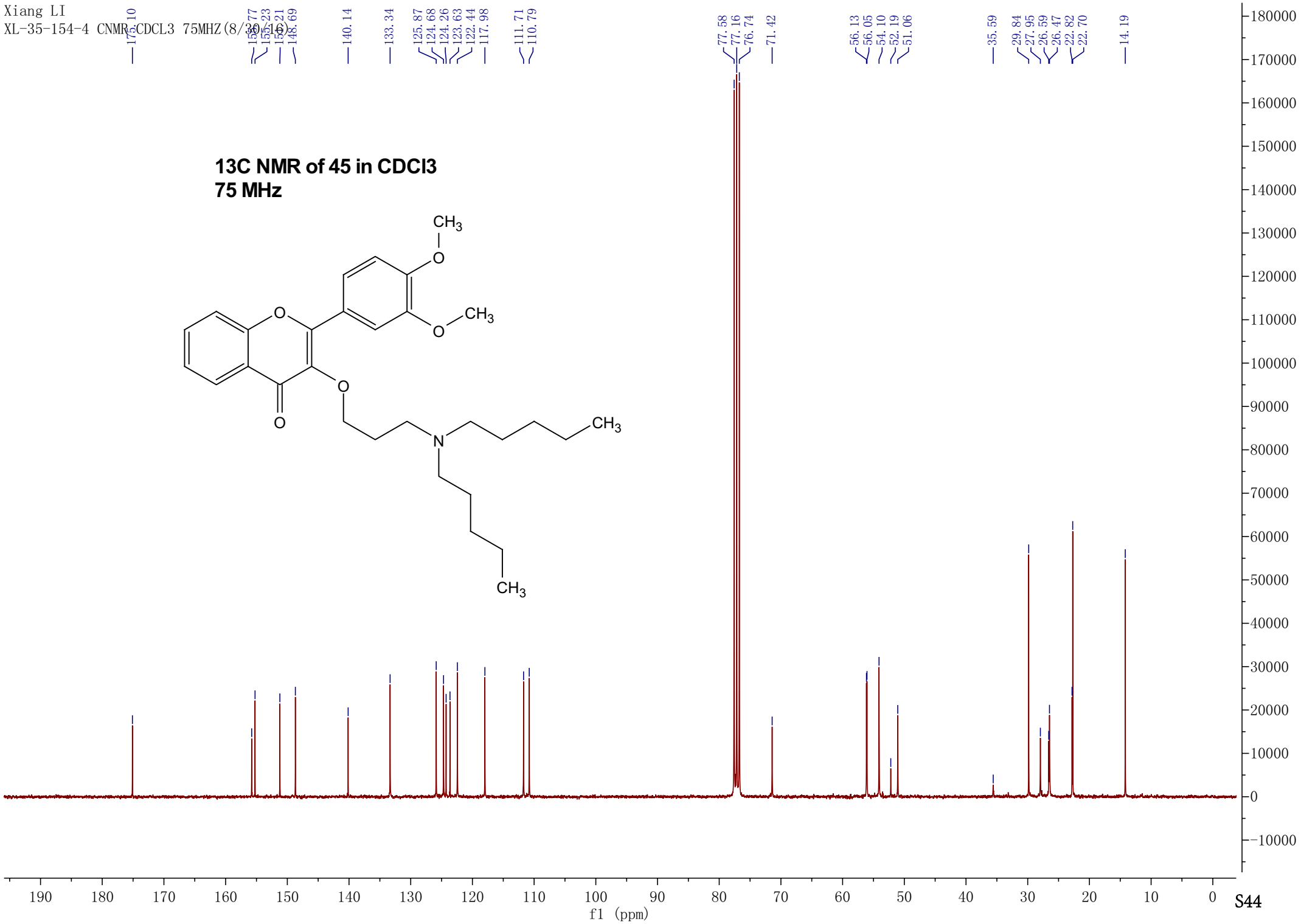

Xiang LI
XL-35-137-5 HNMR CDCL3 300MHZ (7/28/16)
1H NMR of 41 in CDCl3
300 MHz
f1 (ppm)
S41

Xiang LI
XL-35-137-5 CNMR CDCL3 75MHZ(7/28/16)

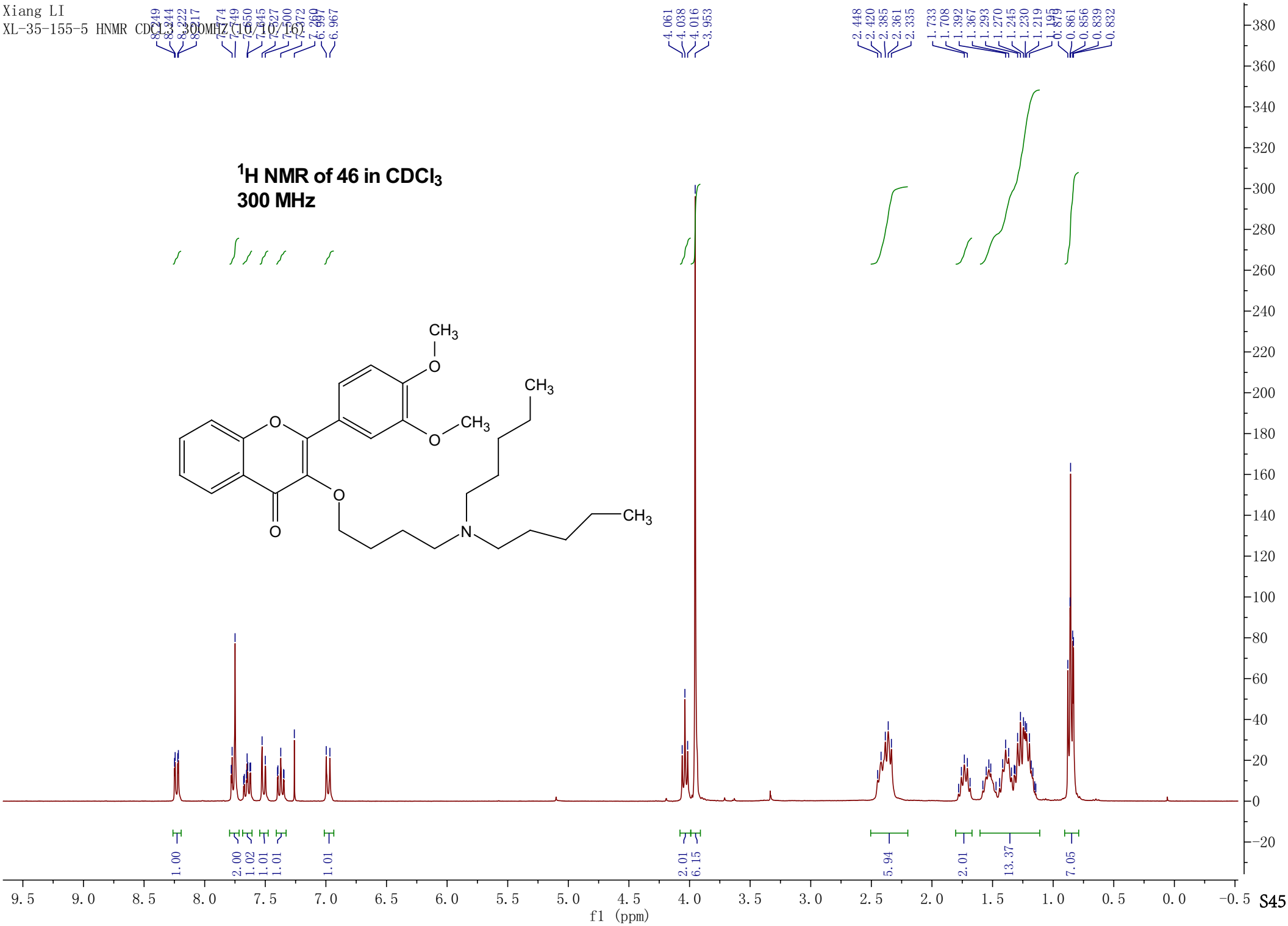



Xiang LI
XL-35-154-4 HNMR CDCL3 300MHZ(8/28/16)
^{1}H NMR of 45 in $CDCl_3$
300 MHz
CH3
O
CH3
O
O
O
O
N
CH3
CH3
f1 (ppm)

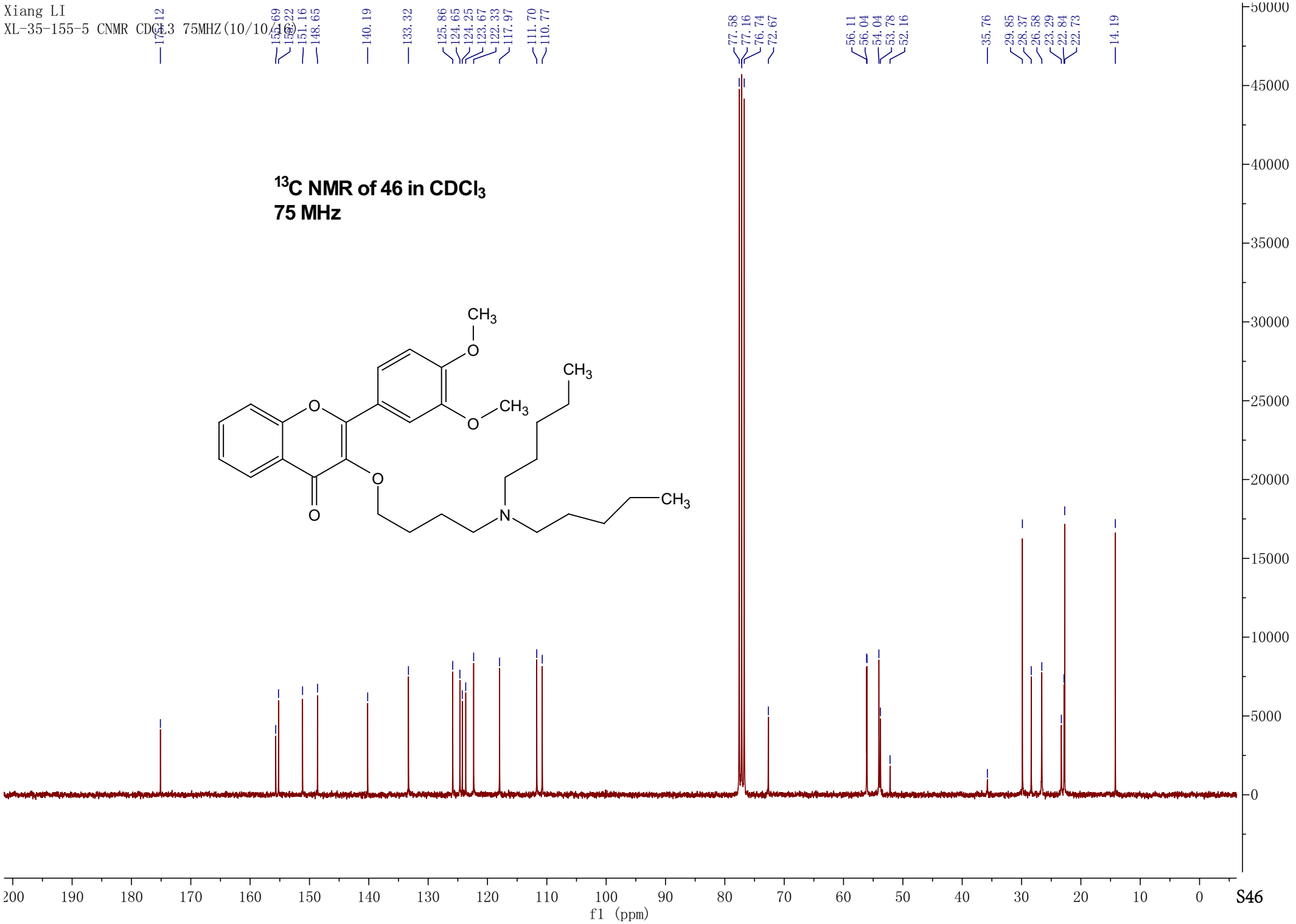
Xiang LI
XL-35-154-4 CNMR CDCL3 75MHZ(8/30/16)



Xiang LI
XL-35-155-5 HNMR CDCl3 300MHZ(10/10/16)

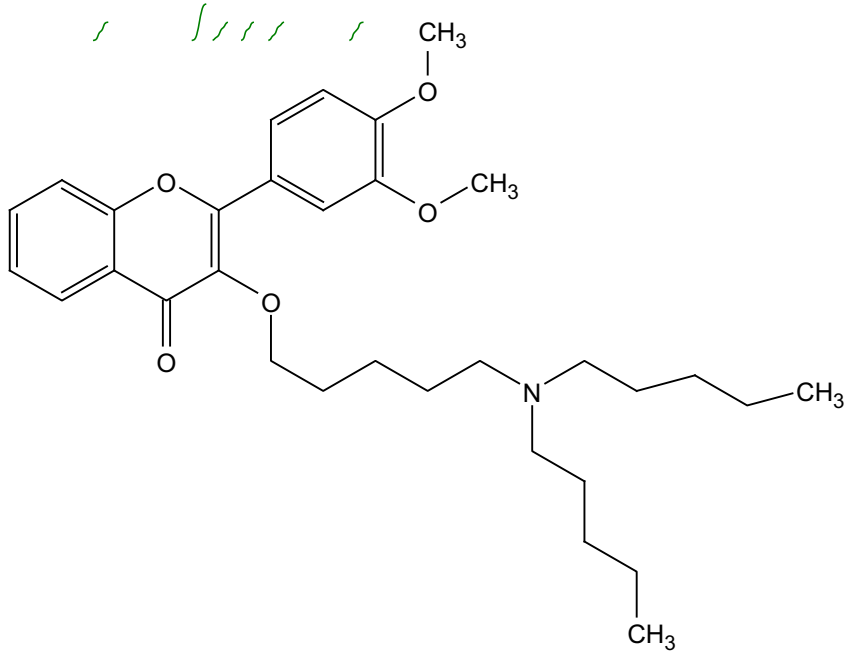


Xiang LI
XL-35-155-5 CNMR CDCL3 75MHZ(10/10/16)



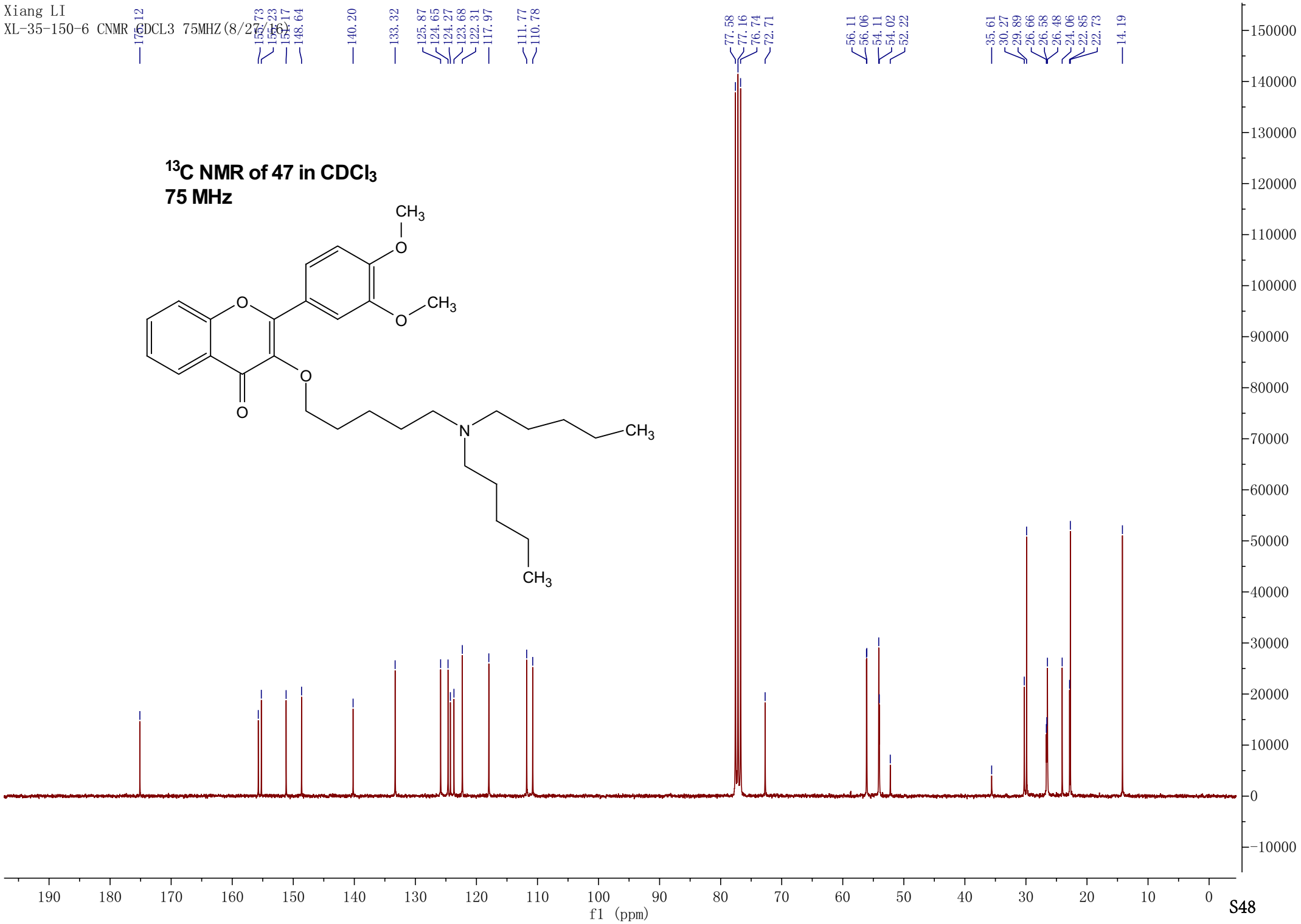
Xiang LI
XL-35-150-6 HNMR CDCl3 300MHZ(8/27/16)

^{1}H NMR of 47 in $CDCl_3$
300 MHz

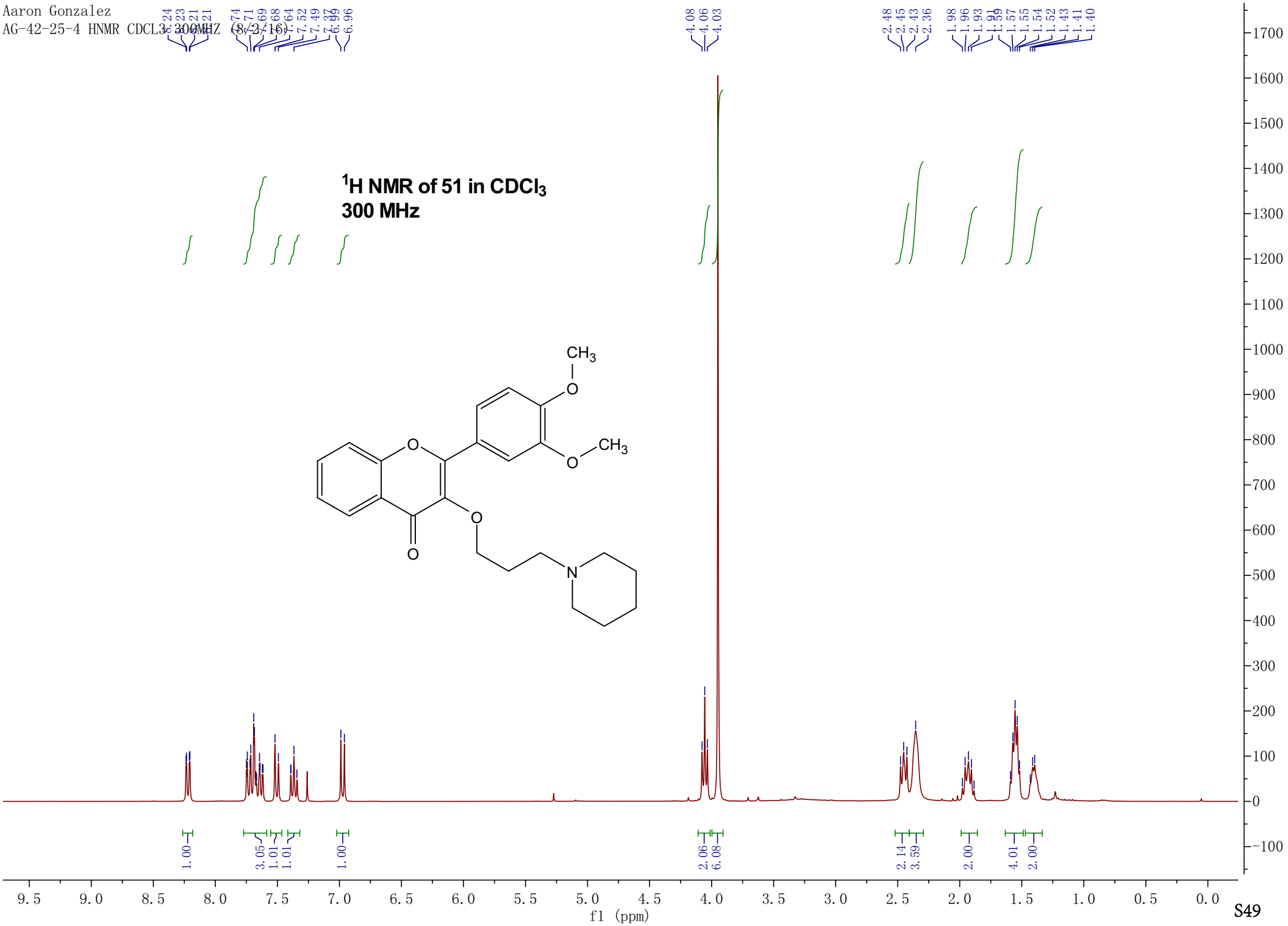


f1 (ppm)

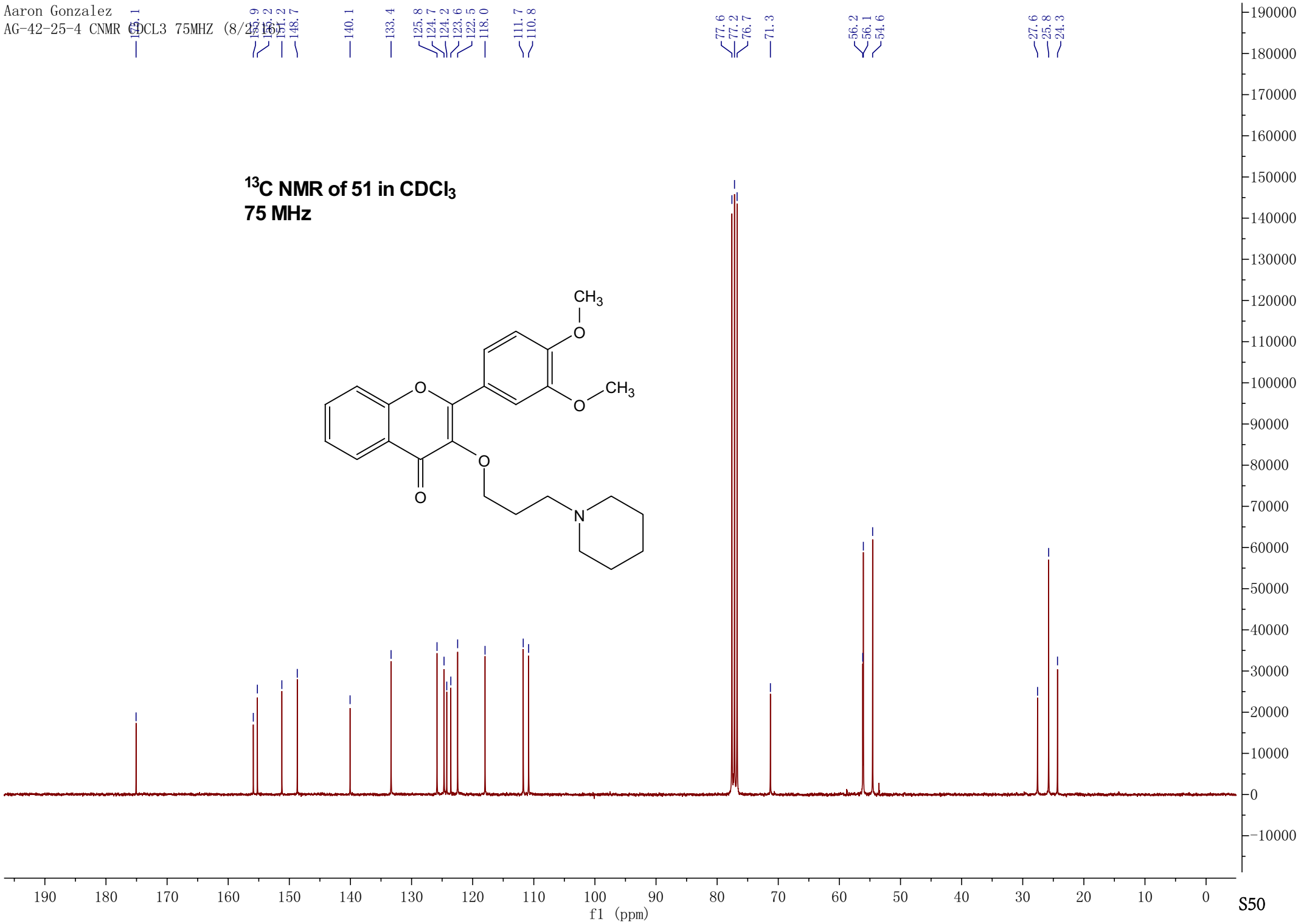
Xiang LI
XL-35-150-6 CNMR CDCL3 75MHZ(8/27/46)

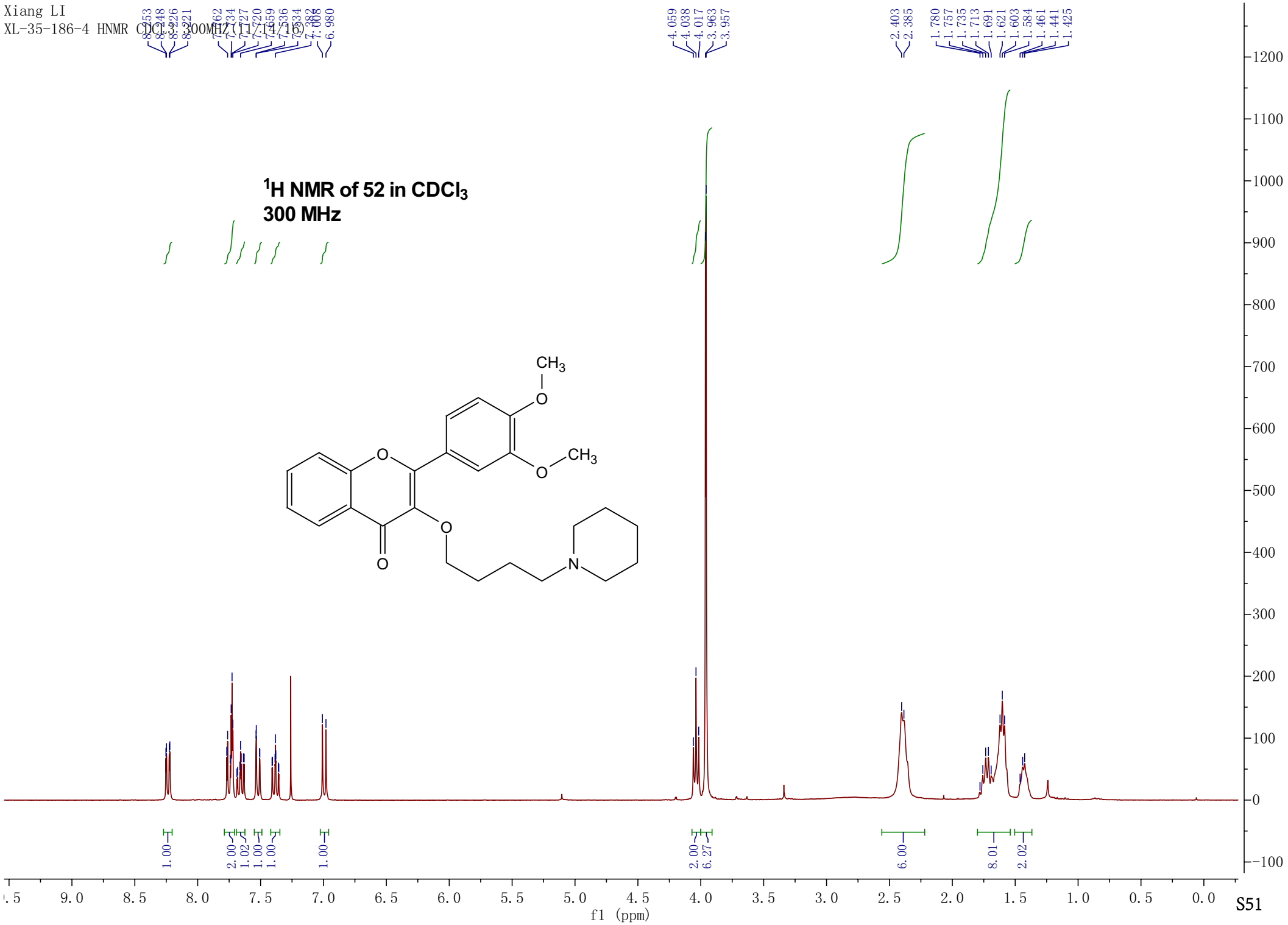


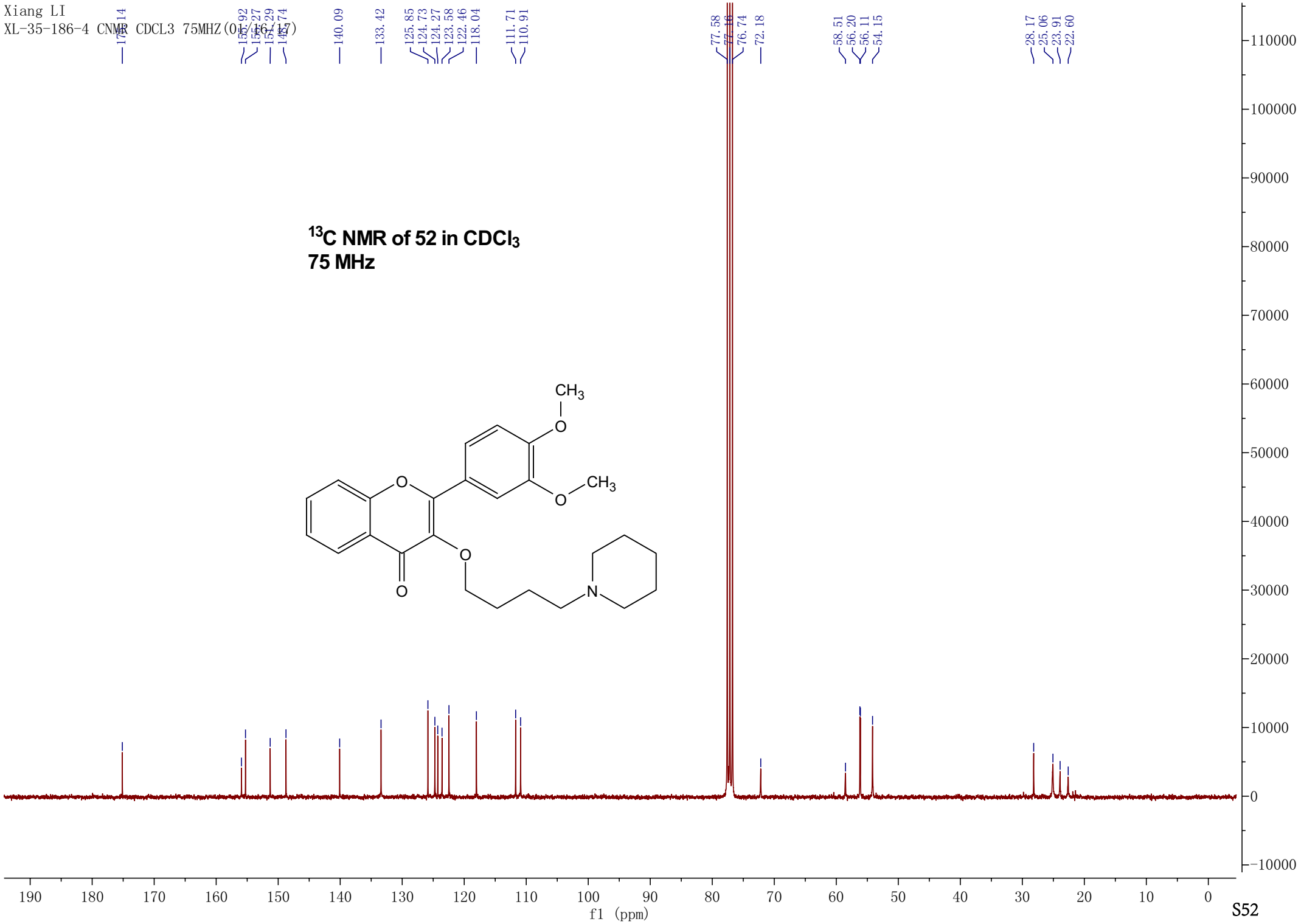
Aaron Gonzalez
AG-42-25-4 HNMR CDCL3 300MHZ (8/2/16)

