

## Supplementary Data

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

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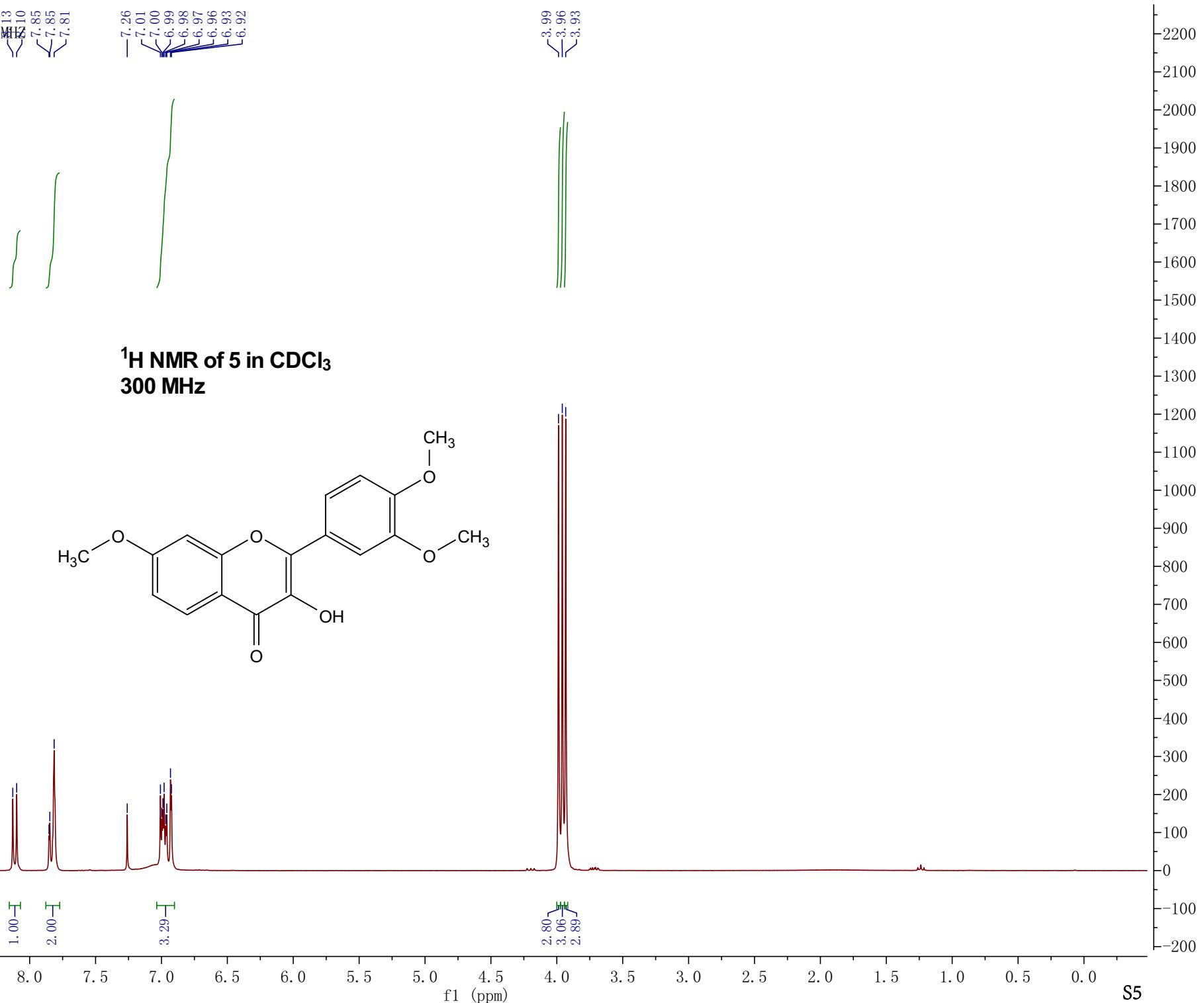
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—172.63

—167.29

—157.29

 $\sim$ 150.68  
 $\sim$ 148.98  
 $\sim$ 144.72

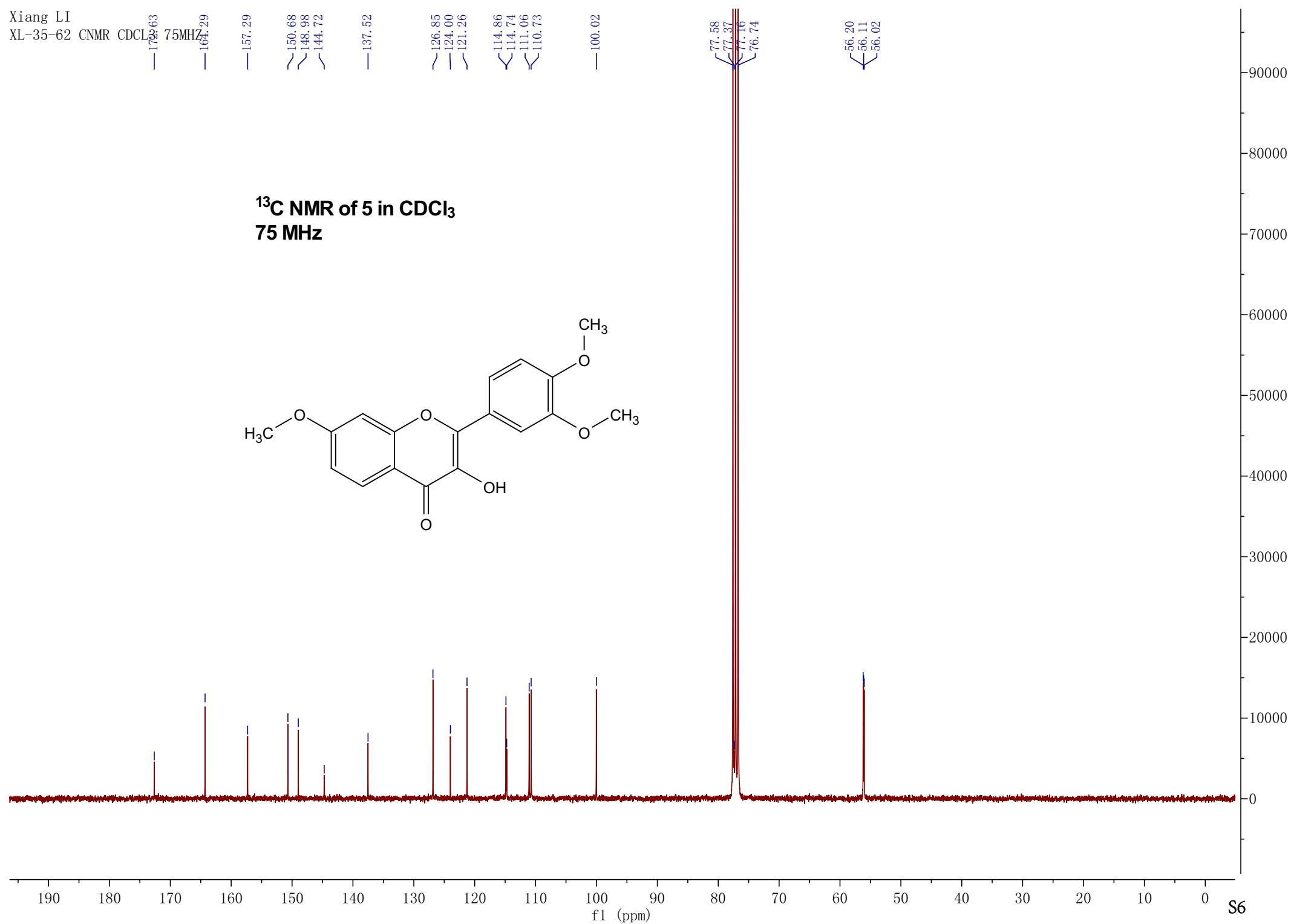
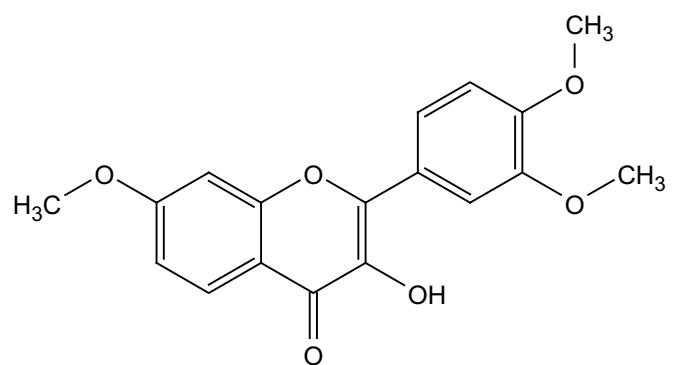
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 $\sim$ 126.85  
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—114.74  
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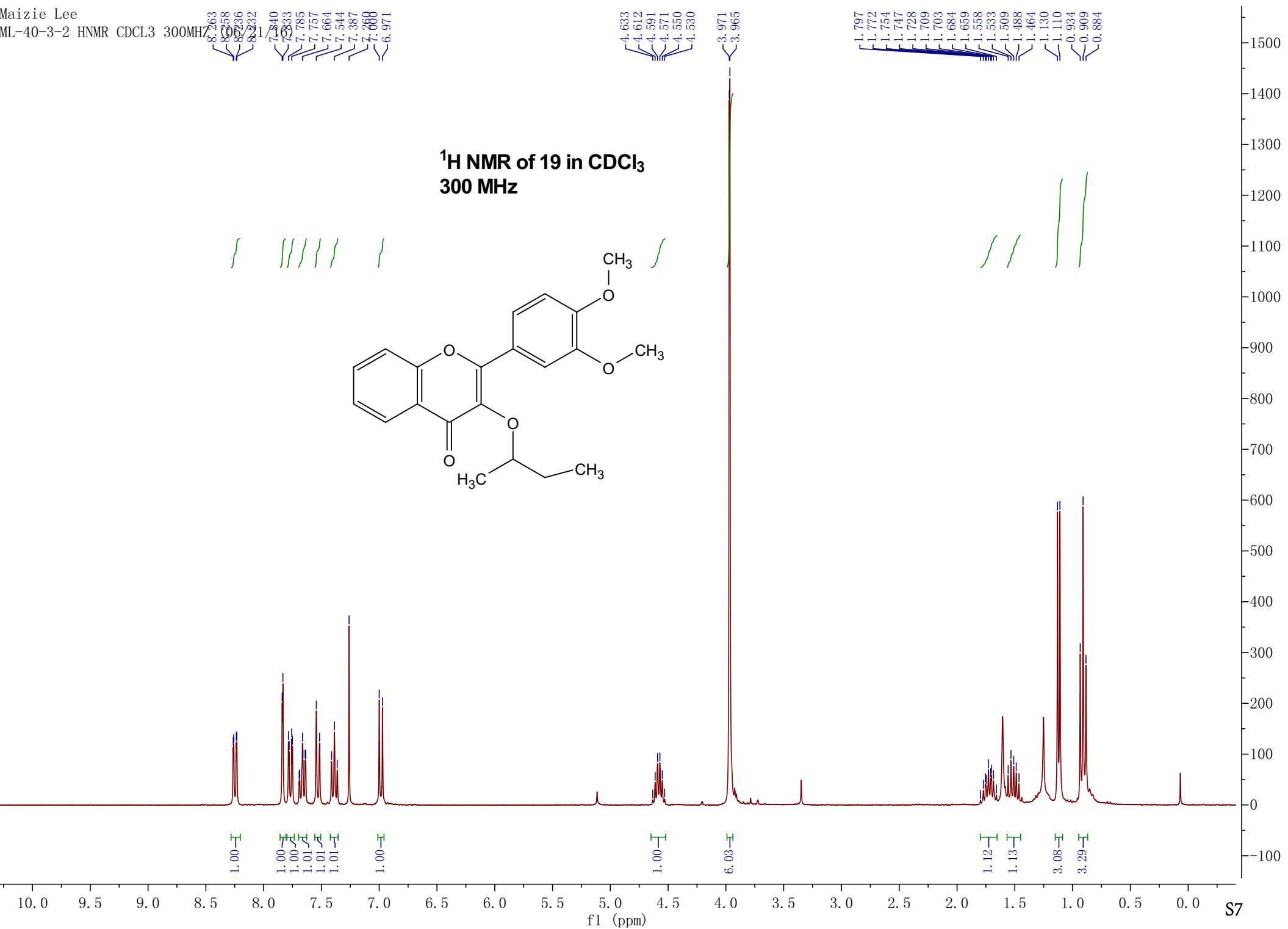
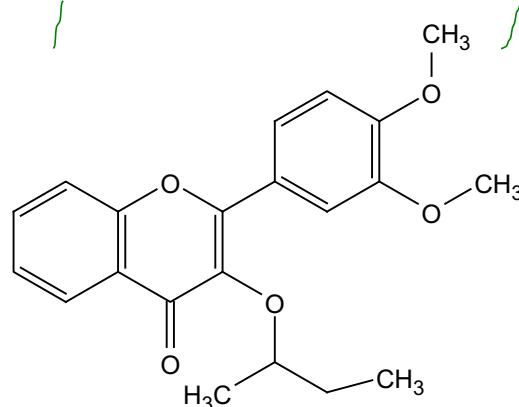
—100.02

77.58  
77.37  
77.16  
76.7456.20  
56.11  
56.02

**<sup>13</sup>C NMR of 5 in CDCl<sub>3</sub>**  
**75 MHz**



**<sup>1</sup>H NMR of 19 in CDCl<sub>3</sub>  
300 MHz**



— 176.48  
— 156.16  
— 154.27  
— 151.00  
— 148.39

— 138.80  
— 133.26  
— 125.94  
— 124.62  
— 124.24  
— 124.22  
— 122.45  
— 117.99

— 112.45  
— 110.64

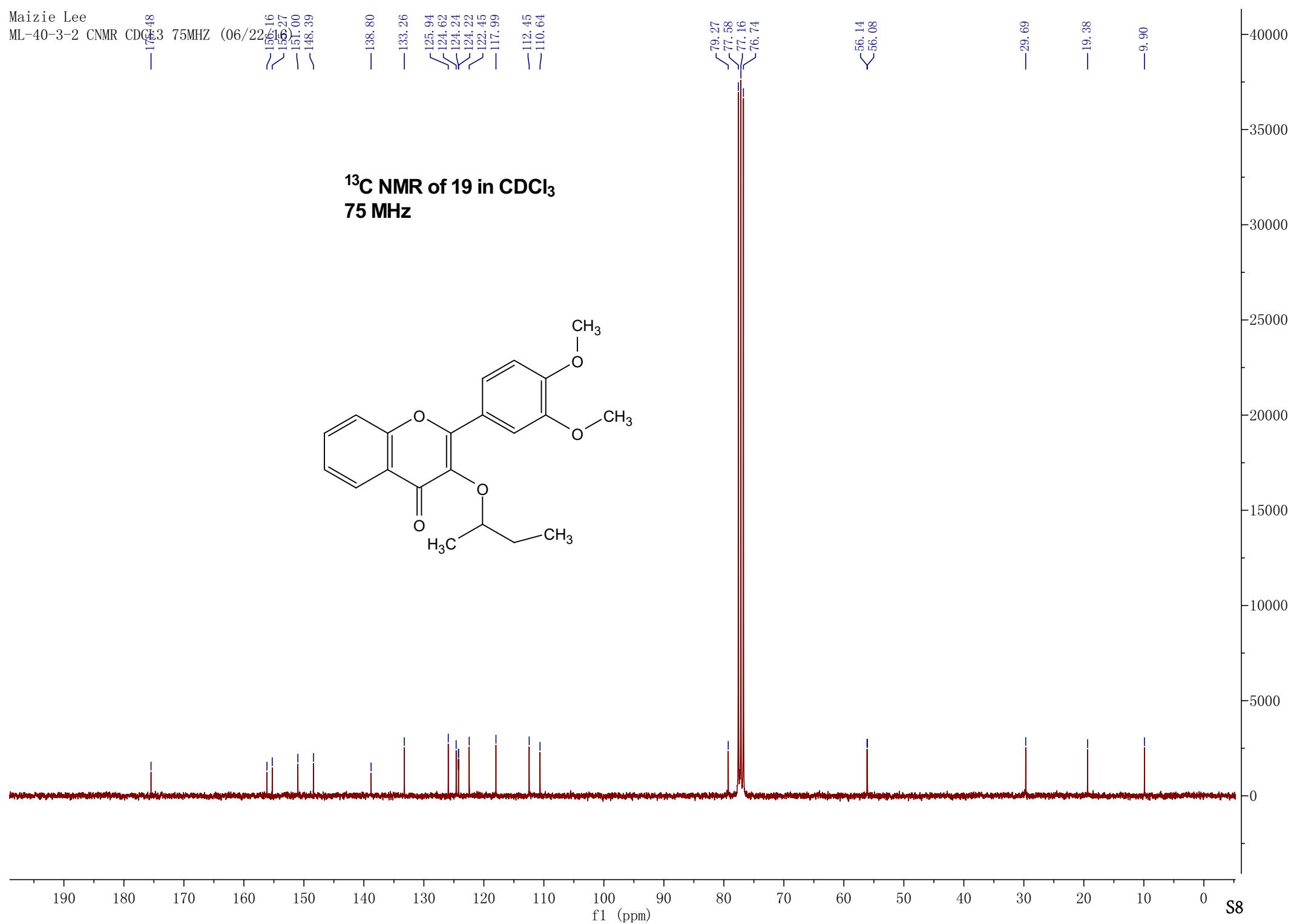
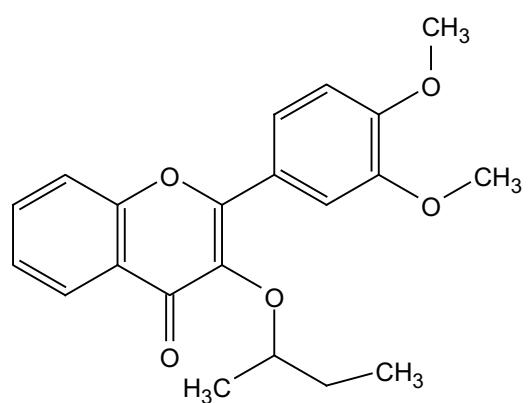
— 56.14  
— 56.08

— 29.69

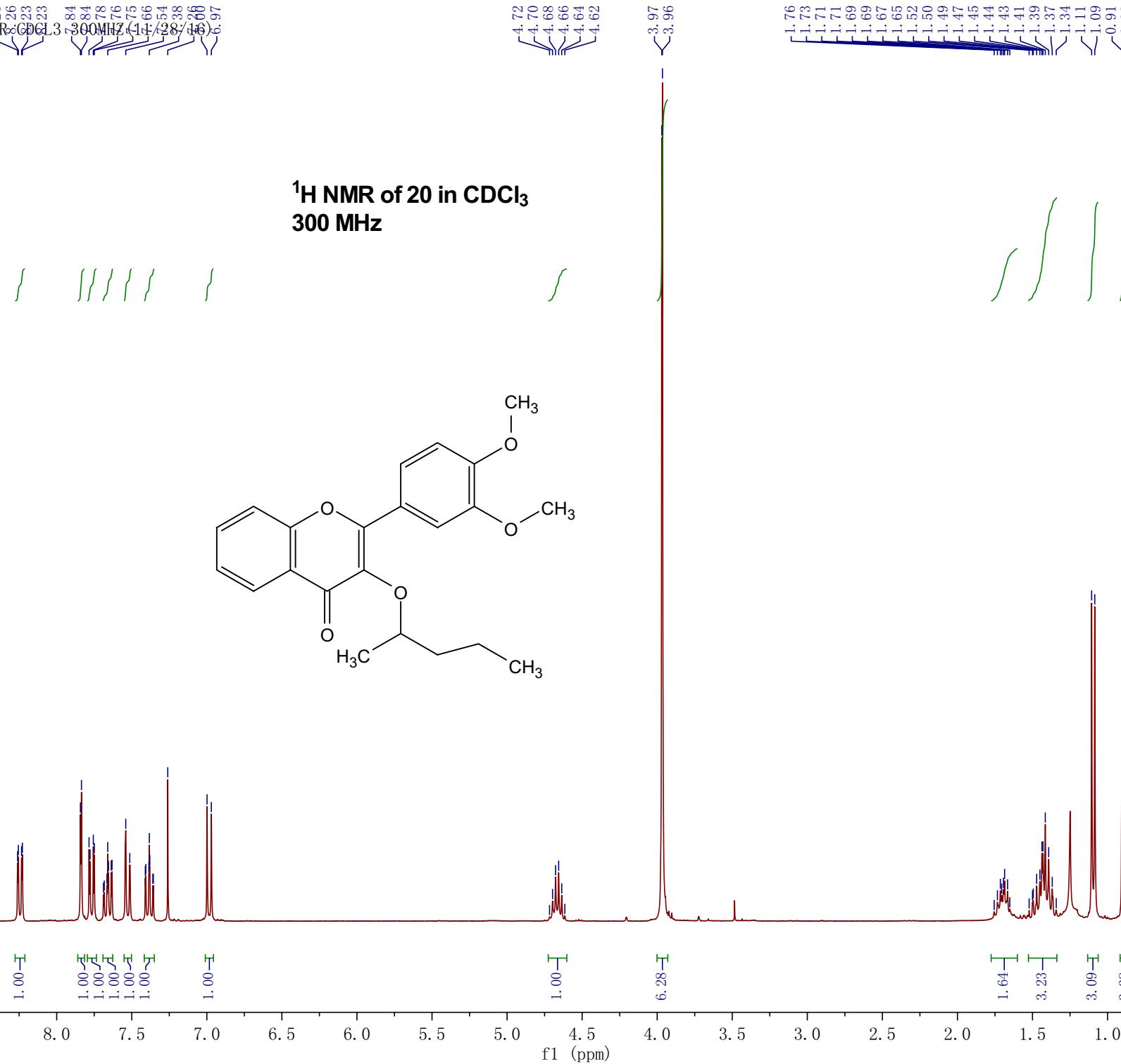
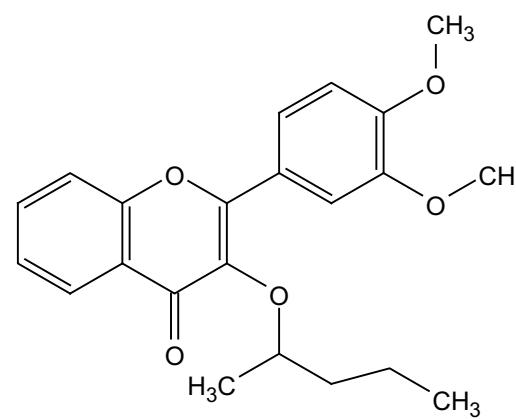
— 19.38