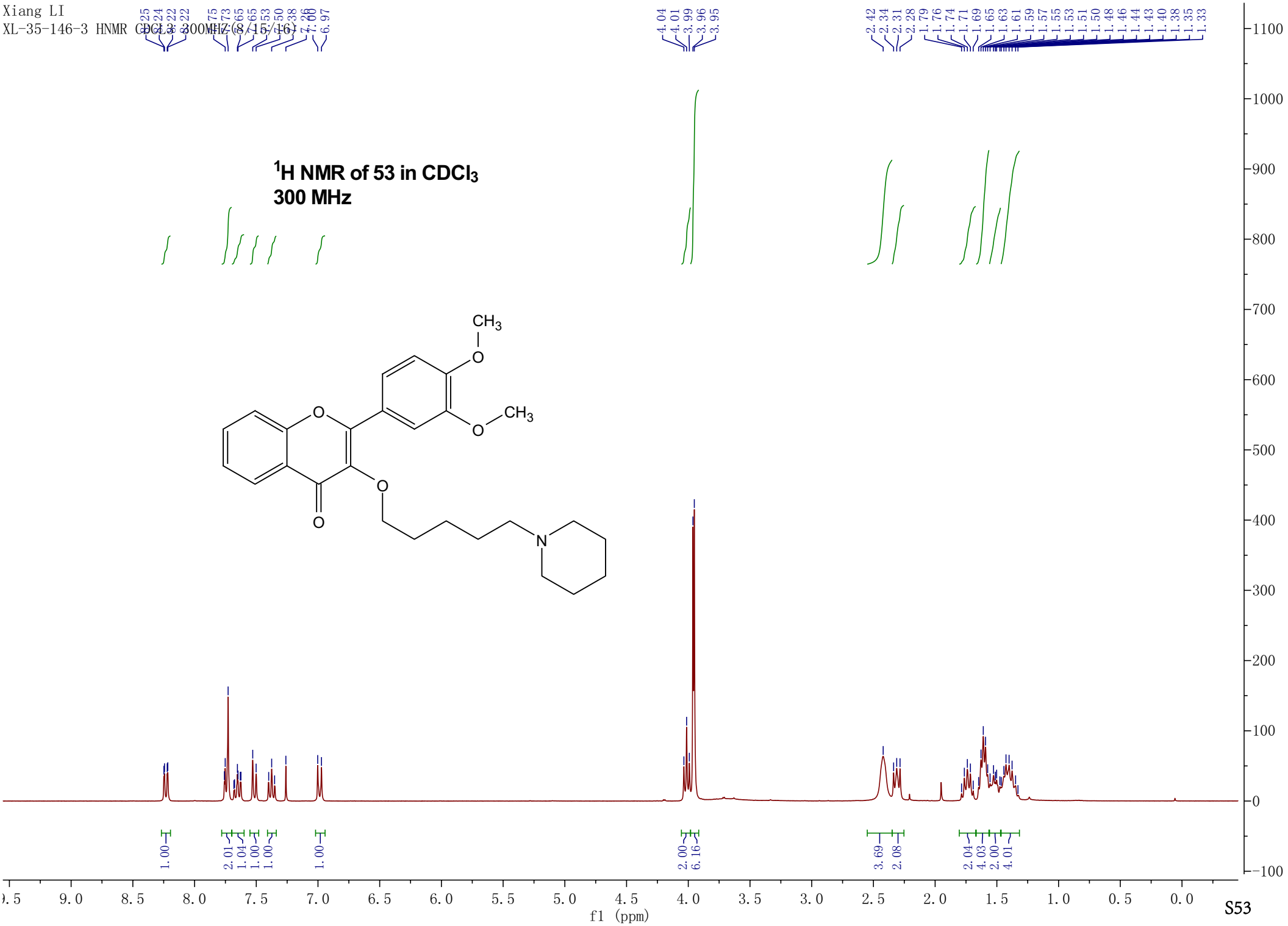


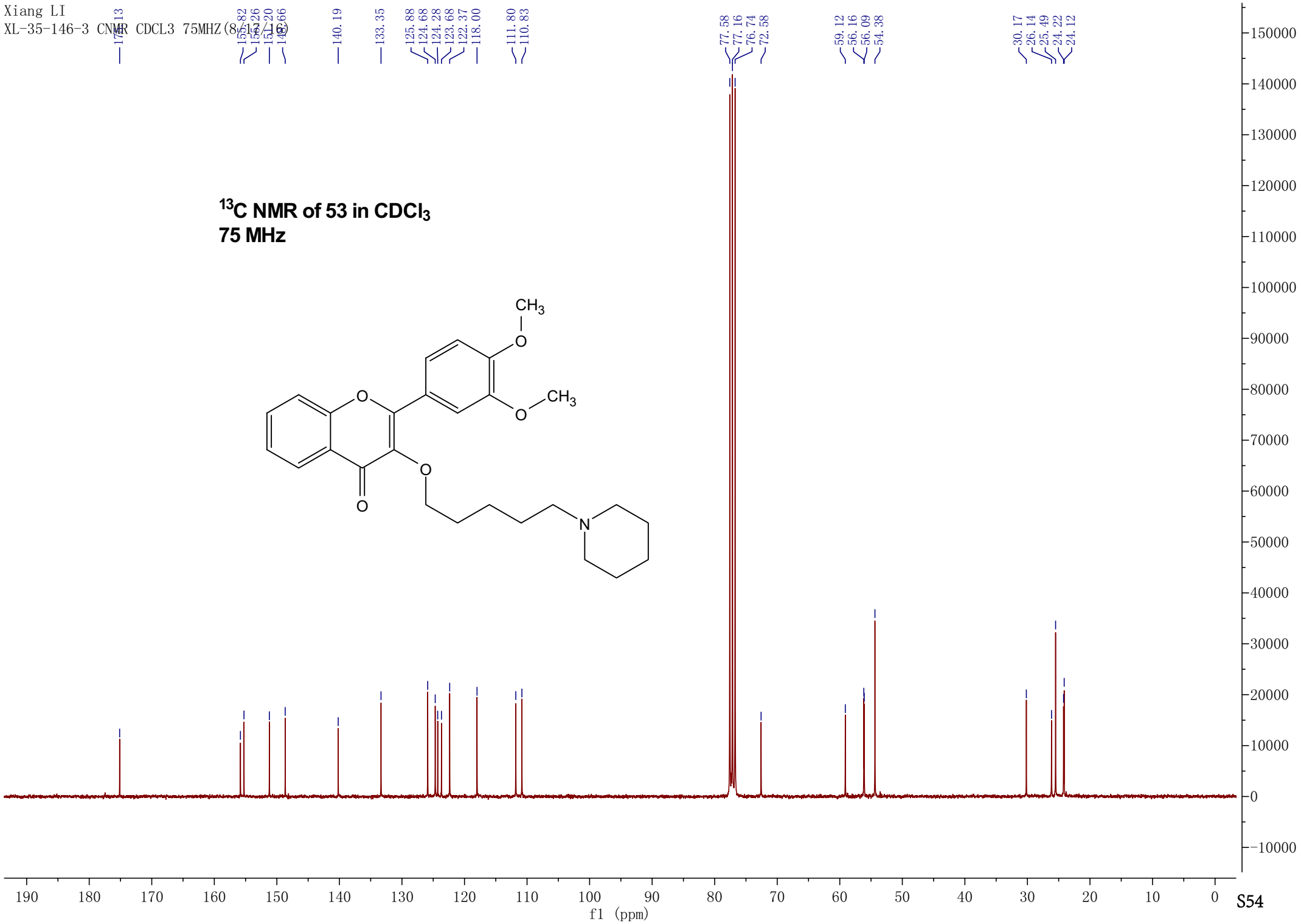
Aaron Gonzalez
AG-42-25-4 CNMR CDCL3 75MHZ (8/2/16)



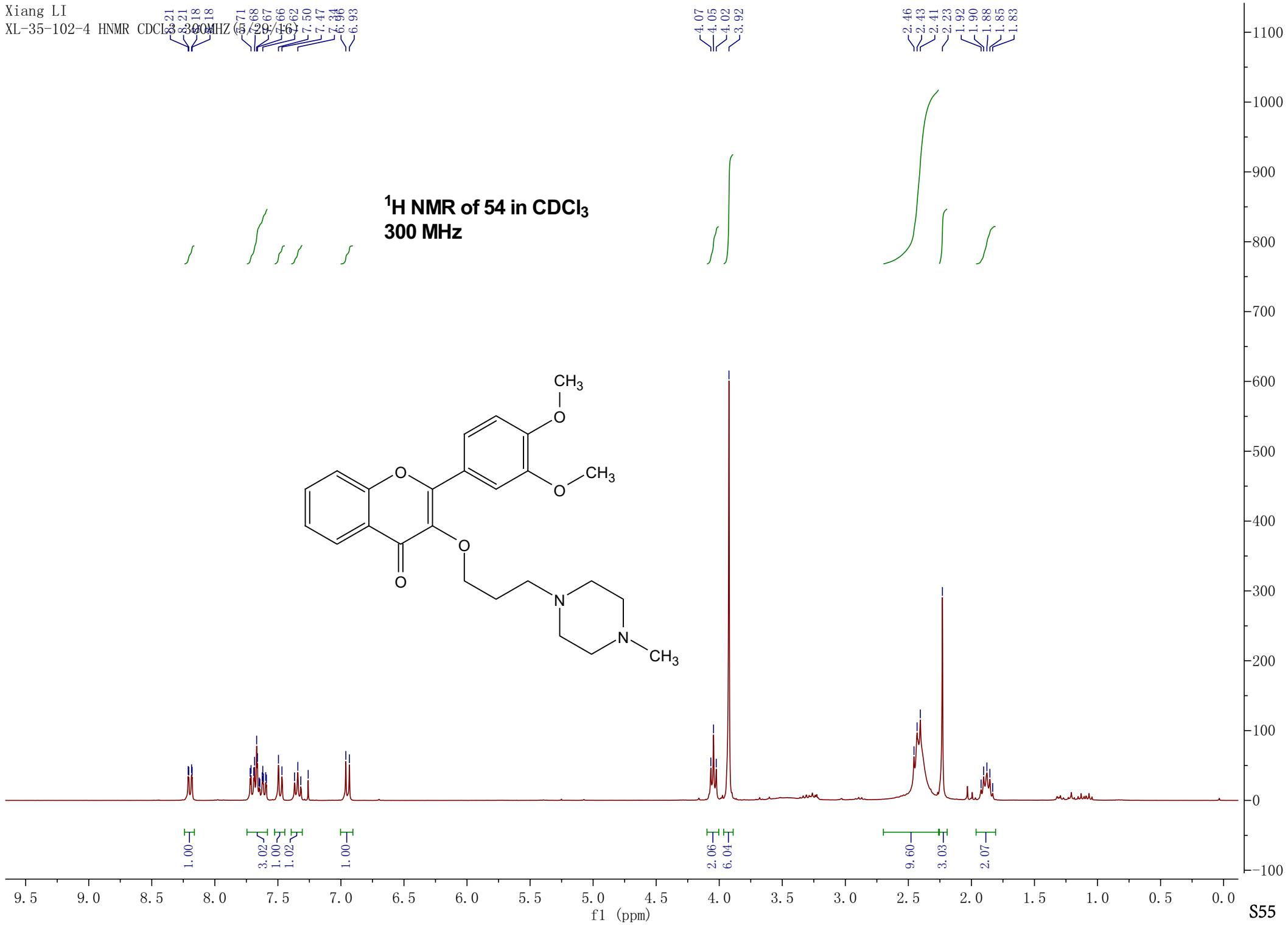

Xiang LI
XL-35-186-4 HNMR CDCl3 300MHZ (11/14/16)
8.253
8.248
8.226
8.221
7.462
7.434
7.427
7.420
7.359
7.336
7.334
7.308
7.302
6.980
4.059
4.038
4.017
3.963
3.957
2.403
2.385
1.780
1.757
1.735
1.713
1.691
1.621
1.603
1.584
1.461
1.441
1.425
1H NMR of 52 in CDCl3
300 MHz
CH3
O
O
CH3
O
O
O
N
1.00
2.00
1.02
1.00
1.00
1.00
2.00
6.27
6.00
8.01
2.02
f1 (ppm)
S51


Xiang LI
XL-35-186-4 CNMR CDCL3 75MHZ(01/16/17)
175.14
155.92
155.27
154.29
149.74
140.09
133.42
125.85
124.73
124.27
123.58
122.46
118.04
111.71
110.91
77.58
77.16
76.74
72.18
58.51
56.20
56.11
54.15
28.17
25.06
23.91
22.60
13C NMR of 52 in CDCl3
75 MHz
CH3
O
O
CH3
O
O
O
N
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

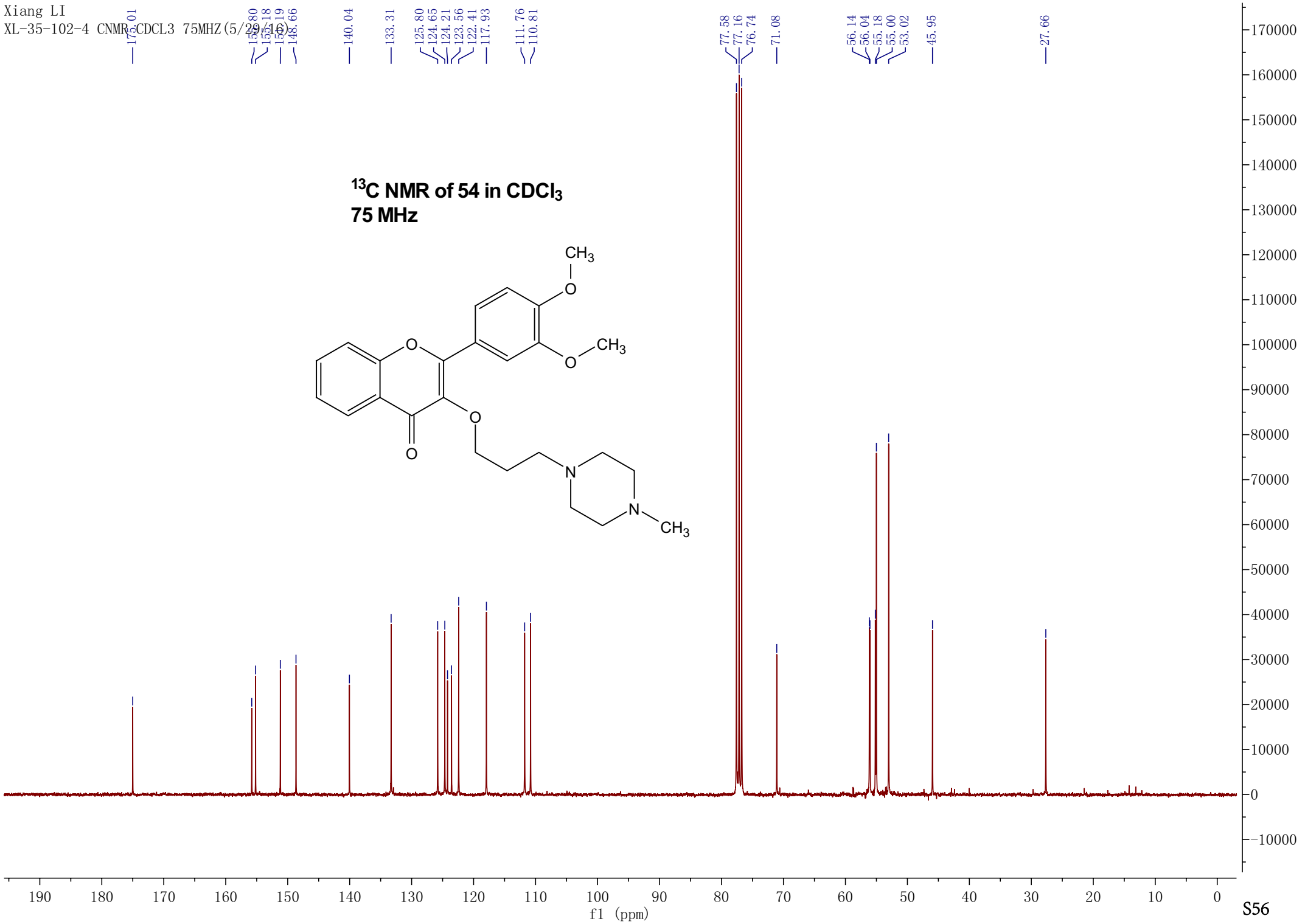

Xiang LI
XL-35-146-3 HNMR CDCL3 300MHZ(8/15/16)
^{1}H NMR of 53 in $CDCl_3$
300 MHz
f1 (ppm)


Xiang LI
XL-35-146-3 CNMR CDCL3 75MHZ(8-15-16)
175.13
155.82
155.26
153.20
149.66
140.19
133.35
125.88
124.68
124.28
123.68
122.37
118.00
111.80
110.83
77.58
77.16
76.74
72.58
59.12
56.16
56.09
54.38
30.17
26.14
25.49
24.22
24.12
13C NMR of 53 in CDCl3
75 MHz
CH3
O
O
CH3
O
O
O
N
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

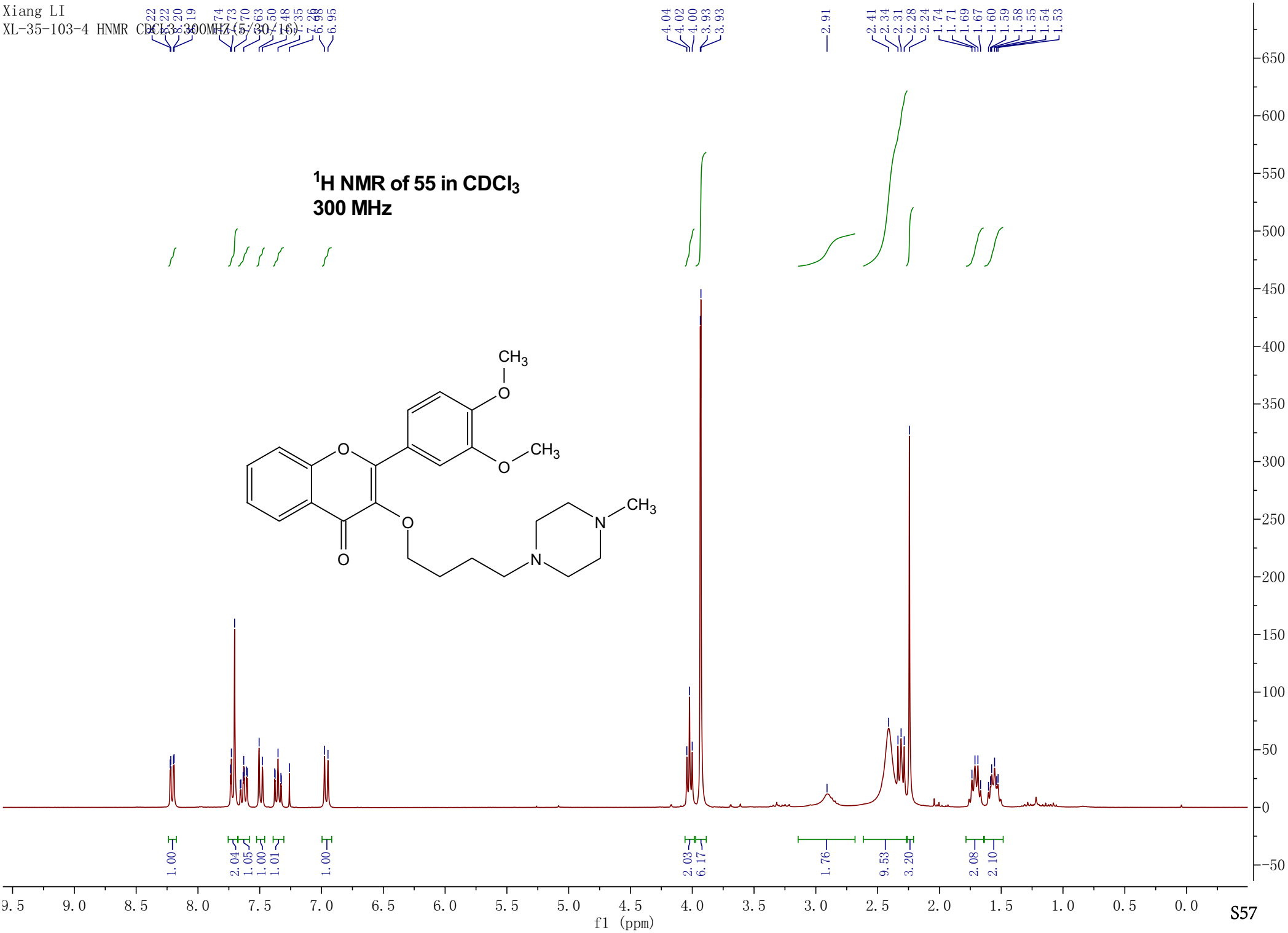
Xiang LI
XL-35-102-4 HNMR CDCl3 300MHZ(5/20/16)



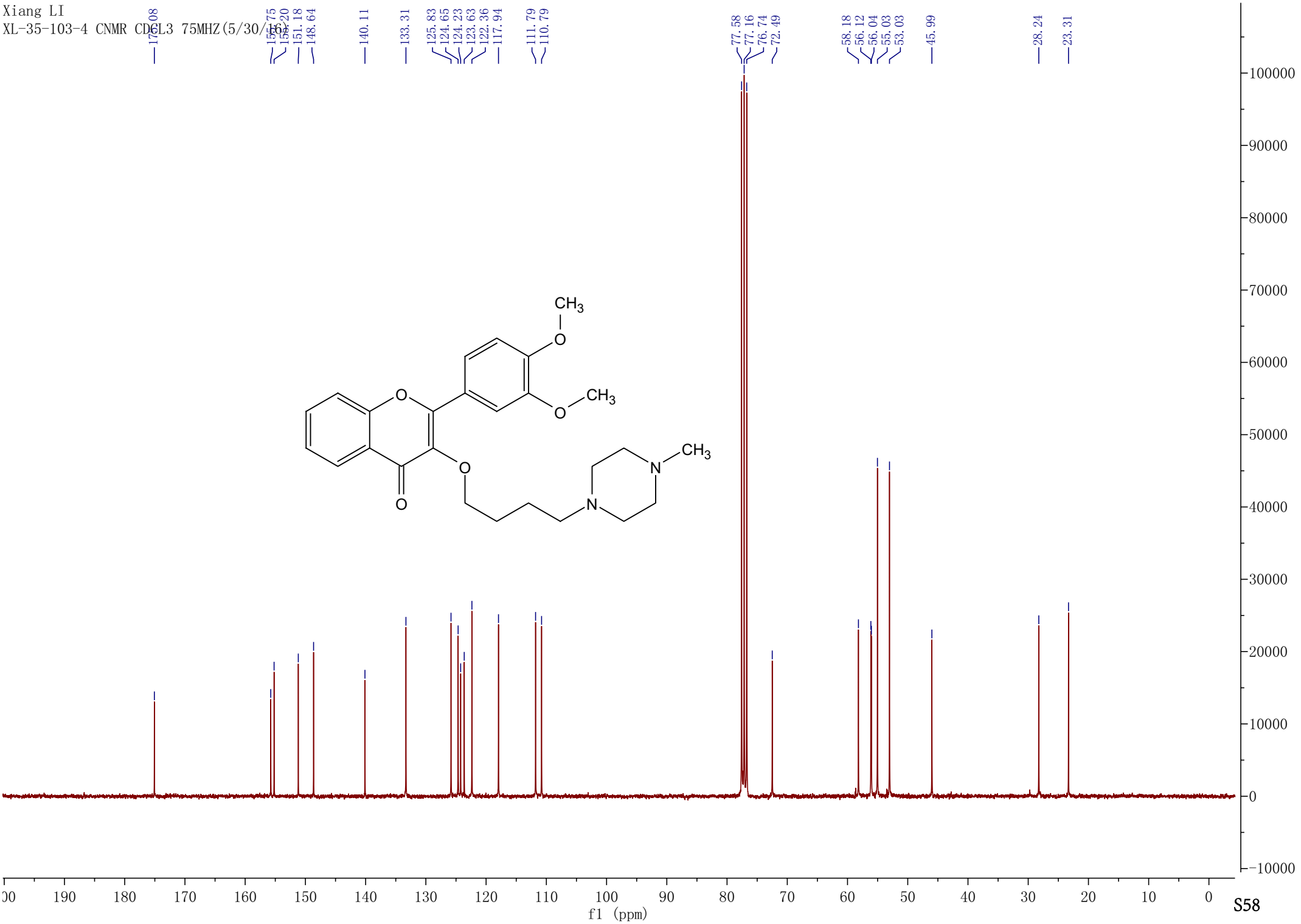
^{1}H NMR of 54 in $CDCl_3$
300 MHz


Xiang LI
XL-35-102-4 CNMR CDCL3 75MHZ(5/29/16)
177.01
155.80
155.18
153.19
148.66
140.04
133.31
125.80
124.65
124.21
123.56
122.41
117.93
111.76
110.81
77.58
77.16
76.74
71.08
56.14
56.04
55.18
55.00
53.02
45.95
27.66
13C NMR of 54 in CDCl3
75 MHz
CH3
O
O
CH3
O
O
O
N
N
CH3
f1 (ppm)

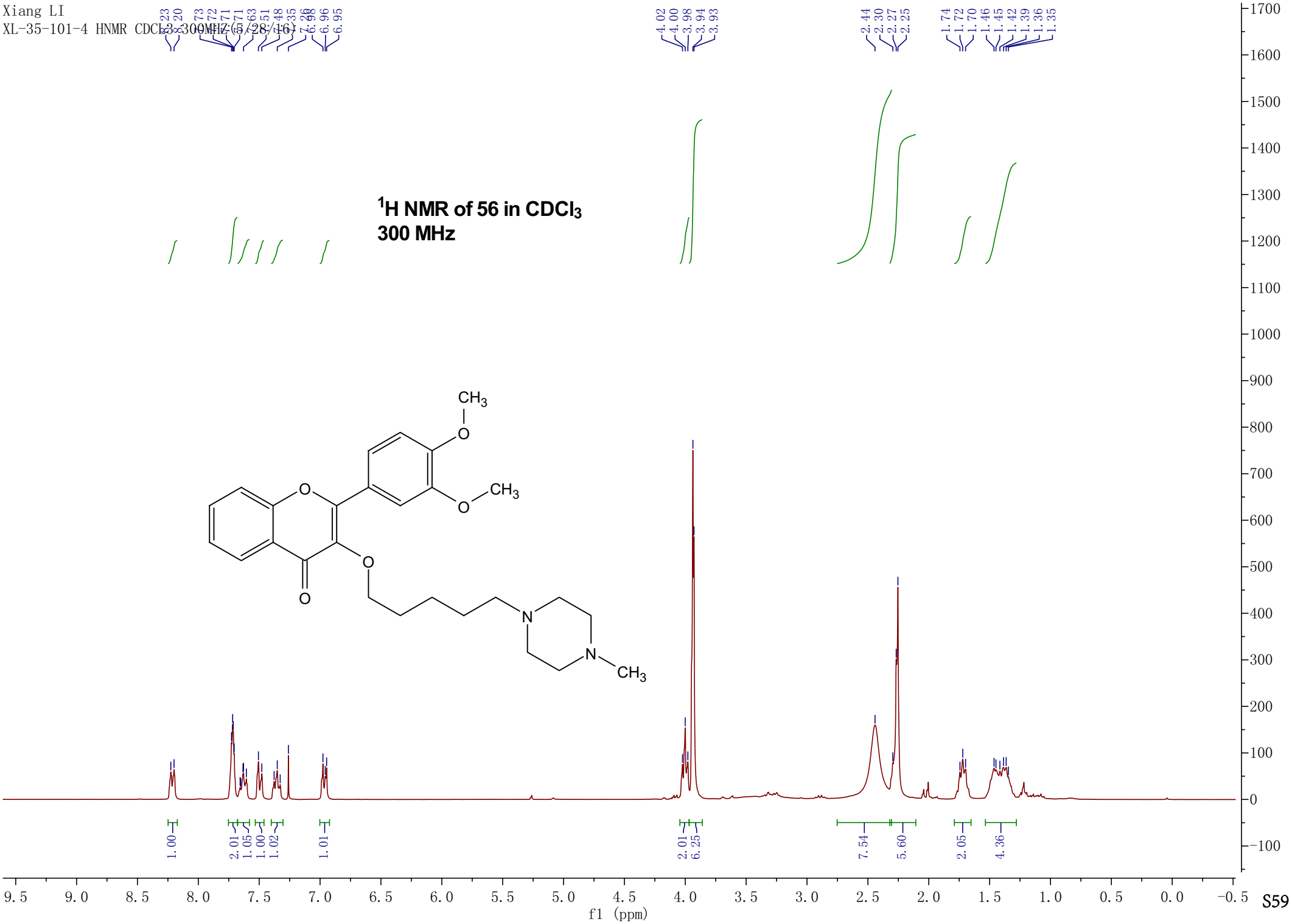
Xiang LI
XL-35-103-4 HNMR CDCl3 300MHz (5/30/16)



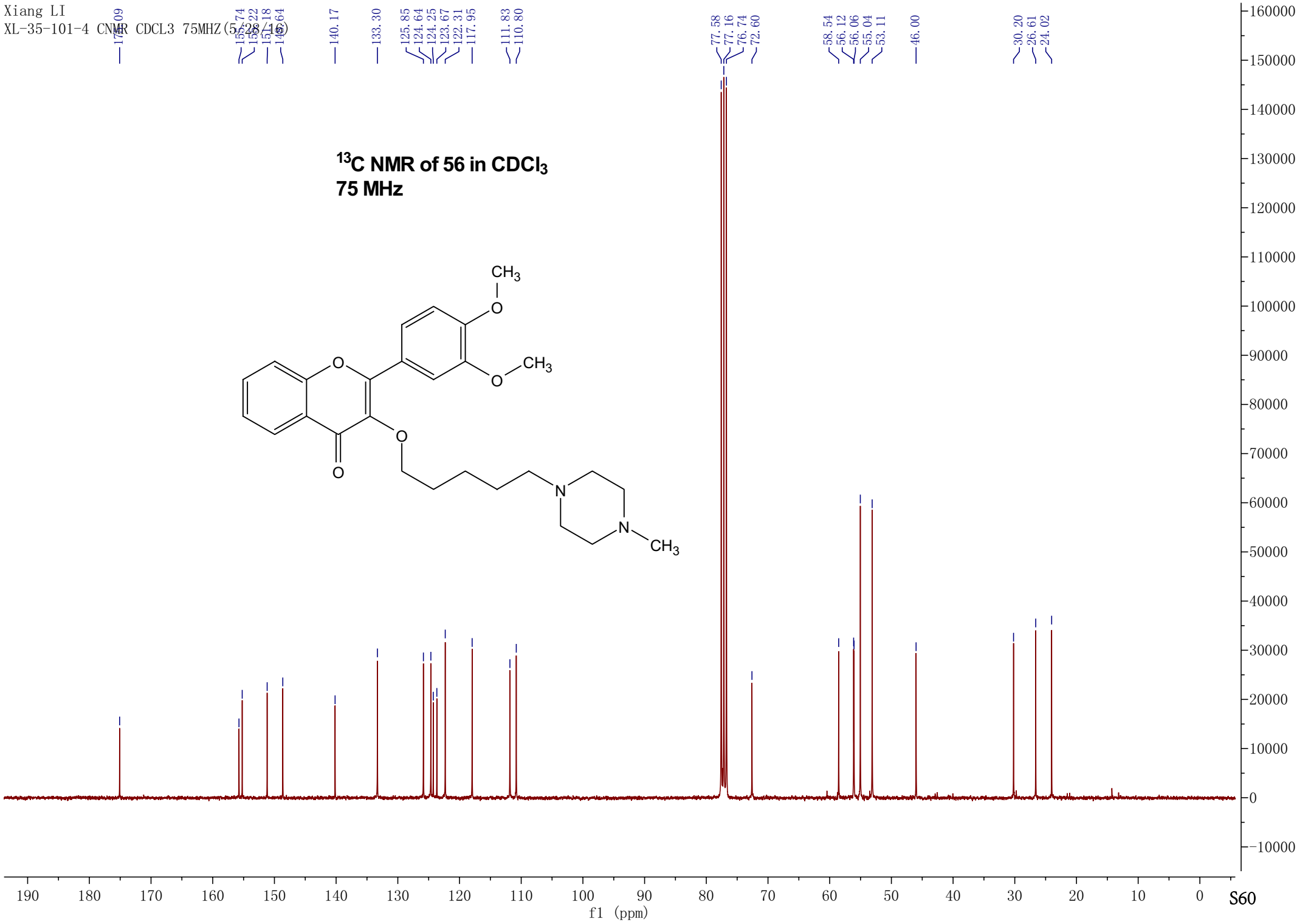
Xiang LI
XL-35-103-4 CNMR CDCL3 75MHZ(5/30/16)



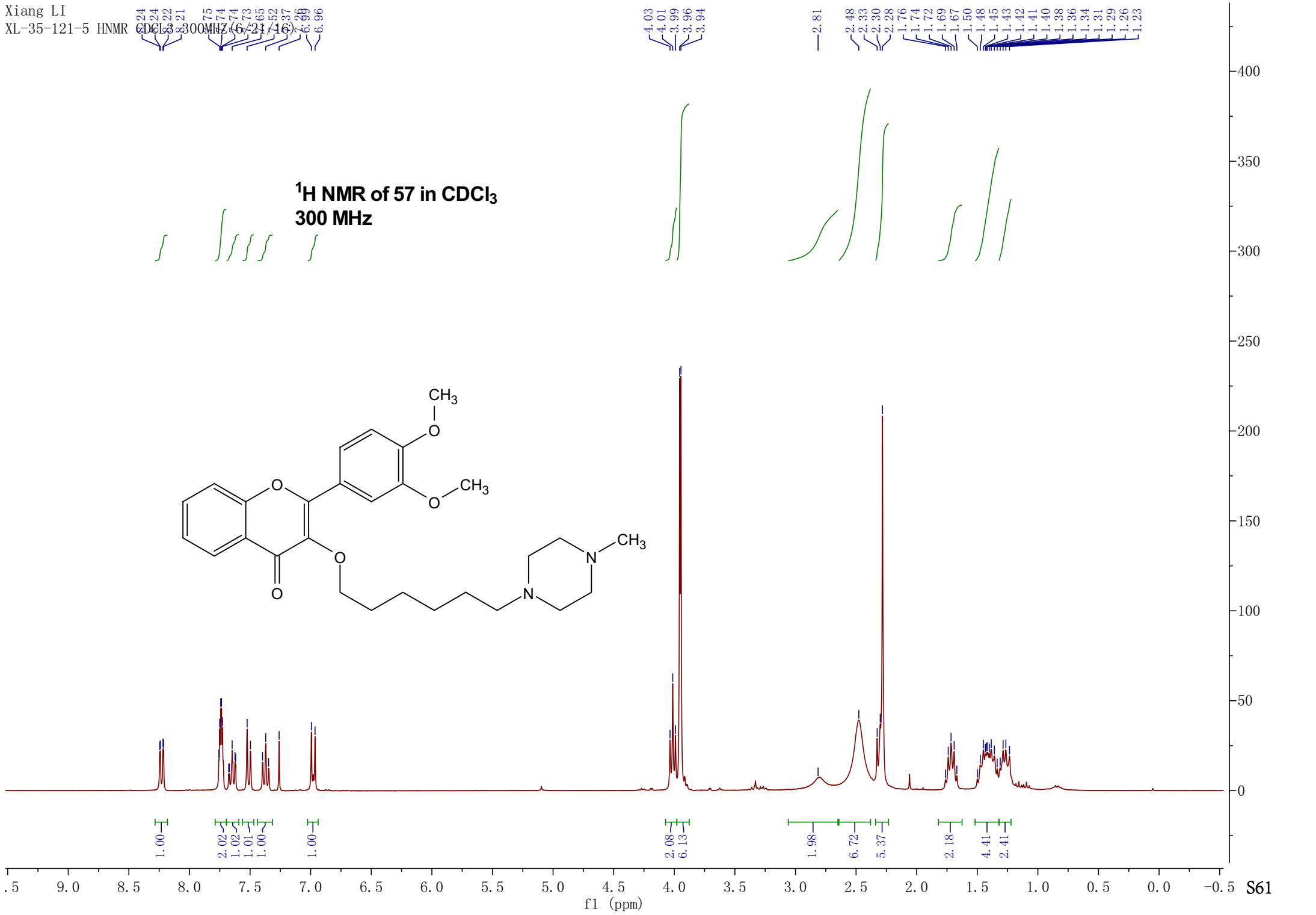
Xiang LI
XL-35-101-4 HNMR CDCl3 300MHz (5/28/16)

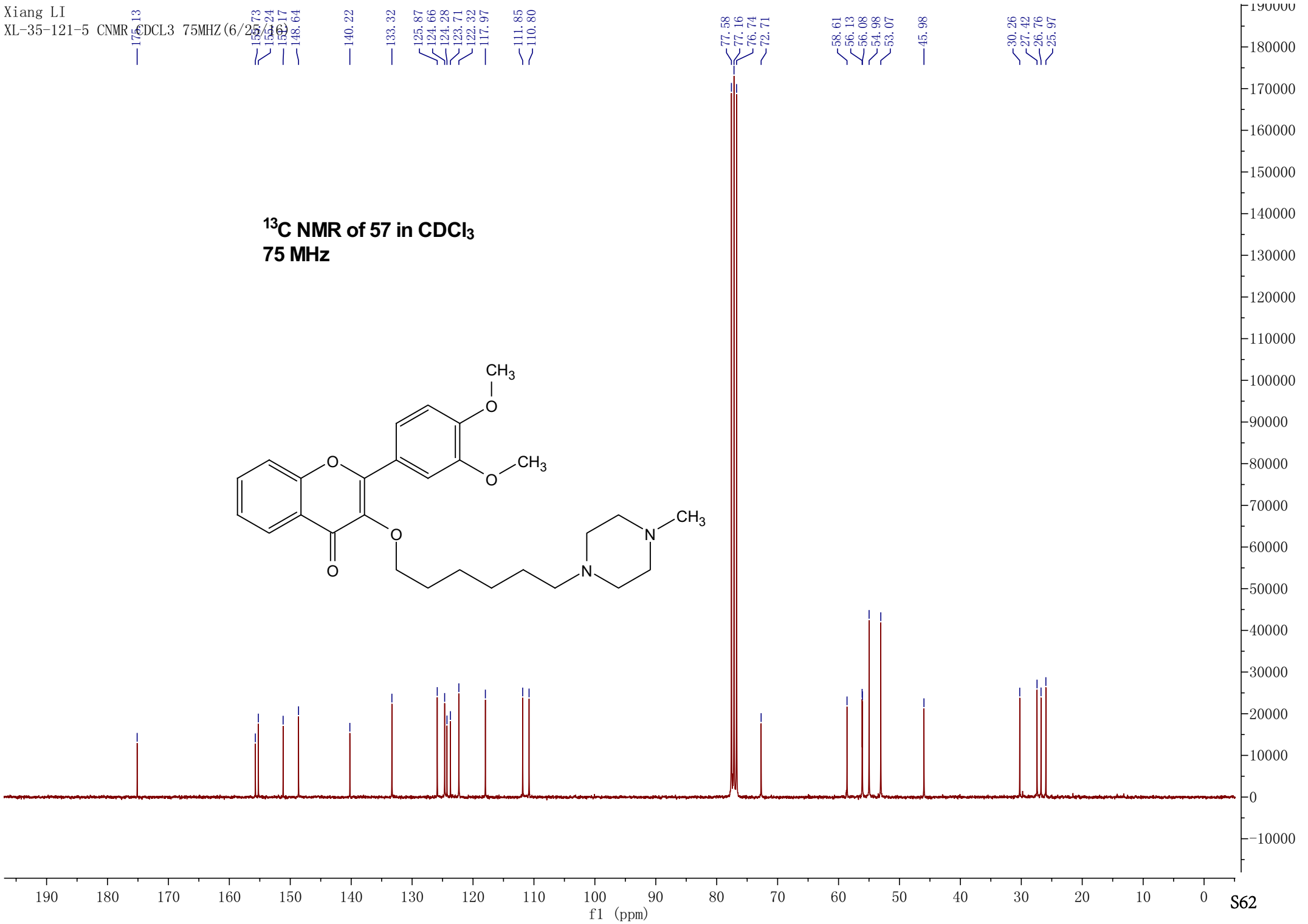


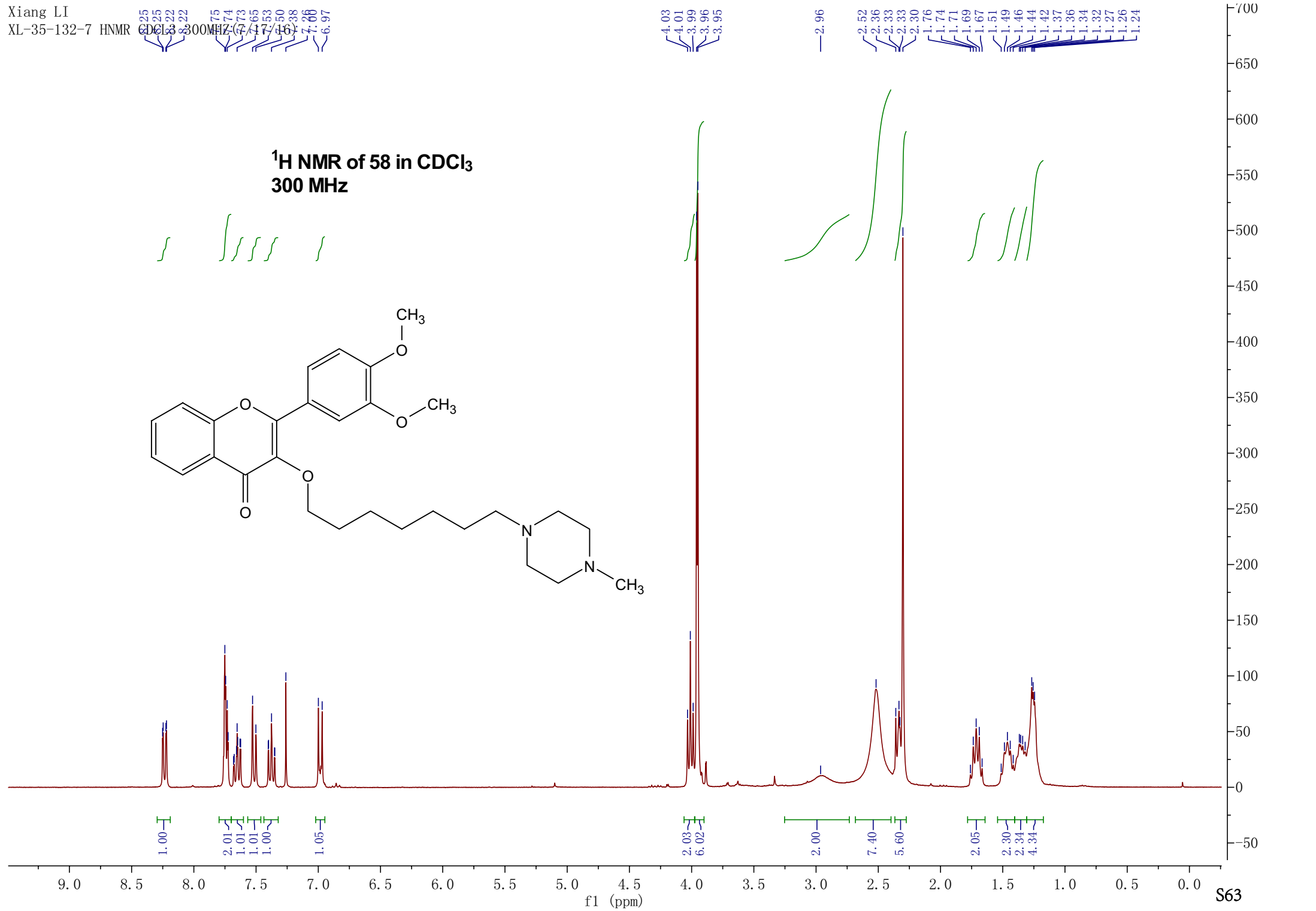
Xiang LI
XL-35-101-4 CNMR CDCL3 75MHZ(5.28/16)

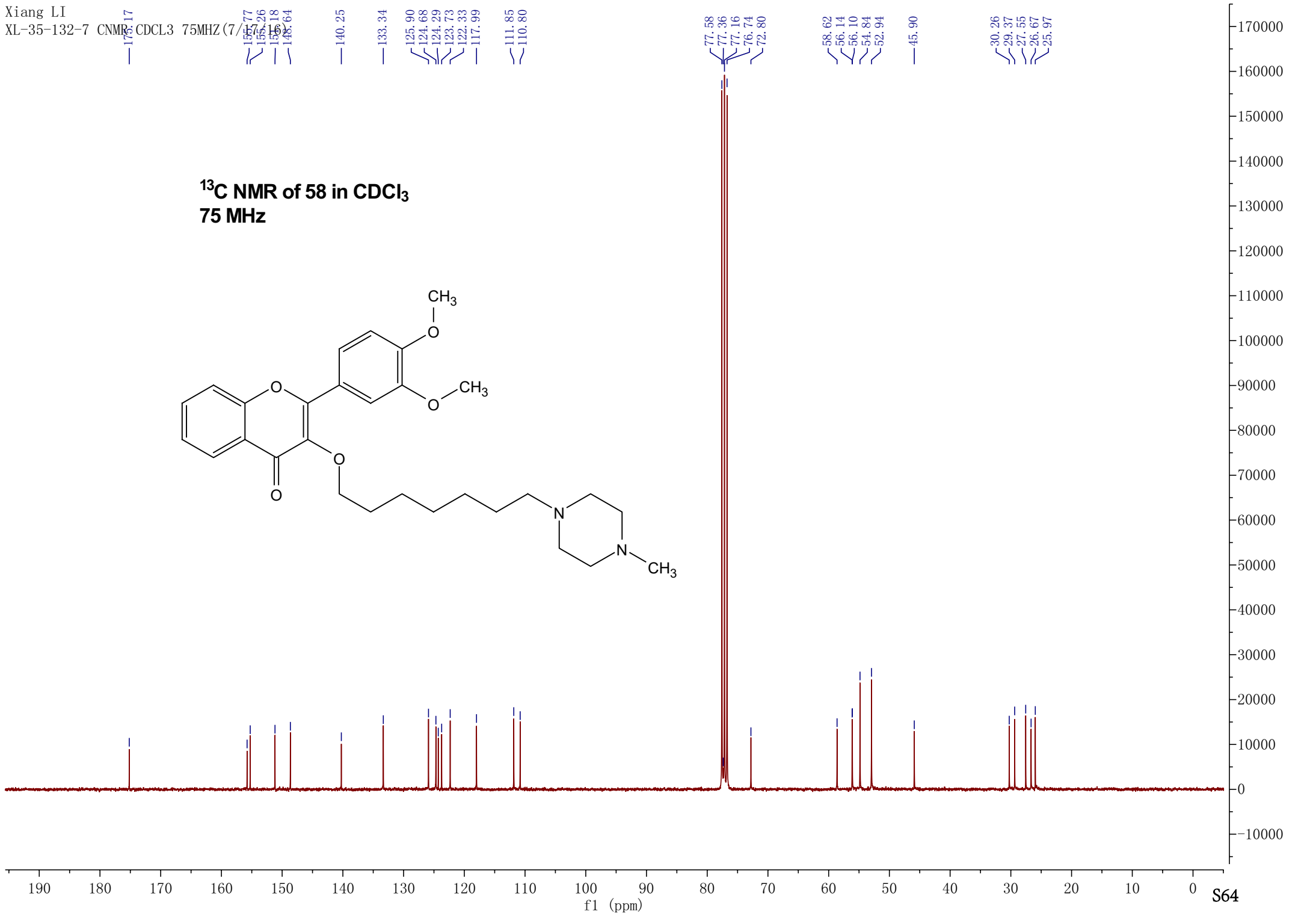


S60

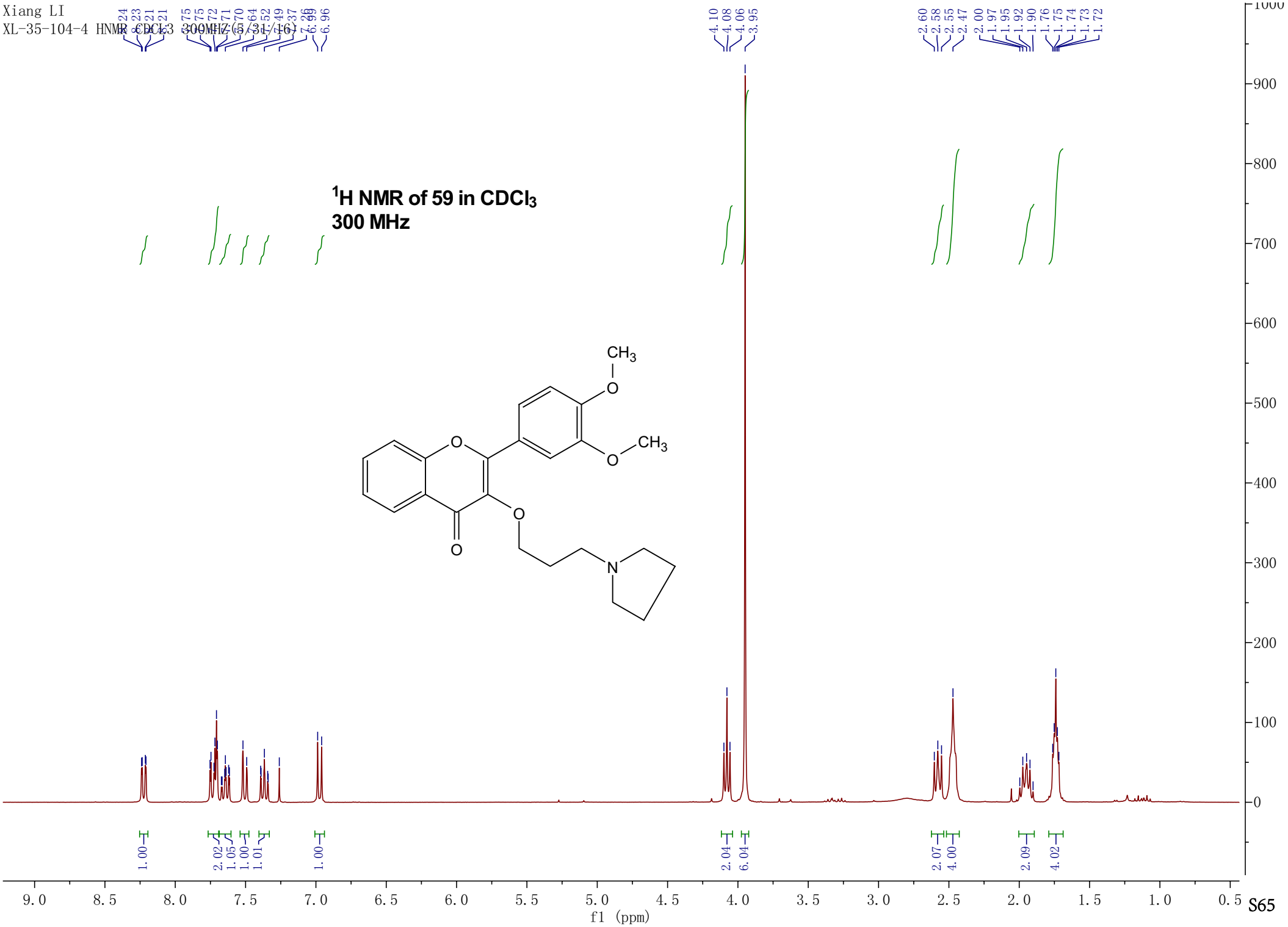

Xiang LI
XL-35-121-5 HNMR CDCl3 300MHz (6/21/16)
^{1}H NMR of 57 in CDCl$_3$
300 MHz
f1 (ppm)


Xiang LI
XL-35-121-5 CNMR CDCL3 75MHZ(6/25/16)
177.13
155.73
155.24
153.17
148.64
140.22
133.32
125.87
124.66
124.28
123.71
122.32
117.97
111.85
110.80
77.58
77.16
76.74
72.71
58.61
56.13
56.08
54.98
53.07
45.98
30.26
27.42
26.76
25.97
13C NMR of 57 in CDCl3
75 MHz
CH3
O
O
CH3
O
O
O
N
CH3
N
f1 (ppm)

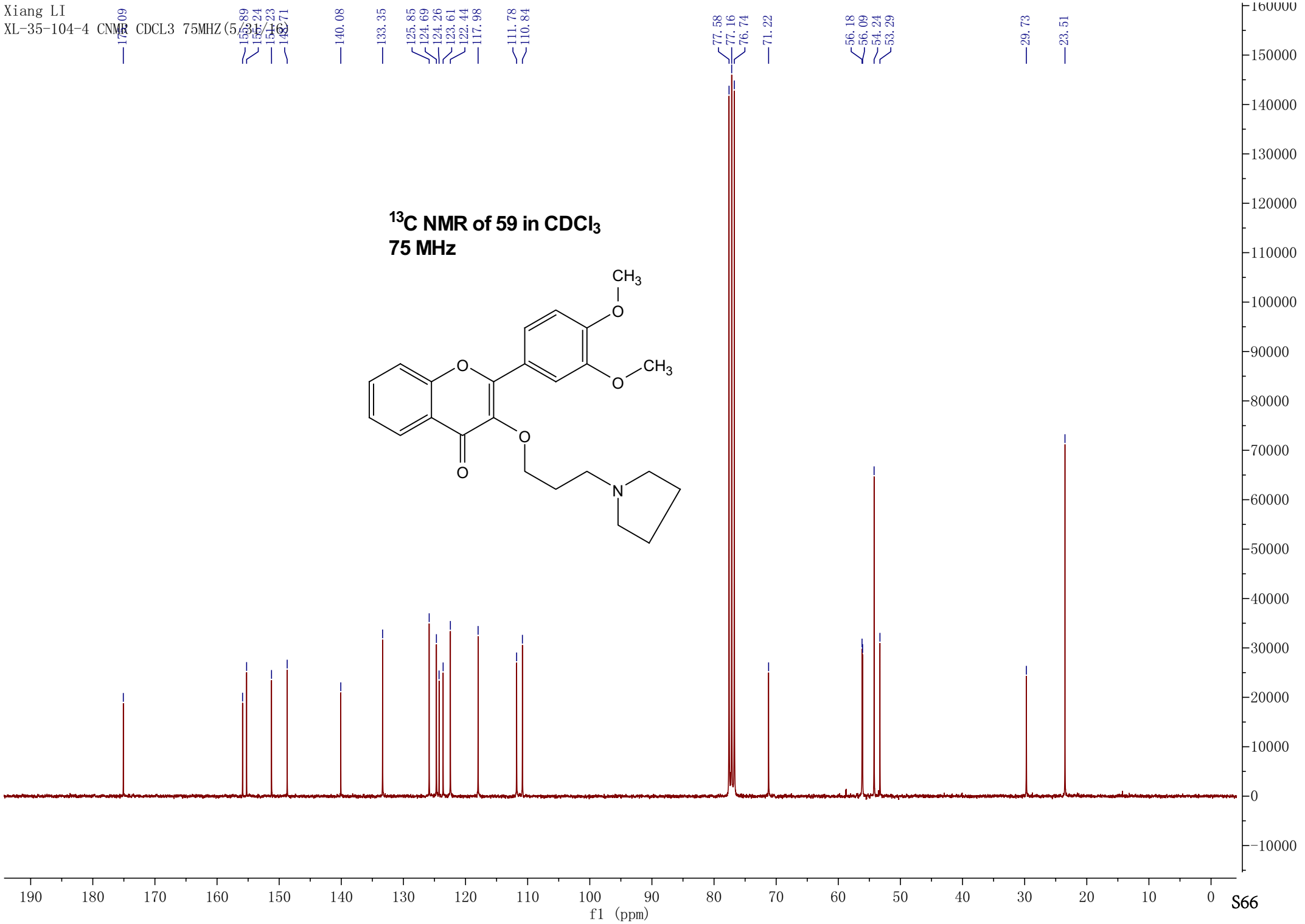

Xiang LI
XL-35-132-7 HNMR CDCl3 300MHZ (7/17/16)
1H NMR of 58 in CDCl3
300 MHz
f1 (ppm)