— 9.90

**<sup>13</sup>C NMR of 19 in CDCl<sub>3</sub>**  
**75 MHz**

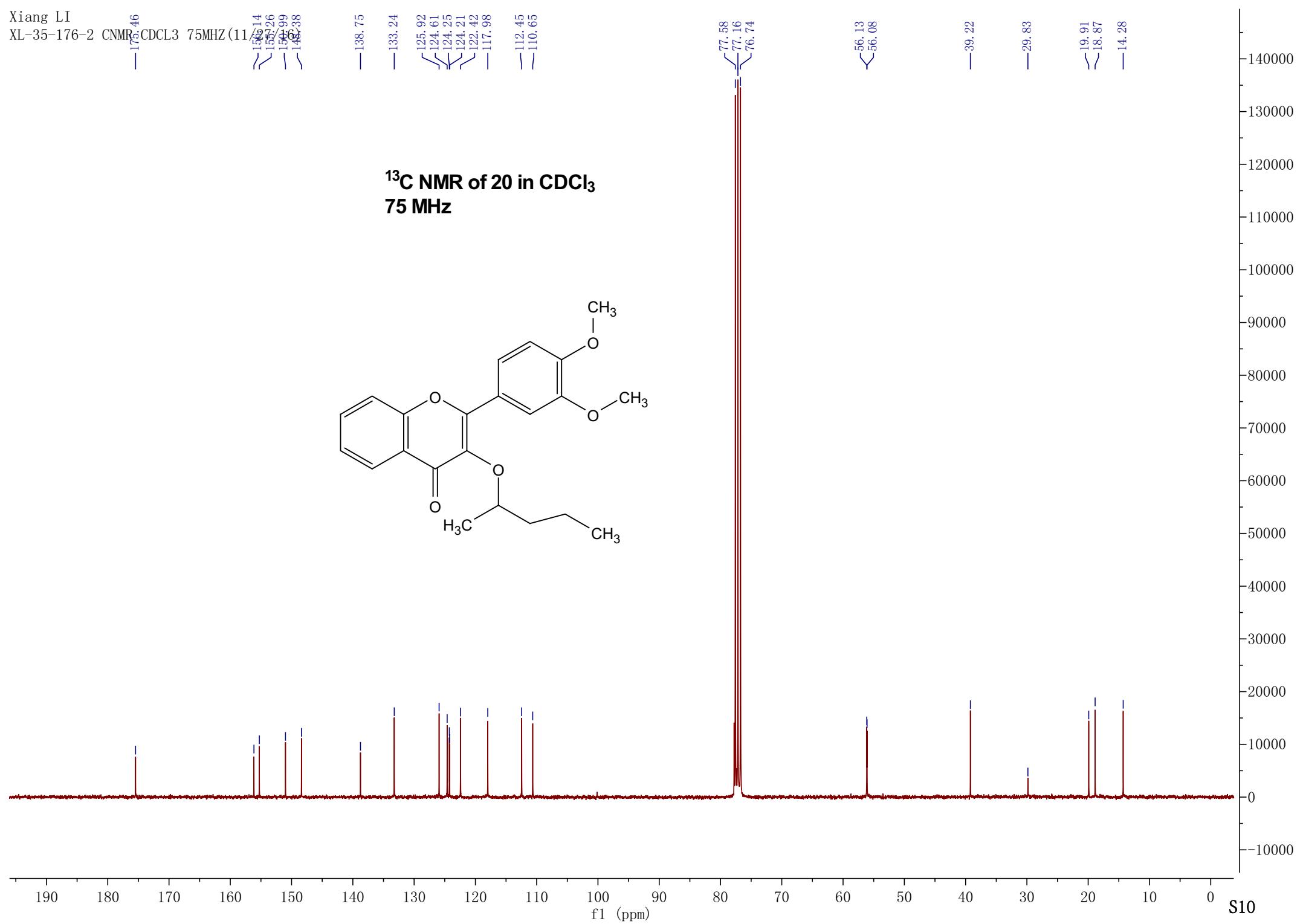
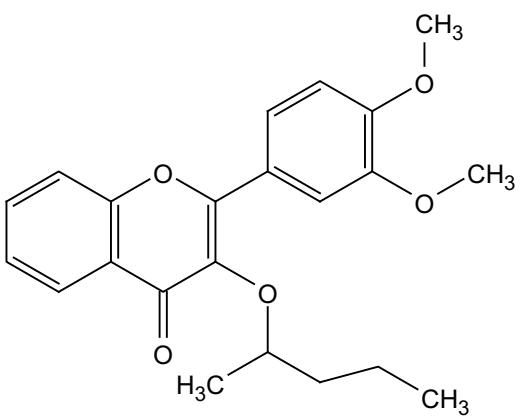


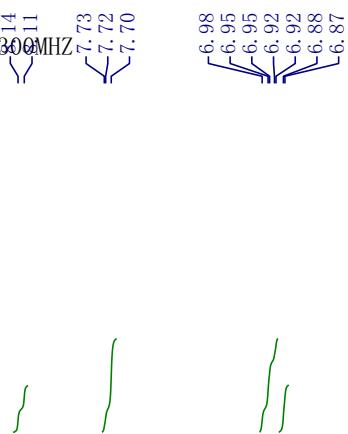
**<sup>1</sup>H NMR of 20 in CDCl<sub>3</sub>**  
**300 MHz**



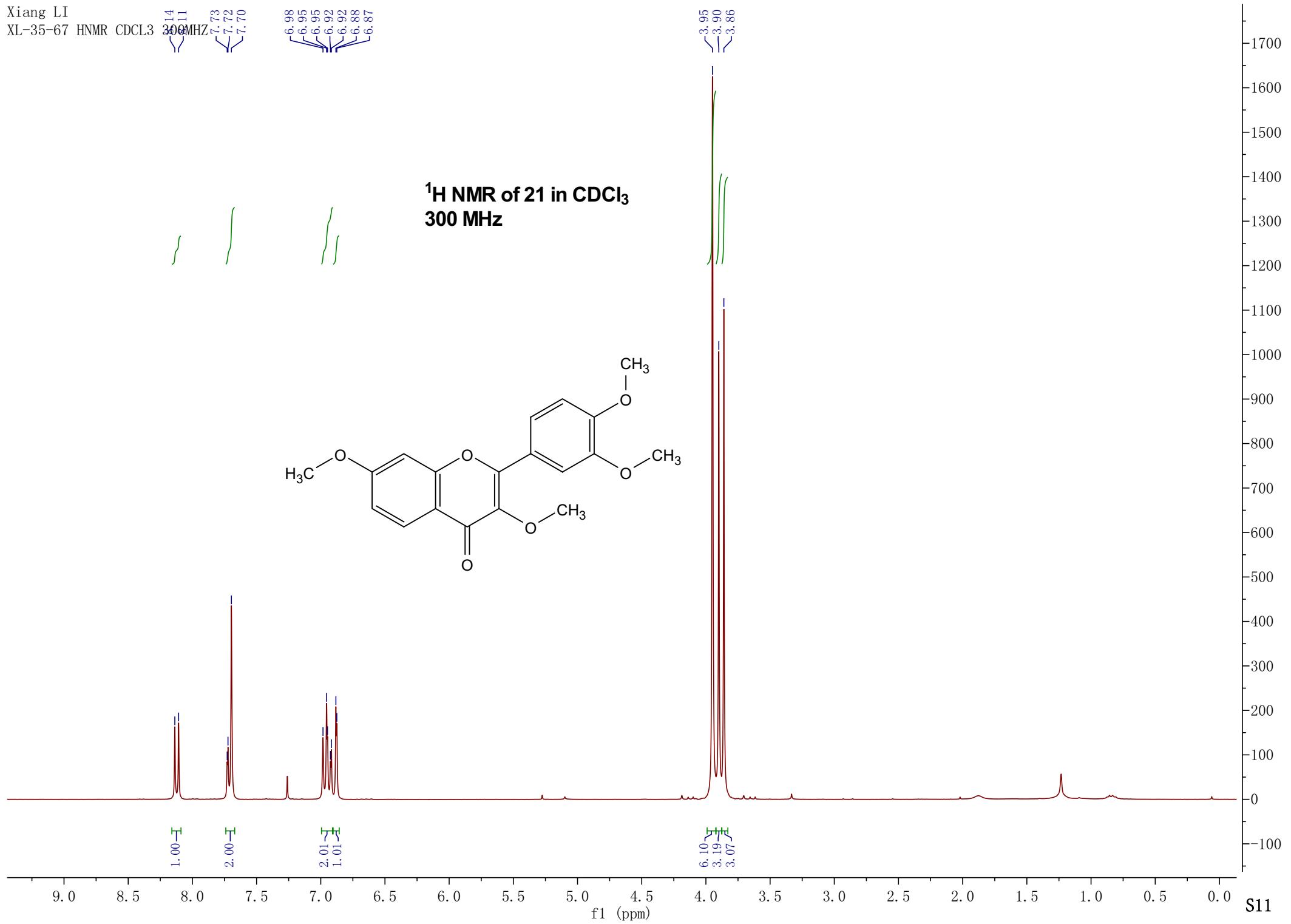
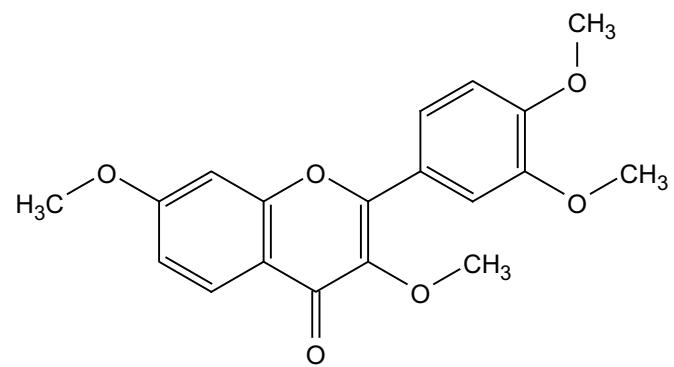
—175.46  
—158.14  
—157.26  
—156.99  
—146.66  
—142.38

**<sup>13</sup>C NMR of 20 in CDCl<sub>3</sub>**  
**75 MHz**





**<sup>1</sup>H NMR of 21 in CDCl<sub>3</sub>  
300 MHz**



—174.48

—164.03

~156.95  
~155.08  
~151.09  
~148.76

—140.81

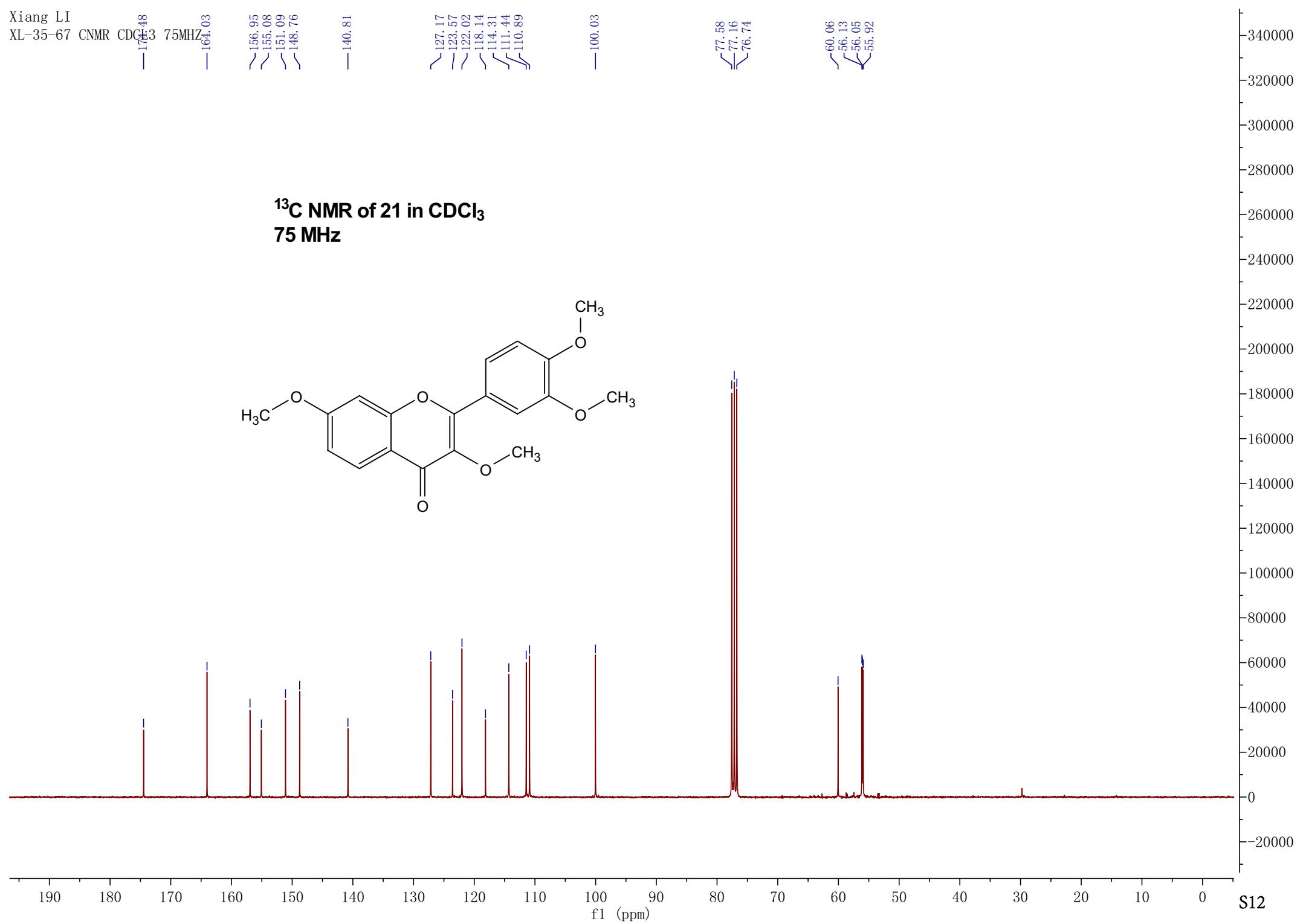
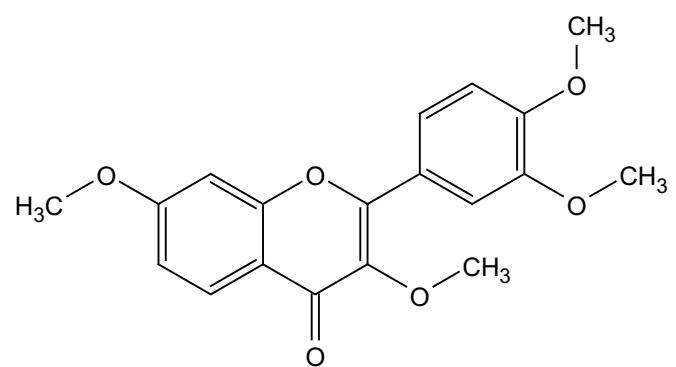
~127.17  
~123.57  
~122.02  
~118.14  
~114.31  
~111.44  
~110.89

—100.03

~77.58  
~77.16  
~76.74

~60.06  
~56.13  
~56.05  
~55.92

**<sup>13</sup>C NMR of 21 in CDCl<sub>3</sub>**  
**75 MHz**

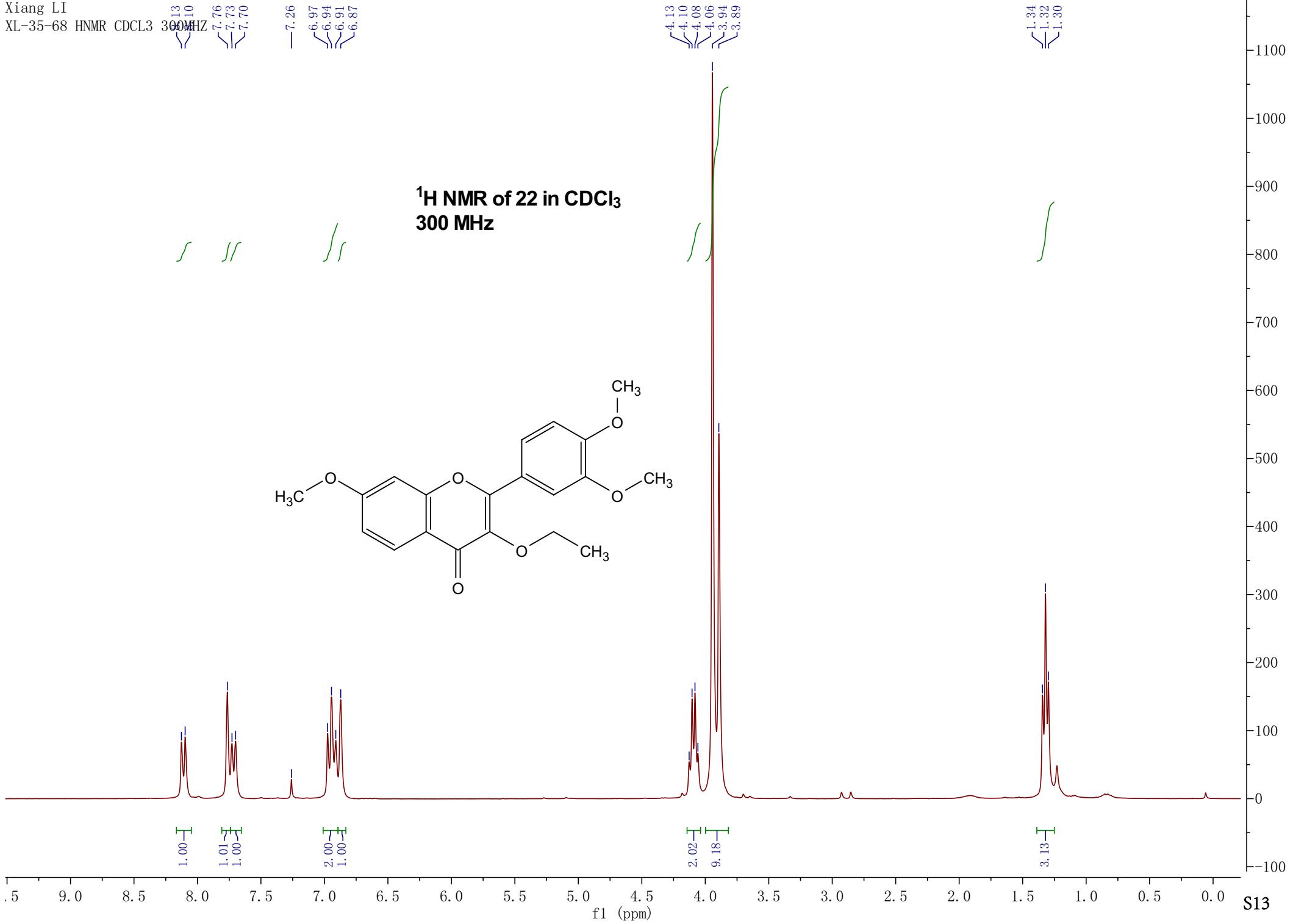
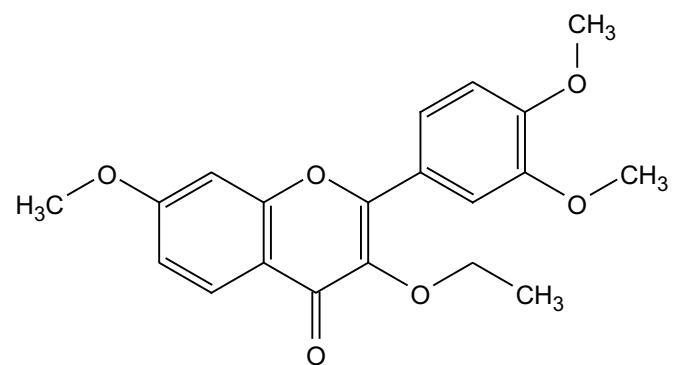


13  
10  
7.76  
7.73  
7.70  
7.26  
6.97  
6.94  
6.91  
6.87

4.13  
4.10  
4.08  
4.06  
3.94  
3.89

1.34  
1.32  
1.30

**<sup>1</sup>H NMR of 22 in CDCl<sub>3</sub>**  
**300 MHz**



—176.62  
—163.97  
—156.93  
—155.23  
—150.96  
—148.59

—139.80

~127.16  
~123.82  
~121.94  
~118.11  
~114.25  
~111.69  
~110.75

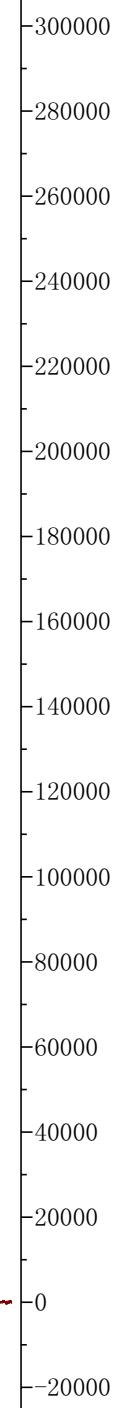
—99.99

77.58  
77.16  
76.74

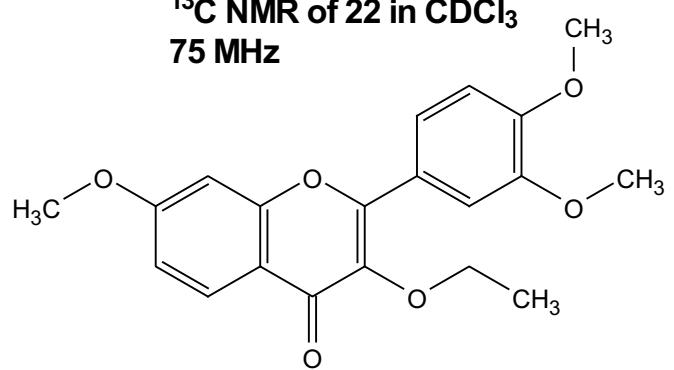
—68.35

56.09  
56.02  
55.90

—15.79



**<sup>13</sup>C NMR of 22 in CDCl<sub>3</sub>**  
**75 MHz**



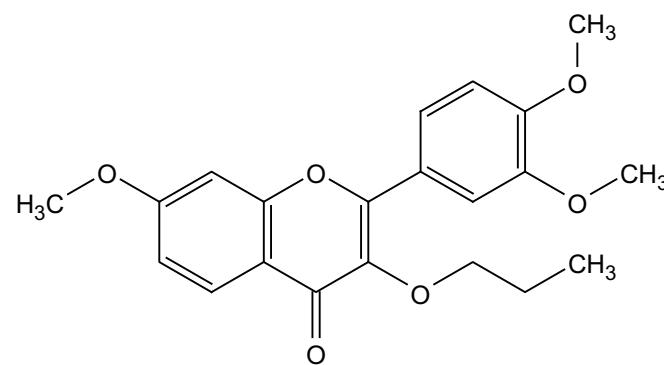
8.94  
8.123  
7.729  
7.723  
7.716  
7.688  
7.681  
7.260  
6.971  
6.943  
6.937  
6.914  
6.907  
6.873  
6.865