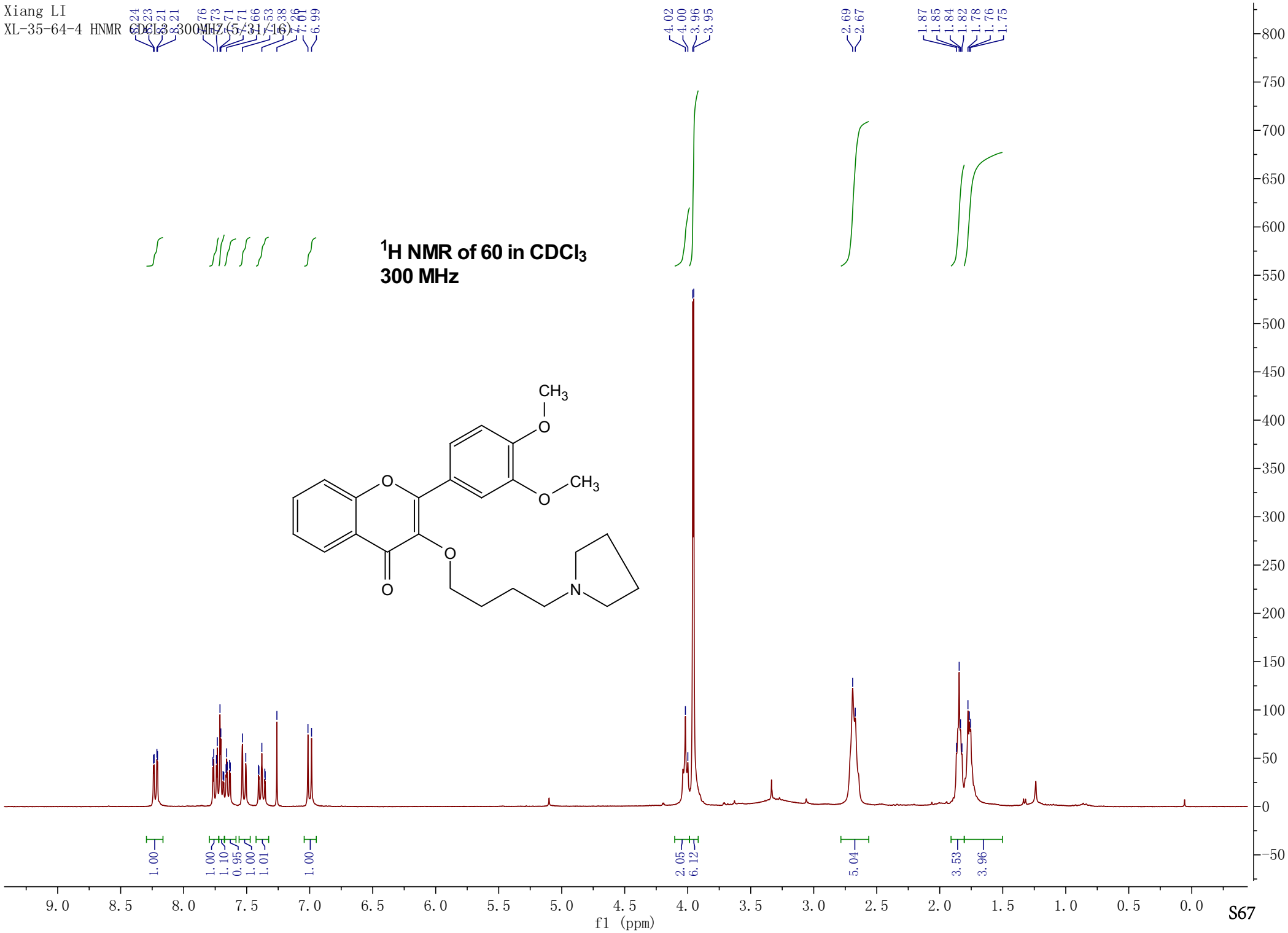

Xiang LI
XL-35-132-7 CNMR CDCL3 75MHZ(7/17/16)
175.17
155.77
155.26
155.18
148.64
140.25
133.34
125.90
124.68
124.29
123.73
122.33
117.99
111.85
110.80
77.58
77.36
77.16
76.74
72.80
58.62
56.14
56.10
54.84
52.94
45.90
30.26
29.37
27.55
26.67
25.97
13C NMR of 58 in CDCl3
75 MHz
CH3
O
O
CH3
O
O
O
N
N
CH3
f1 (ppm)

Xiang LI
XL-35-104-4 HNMR CDCl3 300MHZ(5/31/16)

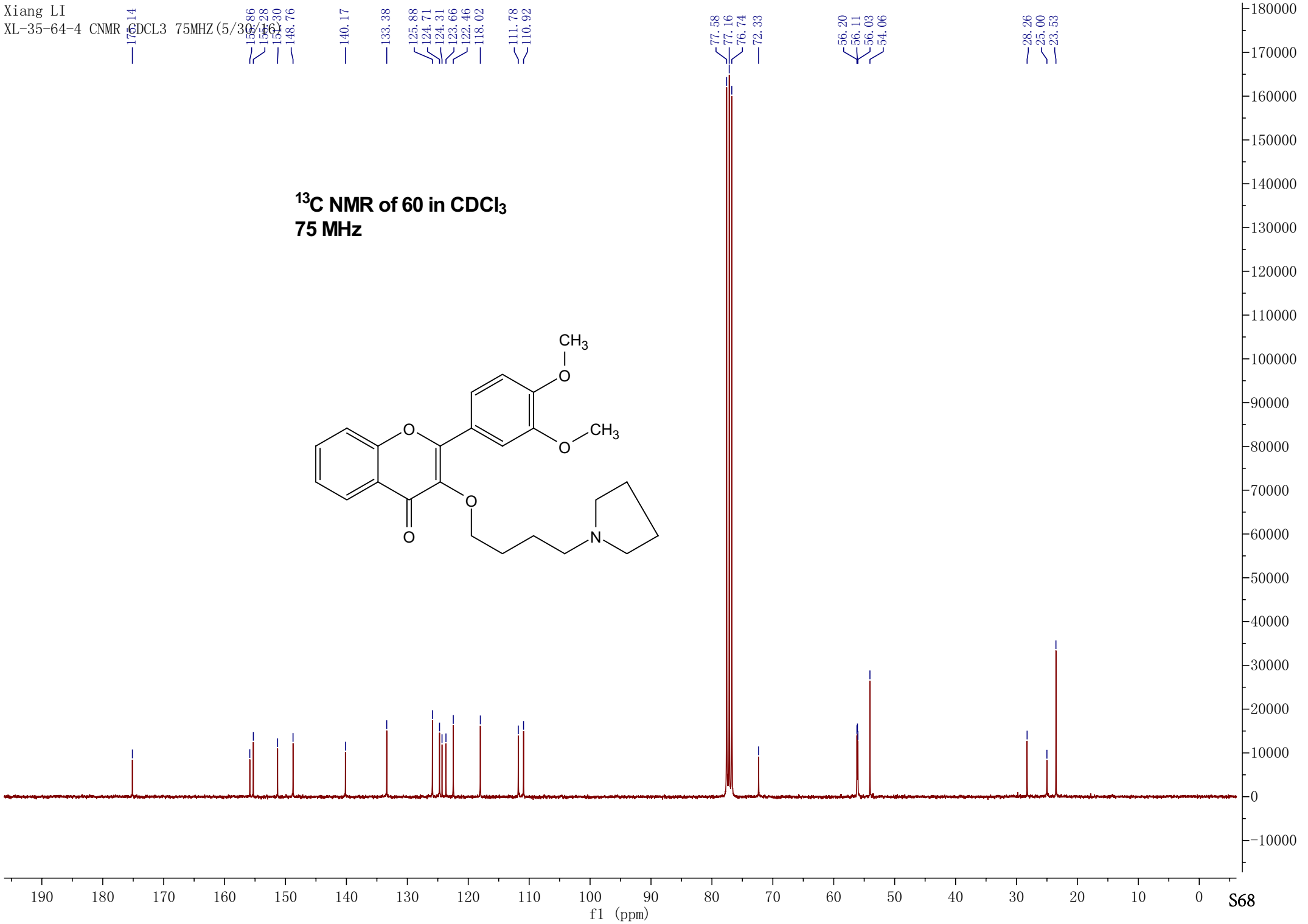


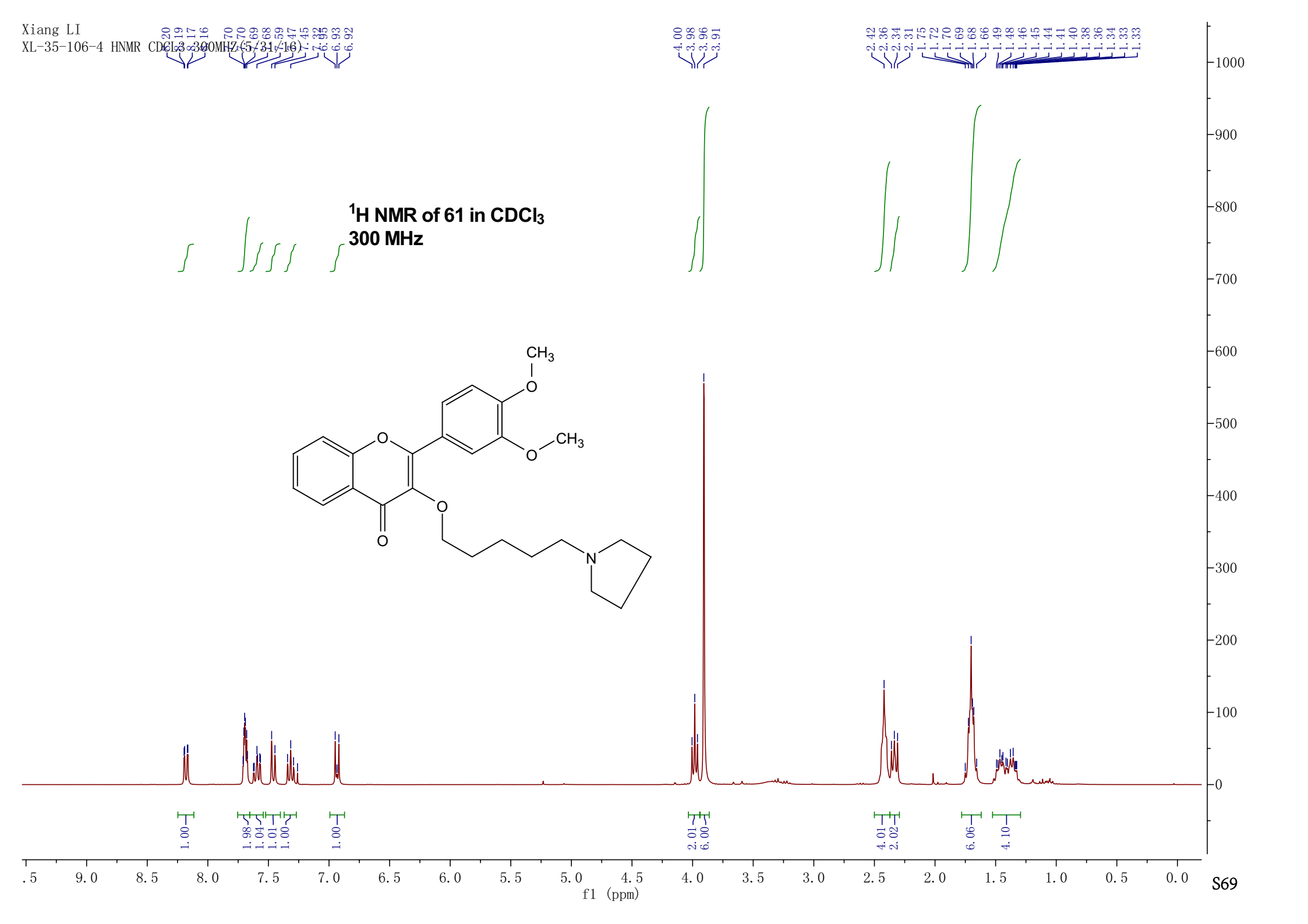
Xiang LI
XL-35-104-4 CNMR CDCL3 75MHZ(5/31/16)



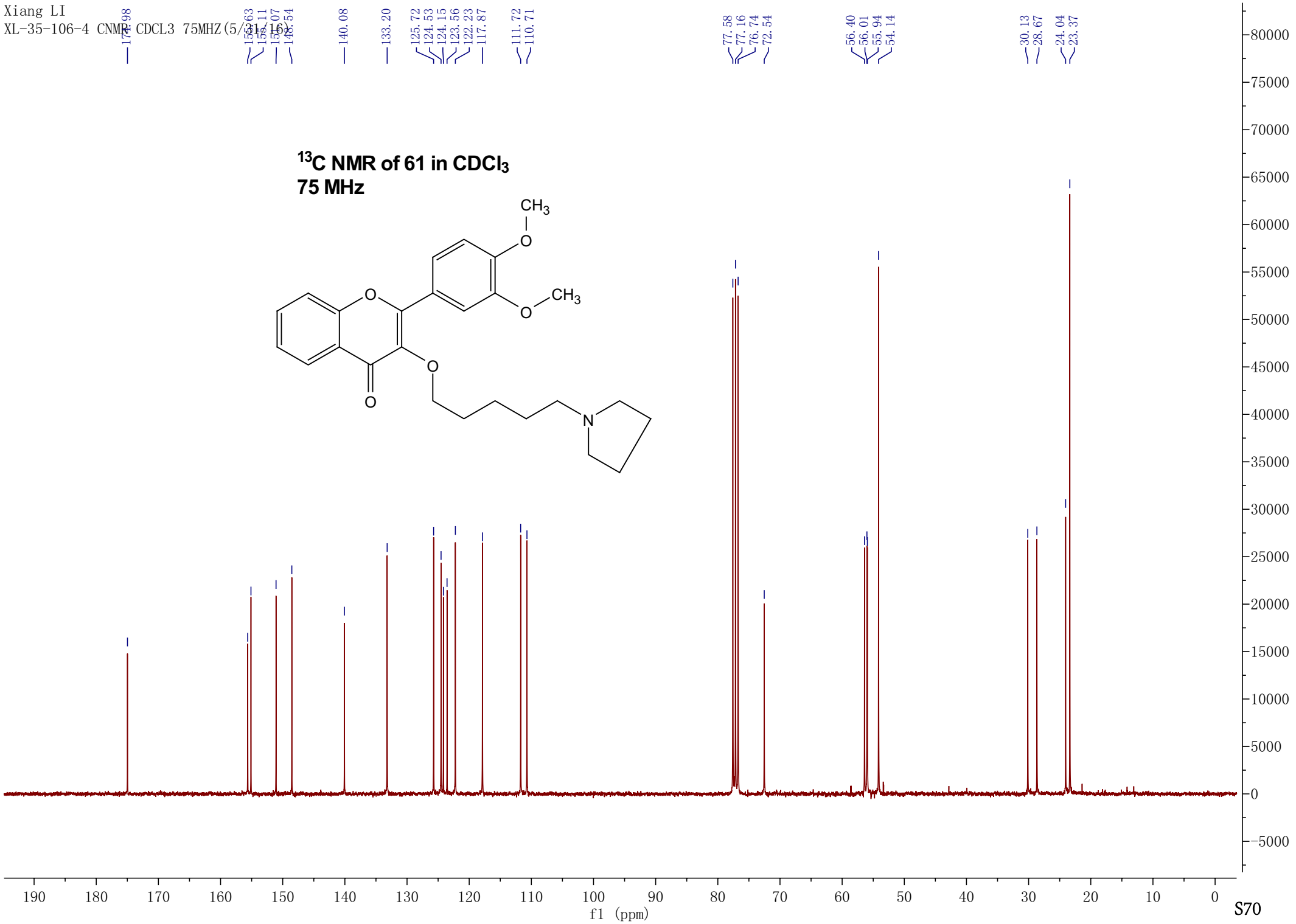

Xiang LI
XL-35-64-4 HNMR CDCl3 300MHz (5/31/16)
7.24
7.23
7.21
7.21
7.76
7.73
7.71
7.71
7.66
7.53
7.38
7.26
7.01
6.99
4.02
4.00
3.96
3.95
2.69
2.67
1.87
1.85
1.84
1.82
1.78
1.76
1.75
1H NMR of 60 in CDCl3
300 MHz
CH3
O
O
CH3
O
O
O
N
1.00
1.00
1.10
0.95
1.00
1.01
1.00
2.05
6.12
5.04
3.53
3.96
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50

Xiang LI
XL-35-64-4 CNMR CDCL3 75MHZ(5/30/16)

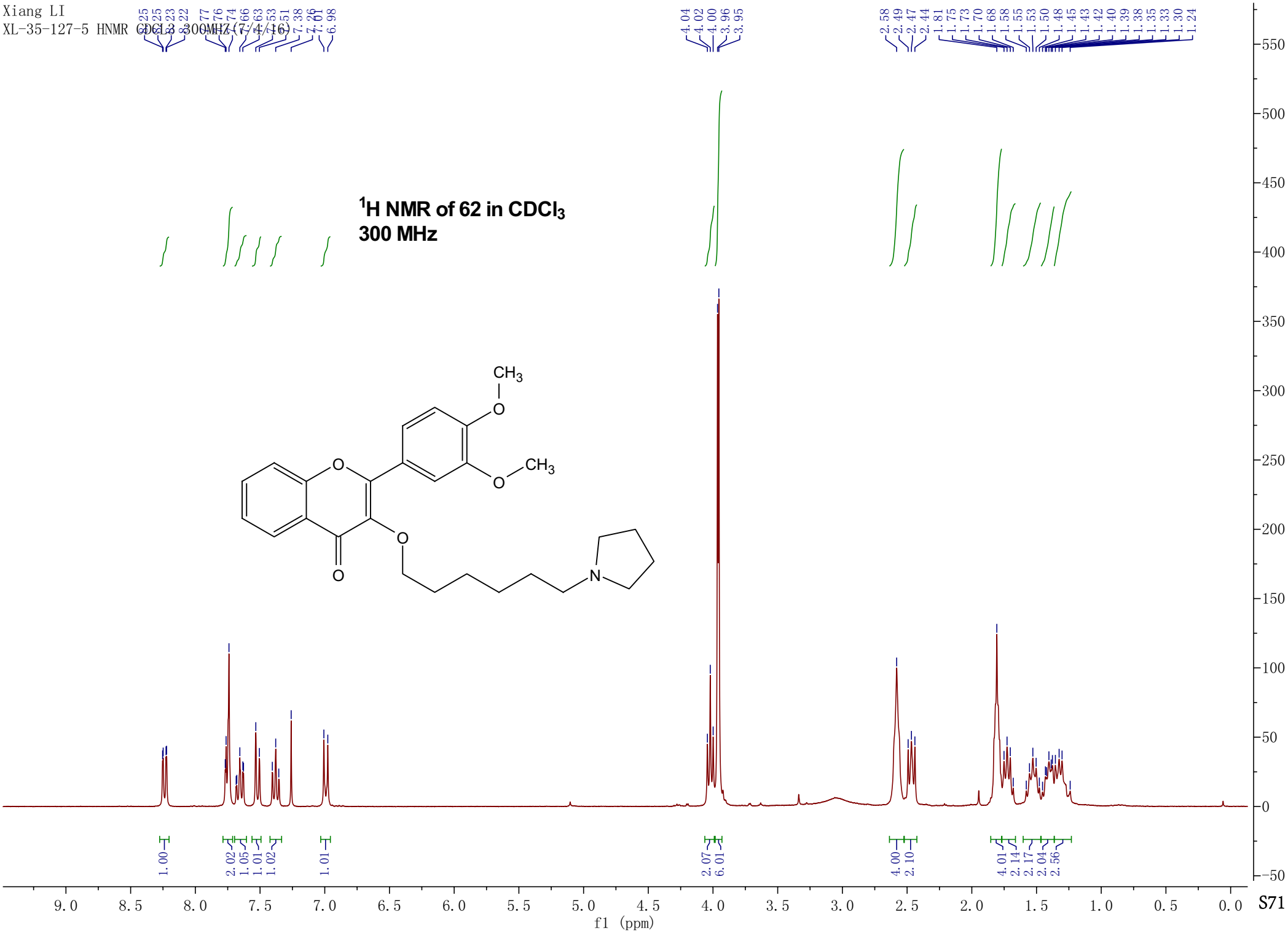



Xiang LI
XL-35-106-4 HNMR CDCl3 300MHZ(5/31/16)
1H NMR of 61 in CDCl3
300 MHz
f1 (ppm)

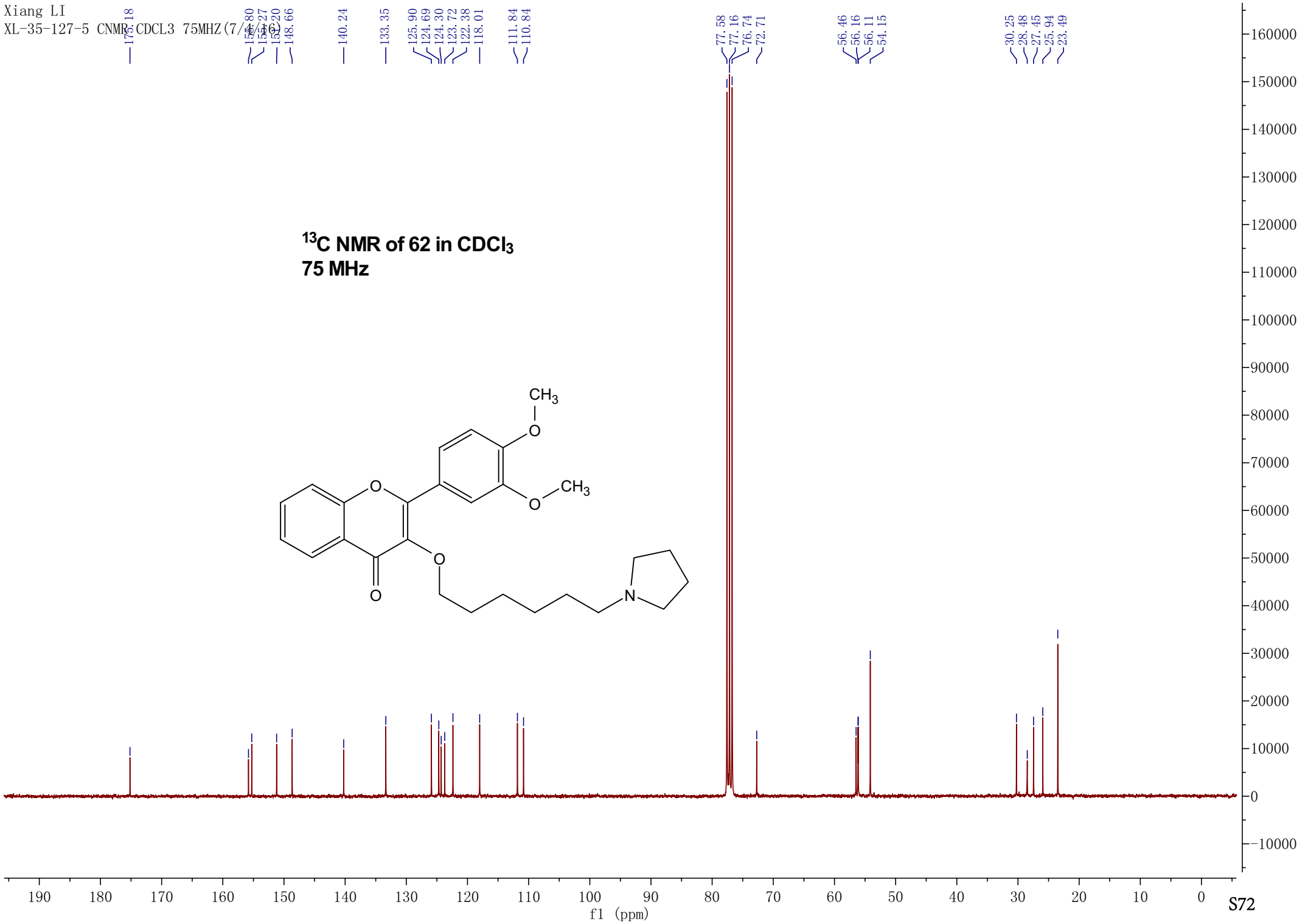
Xiang LI
XL-35-106-4 CNMR CDCL3 75MHZ(5/31/16)

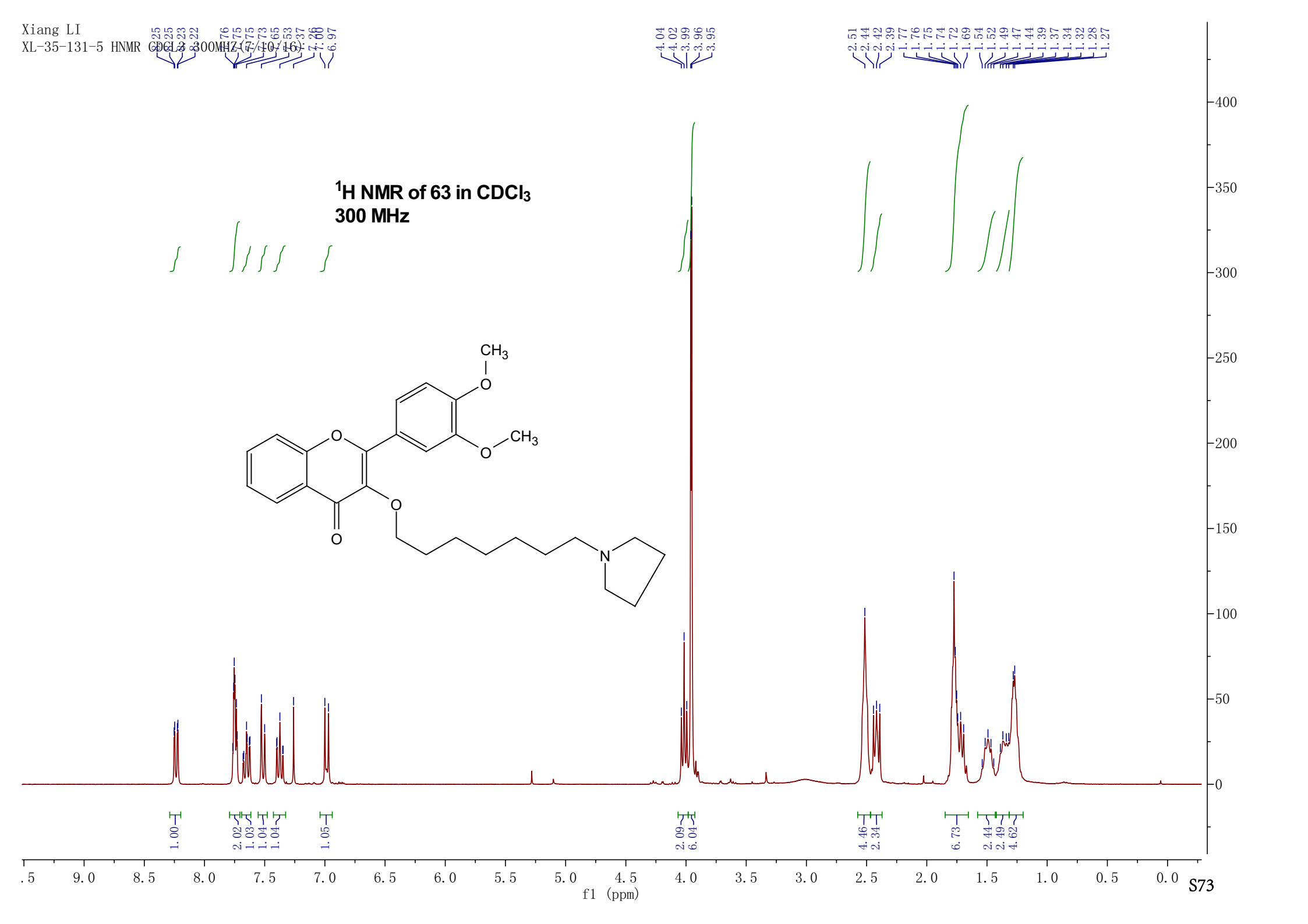


Xiang LI
XL-35-127-5 HNMR CDCL3 300MHZ(7/4/16)

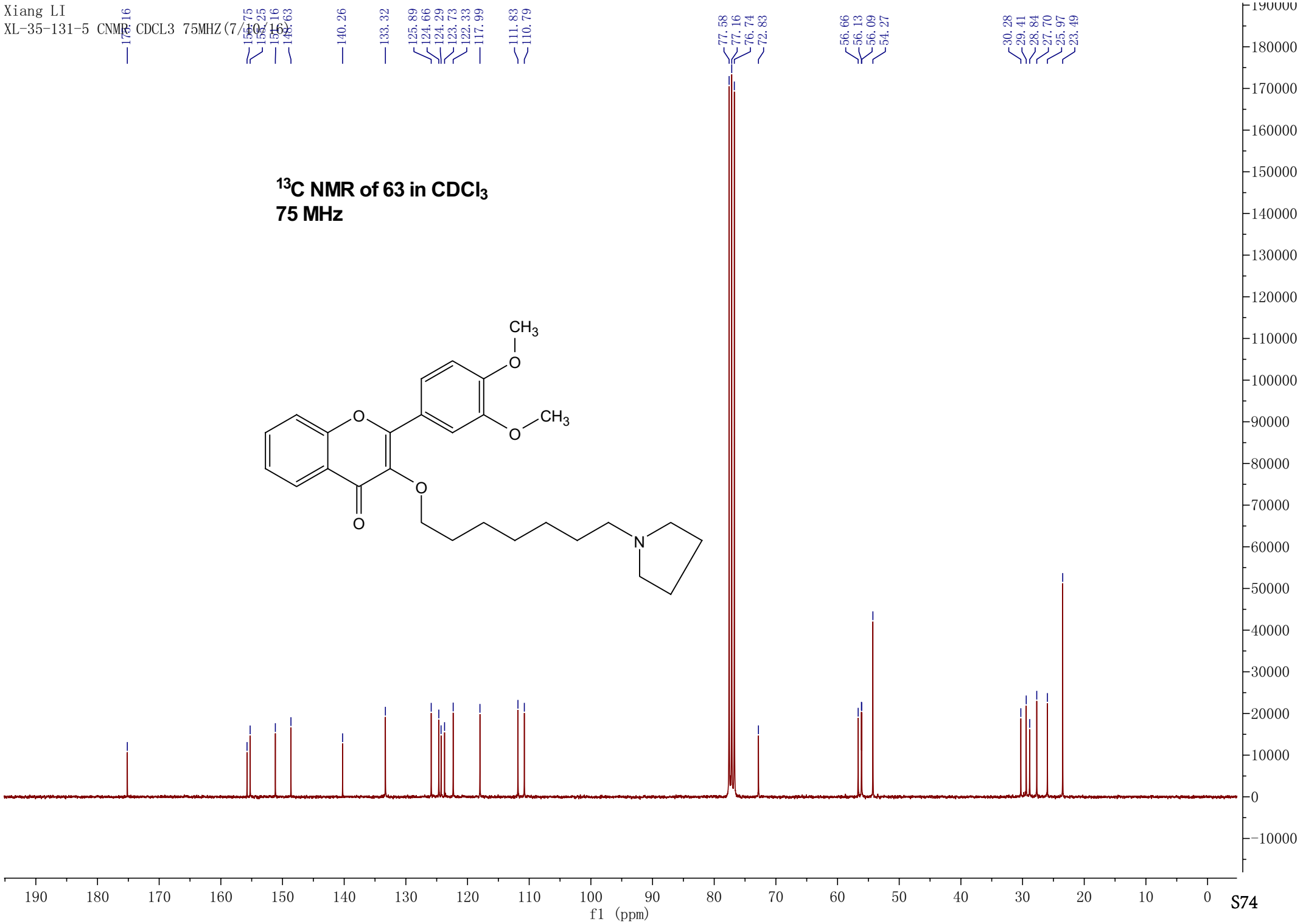


Xiang LI
XL-35-127-5 CNMR CDCL3 75MHZ(7/4/16)