3.992  
3.969  
3.941  
3.890

1.790  
1.765  
1.742  
1.717  
1.694  
1.670

0.945  
0.920  
0.895

**<sup>1</sup>H NMR of 23 in CDCl<sub>3</sub>**  
**300 MHz**



{ { } }

{ }

{ }

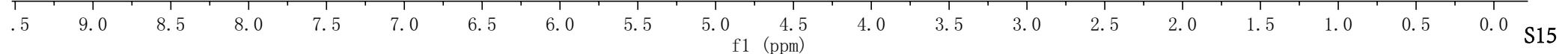
{ }

1.00  
2.05  
2.08  
1.02

2.07  
6.19  
3.19

2.11

3.09



—175.59  
—168.95

~156.93  
~155.17  
~150.95  
~148.57

—140.00

~127.14  
~123.81  
~122.04  
~118.15  
~114.25  
~111.74  
~110.72

—99.98

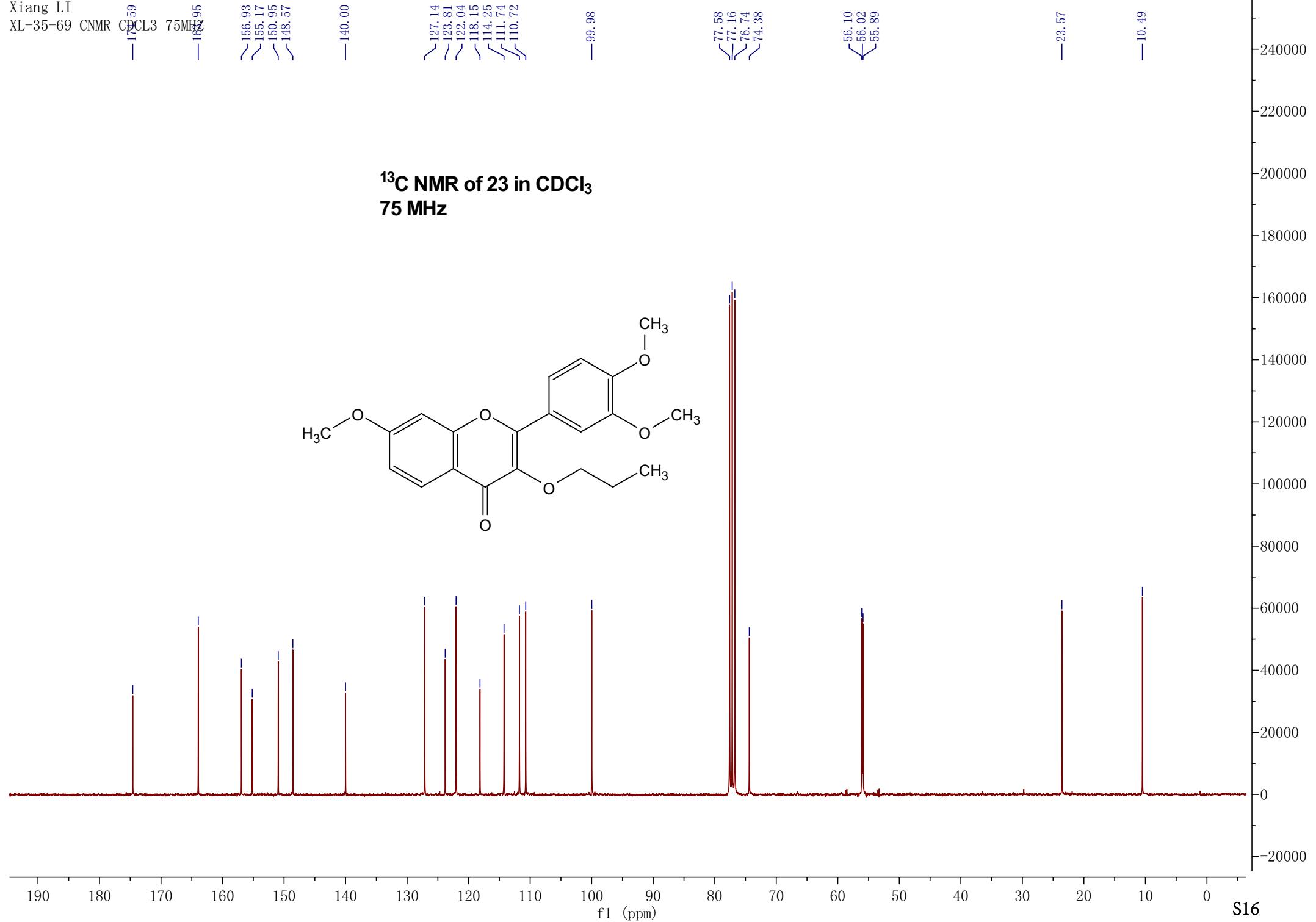
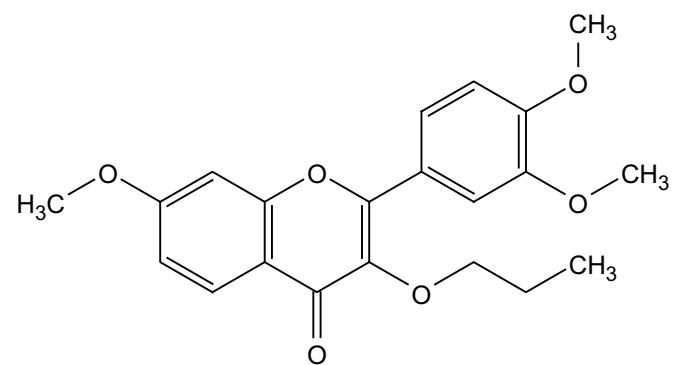
77.58  
77.16  
76.74  
74.38

56.10  
56.02  
55.89

—23.57

—10.49

**<sup>13</sup>C NMR of 23 in CDCl<sub>3</sub>**  
**75 MHz**

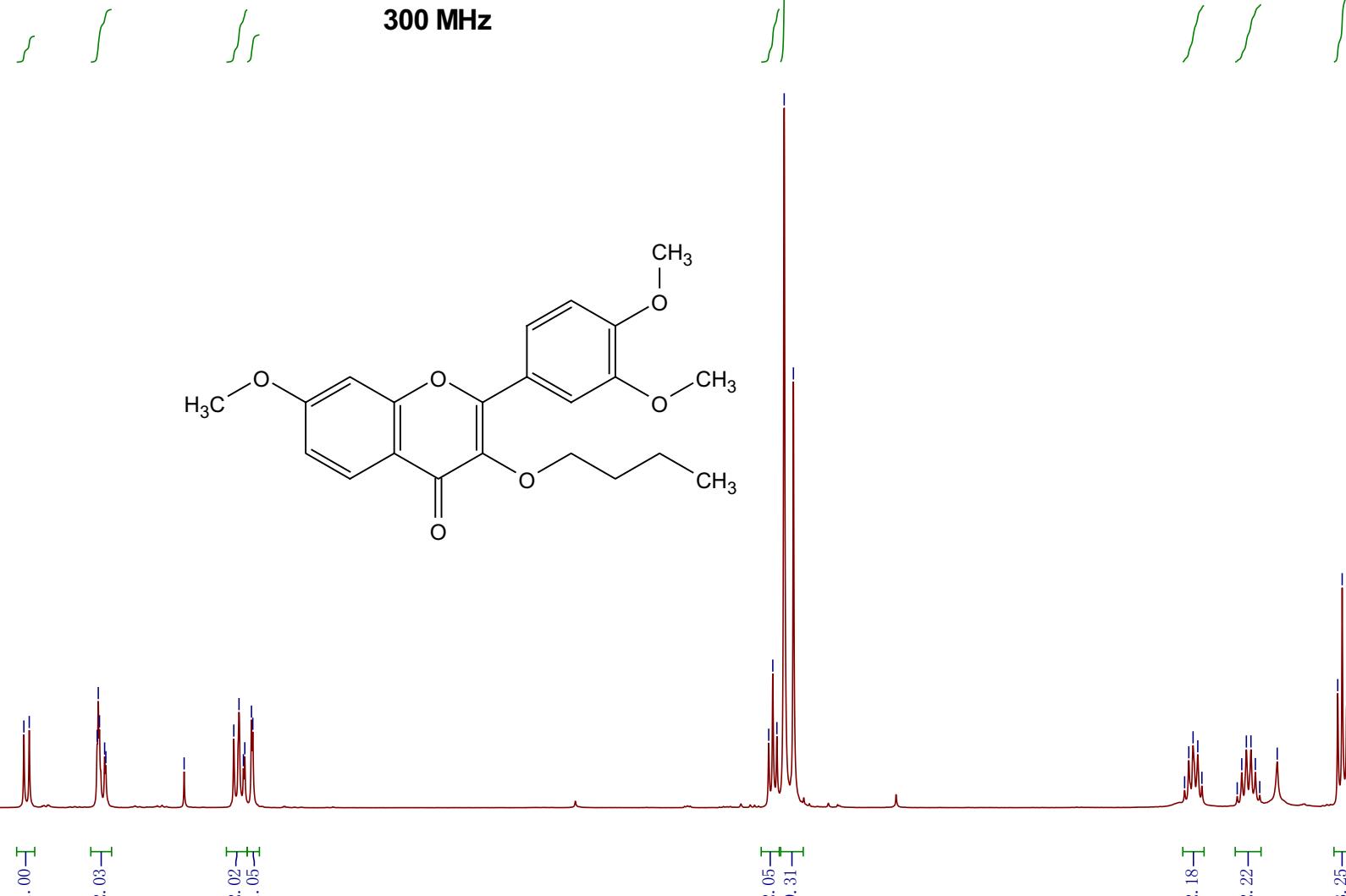
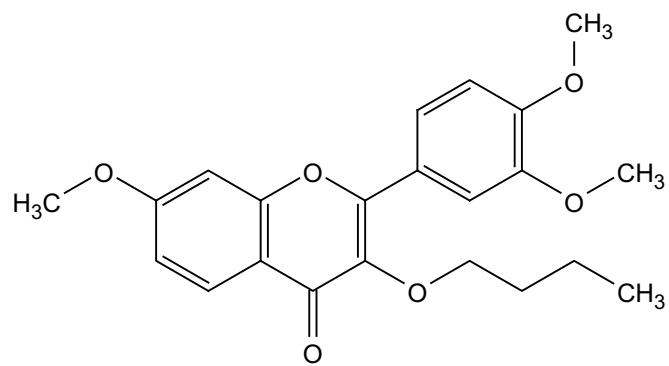


8.442  
8.113  
7.739  
7.733  
7.726  
7.698  
7.691  
7.260  
6.987  
6.958  
6.934  
6.926  
6.889  
6.882

4.041  
4.018  
3.996  
3.955  
3.905

1.750  
1.727  
1.704  
1.678  
1.655  
1.461  
1.436  
1.410  
1.385  
1.361  
1.337  
1.240  
0.907  
0.883  
0.858

**<sup>1</sup>H NMR of 24 in CDCl<sub>3</sub>**  
**300 MHz**



Xiang LI  
XL-35-70 €NMR CDCl<sub>3</sub> 75MHz

— 174.54  
— 163.88  
— 155.15  
— 150.88  
— 148.51

— 139.97

— 127.11  
— 123.76  
— 121.95  
— 118.11  
— 114.18  
— 111.68  
— 110.66

— 99.93

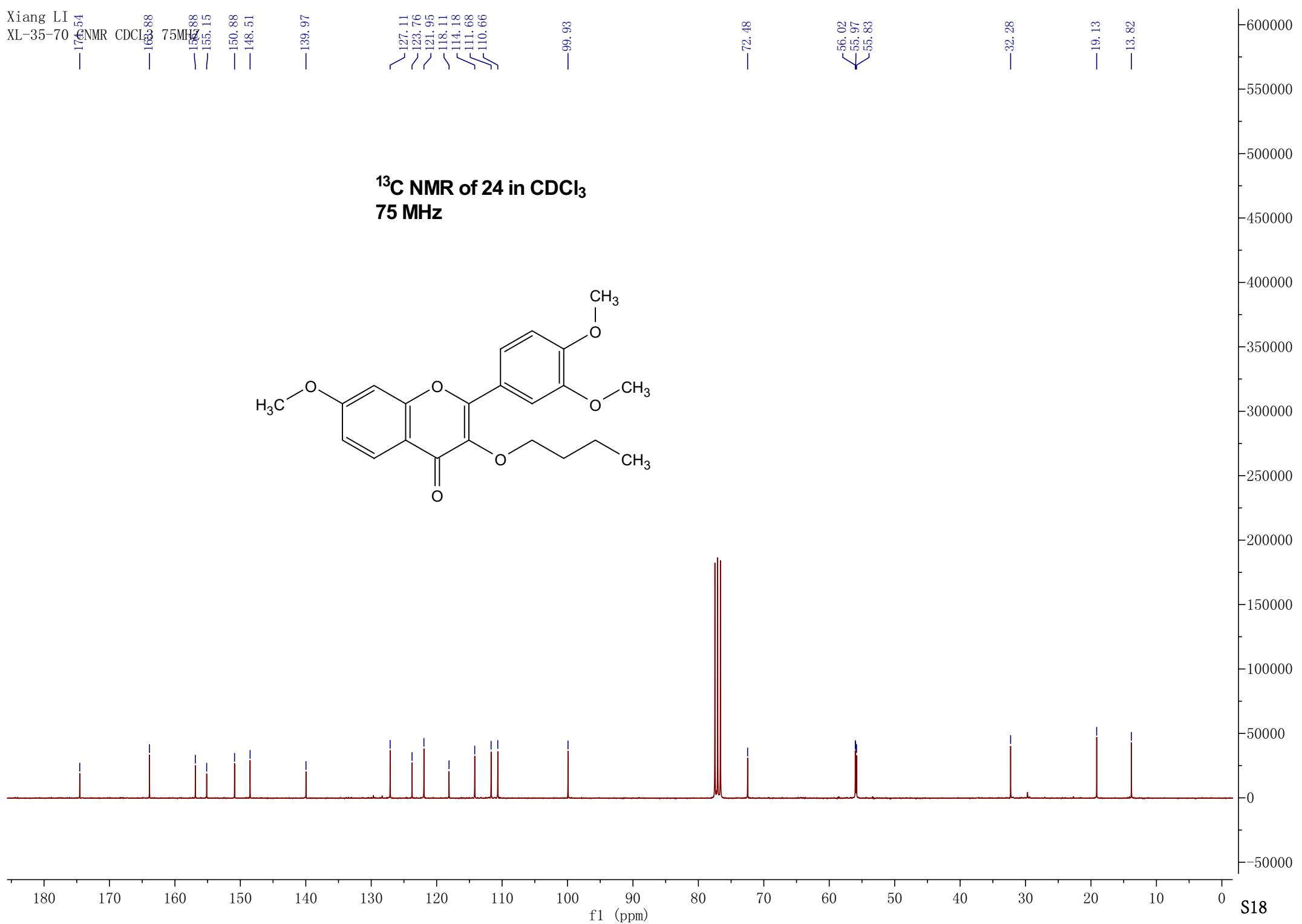
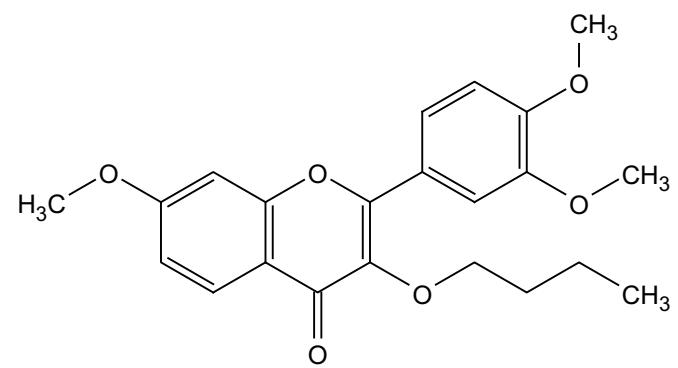
— 72.48

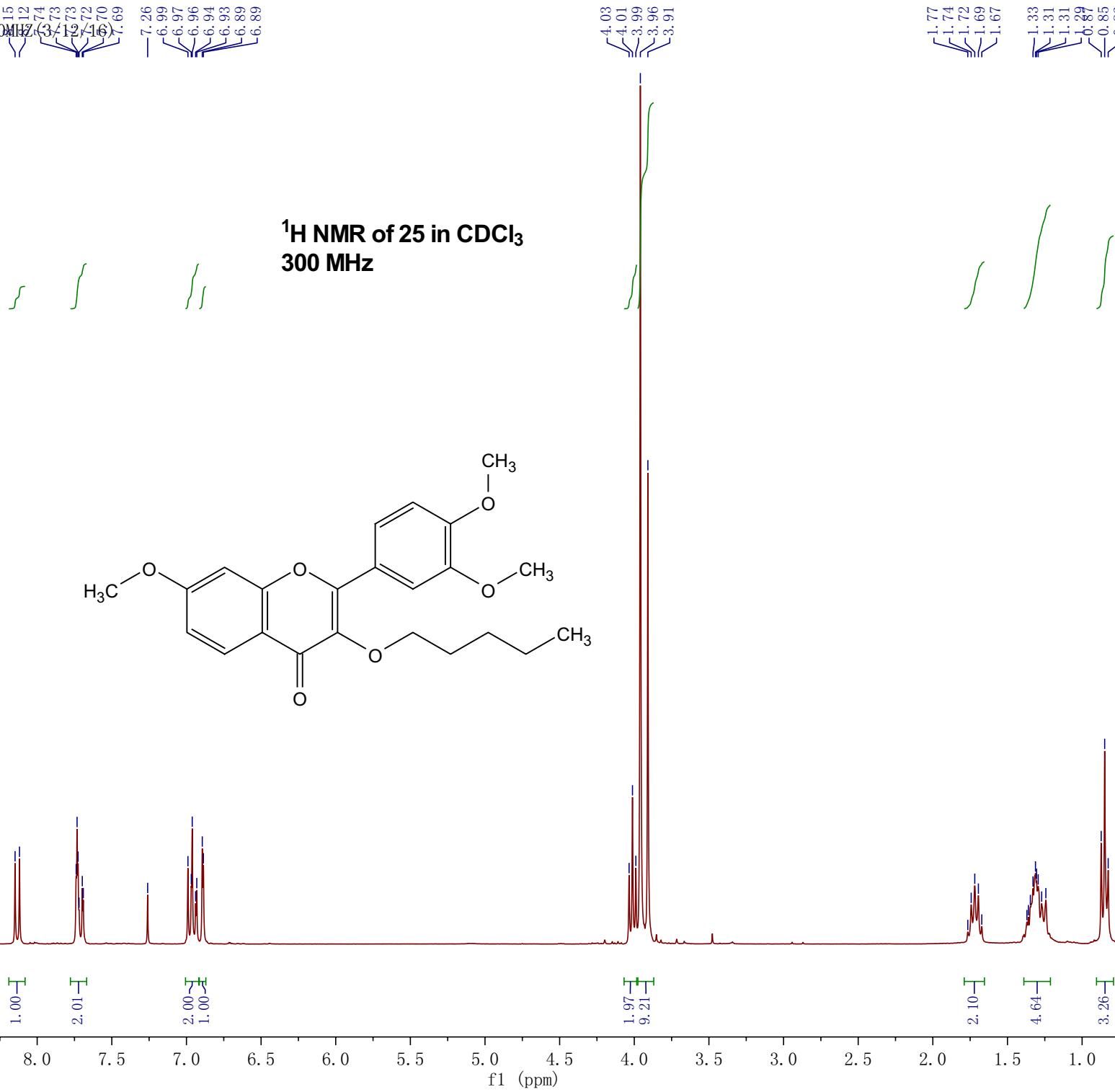
— 56.02  
— 55.97  
— 55.83

— 32.28

— 19.13  
— 13.82

**<sup>13</sup>C NMR of 24 in CDCl<sub>3</sub>**  
**75 MHz**





Xiang LI

XL-35-71 CNMR CDCl<sub>3</sub> 75MHz (3/16)

-176.65  
-167.99  
-154.00  
-153.29  
-151.66  
-150.99  
-148.63

-140.08

~127.23  
~123.88  
~122.07  
~118.23  
~114.30  
~111.80  
~110.76

-100.04

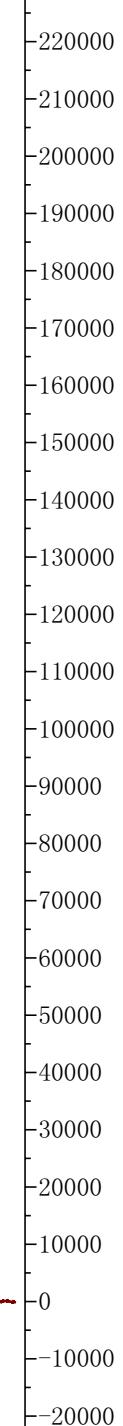
77.58  
77.16  
76.74  
72.89

56.14  
56.08  
55.95

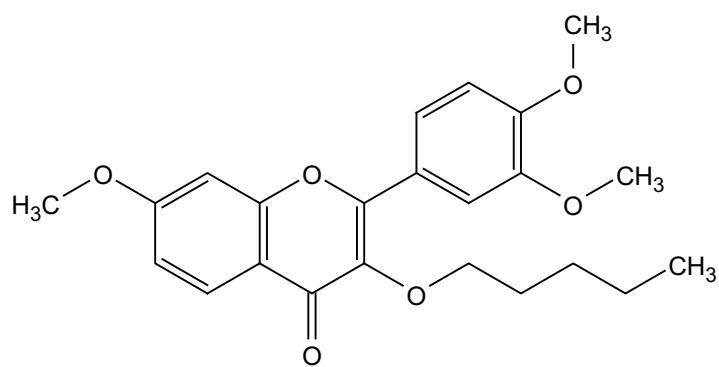
-30.05  
-28.20

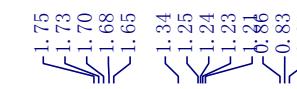
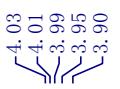
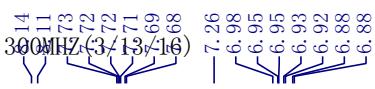
-22.56

-14.12

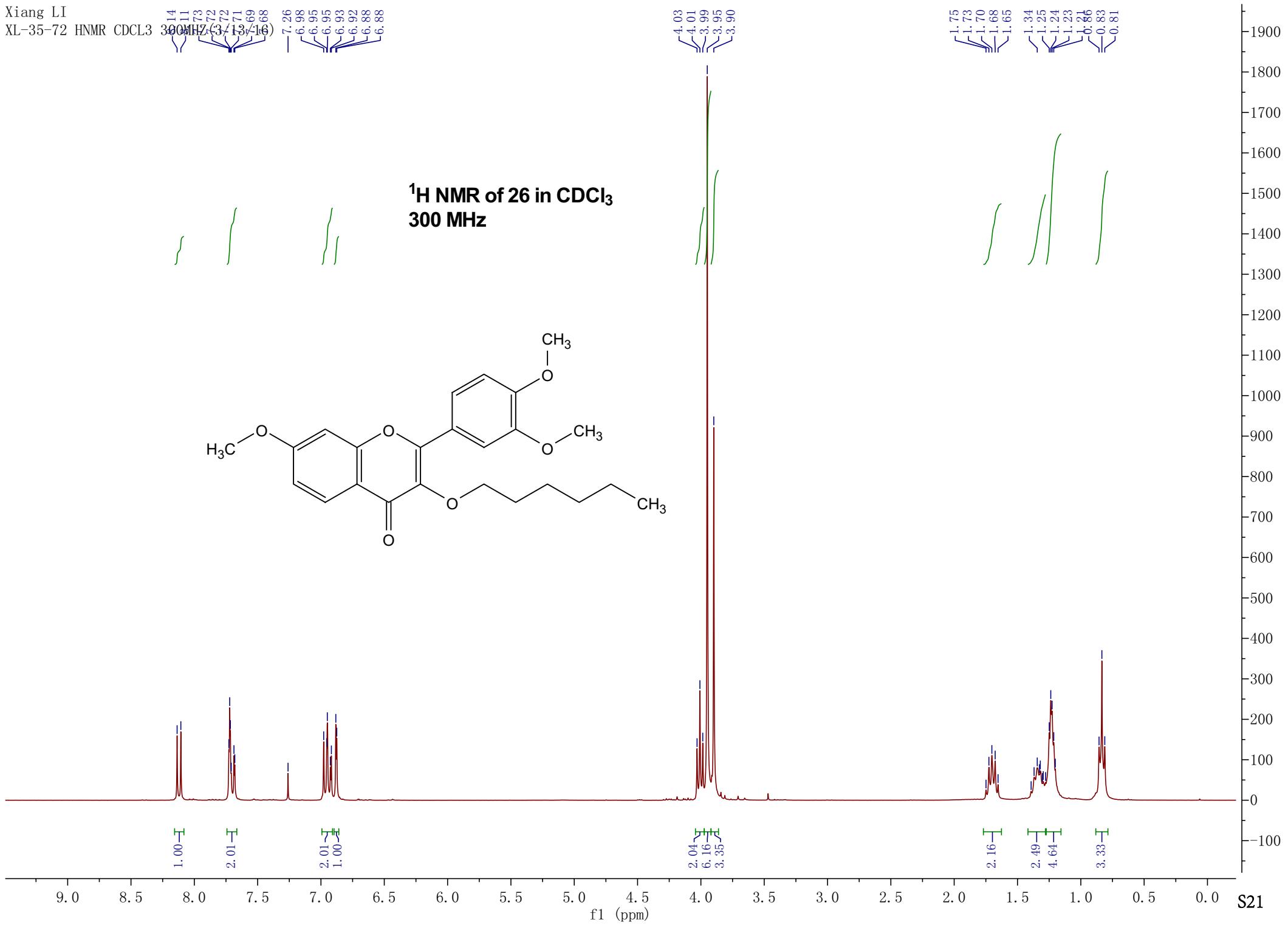
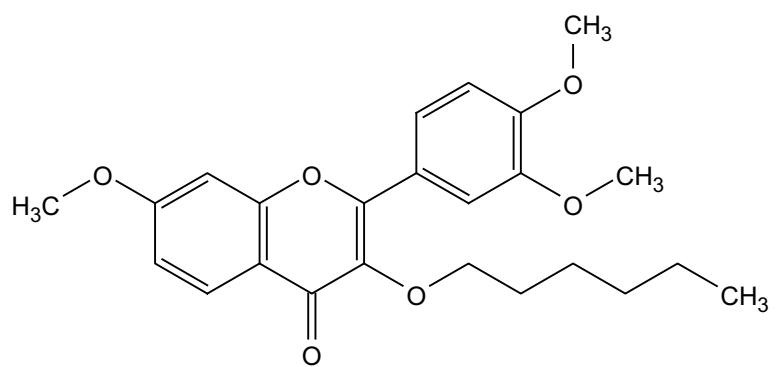


**<sup>13</sup>C NMR of 25 in CDCl<sub>3</sub>  
75 MHz**





**<sup>1</sup>H NMR of 26 in CDCl<sub>3</sub>**  
**300 MHz**



— 174.62  
 — 163.96  
 — 158.26  
 — 152.26  
 — 150.95  
 — 148.59

— 140.04

~ 127.18  
 ~ 123.84  
 ~ 122.05  
 ~ 118.19  
 ~ 114.27  
 ~ 111.76  
 ~ 110.71

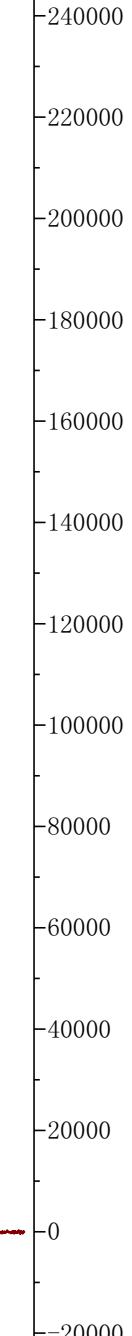
— 100.00

~ 77.58  
 ~ 77.16  
 ~ 76.74  
 ~ 72.91

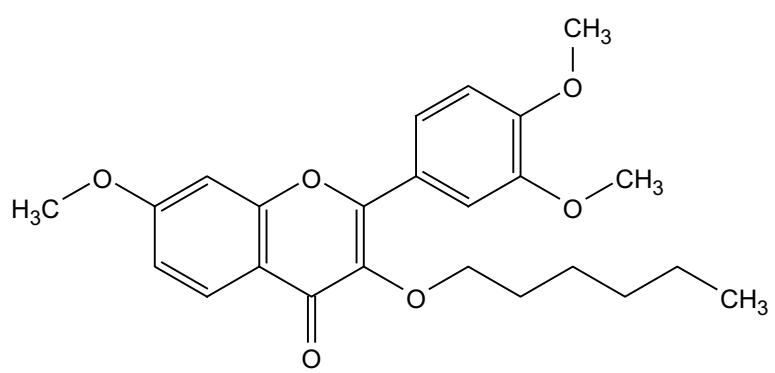
~ 56.11  
 ~ 56.04  
 ~ 55.91

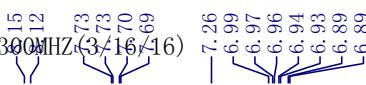
— 31.70  
 — 30.31  
 — 25.73  
 — 22.68

— 14.11



**<sup>13</sup>C NMR of 26 in CDCl<sub>3</sub>**  
**75 MHz**

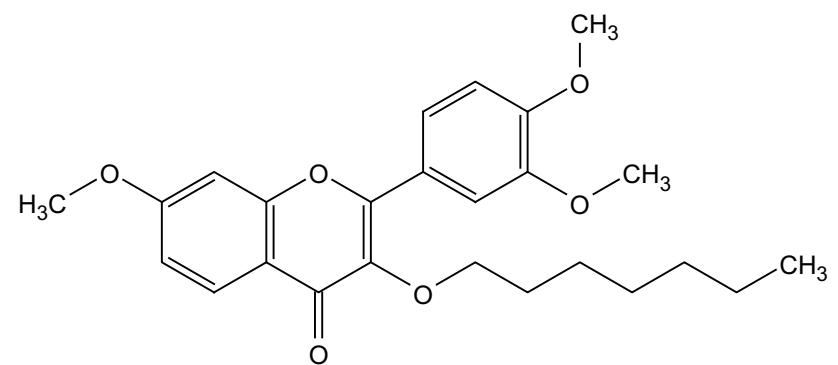




4.04  
4.02  
3.99  
3.96  
3.91

1.76  
1.73  
1.71  
1.68  
1.66

<sup>1</sup>H NMR of 27 in CDCl<sub>3</sub>  
300 MHz



1.00  
2.01  
2.08  
1.00

2.10  
6.27  
3.13

2.19  
2.46  
7.74  
3.33

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5

f1 (ppm)

S23

1900  
1800  
1700  
1600  
1500  
1400  
1300  
1200  
1100  
1000  
900  
800  
700  
600  
500  
400  
300  
200  
100  
0  
-100

—176.67  
 —162.00  
 —155.01  
 —156.31  
 —150.99  
 —148.63

—140.09

~127.25  
 ~123.89  
 ~122.09  
 ~118.24  
 ~114.30  
 ~111.81  
 ~110.74

—100.05

77.58  
 77.16  
 76.74  
 72.96

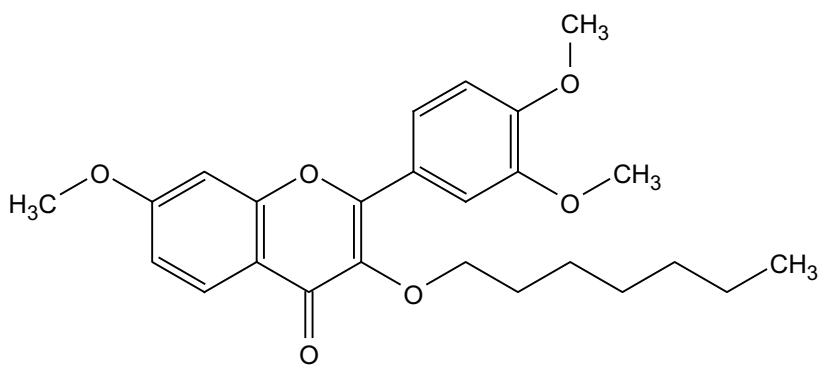
56.15  
 56.07  
 55.95

~31.91  
 ~30.38  
 ~29.20  
 ~26.05  
 ~22.69

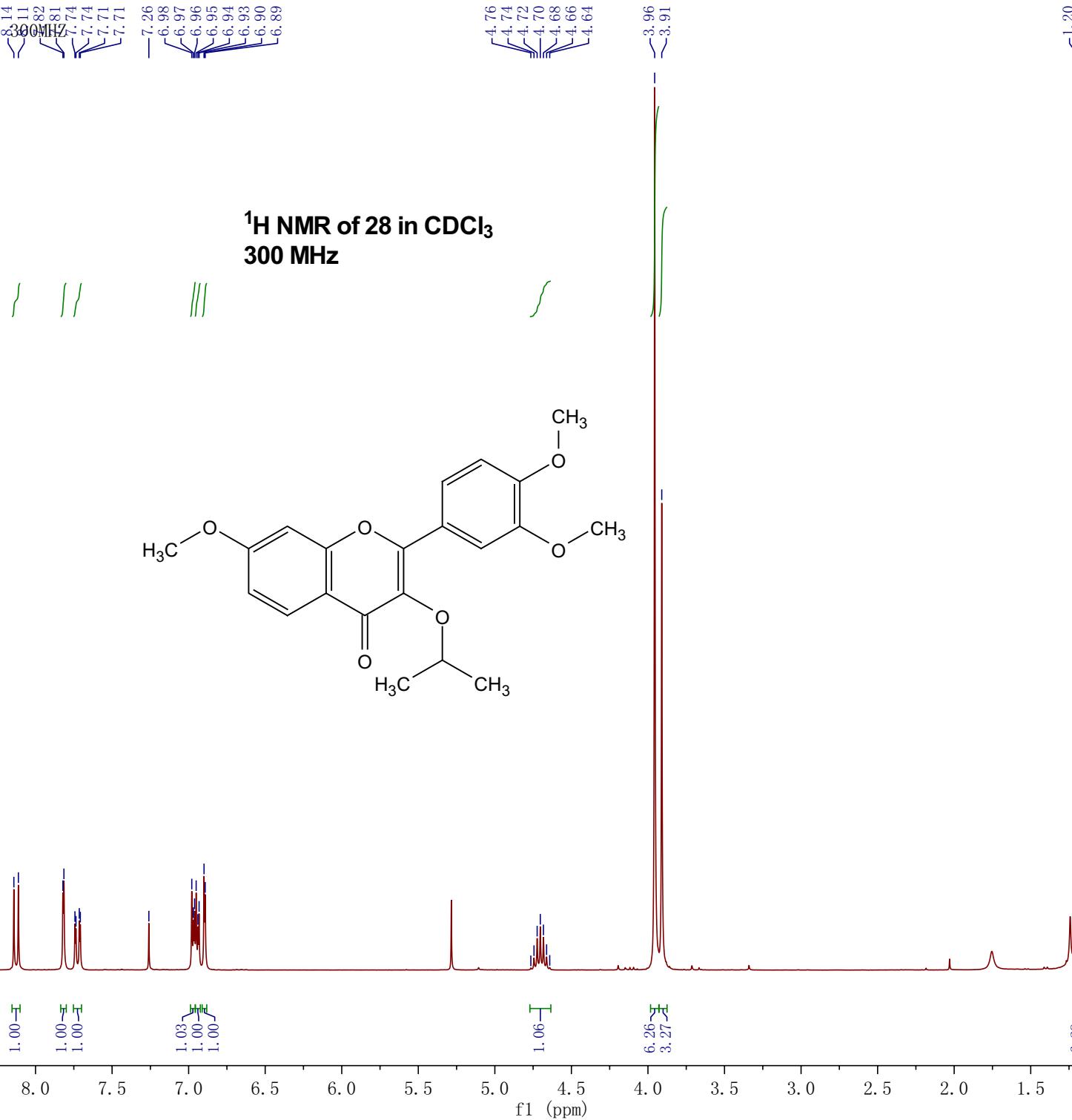
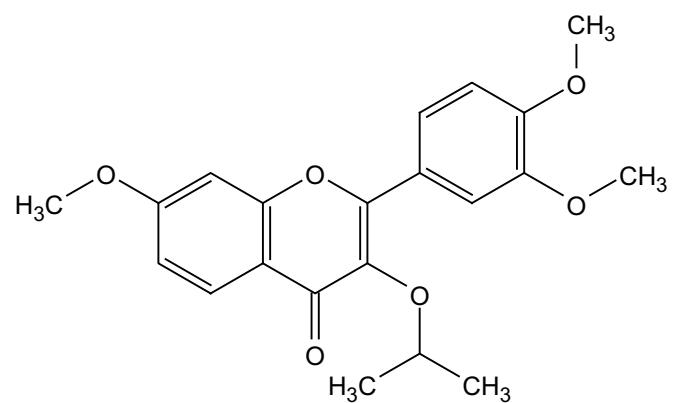
—14.19

210000  
200000  
190000  
180000  
170000  
160000  
150000  
140000  
130000  
120000  
110000  
100000  
90000  
80000  
70000  
60000  
50000  
40000  
30000  
20000  
10000  
0

**<sup>13</sup>C NMR of 27 in CDCl<sub>3</sub>**  
**75 MHz**



**<sup>1</sup>H NMR of 28 in CDCl<sub>3</sub>**  
**300 MHz**



S25

— 177.98  
— 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

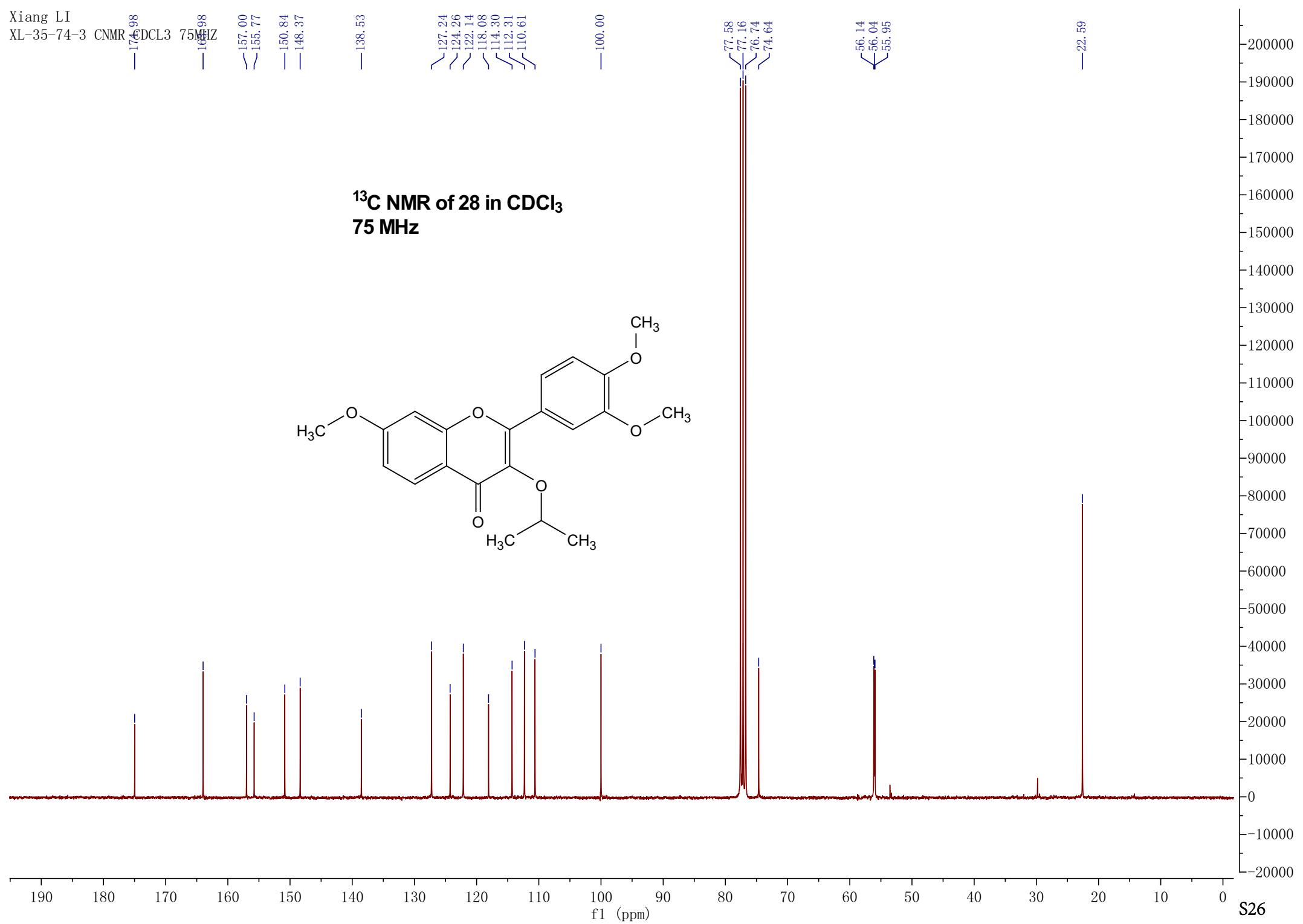
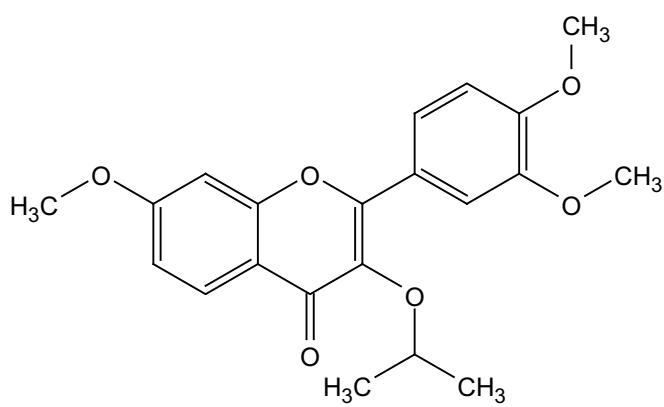
— 100.00