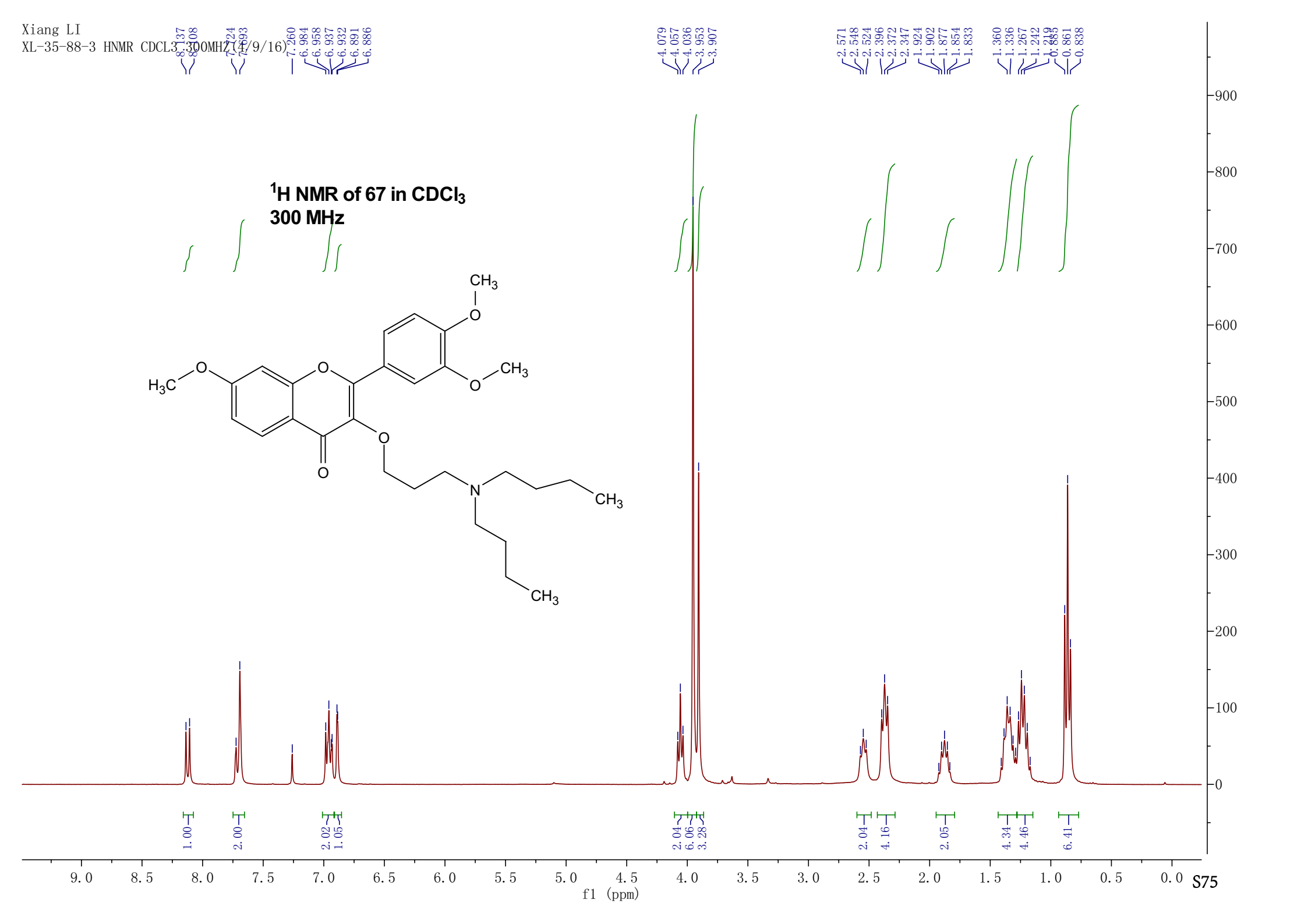


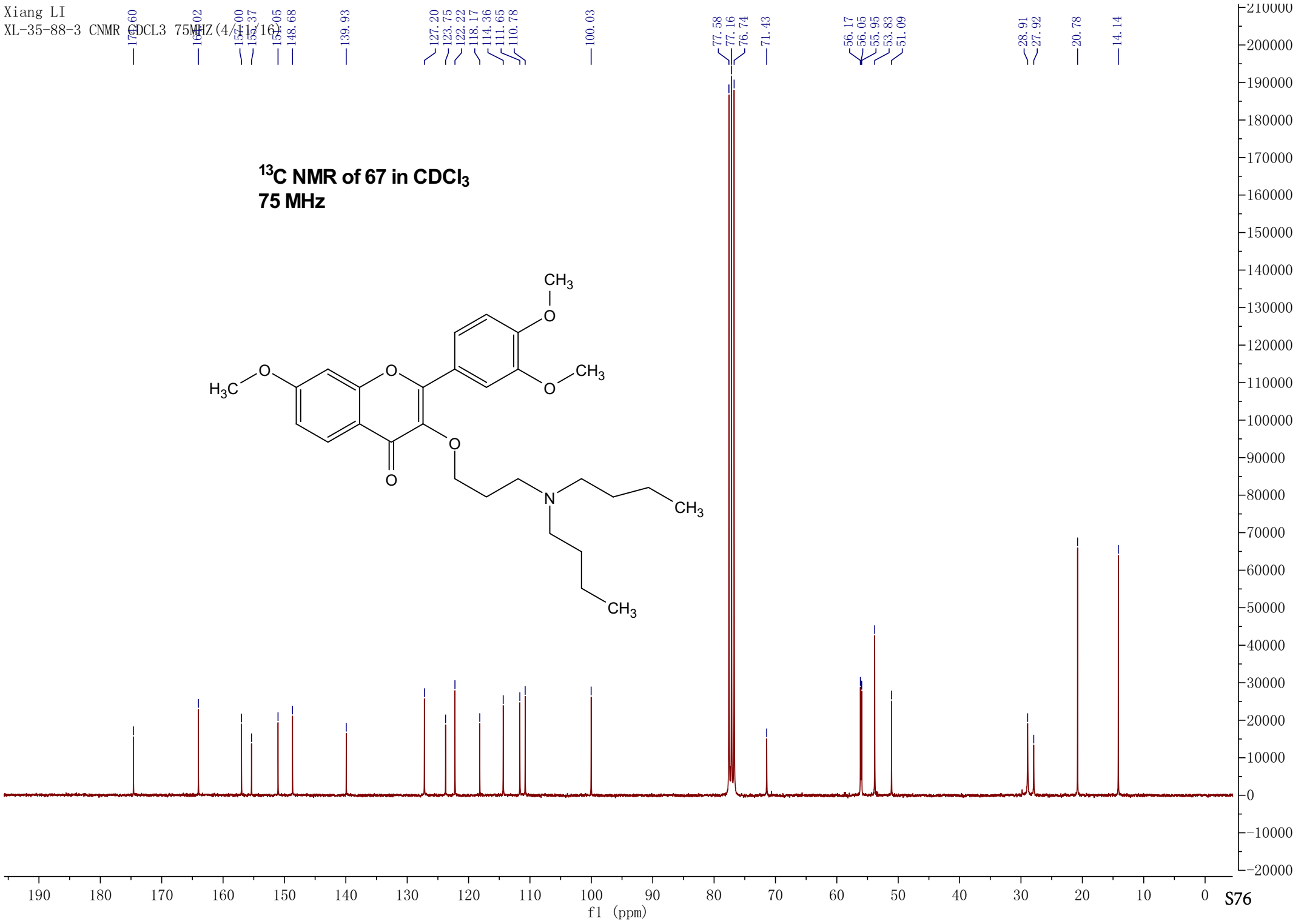

Xiang LI
XL-35-131-5 HNMR CDCL3 300MHZ(7/10/16)
^{1}H NMR of 63 in CDCl$_3$
300 MHz
f1 (ppm)

Xiang LI
XL-35-131-5 CNMR CDCL3 75MHZ(7/10/16)

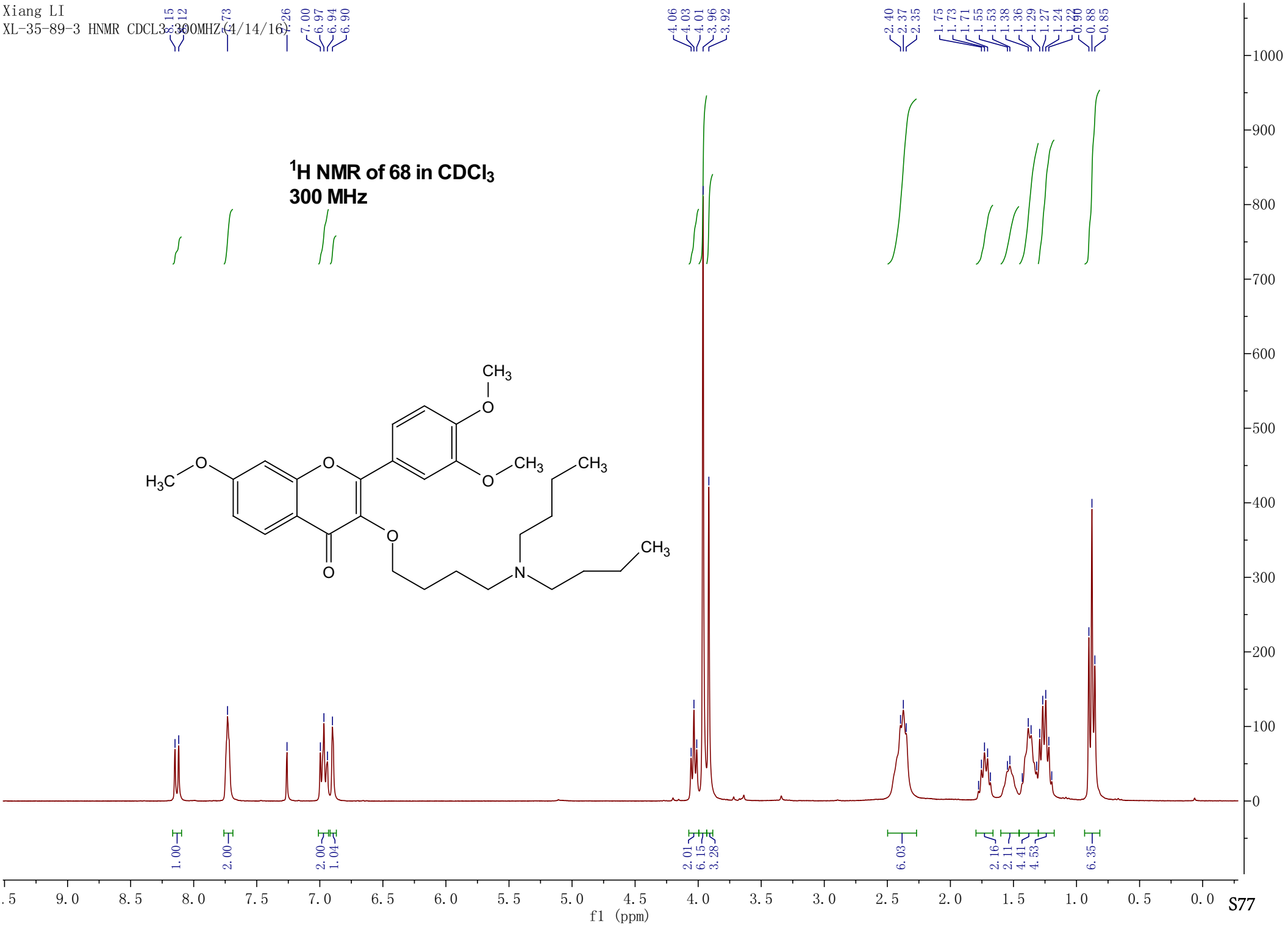


Xiang LI
XL-35-88-3 HNMR CDCL3 300MHZ(4/9/16)

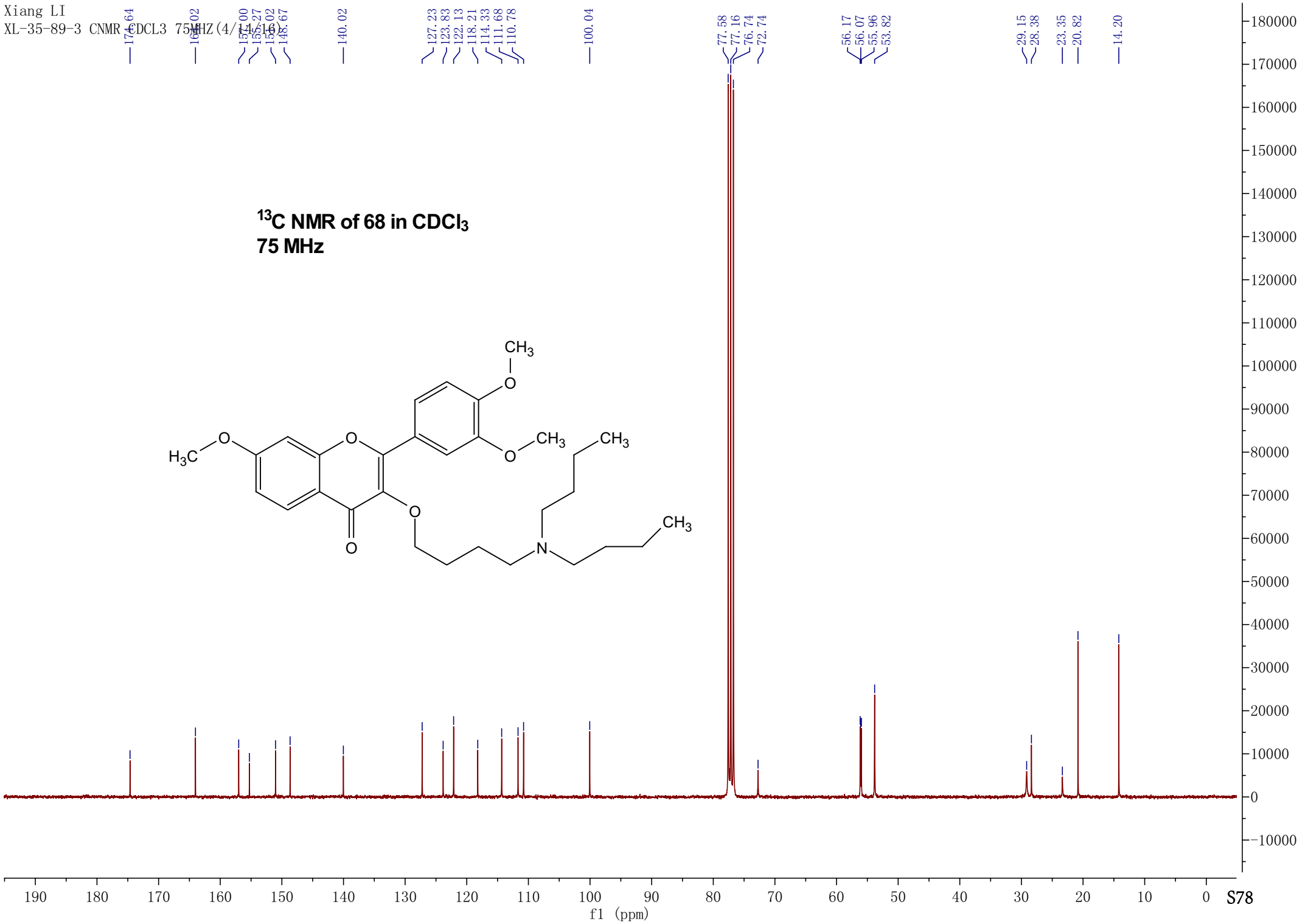


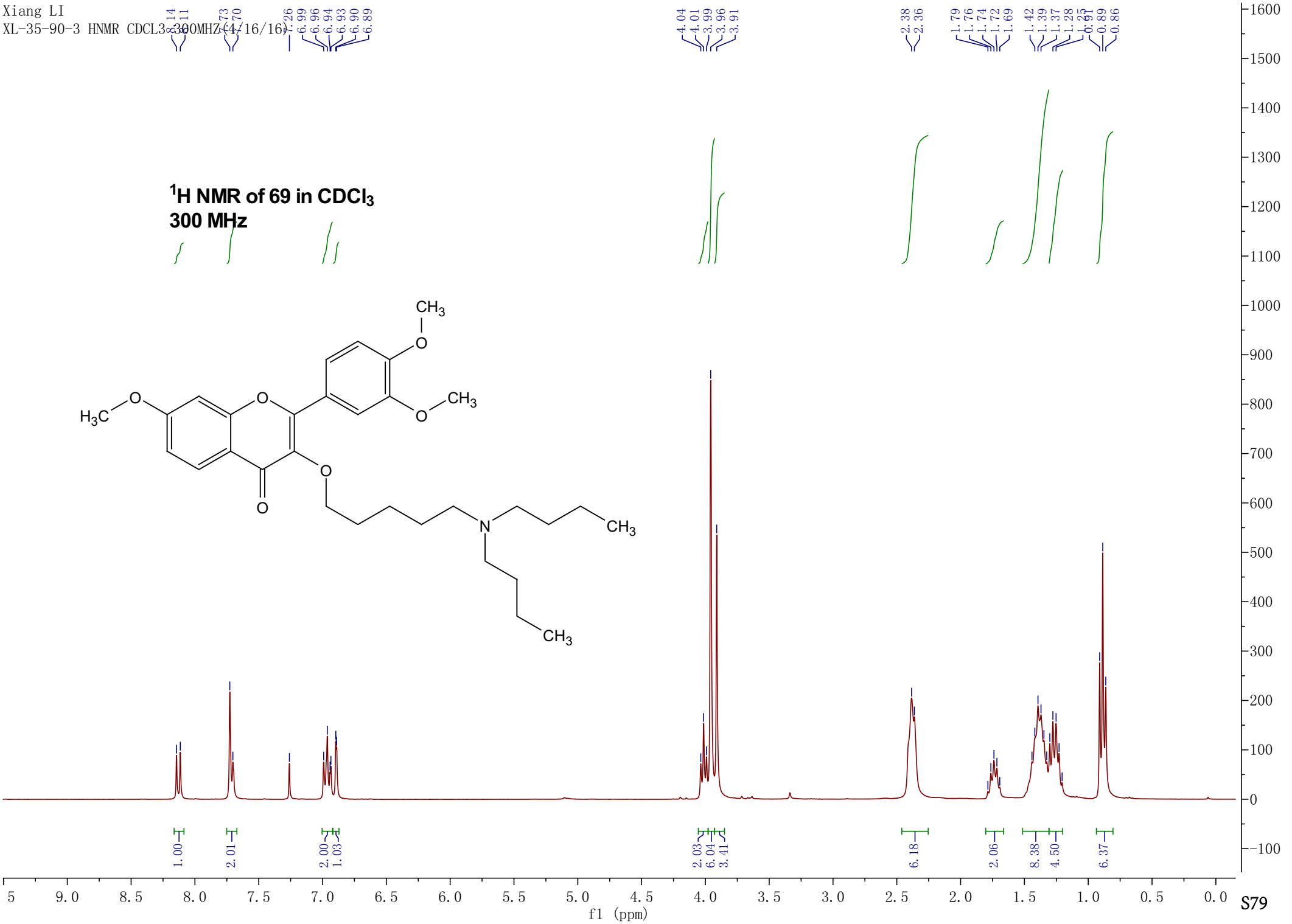

Xiang LI
XL-35-88-3 CNMR CDCL3 75MHZ(4/11/16)
175.60
163.02
157.00
155.37
154.05
148.68
139.93
127.20
123.75
122.22
118.17
114.36
111.65
110.78
100.03
77.58
77.16
76.74
71.43
56.17
56.05
55.95
53.83
51.09
28.91
27.92
20.78
14.14
13C NMR of 67 in CDCl3
75 MHz
CH3
O
H3C
O
O
O
CH3
O
O
N
CH3
CH3
f1 (ppm)
S76

Xiang LI
XL-35-89-3 HNMR CDCL3:300MHZ(4/14/16)



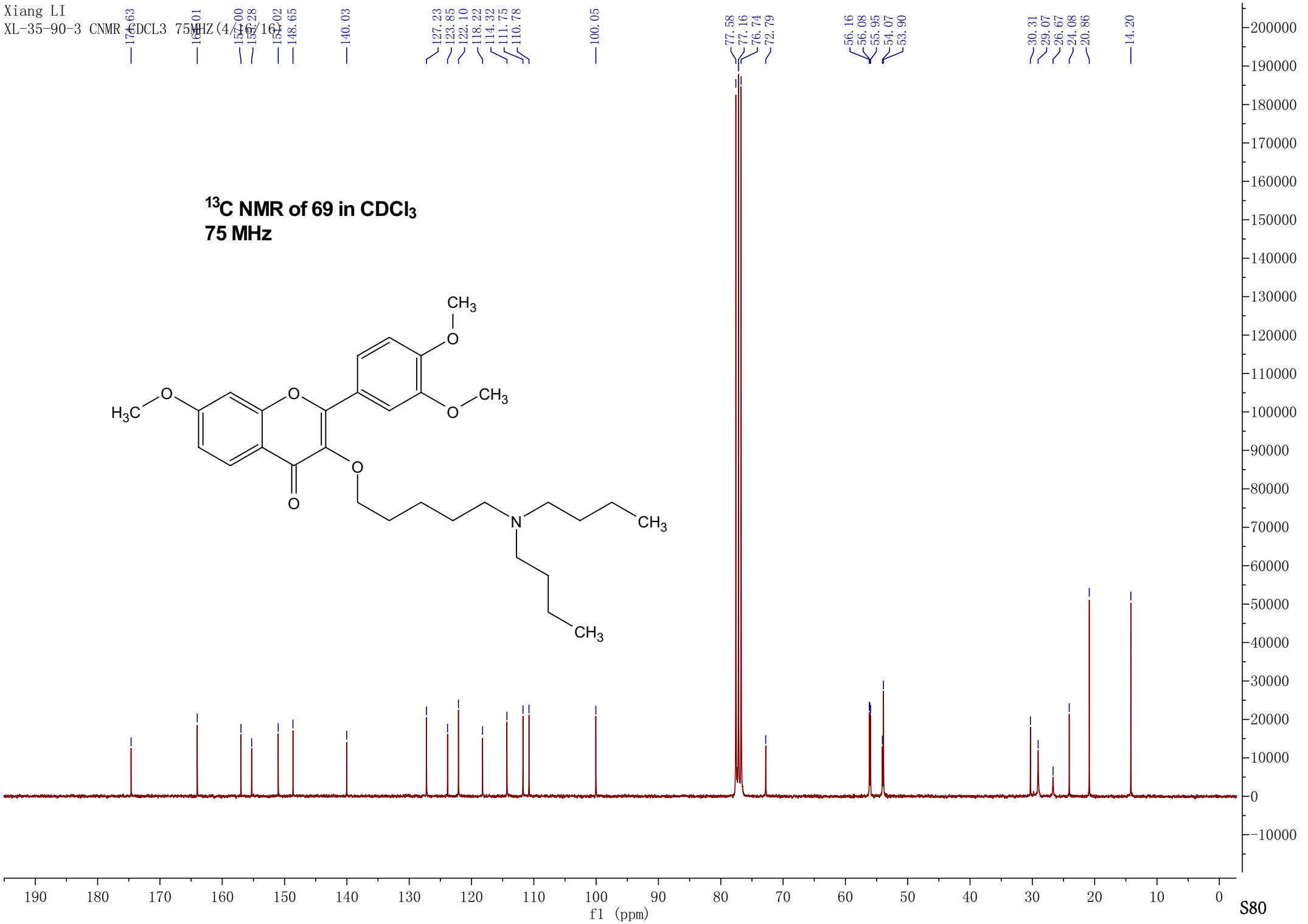
Xiang LI
XL-35-89-3 CNMR CDCL3 75MHZ(4/14/16)



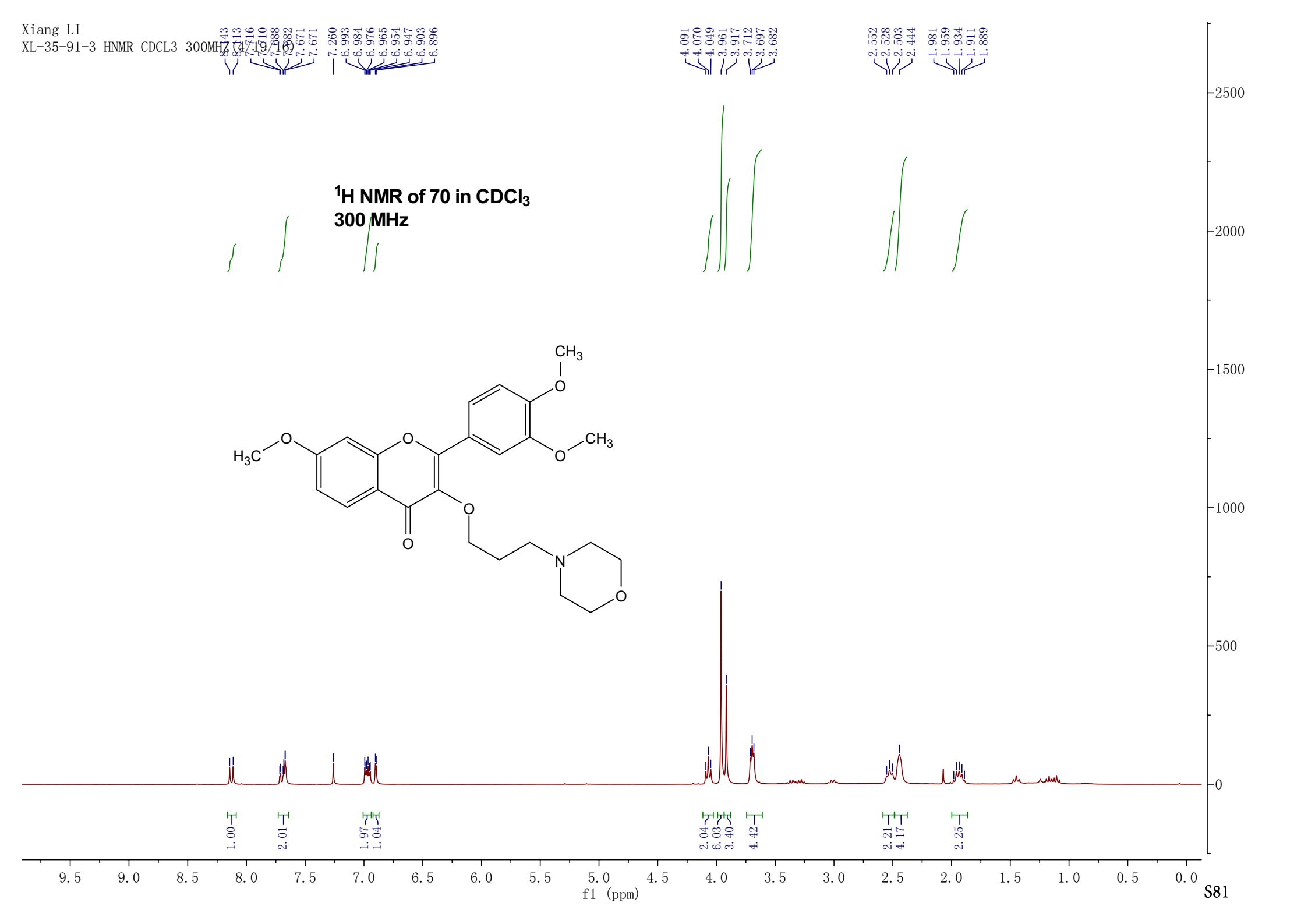


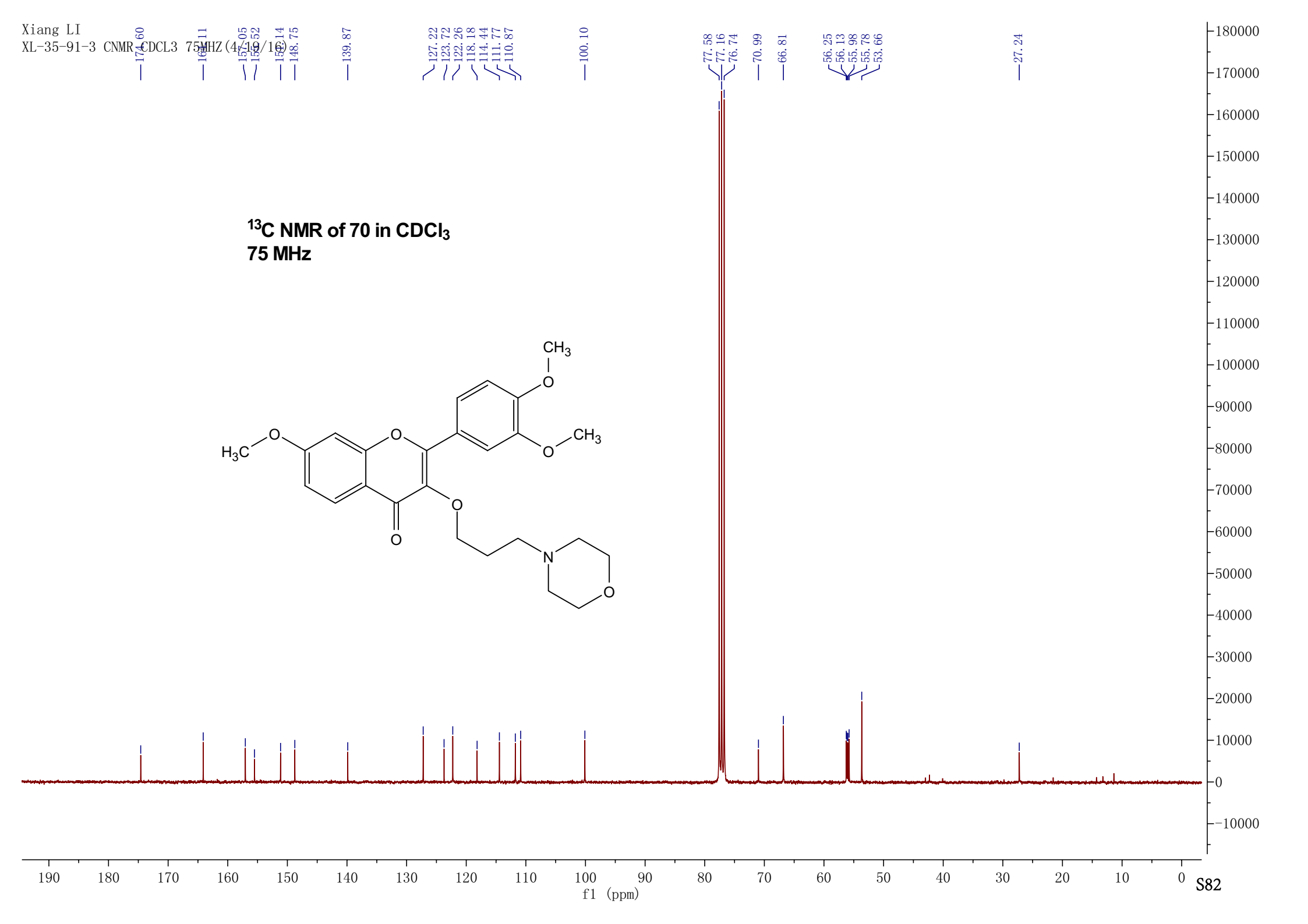
^{1}H NMR of 69 in $CDCl_3$
300 MHz

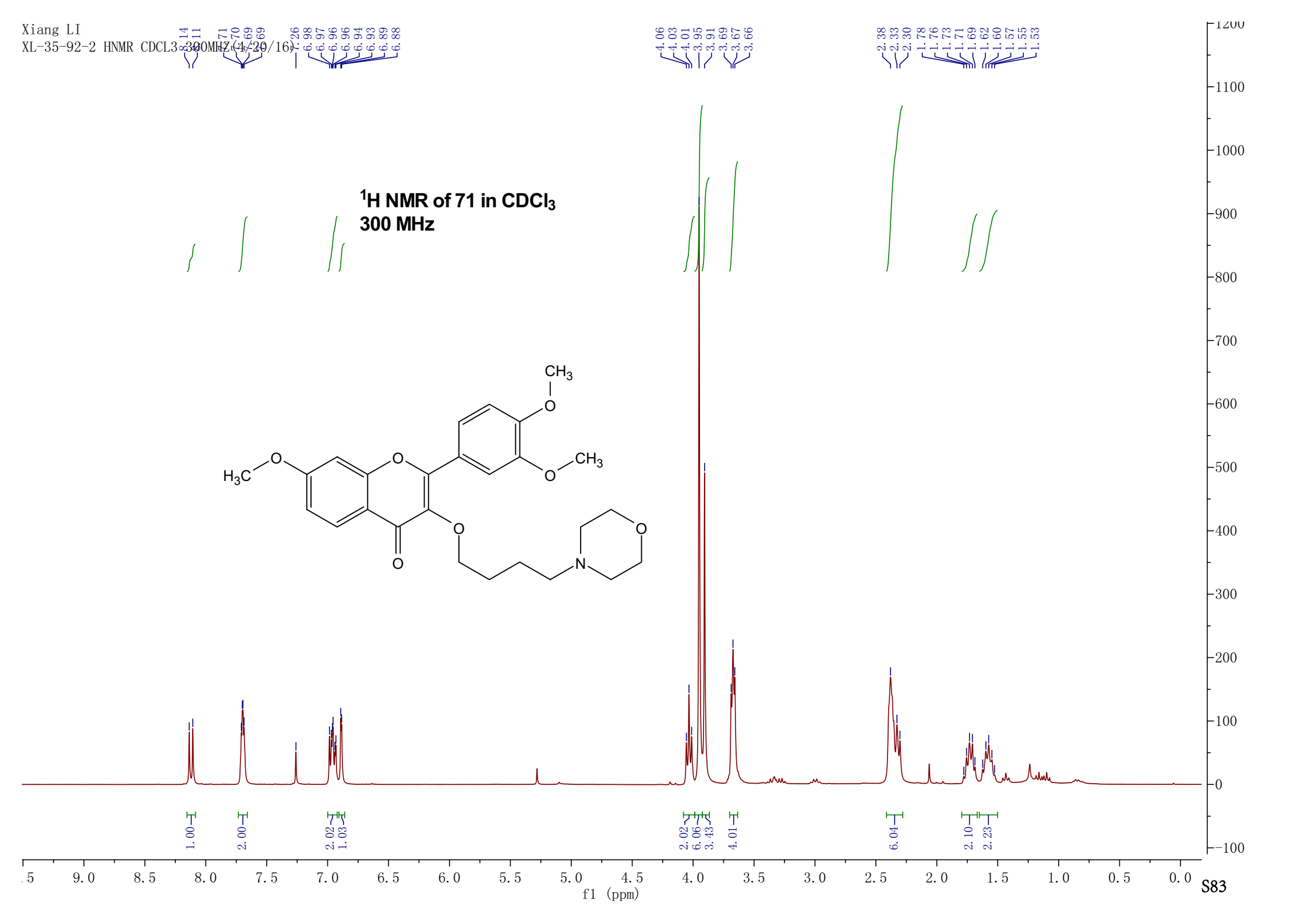
Xiang LI
XL-35-90-3 CNMR CDCL3 75MHZ(4/16/16)



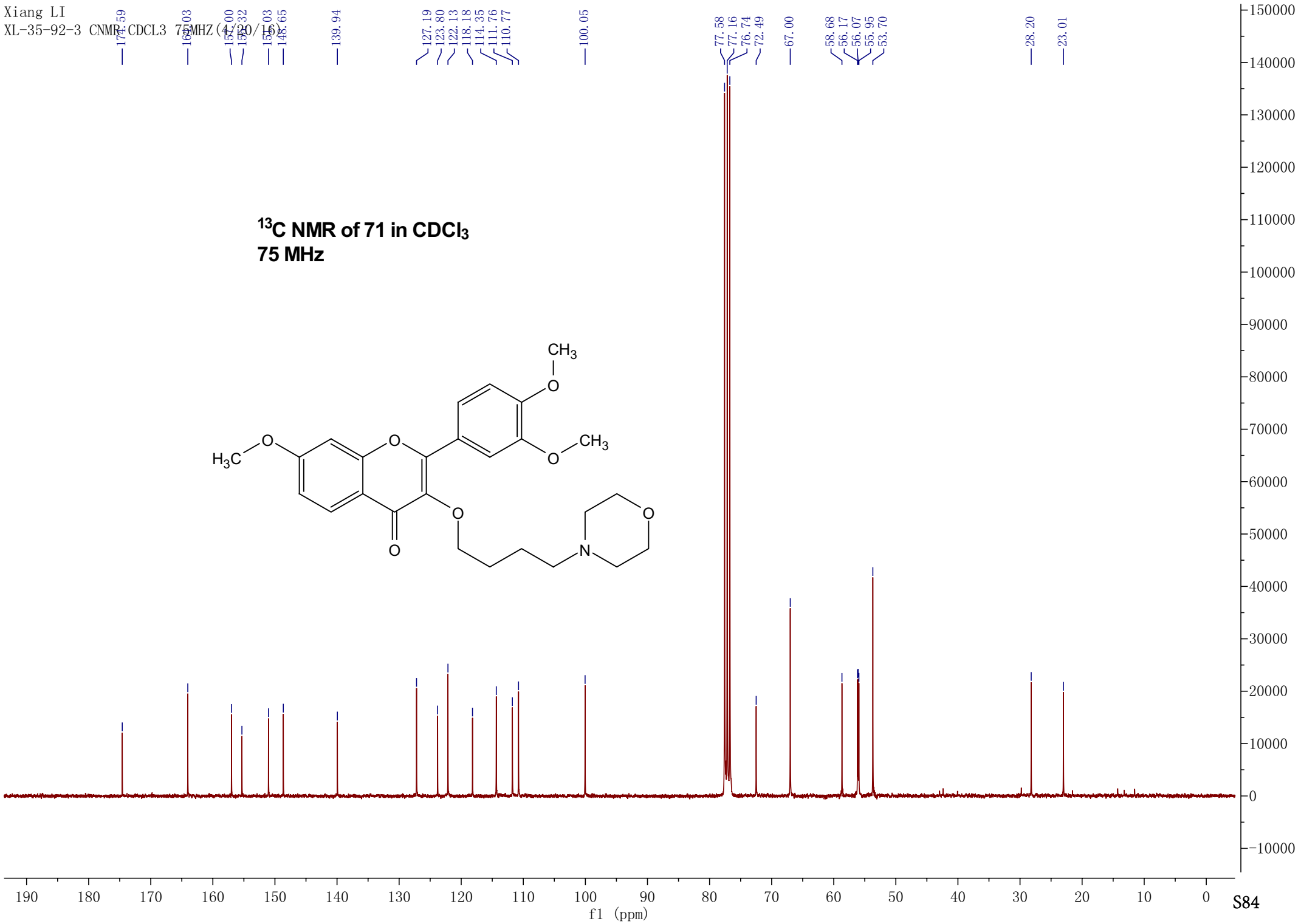
Xiang LI
XL-35-91-3 HNMR CDCL3 300MHZ 7/7/19 16

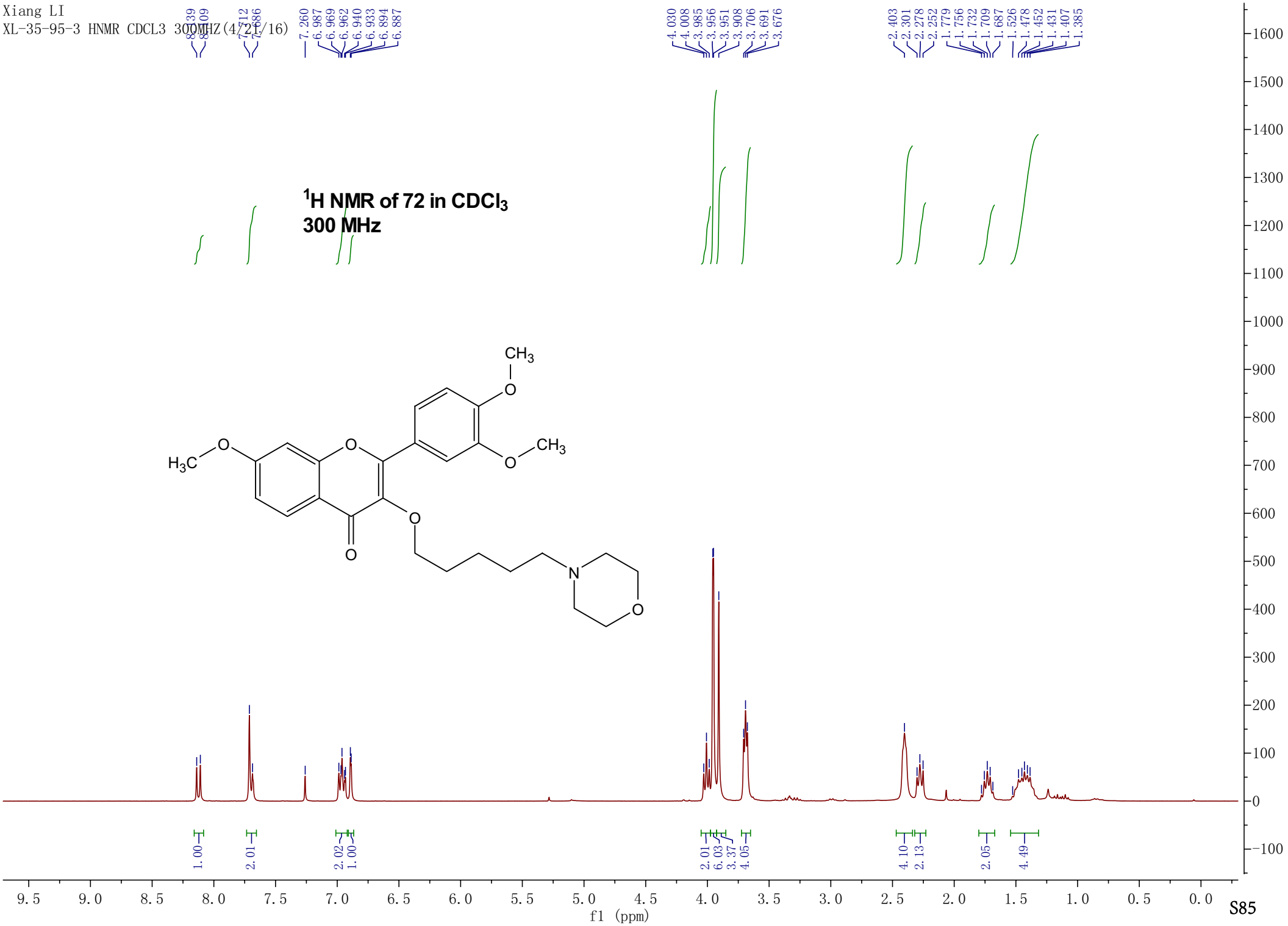



Xiang LI
XL-35-91-3 CNMR-CDCL3 75MHZ(4/19/16)
174.60
166.11
157.05
155.52
153.14
148.75
139.87
127.22
123.72
122.26
118.18
114.44
111.77
110.87
100.10
77.58
77.16
76.74
70.99
66.81
56.25
56.13
55.98
55.78
53.66
27.24
13C NMR of 70 in CDCl3
75 MHz
CH3
O
O
CH3
H3C
O
O
O
O
O
N
O
f1 (ppm)
S82

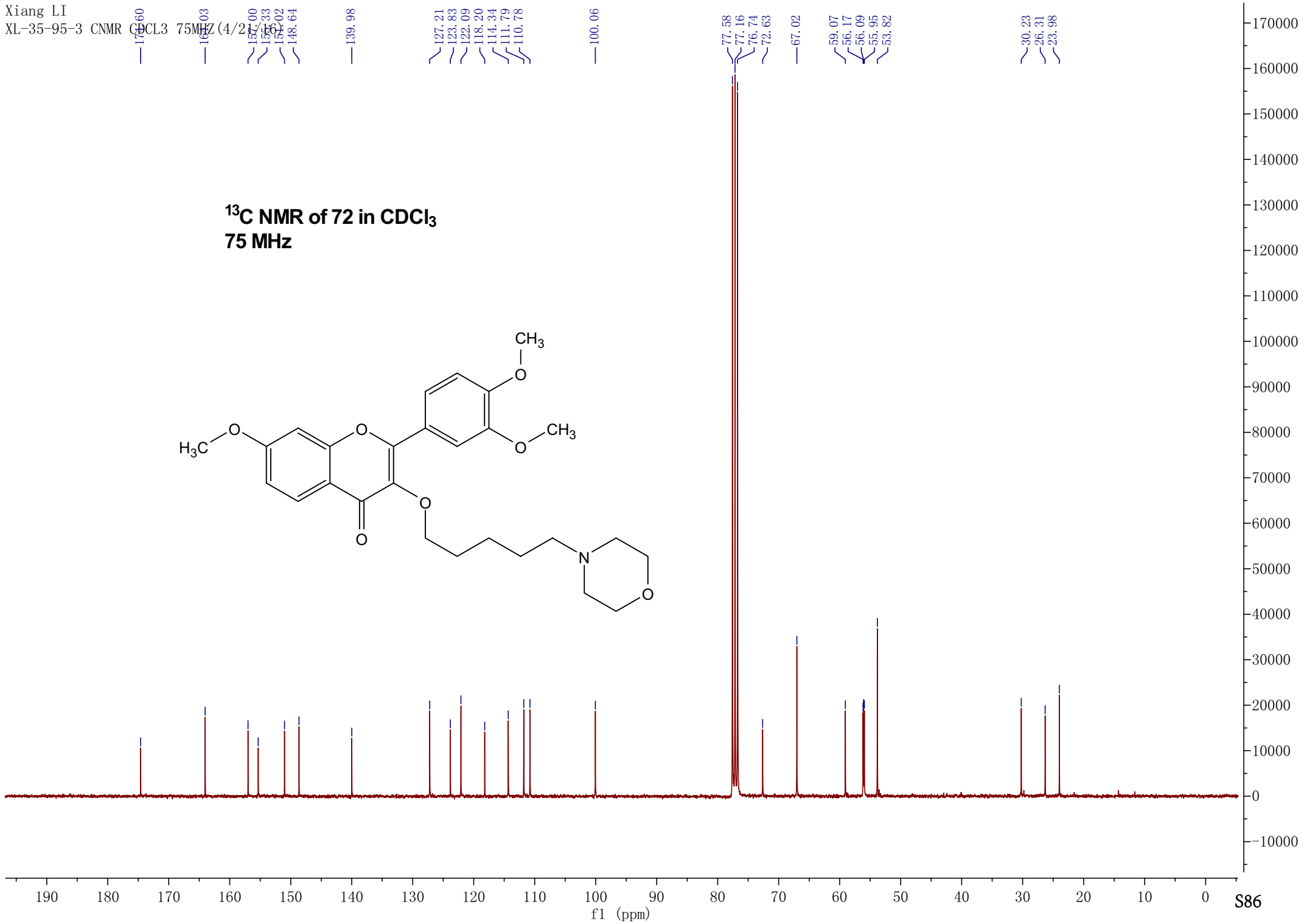

Xiang LI
XL-35-92-2 HNMR CDCL3 300MHZ (4/20/16)
1H NMR of 71 in CDCl3
300 MHz
f1 (ppm)

Xiang LI
XL-35-92-3 CNMR-CDCL3 75MHZ(4/20/16)

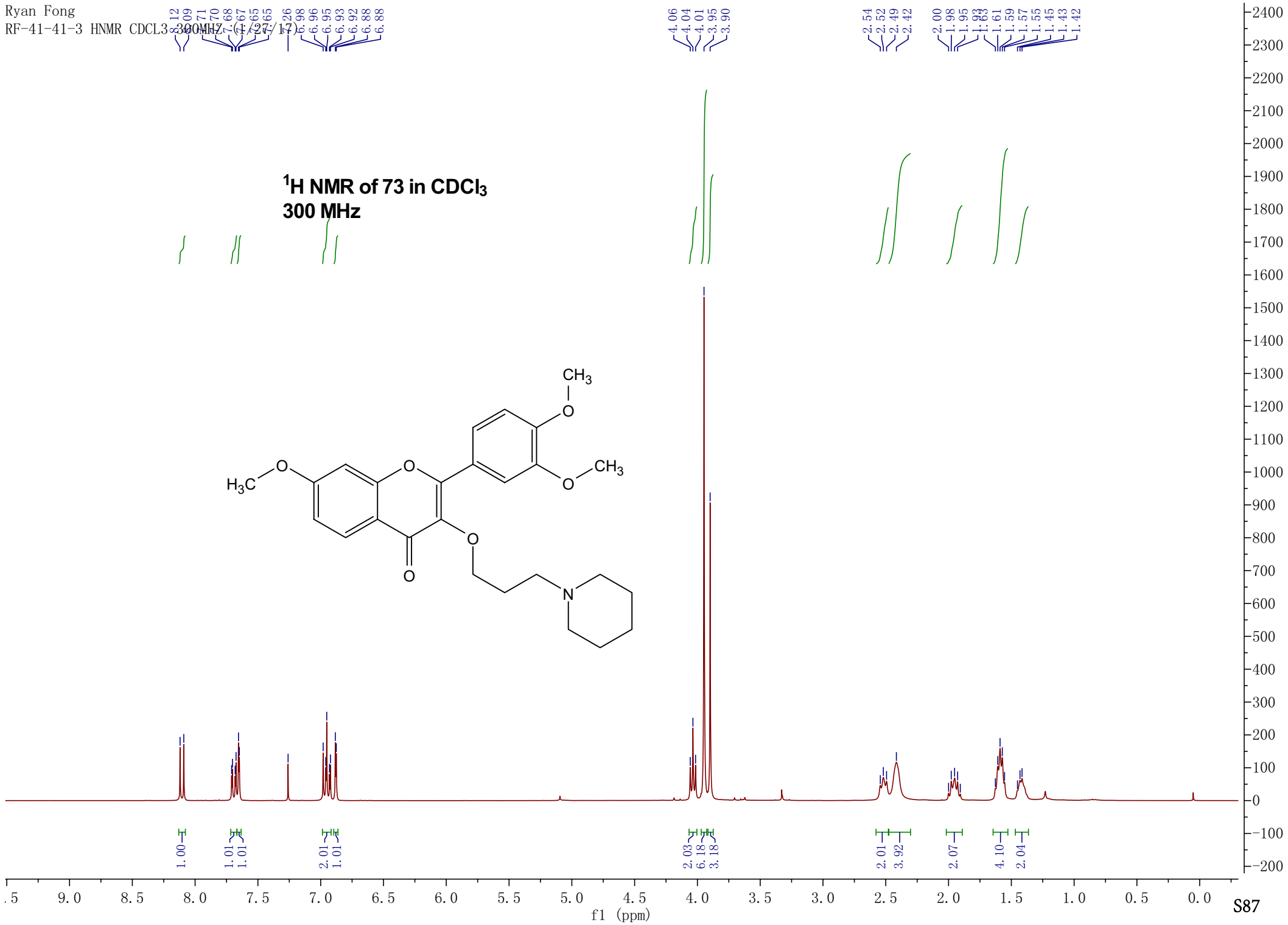




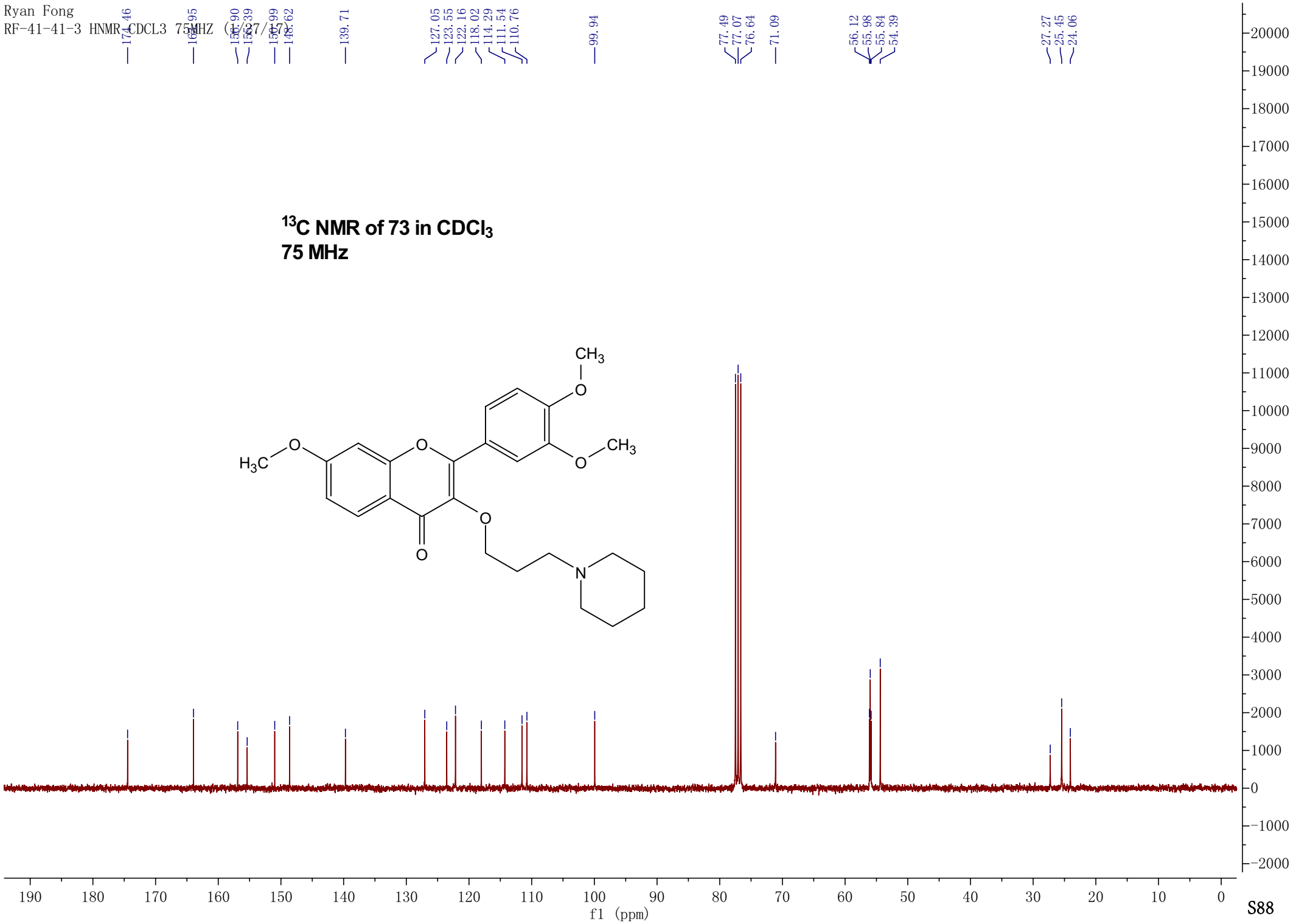
^{1}H NMR of 72 in $CDCl_3$
300 MHz


Xiang LI
XL-35-95-3 CNMR CDCL3 75MHZ(4/21/16)
175.60
160.03
155.00
153.33
151.02
148.64
139.98
127.21
123.83
122.09
118.20
114.34
111.79
110.78
100.06
77.58
77.16
76.74
72.63
67.02
59.07
56.17
56.09
55.95
53.82
30.23
26.31
23.98
13C NMR of 72 in CDCl3
75 MHz
CH3
O
O
H3C
O
O
CH3
O
O
N
O
f1 (ppm)

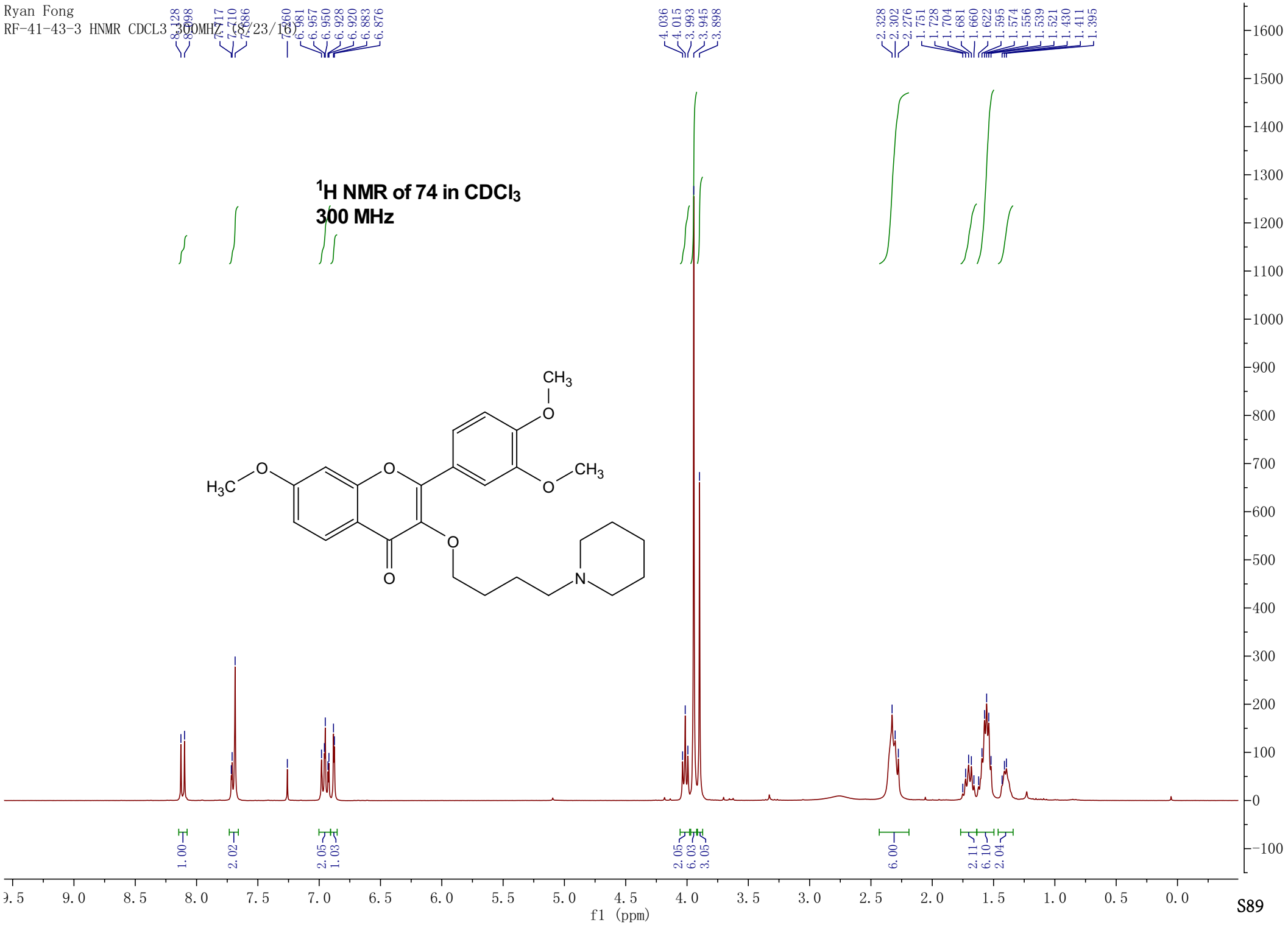
Ryan Fong
RF-41-41-3 HNMR CDCL3 300MHZ (1/27/17)