— 77.58  
— 77.16  
— 76.74  
— 74.64

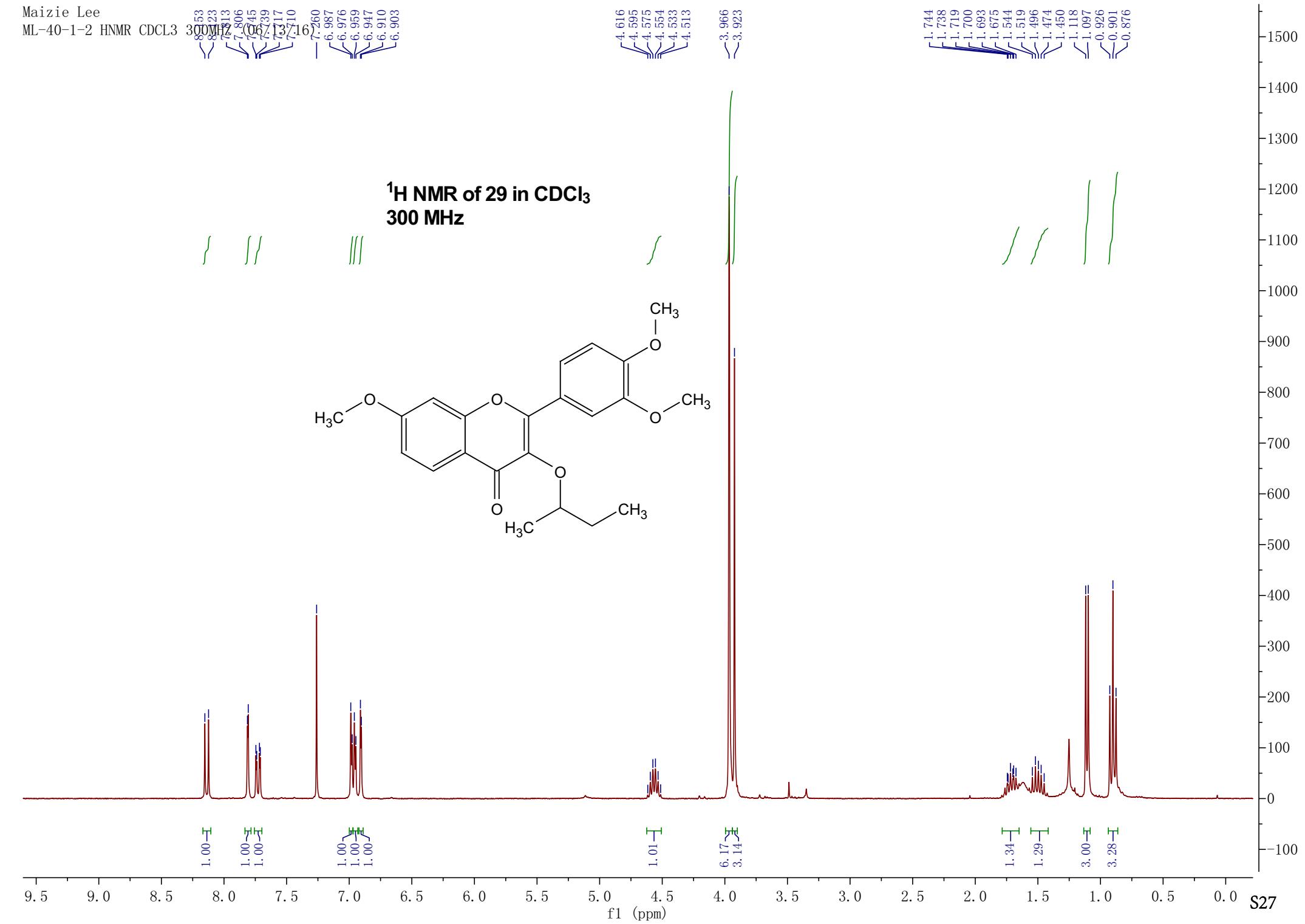
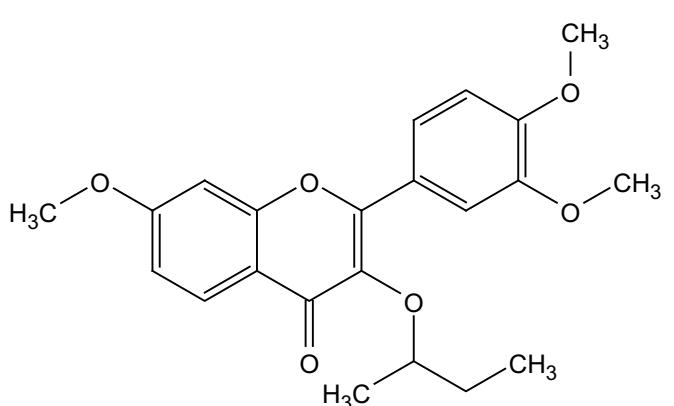
— 56.14  
— 56.04  
— 55.95

— 22.59

**<sup>13</sup>C NMR of 28 in CDCl<sub>3</sub>**  
**75 MHz**



**<sup>1</sup>H NMR of 29 in CDCl<sub>3</sub>**  
**300 MHz**



DCL3 75MHz (06/00-15/16/17/18/1985)

— 138. 57 —

— 99.99 —

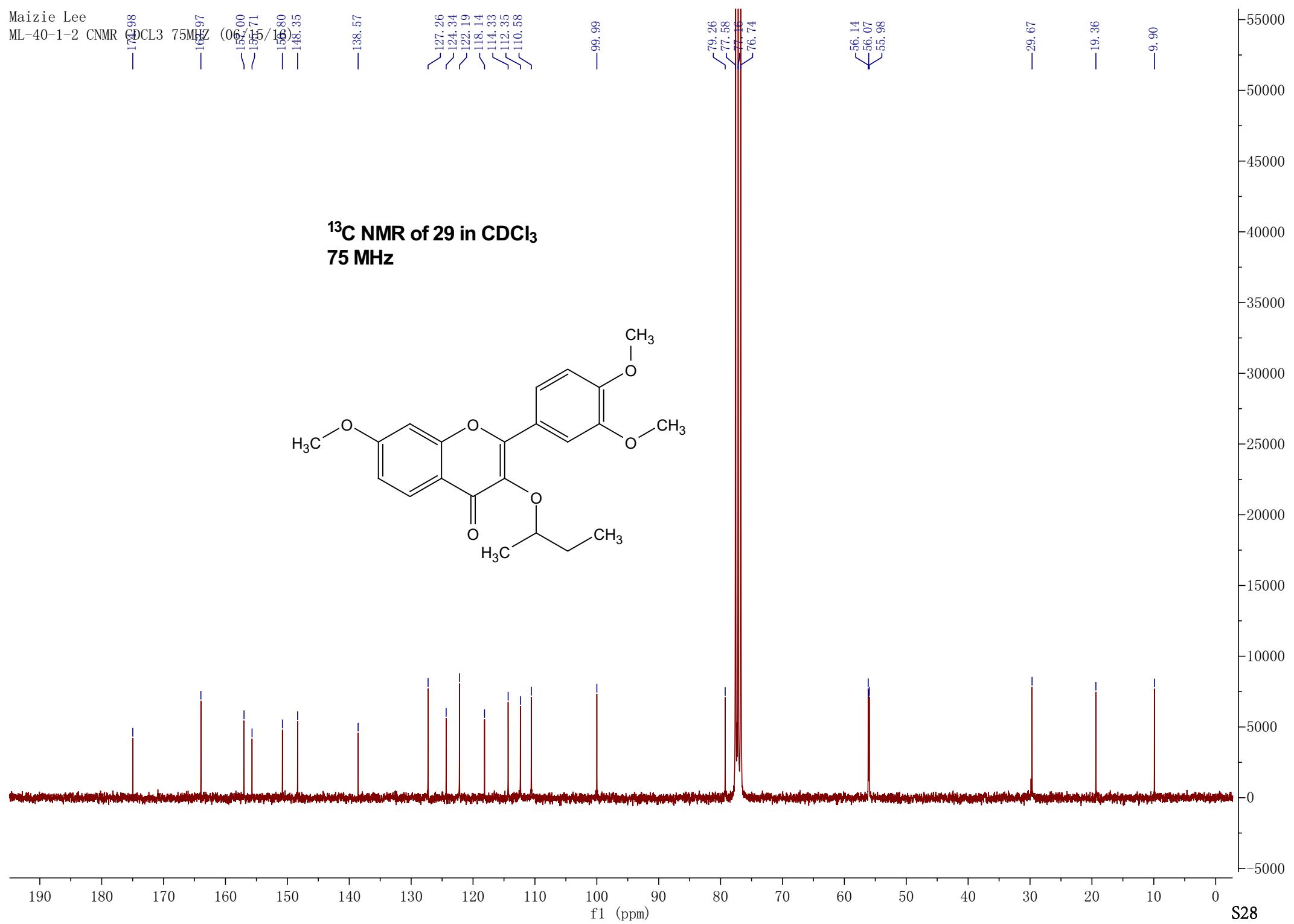
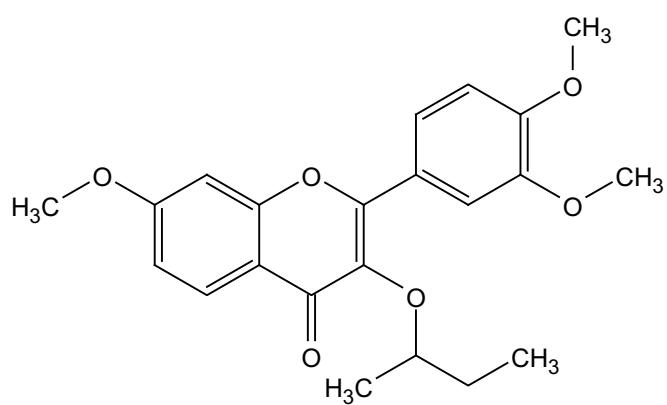
76.74

56. 14  
56. 07  
55. 98

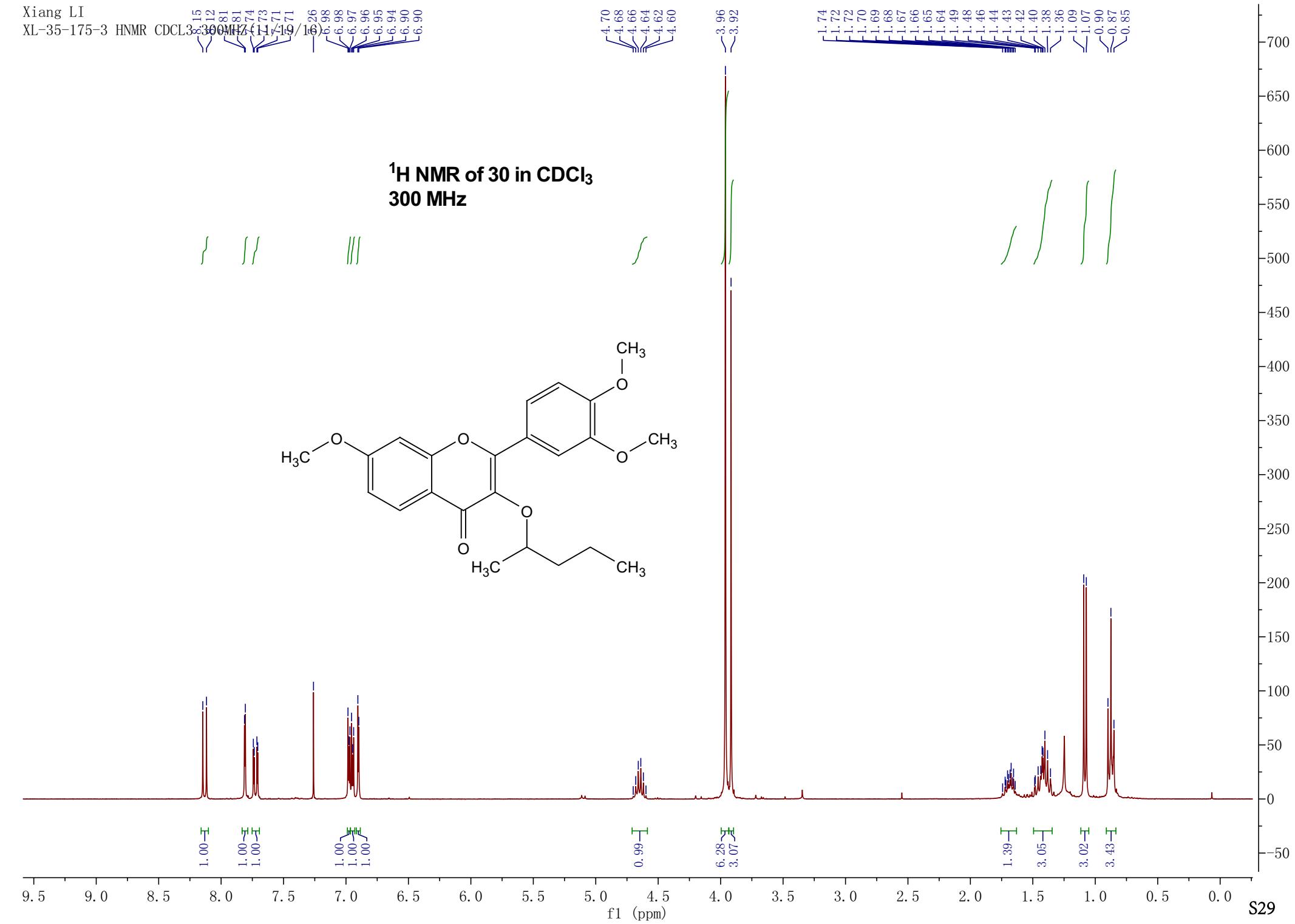
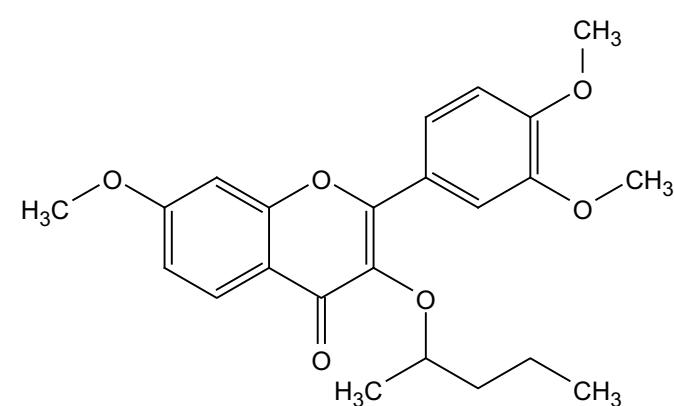
—29.67

a 00

**<sup>13</sup>C NMR of 29 in CDCl<sub>3</sub>  
75 MHz**



**$^1\text{H}$  NMR of 30 in  $\text{CDCl}_3$   
300 MHz**



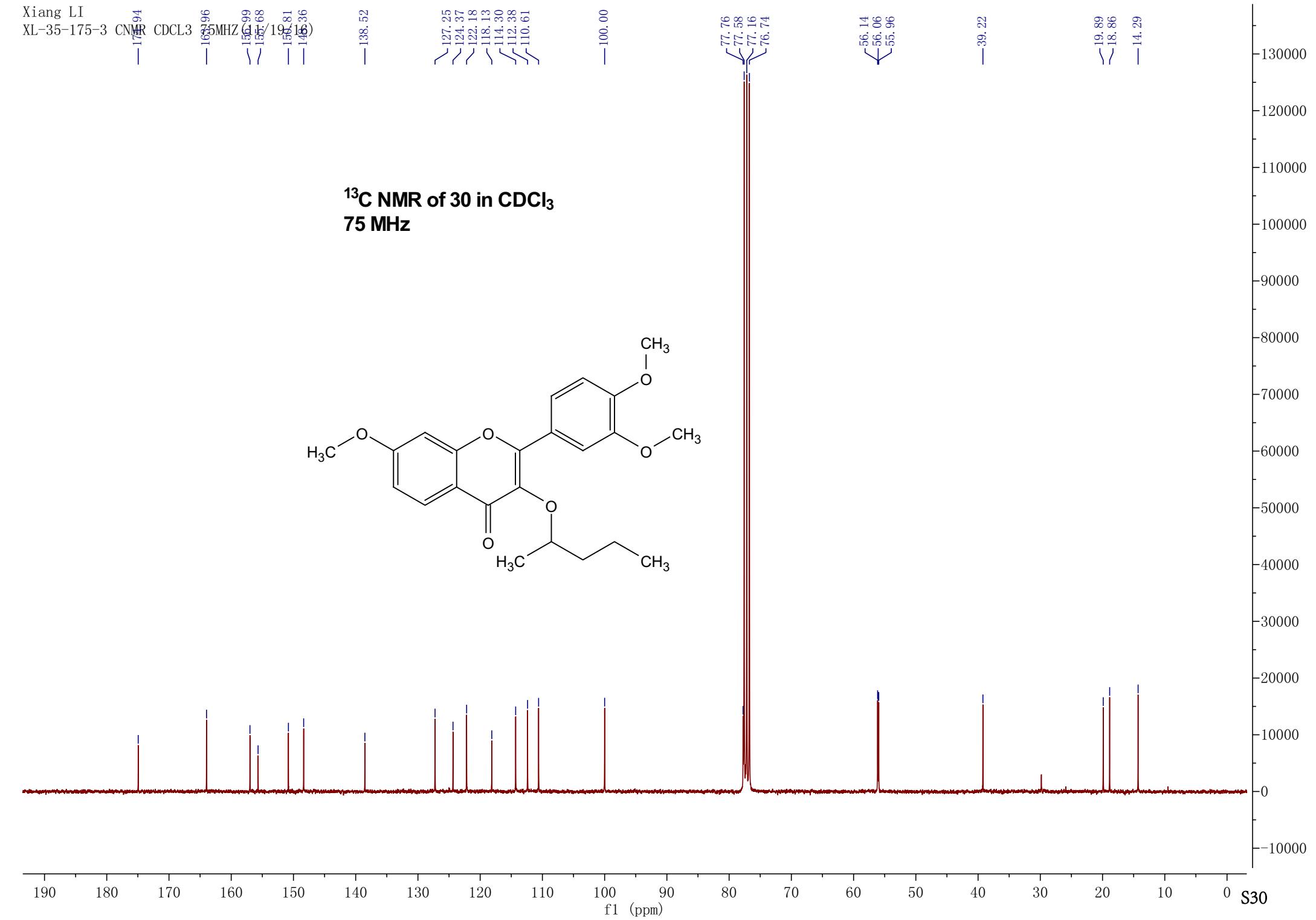
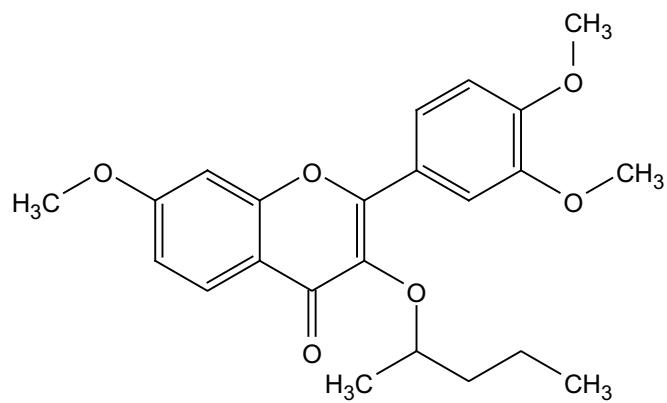
Xiang LI

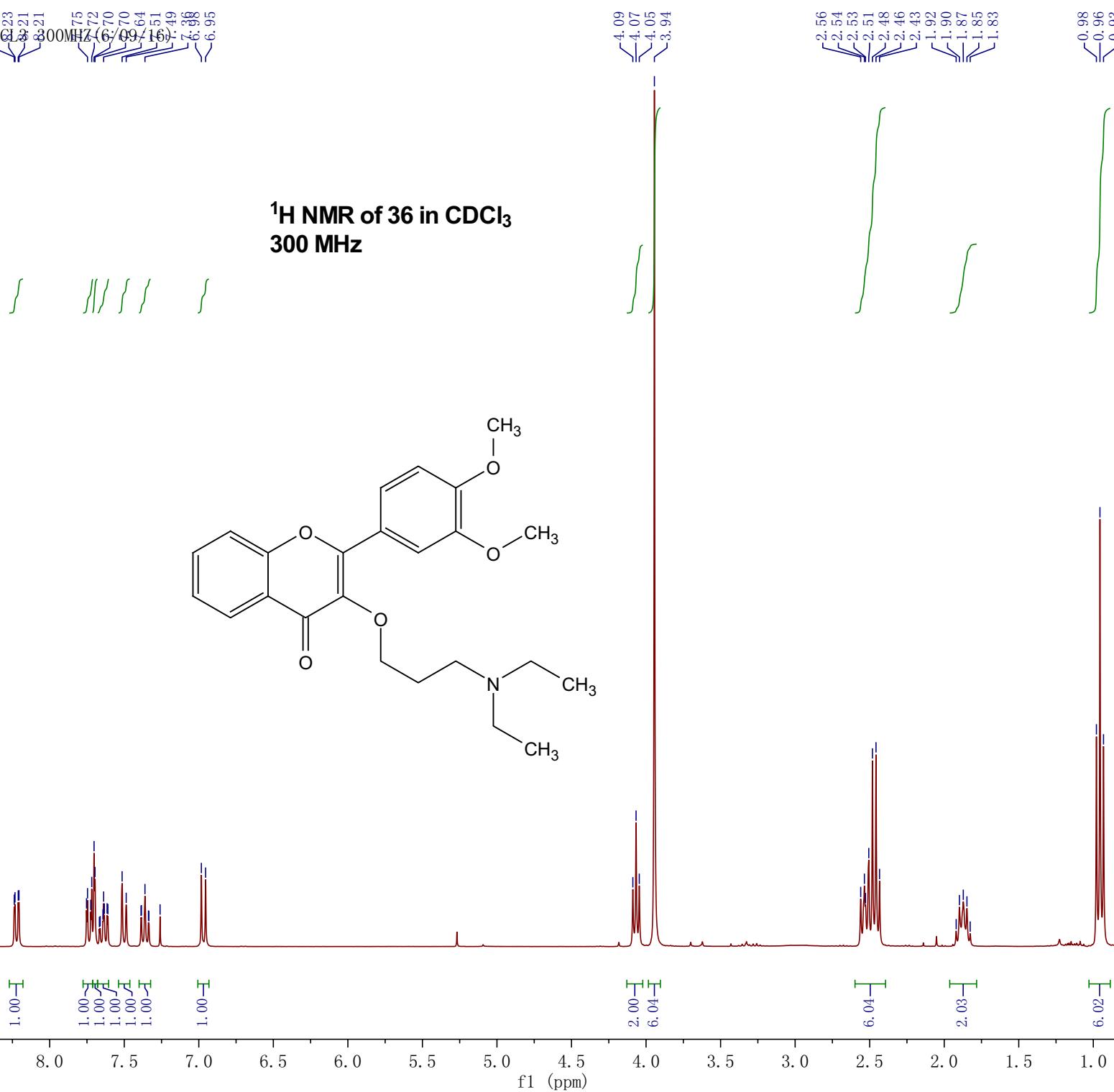
XL-35-175-3 CNW94

CDCl<sub>3</sub> 75 MHZ

— 173.94  
— 163.96  
— 155.99  
— 154.68  
— 154.19  
— 153.81  
— 146.36

**<sup>13</sup>C NMR of 30 in CDCl<sub>3</sub>**  
**75 MHz**





—175.05

<sup>13</sup>C 159.78  
158.19  
158.16  
148.65

—140.09

—133.30

125.81  
124.64  
124.22  
123.59  
122.43  
117.95—111.67  
—110.7777.58  
77.16  
76.74  
—71.3756.11  
56.04  
—49.82  
—46.87