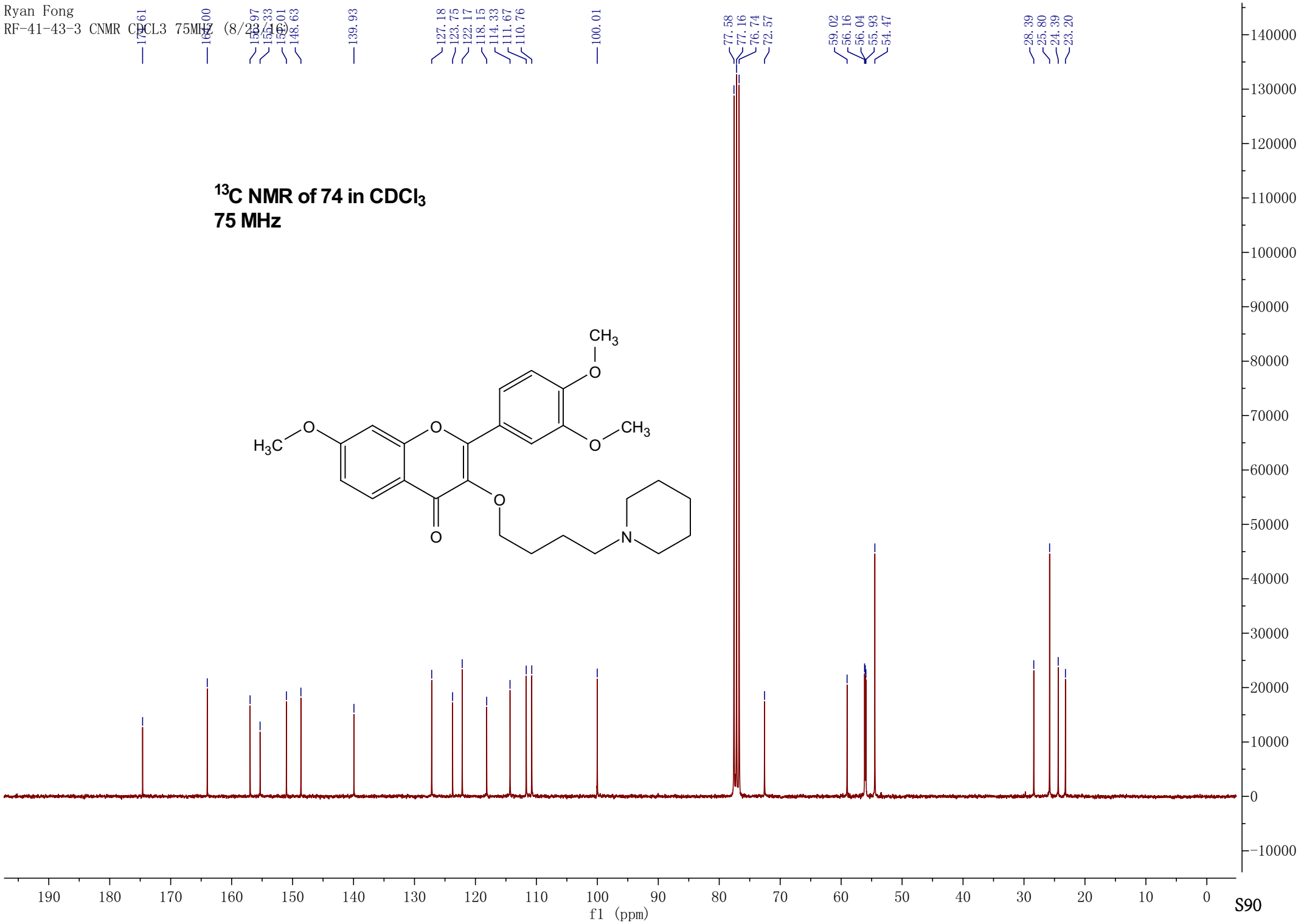
Ryan Fong
RF-41-41-3 HNMR-CDCL3 75MHZ (11/27/17)



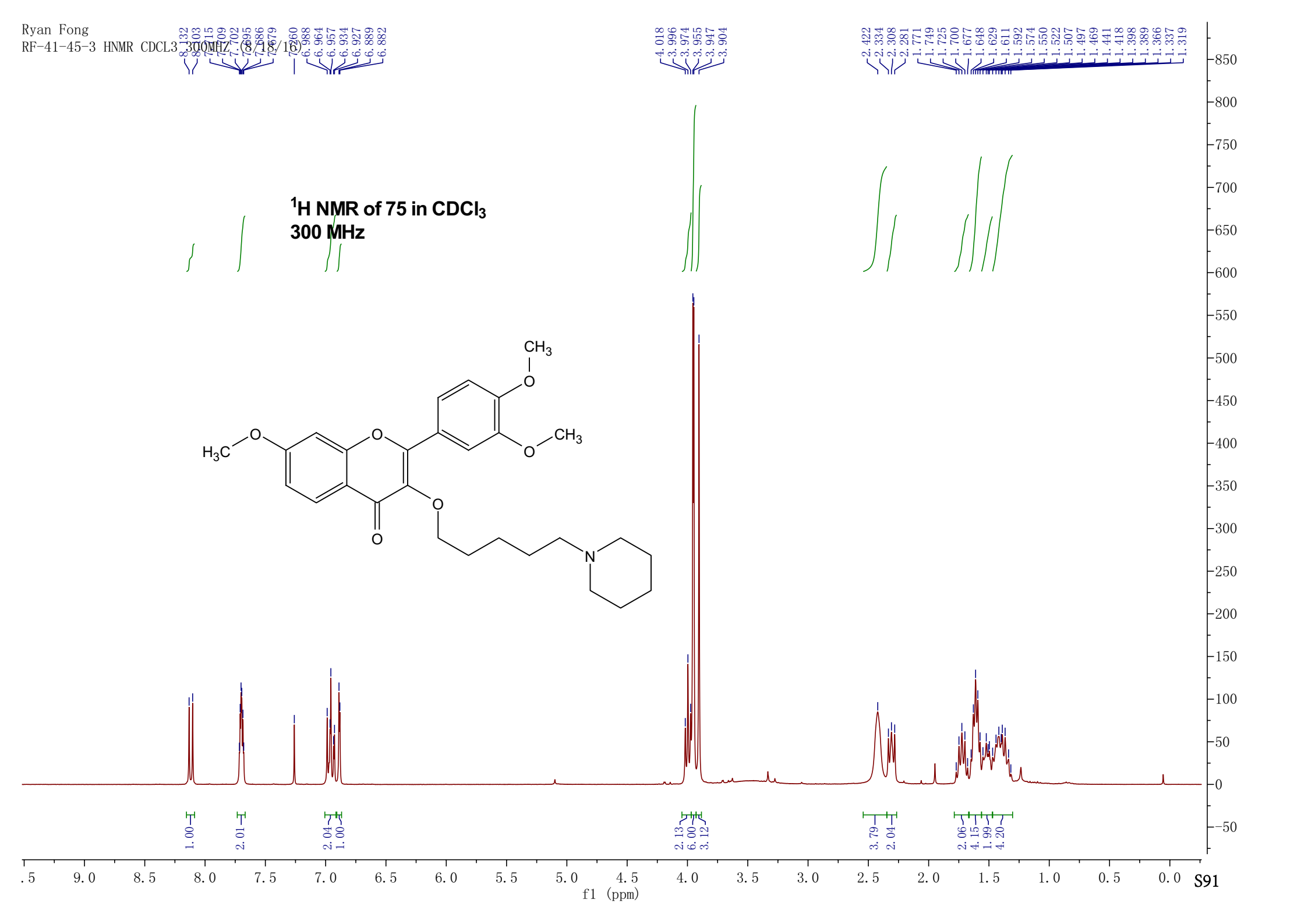
Ryan Fong
RF-41-43-3 HNMR CDCL3 300MHZ (8/23/16)



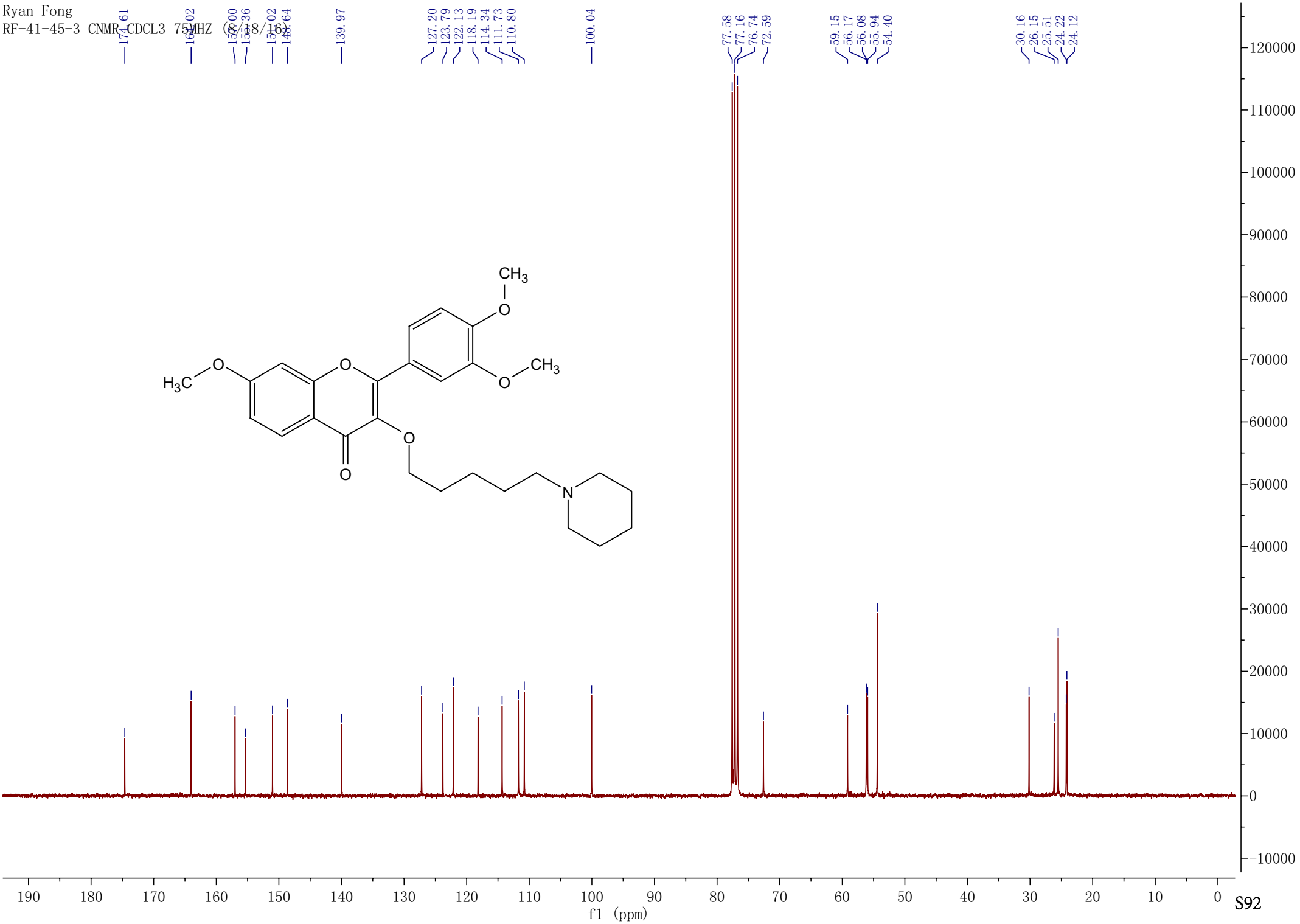
Ryan Fong
RF-41-43-3 CNMR CDCL3 75MHZ (8/23/16)



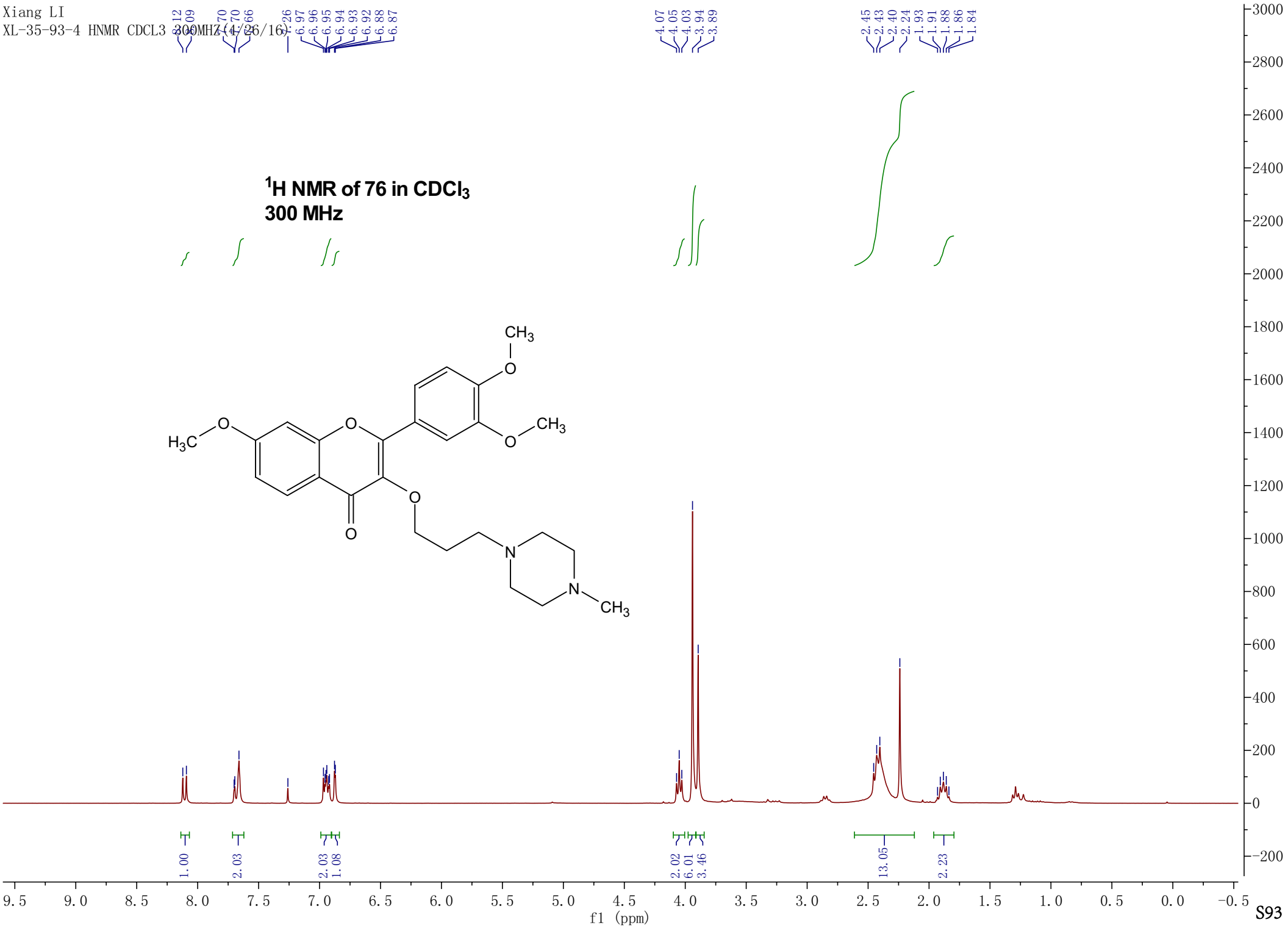
Ryan Fong
RF-41-45-3 HNMR CDCL3 300MHZ (8/18/16)



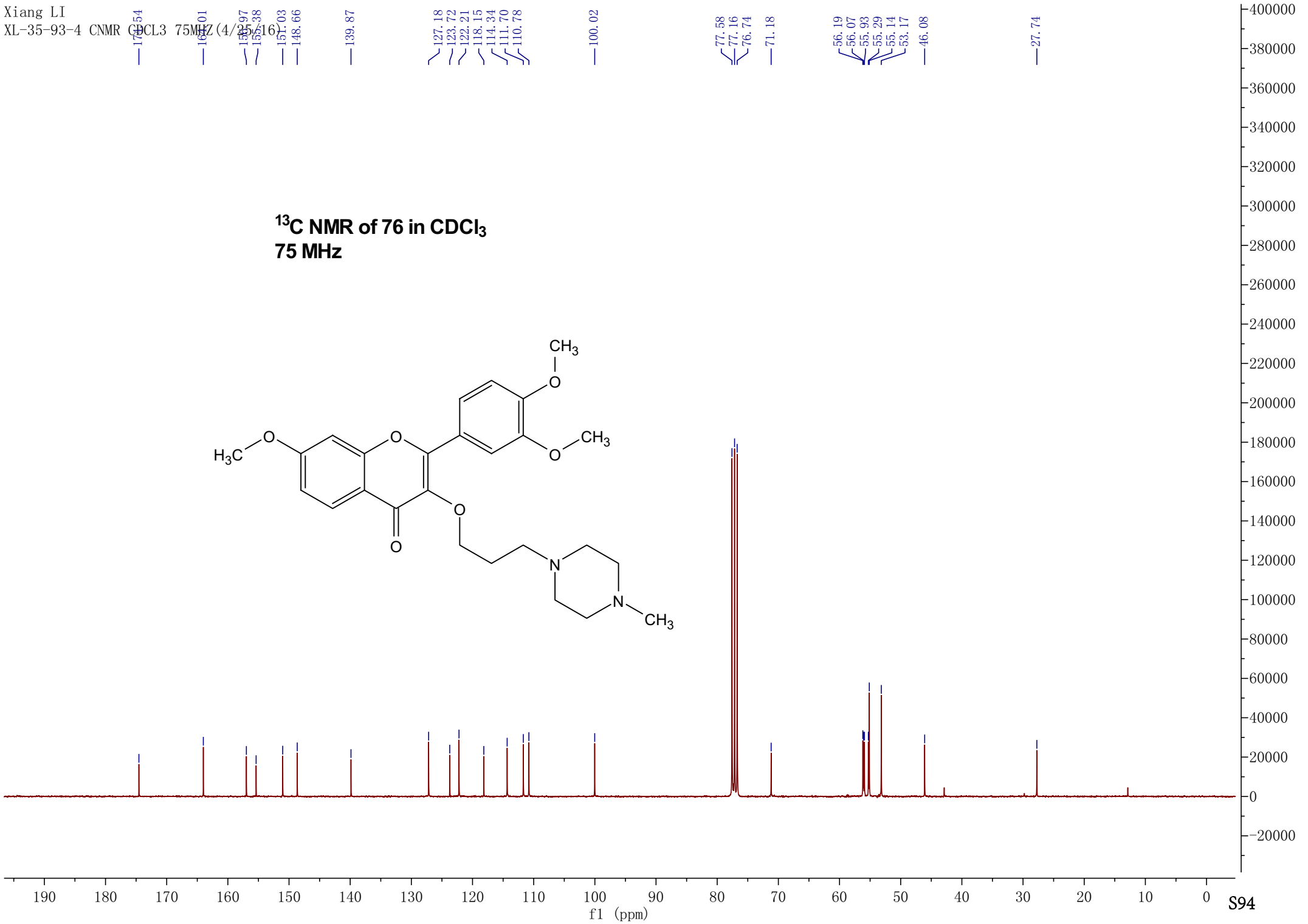
Ryan Fong
RF-41-45-3 CNMR-CDCL3 75MHZ (8/18/16)

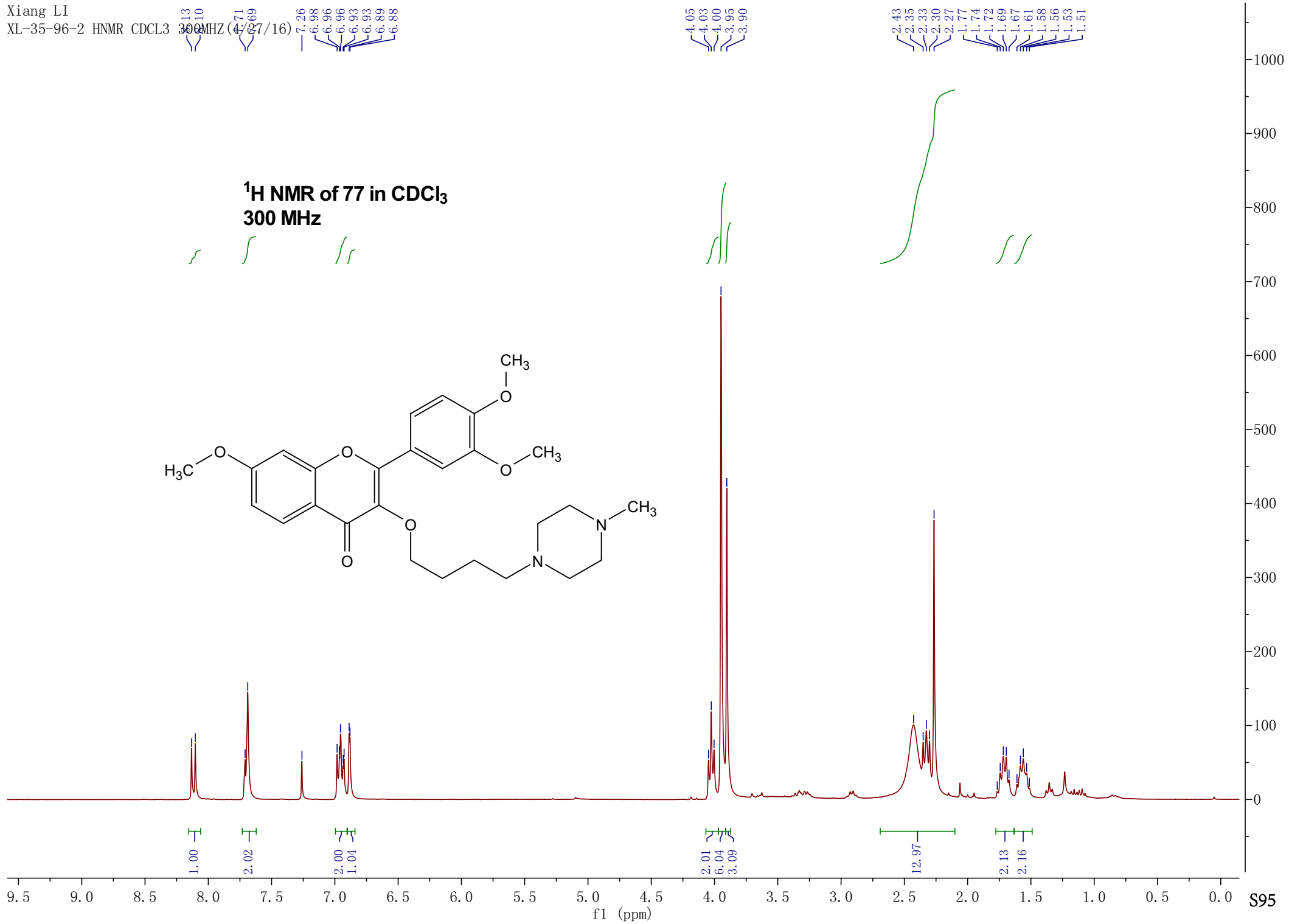


Xiang LI
XL-35-93-4 HNMR CDCL3 300MHZ(4/26/16)

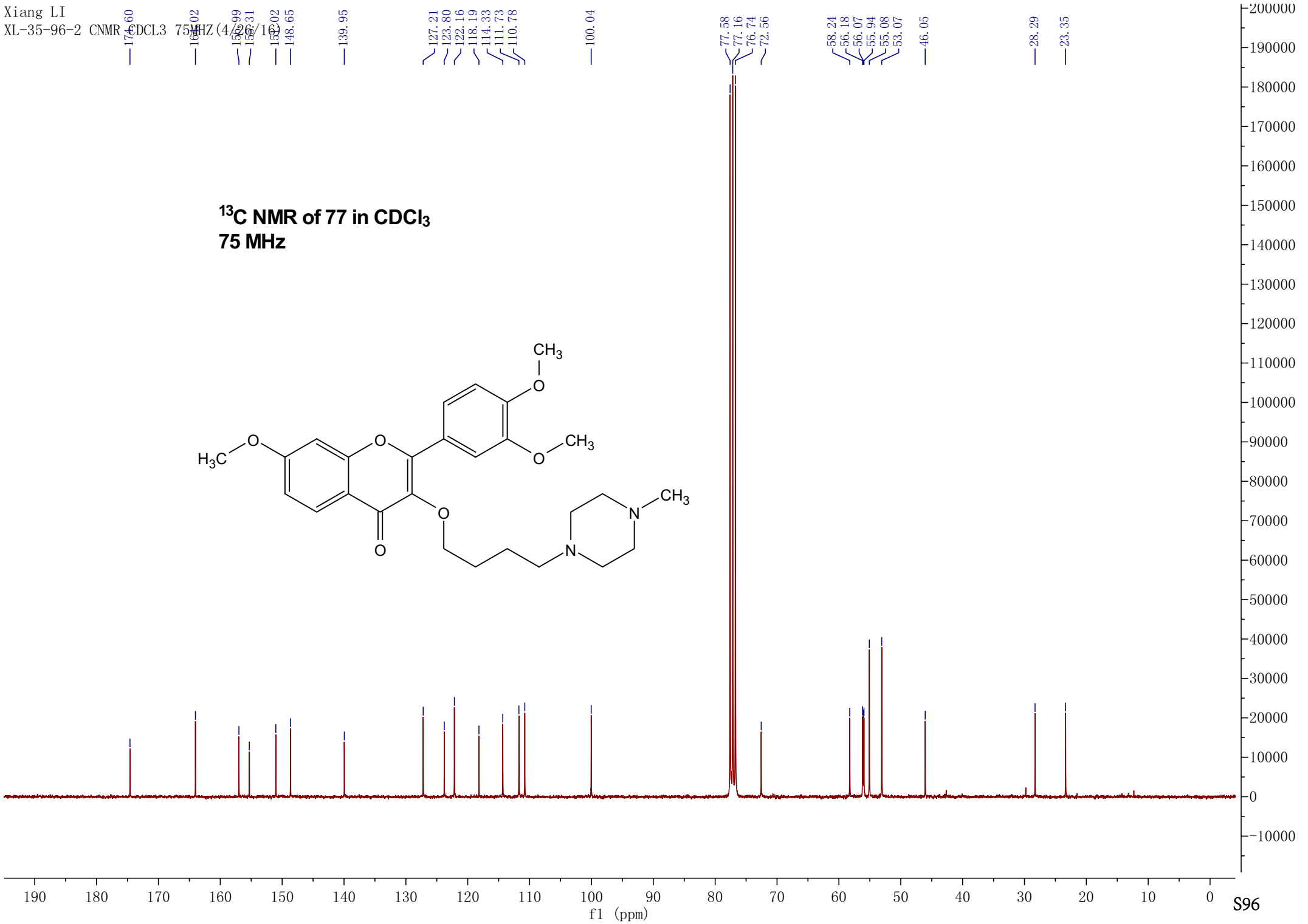


Xiang LI
XL-35-93-4 CNMR CDCL3 75MHZ(4/25/16)