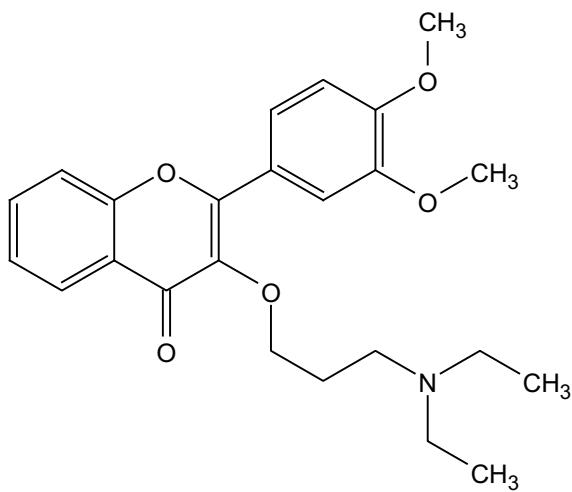
—27.95

—11.60

40000  
35000  
30000  
25000  
20000  
15000  
10000  
5000  
0

S32

**<sup>13</sup>C NMR of 36 in CDCl<sub>3</sub>**  
**75 MHz**



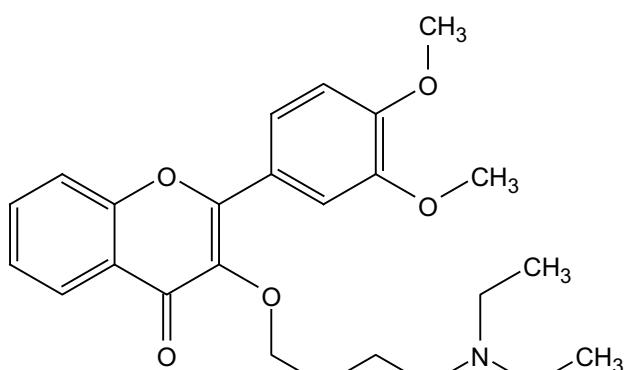
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 f1 (ppm)

12.21  
3.77  
7.76  
7.73  
7.65  
7.64  
7.52  
7.49  
7.39  
7.37  
7.26  
7.06  
6.96

4.06  
4.04  
4.02  
3.95

2.52  
2.50  
2.47  
2.46  
2.45  
2.43  
2.41  
1.74  
1.72  
1.69  
1.67  
1.58  
1.56  
1.53  
1.52  
1.51  
1.06  
0.98  
0.96

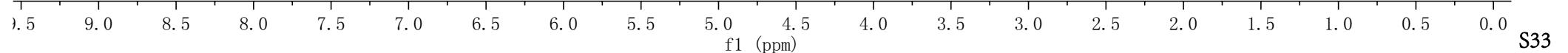
**<sup>1</sup>H NMR of 37 in CDCl<sub>3</sub>**  
**300 MHz**



1.00  
2.00  
1.02  
1.00  
1.01  
1.00

2.00  
6.00  
6.01

2.01  
2.01  
6.03



700  
650  
600  
550  
500  
450  
400  
350  
300  
250  
200  
150  
100  
50  
0  
-50

Xiang LI

XL-35-117-5 CN<sup>13</sup>C NMR CDCl<sub>3</sub> 75MHz

176  
155.21  
155.17  
146.64

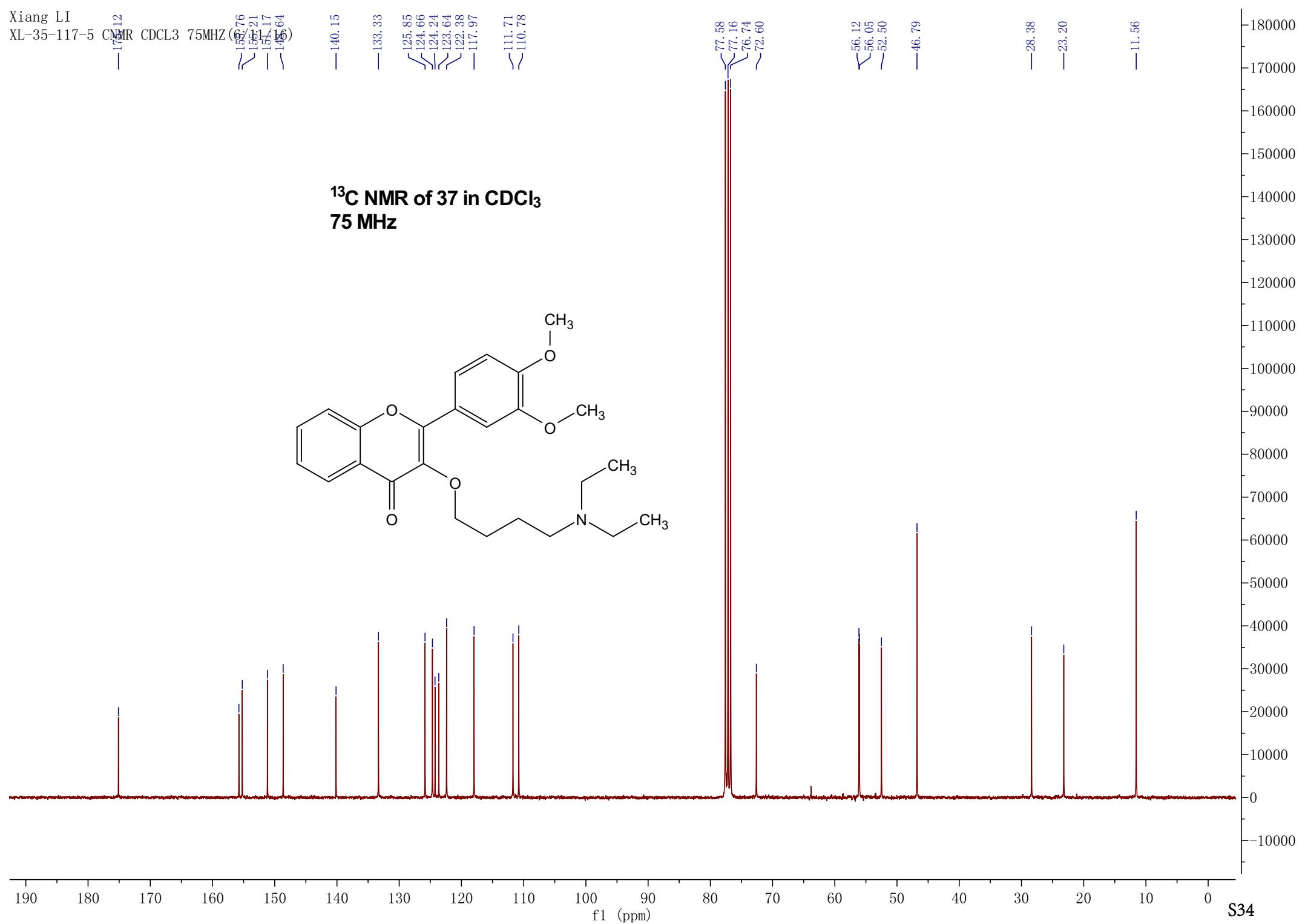
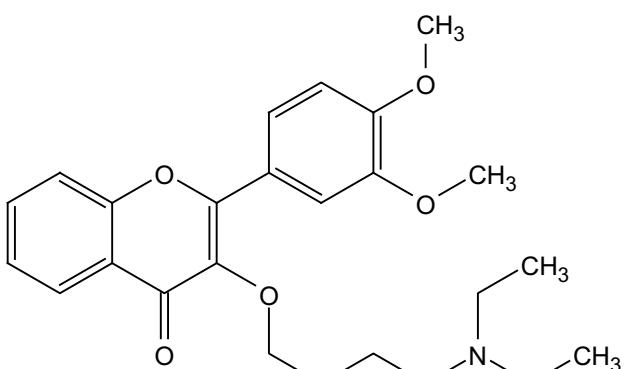
140.15

133.33

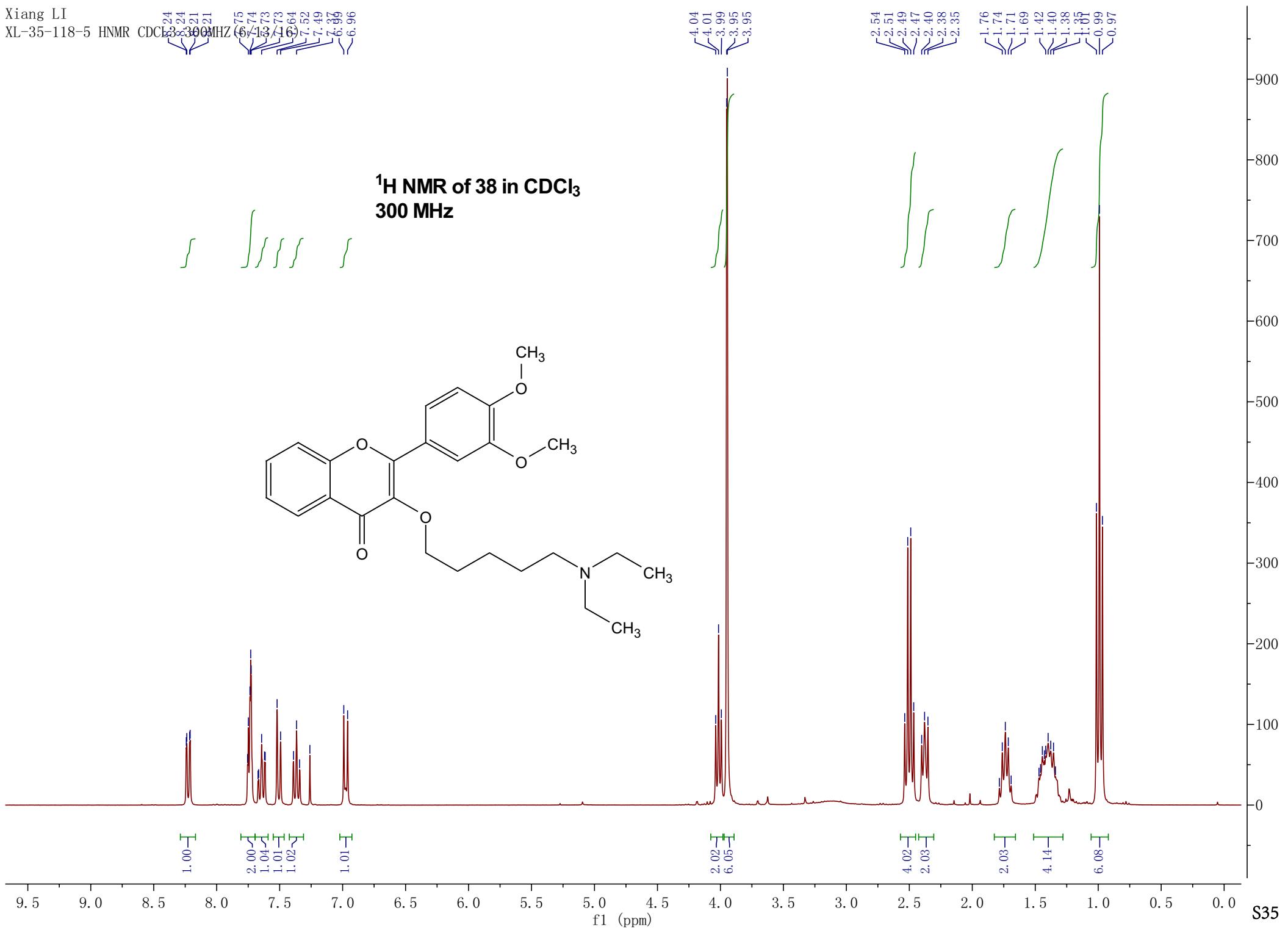
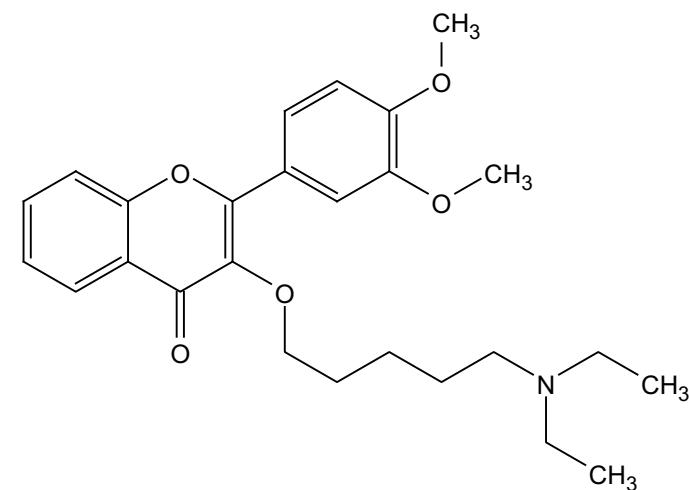
125.85  
124.66  
124.24  
123.64  
122.38  
117.97

111.71  
110.78

**<sup>13</sup>C NMR of 37 in CDCl<sub>3</sub>  
75 MHz**



**<sup>1</sup>H NMR of 38 in CDCl<sub>3</sub>  
300 MHz**



—173.11

—155.76  
—155.22  
—155.15  
—148.62

—140.18

—133.32

125.85  
124.65  
124.25  
123.66  
122.32  
—117.97

—111.76  
—110.76

—77.58  
—77.16  
—76.74  
—72.69

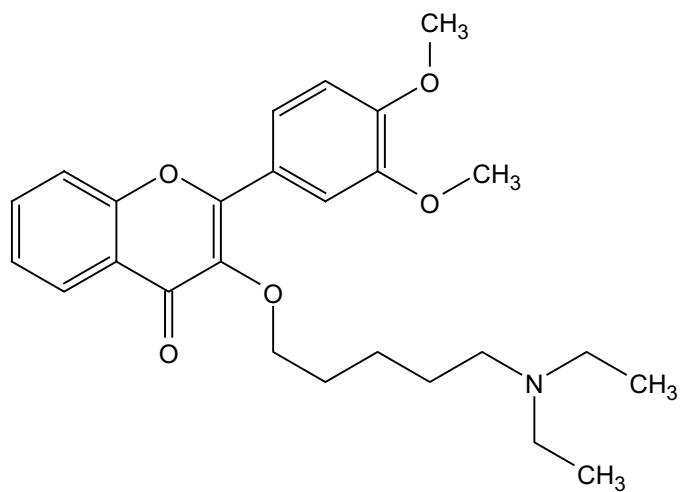
—56.11  
—56.05  
—52.74

—46.86

—30.25  
—26.55  
—24.11

—11.53

**<sup>13</sup>C NMR of 38 in CDCl<sub>3</sub>**  
**75 MHz**



1.25  
1.23  
1.22  
1.76  
1.73  
1.71  
1.70  
1.66  
1.64  
1.54  
1.38  
1.26  
1.01  
6.98

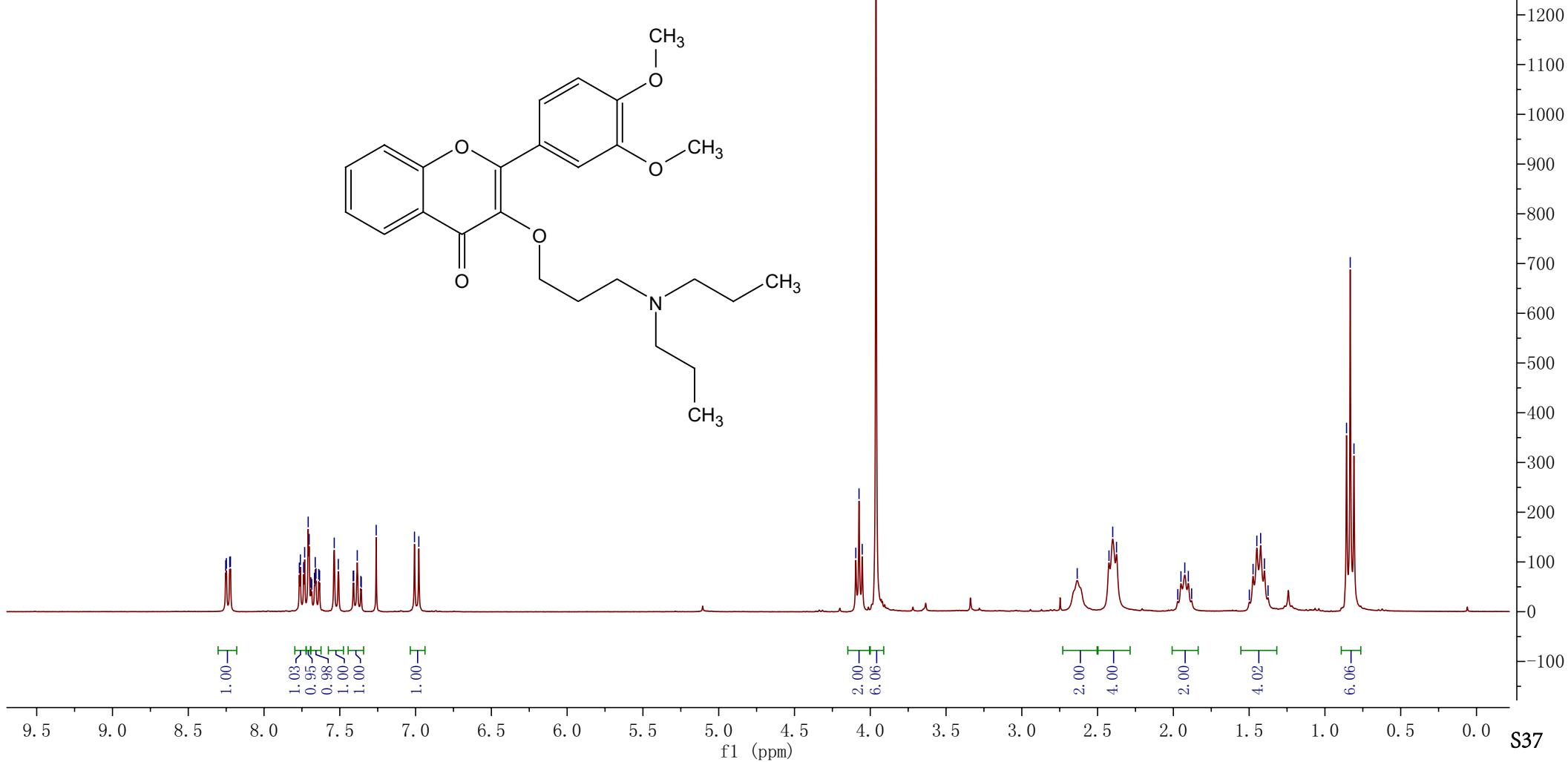
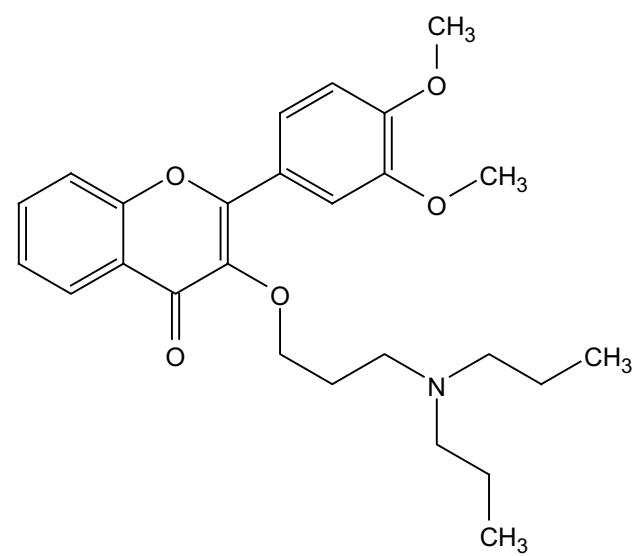
4.10  
4.07  
4.05  
3.96

2.63  
2.42  
2.38  
1.97  
1.95  
1.92  
1.90  
1.88  
1.50  
1.47  
1.45  
1.42  
1.40  
1.38  
0.86  
0.83  
0.81

**<sup>1</sup>H NMR of 39 in CDCl<sub>3</sub>**  
**300 MHZ**

ʃ      // / { }

ʃ      // / { }



<sup>13</sup>C NMR chemical shifts (ppm): 159.92, 155.28, 154.28, 154.16, 148.76

—140.13

—133.40

125.89, 124.74, 124.29, 123.61, 122.50, 118.02

—111.73, —110.87

77.58, 77.16, 76.74, —71.26

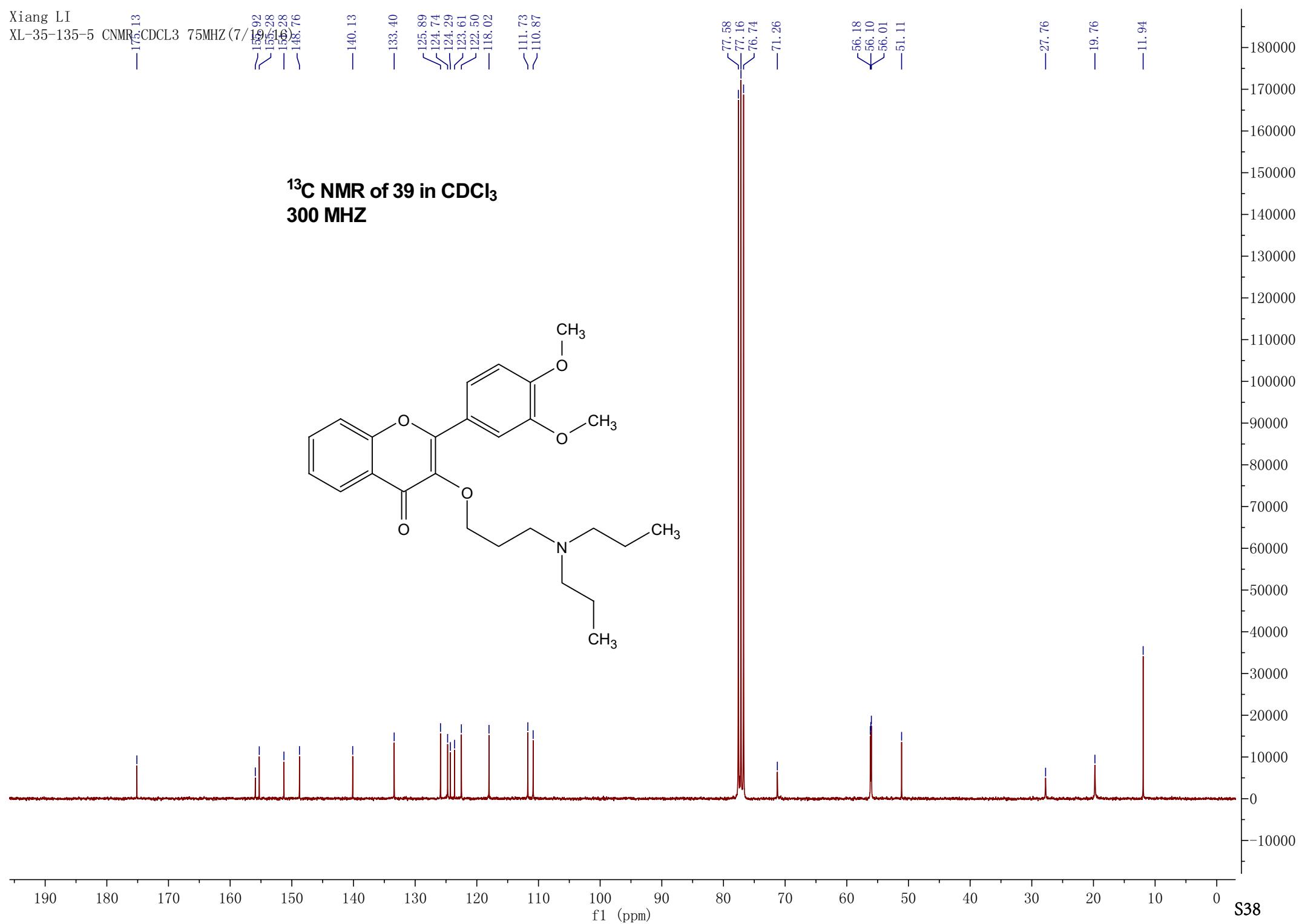
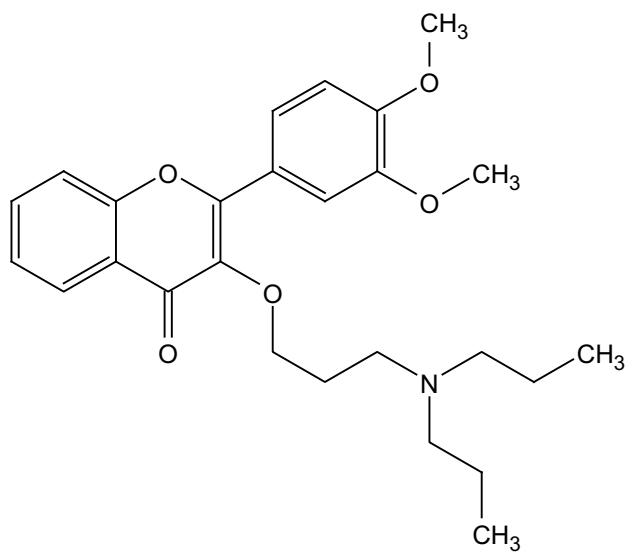
56.18, 56.10, 56.01, —51.11