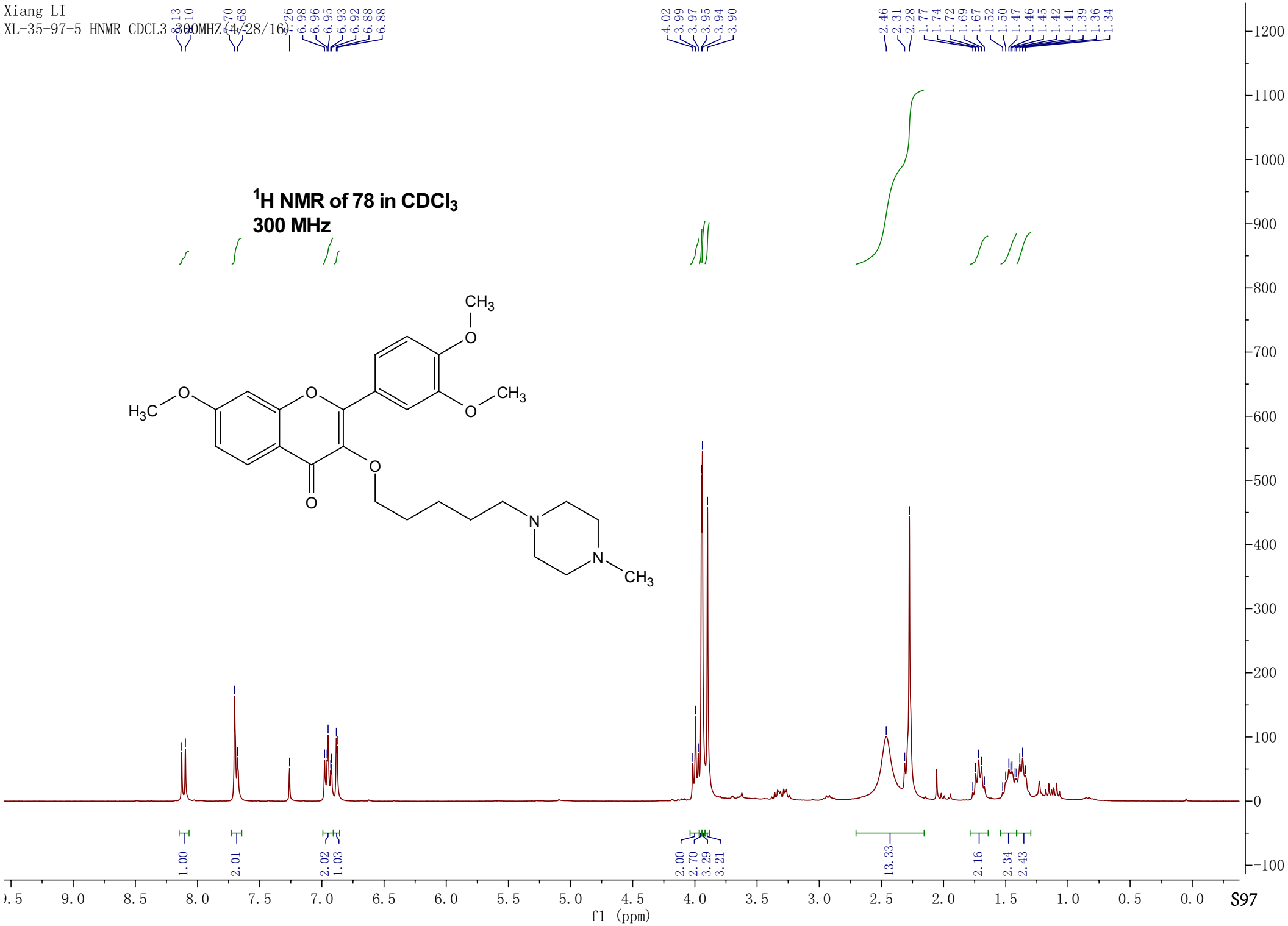


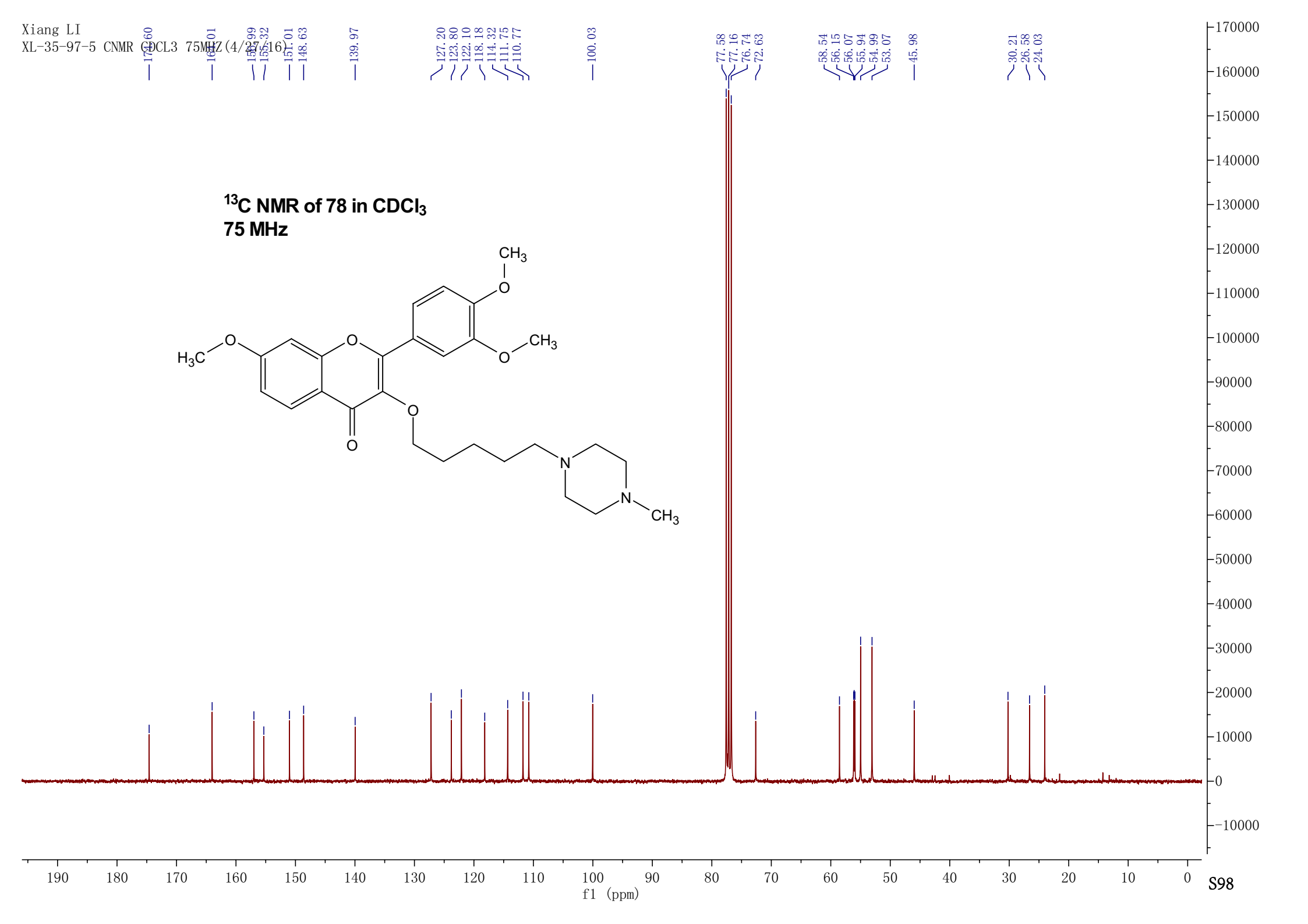

Xiang LI
XL-35-96-2 HNMR CDCL3 300MHZ(4/27/16)
^{1}H NMR of 77 in CDCl$_3$
300 MHz
f1 (ppm)

Xiang LI
XL-35-96-2 CNMR CDCL3 75MHZ(4/26/16)

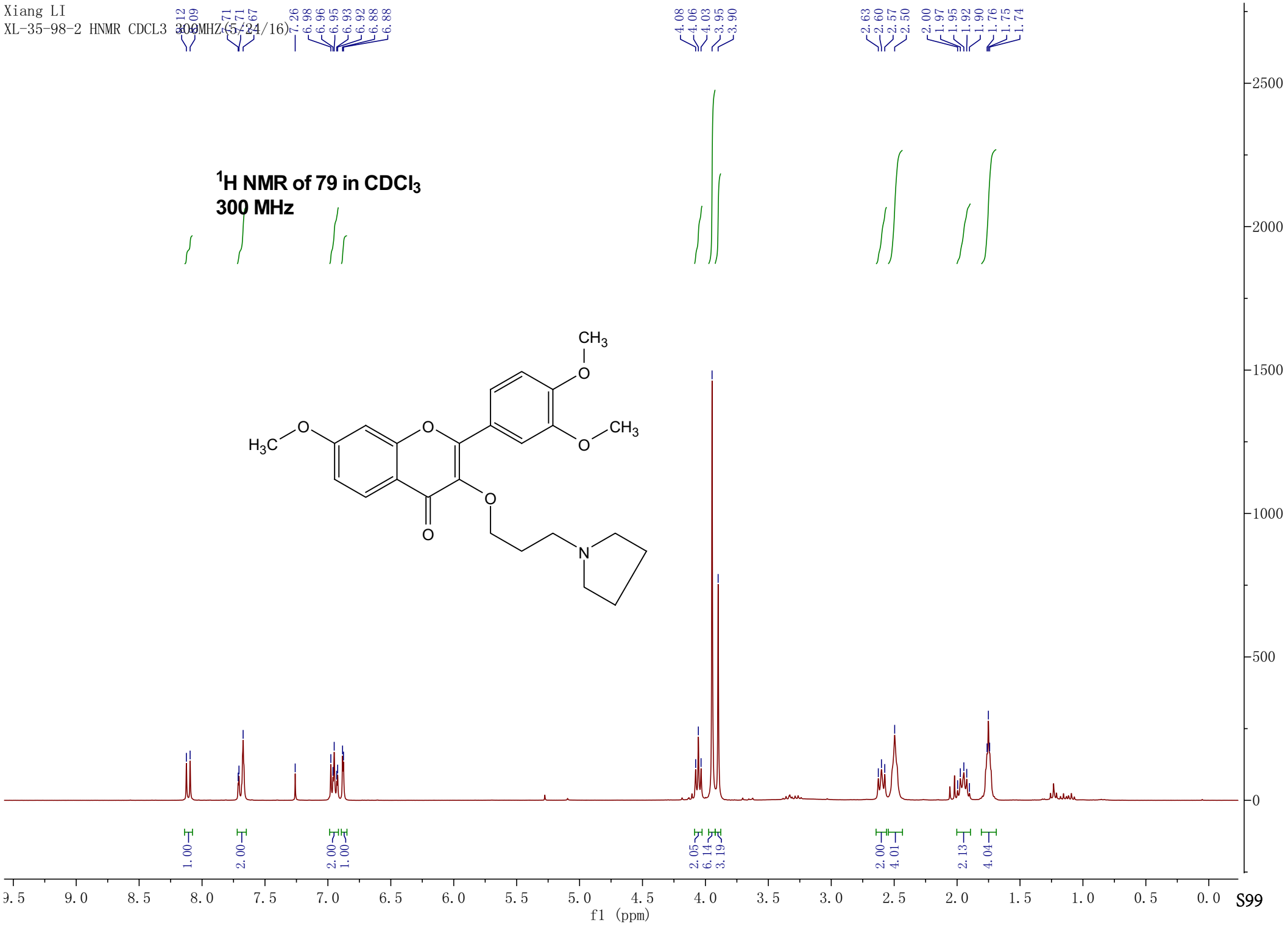


Xiang LI
XL-35-97-5 HNMR CDCL3 300MHZ(4-28/16)

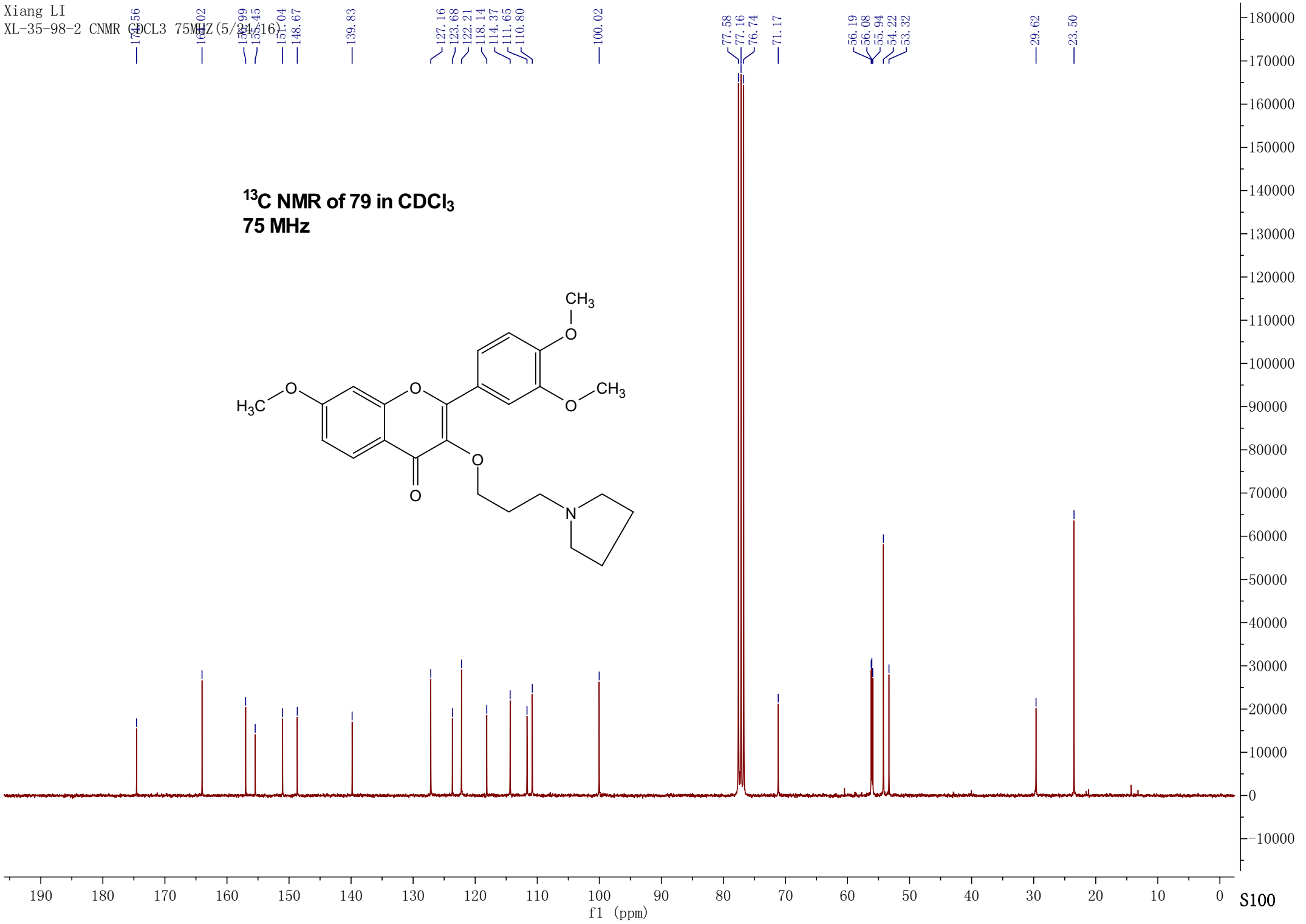



Xiang LI
XL-35-97-5 CNMR CDCL3 75MHZ(4/27/16)
175.60
165.01
155.99
155.32
151.01
148.63
139.97
127.20
123.80
122.10
118.18
114.32
111.75
110.77
100.03
77.58
77.16
76.74
72.63
58.54
56.15
56.07
55.94
54.99
53.07
45.98
30.21
26.58
24.03
13C NMR of 78 in CDCl3
75 MHz
CH3
O
H3C
O
O
CH3
O
O
O
N
N
CH3
f1 (ppm)
S98

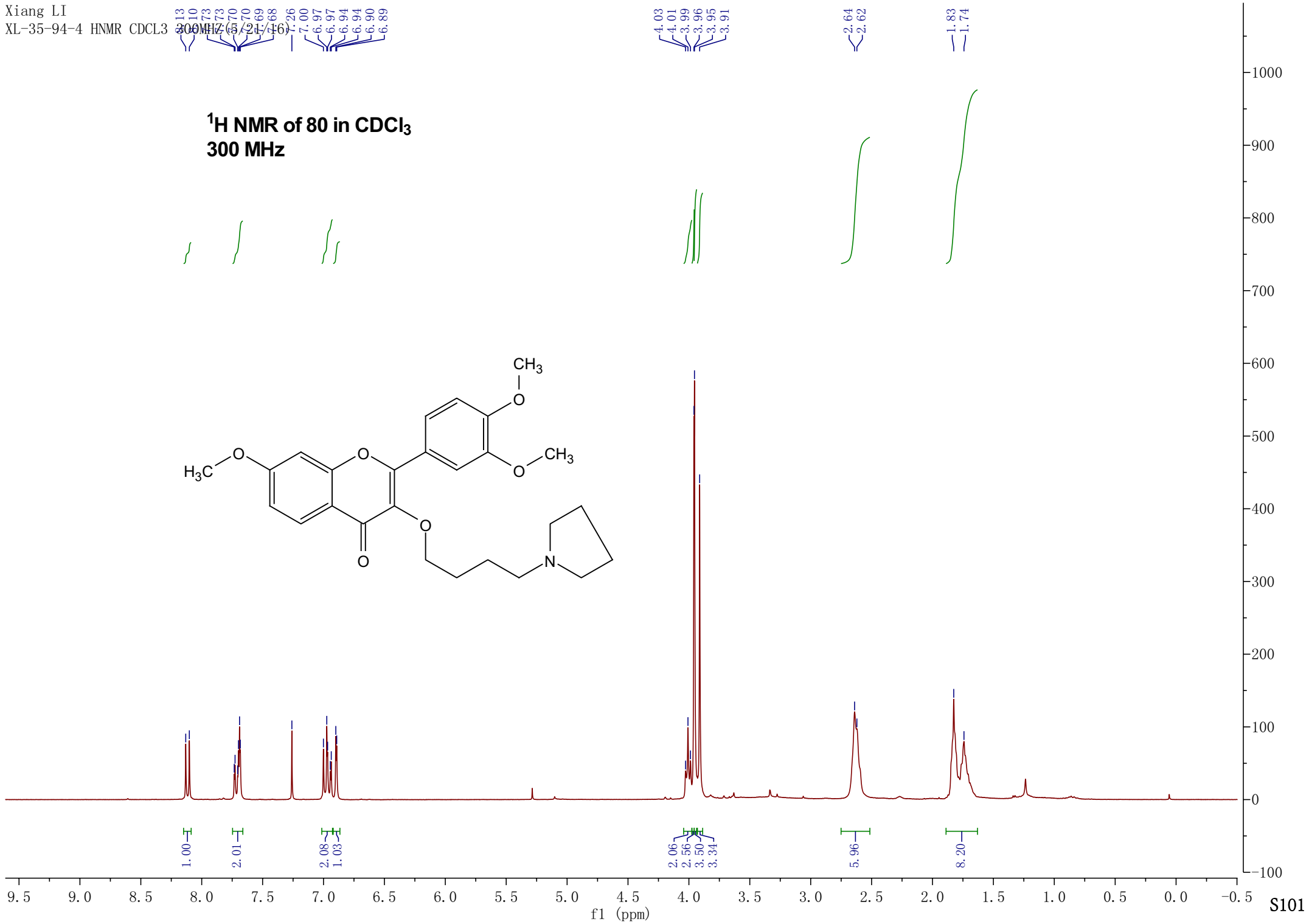
Xiang LI
XL-35-98-2 HNMR CDCL3 300MHZ(5/24/16)



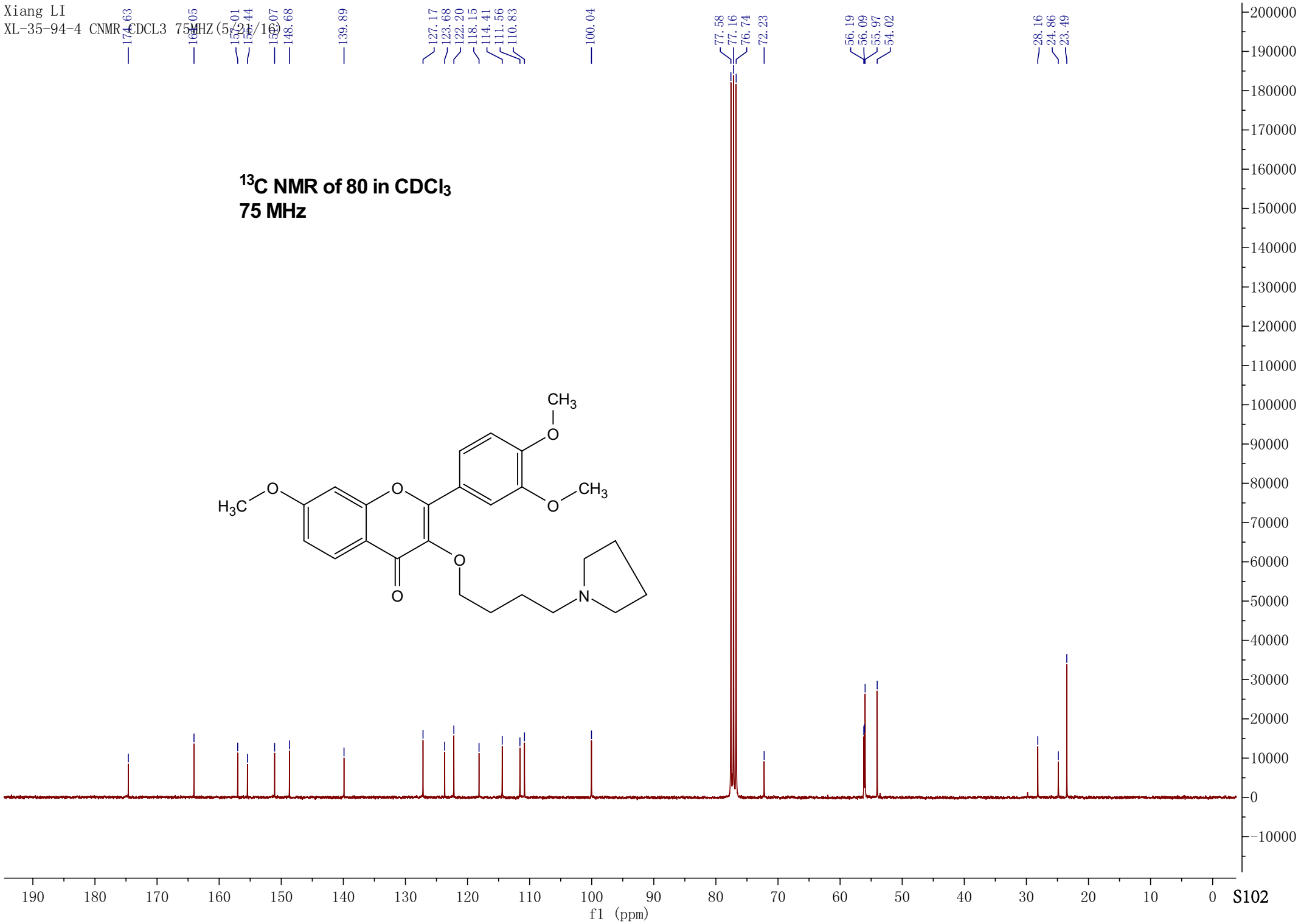
Xiang LI
XL-35-98-2 CNMR CDCL3 75MHZ(5/24/16)



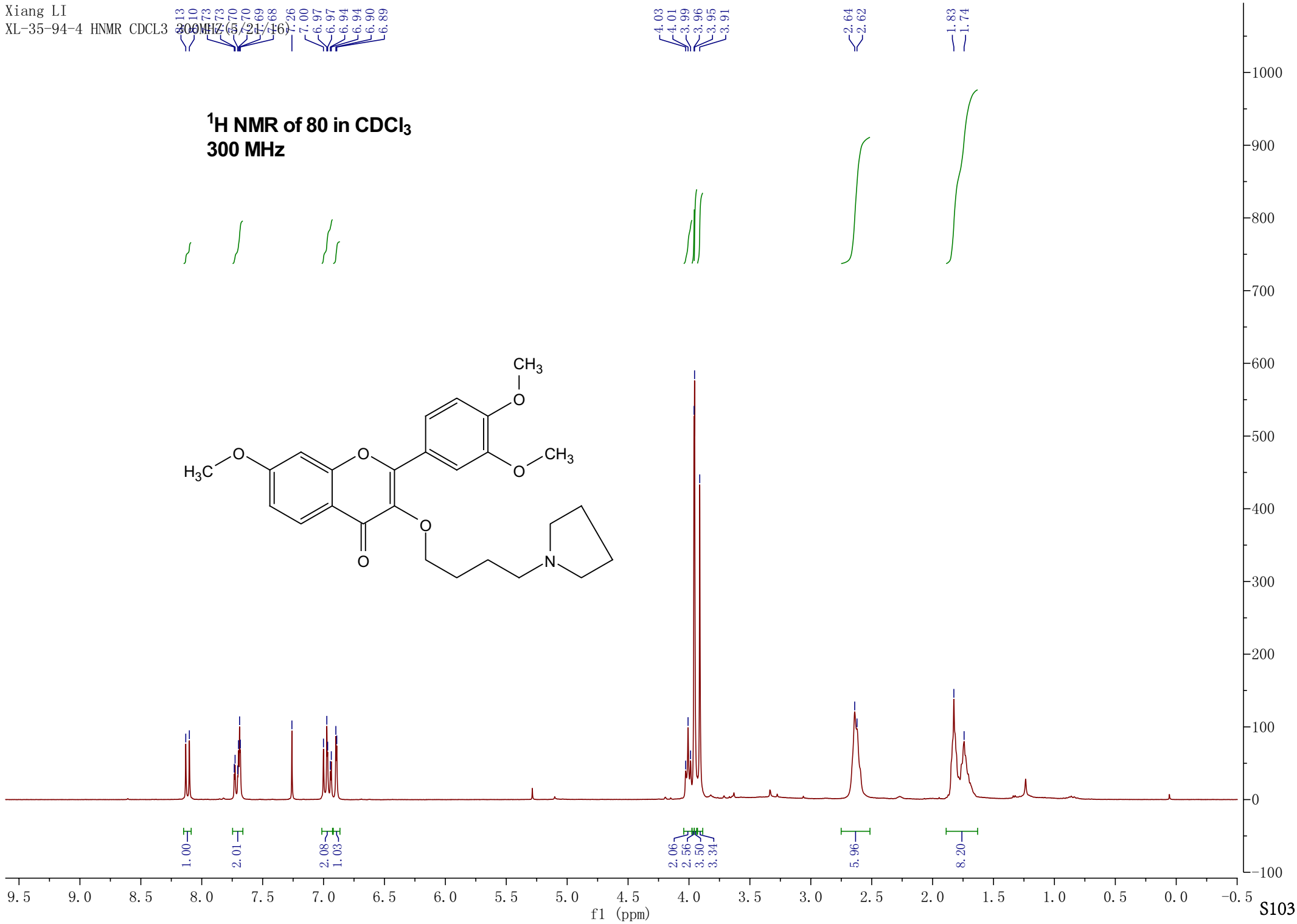
Xiang LI
XL-35-94-4 HNMR CDCL3 300MHZ(5/24/16)

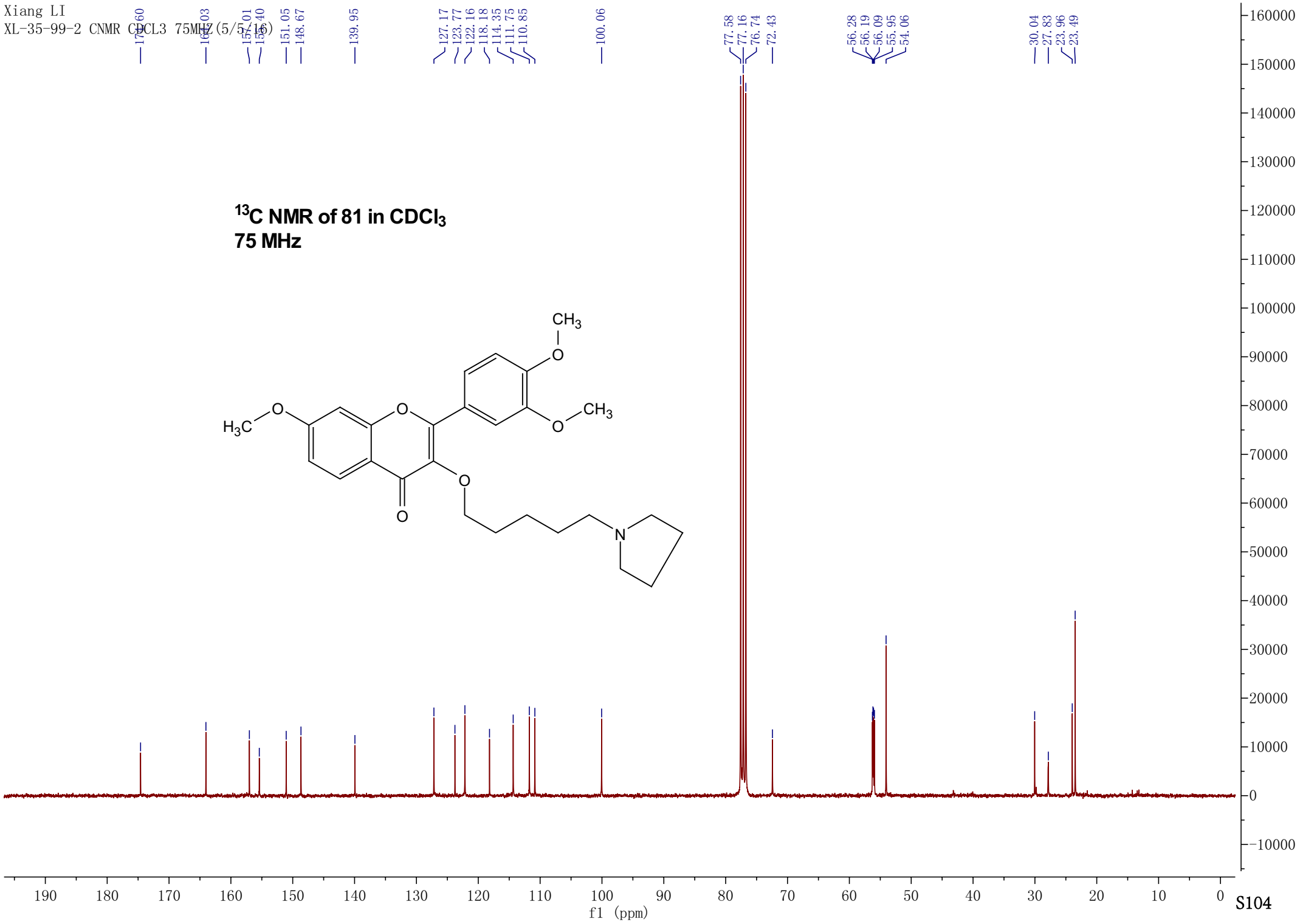


Xiang LI
XL-35-94-4 CNMR-CDCL3 75MHZ(5/24/16)



Xiang LI
XL-35-94-4 HNMR CDCL3 300MHZ(5/24/16)




Xiang LI
XL-35-99-2 CNMR CDCL3 75MHZ(5/5/16)
175.60
163.03
157.01
155.40
151.05
148.67
139.95
127.17
123.77
122.16
118.18
114.35
111.75
110.85
100.06
77.58
77.16
76.74
72.43
56.28
56.19
56.09
55.95
54.06
30.04
27.83
23.96
23.49
13C NMR of 81 in CDCl3
75 MHz
CH3
O
O
CH3
H3C
O
O
O
O
N
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)