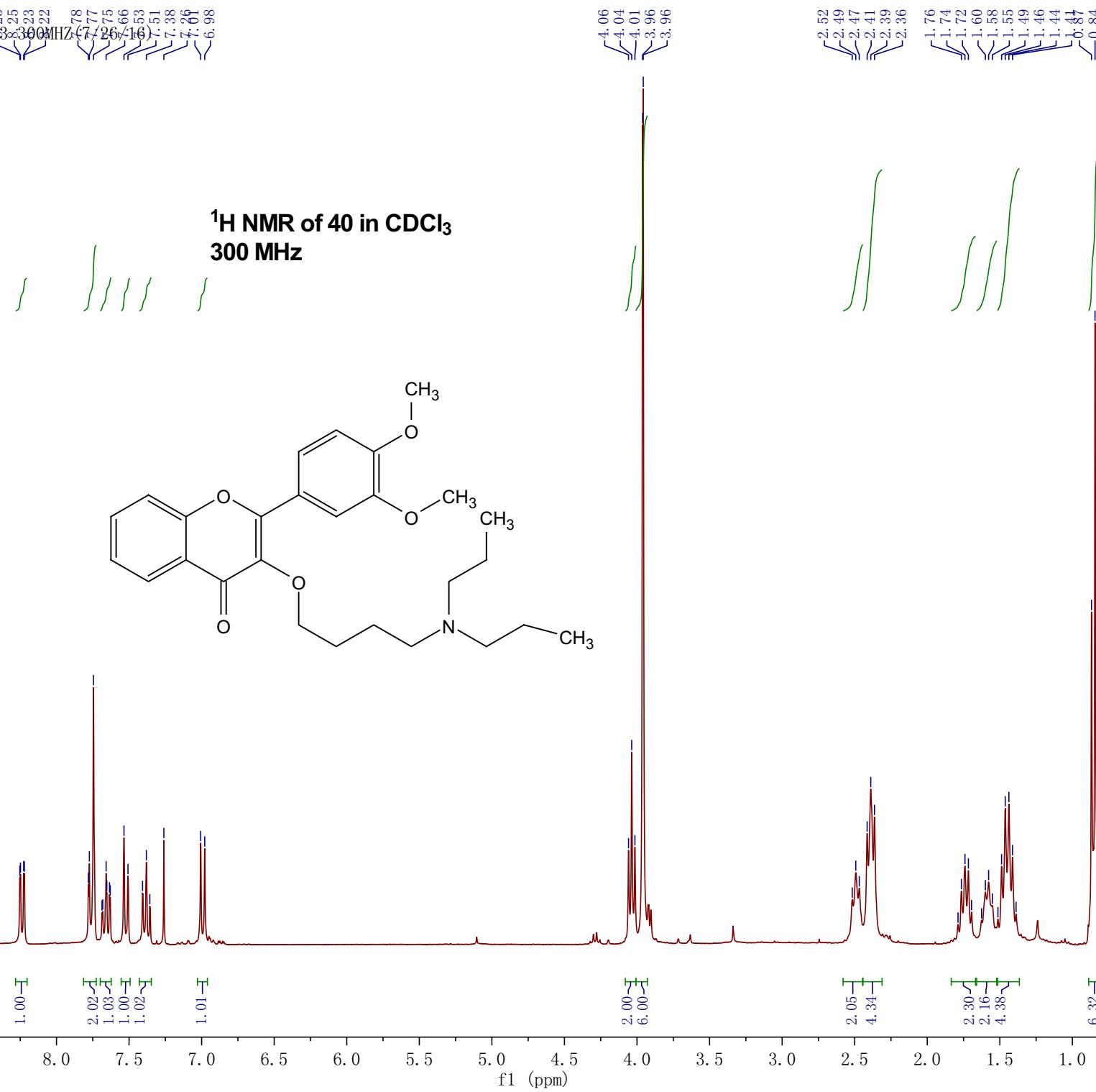
—27.76

—19.76

—11.94

<sup>13</sup>C NMR of 39 in CDCl<sub>3</sub>  
300 MHz





Xiang LI

XL-35-136-6 CNMR CDCl<sub>3</sub> 75MHz (7/80)

-178.15  
-158.26  
-155.24  
-148.71

-140.18

-133.36

125.89  
124.69  
124.29  
123.67  
122.39  
118.00

111.75  
110.85

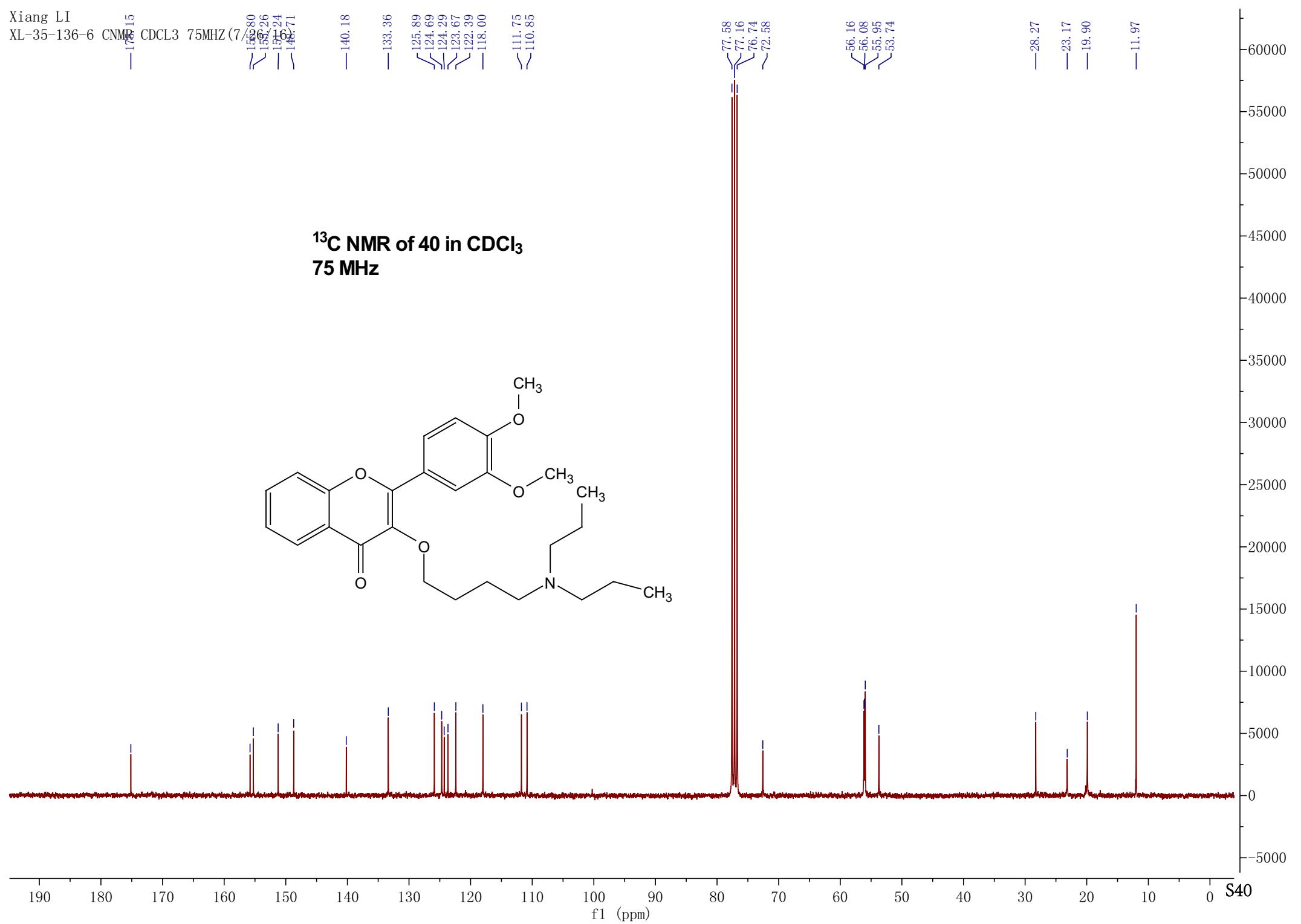
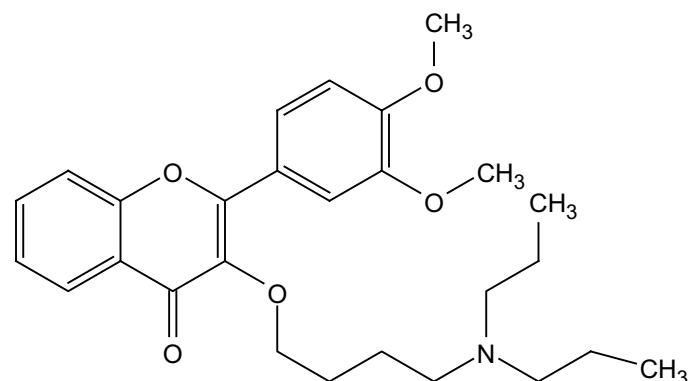
77.58  
77.16  
76.74  
72.58

56.16  
56.08  
55.95  
53.74

-28.27  
-23.17  
-19.90

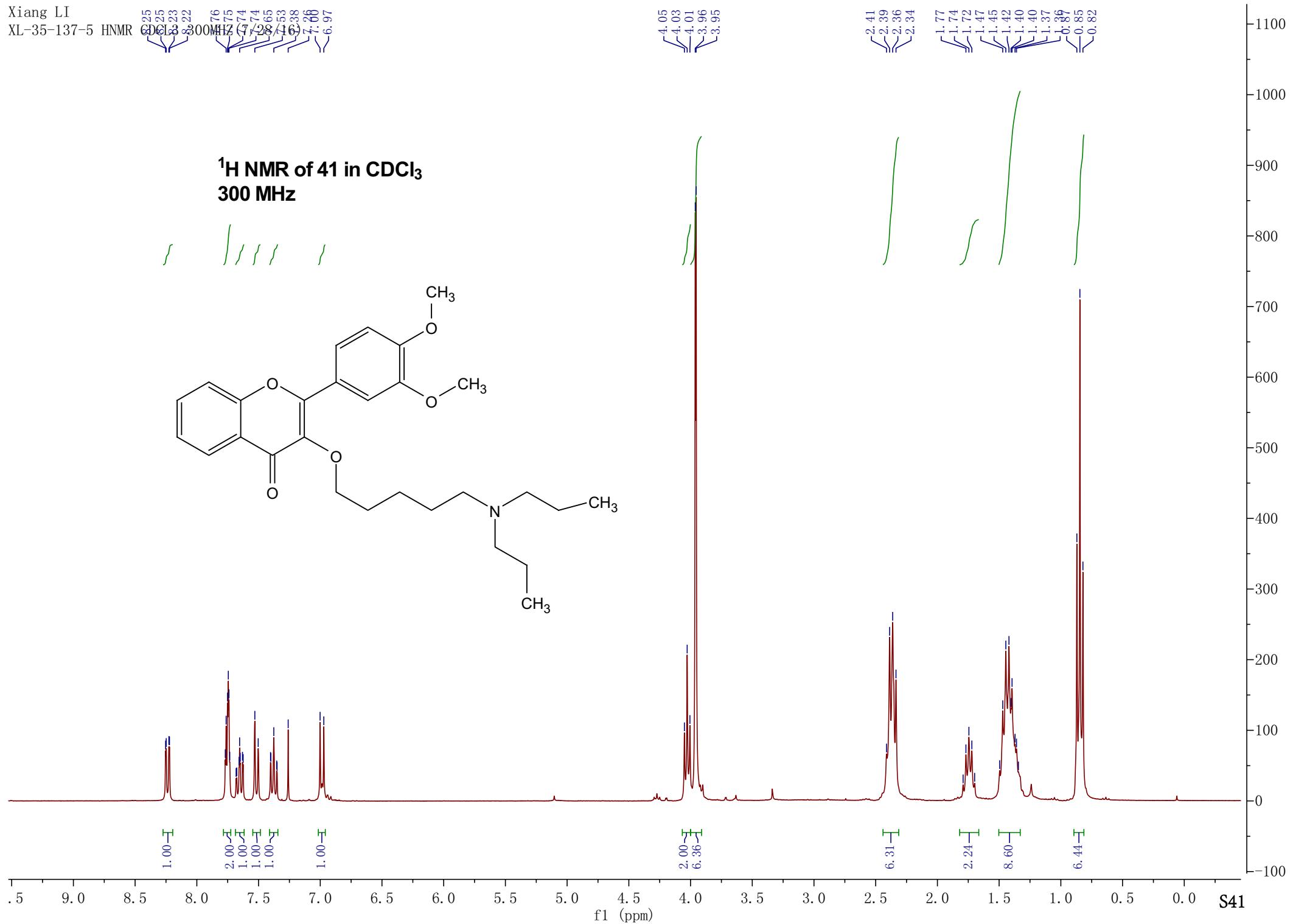
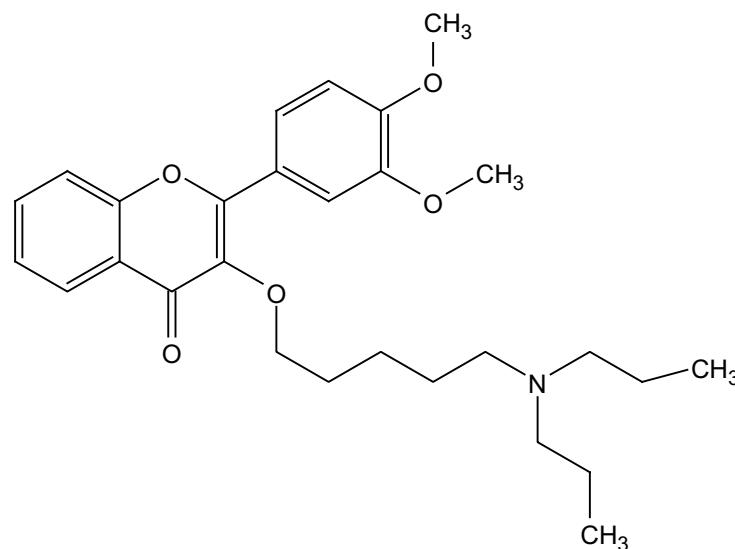
-11.97

**<sup>13</sup>C NMR of 40 in CDCl<sub>3</sub>**  
**75 MHz**





<sup>1</sup>H NMR of 41 in CDCl<sub>3</sub>  
300 MHz



-178.14

 $\sim$ 153.75  
153.26  
153.20  
148.67

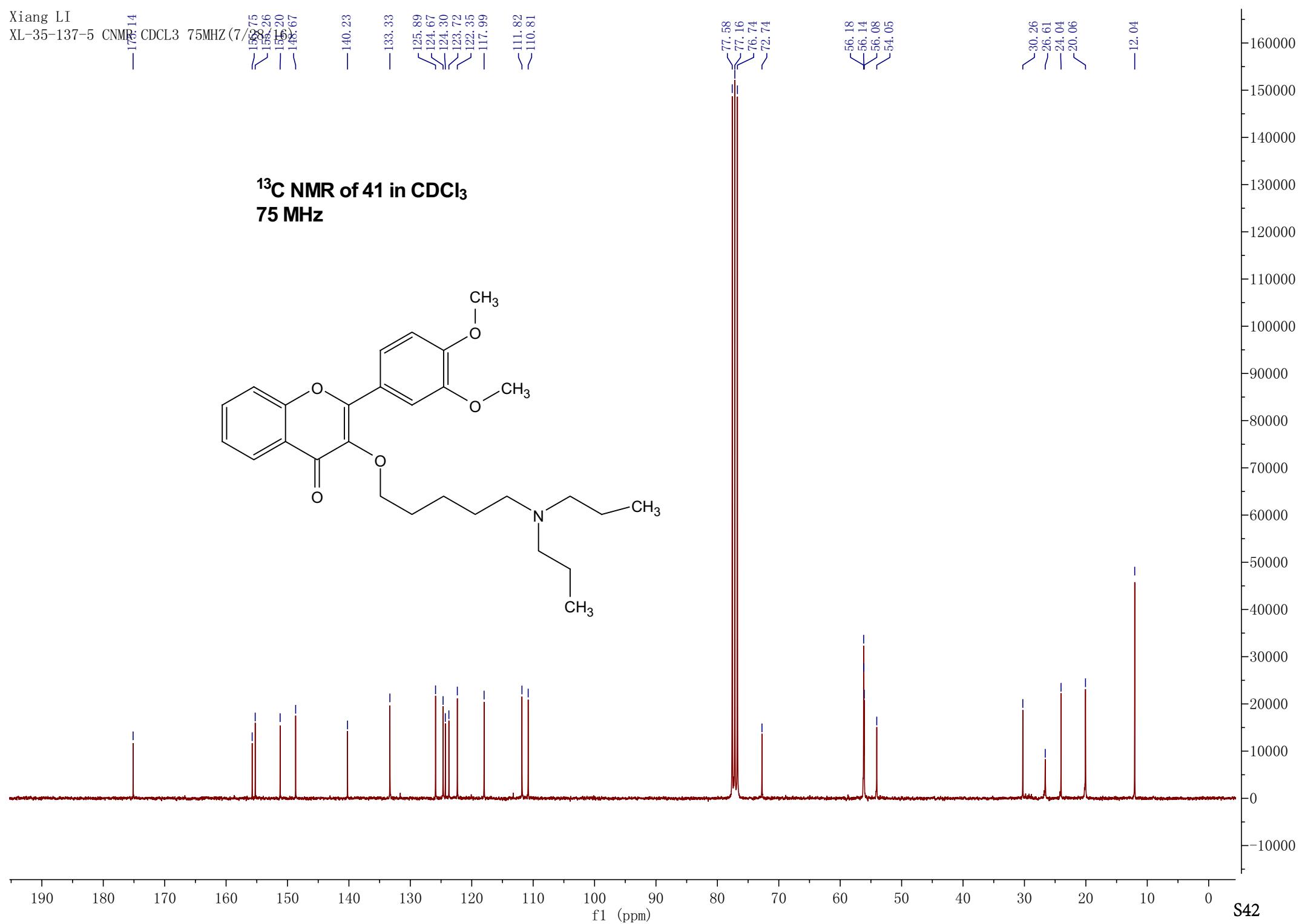
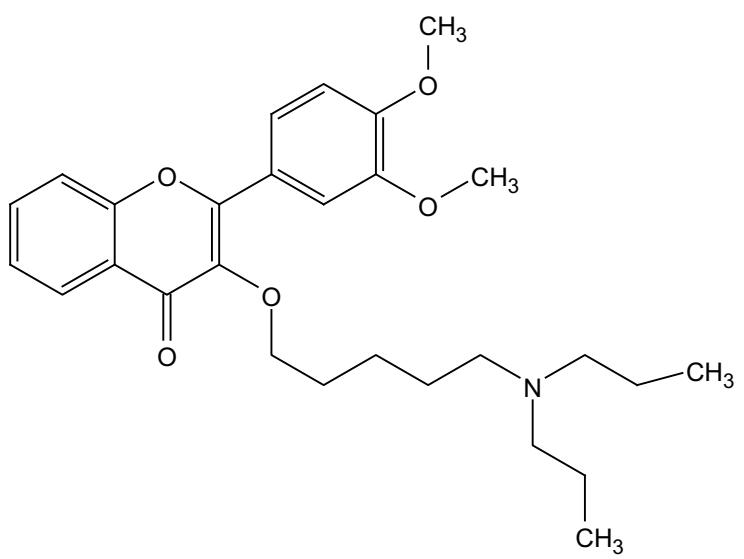
-140.23

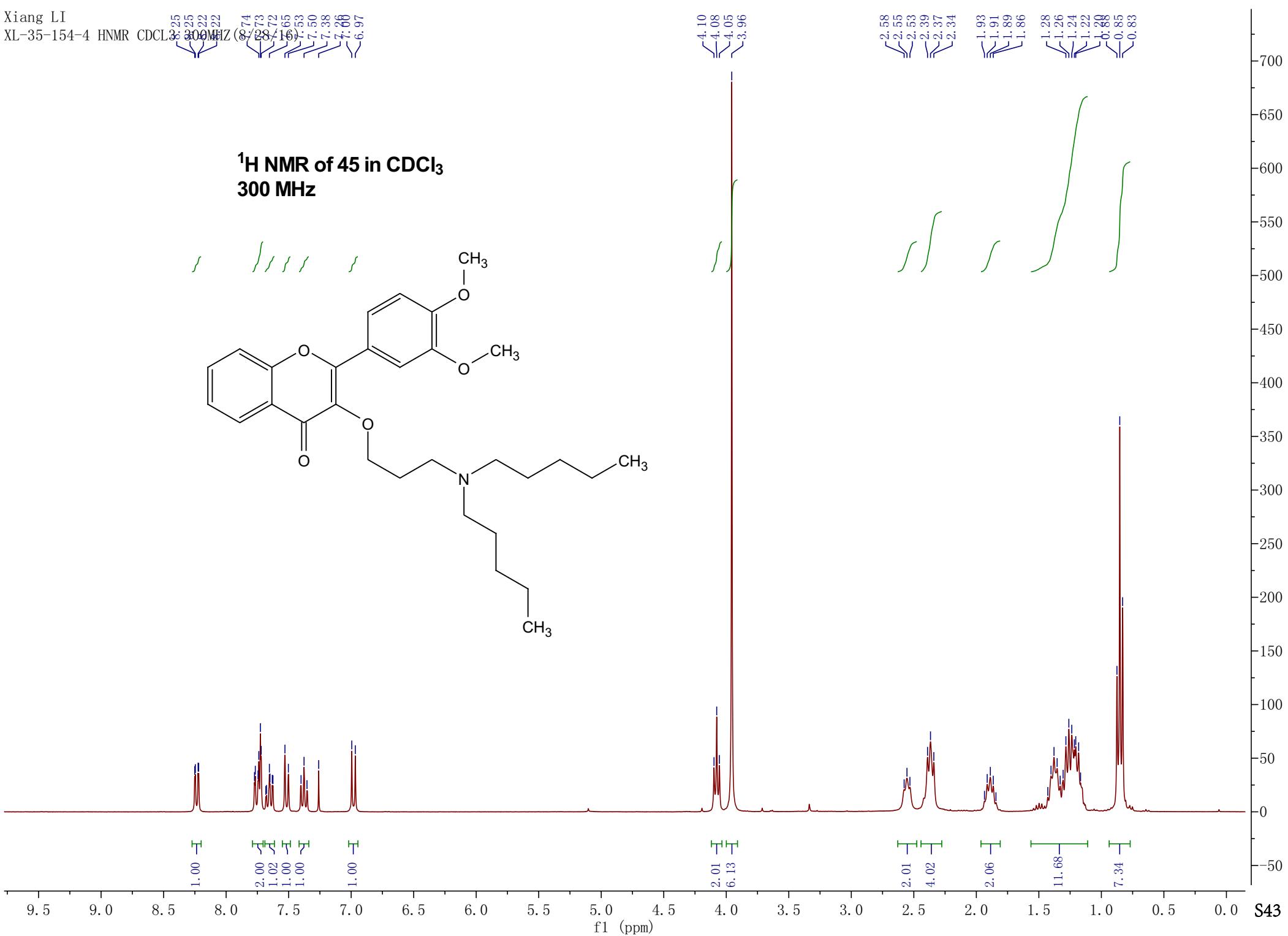
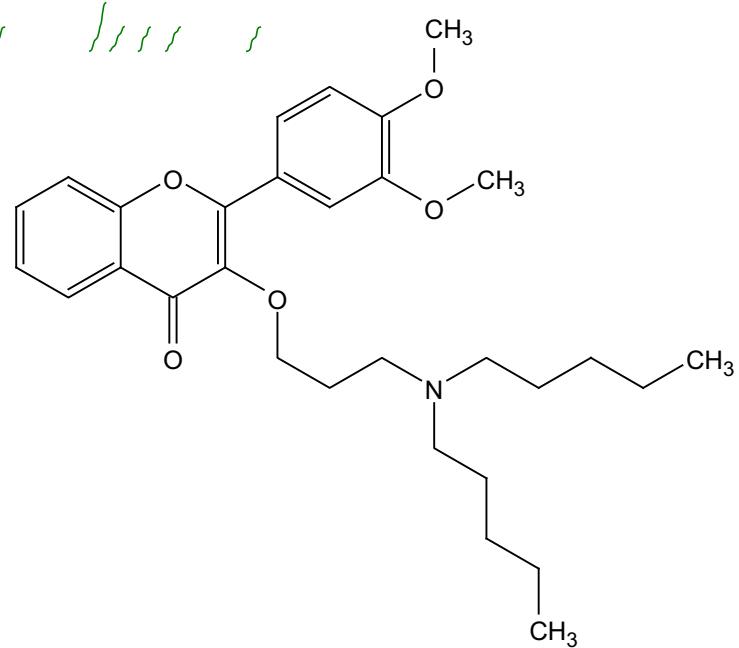
-133.33

125.89  
124.67  
124.30  
123.72  
122.35  
-117.99 $\sim$ 111.82  
 $\sim$ 110.8177.58  
77.16  
76.74  
72.7456.18  
56.14  
56.08  
54.05 $\sim$ 30.26  
26.61  
24.04  
20.06

-12.04

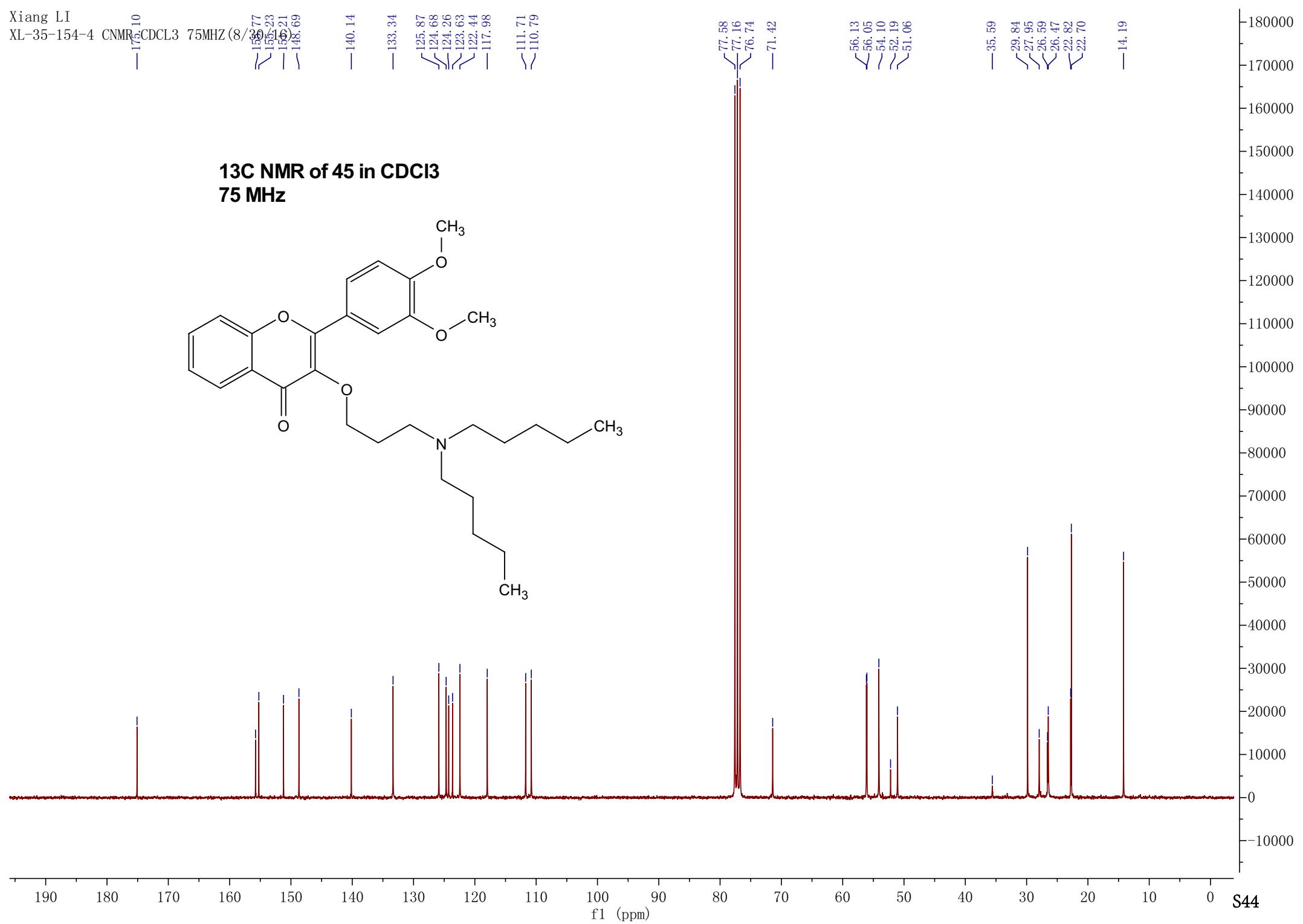
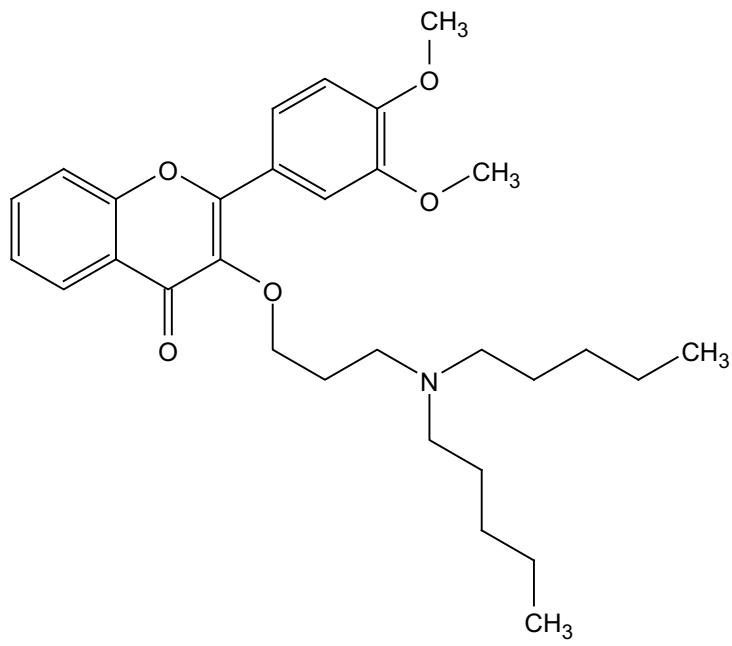
**<sup>13</sup>C NMR of 41 in CDCl<sub>3</sub>**  
**75 MHz**





## **<sup>13</sup>C NMR of 45 in CDCl<sub>3</sub>**

**75 MHz**

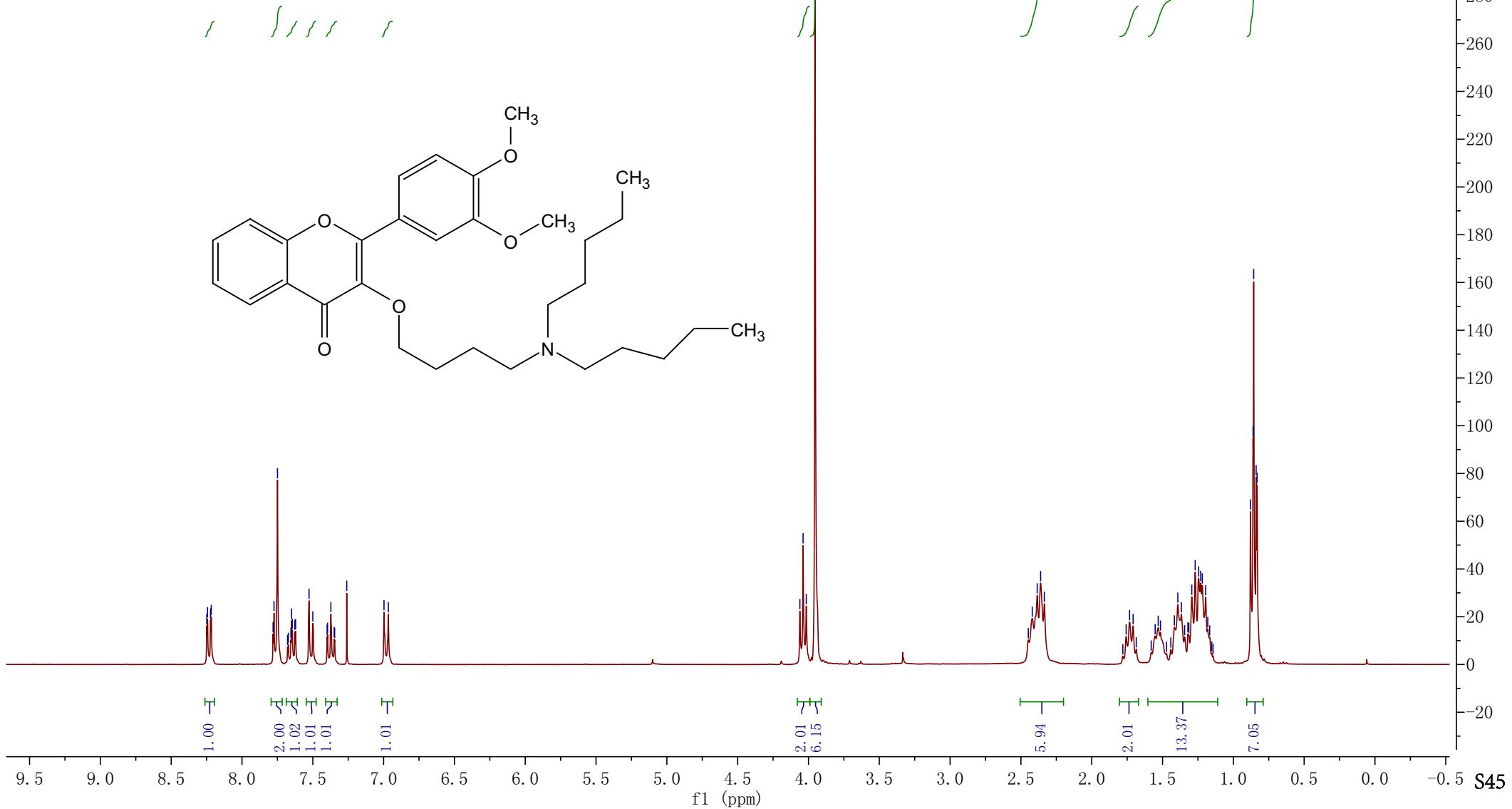
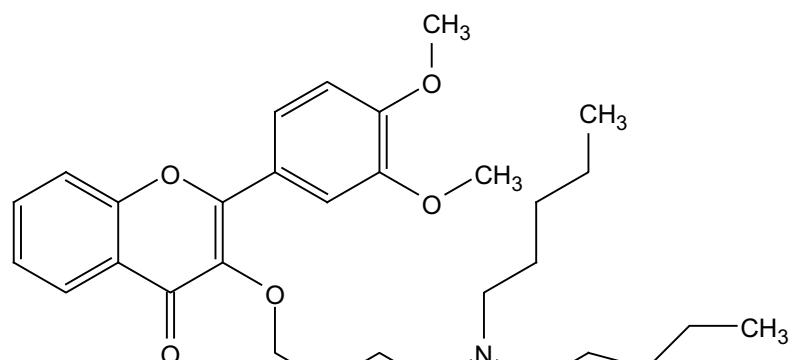


8.49  
8.344  
8.222  
8.17  
7.74  
7.49  
7.50  
7.45  
7.27  
7.00  
6.972  
6.967

4.061  
4.038  
4.016  
3.953

2.448  
2.420  
2.385  
2.361  
2.335  
1.733  
1.708  
1.392  
1.367  
1.293  
1.270  
1.245  
1.230  
1.219  
0.895  
0.861  
0.856  
0.839  
0.832

**<sup>1</sup>H NMR of 46 in CDCl<sub>3</sub>**  
**300 MHz**



—173.12

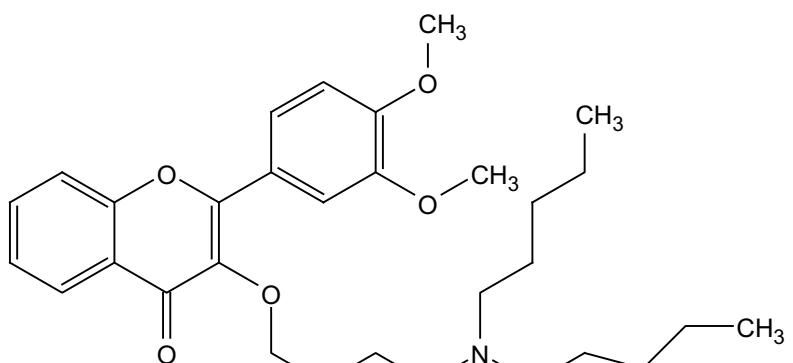
—155.69  
—155.22  
—151.16  
—148.65

—140.19

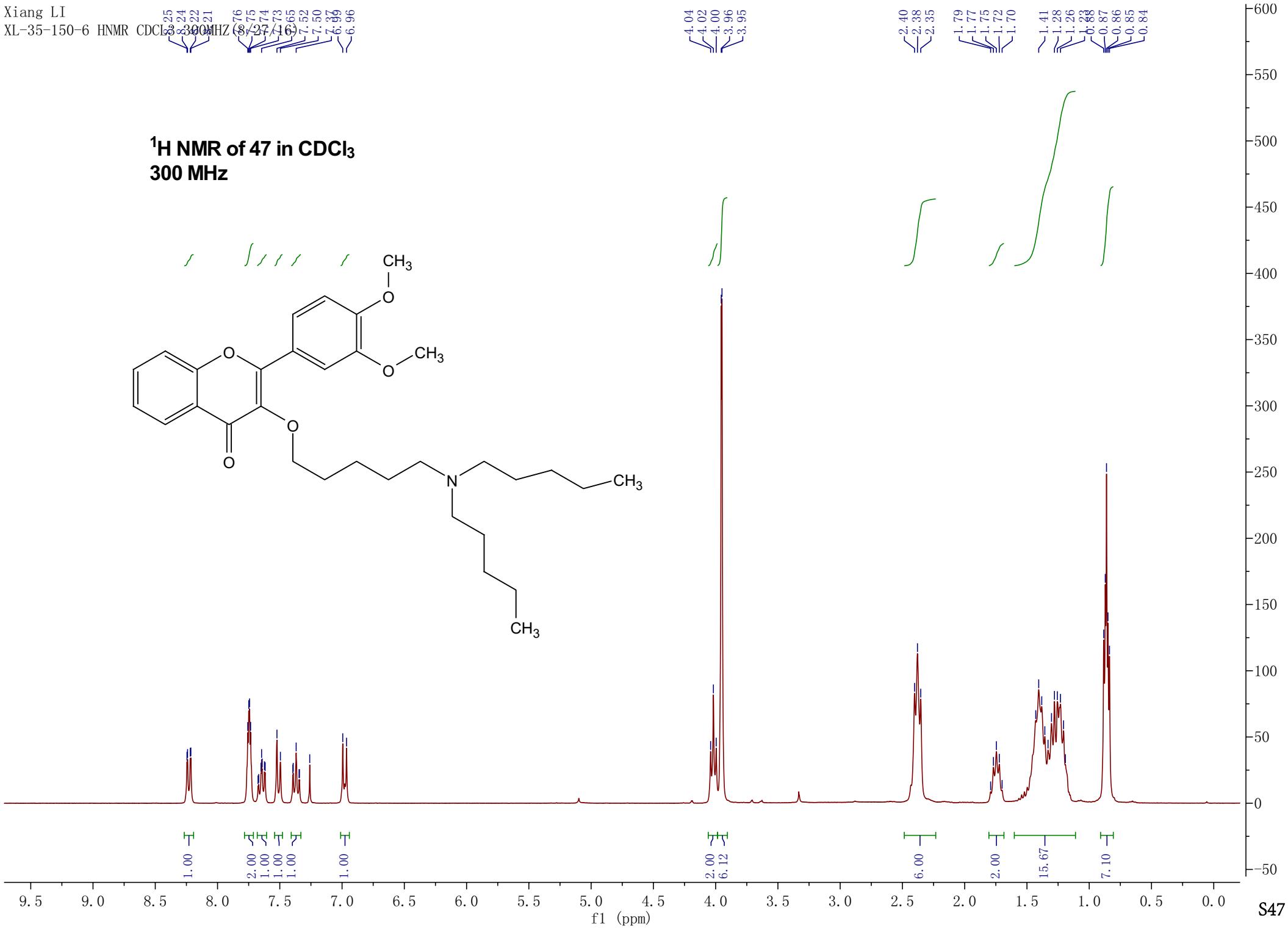
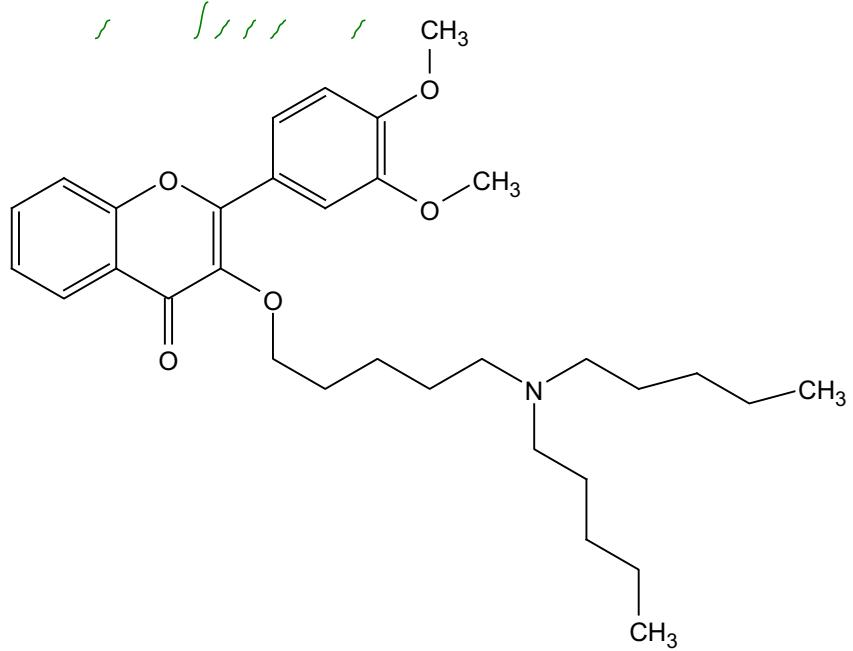
—133.32  
—125.86  
—124.65  
—124.25  
—123.67  
—122.33  
—117.97  
—111.70  
—110.77—77.58  
—77.16  
—76.74  
—72.67—56.11  
—56.04  
—54.04  
—53.78  
—52.16—35.76  
—29.85  
—28.37  
—26.58  
—23.29  
—22.84  
—22.73

—14.19

**<sup>13</sup>C NMR of 46 in CDCl<sub>3</sub>**  
**75 MHz**



**<sup>1</sup>H NMR of 47 in CDCl<sub>3</sub>**  
**300 MHz**



S47

—176.12

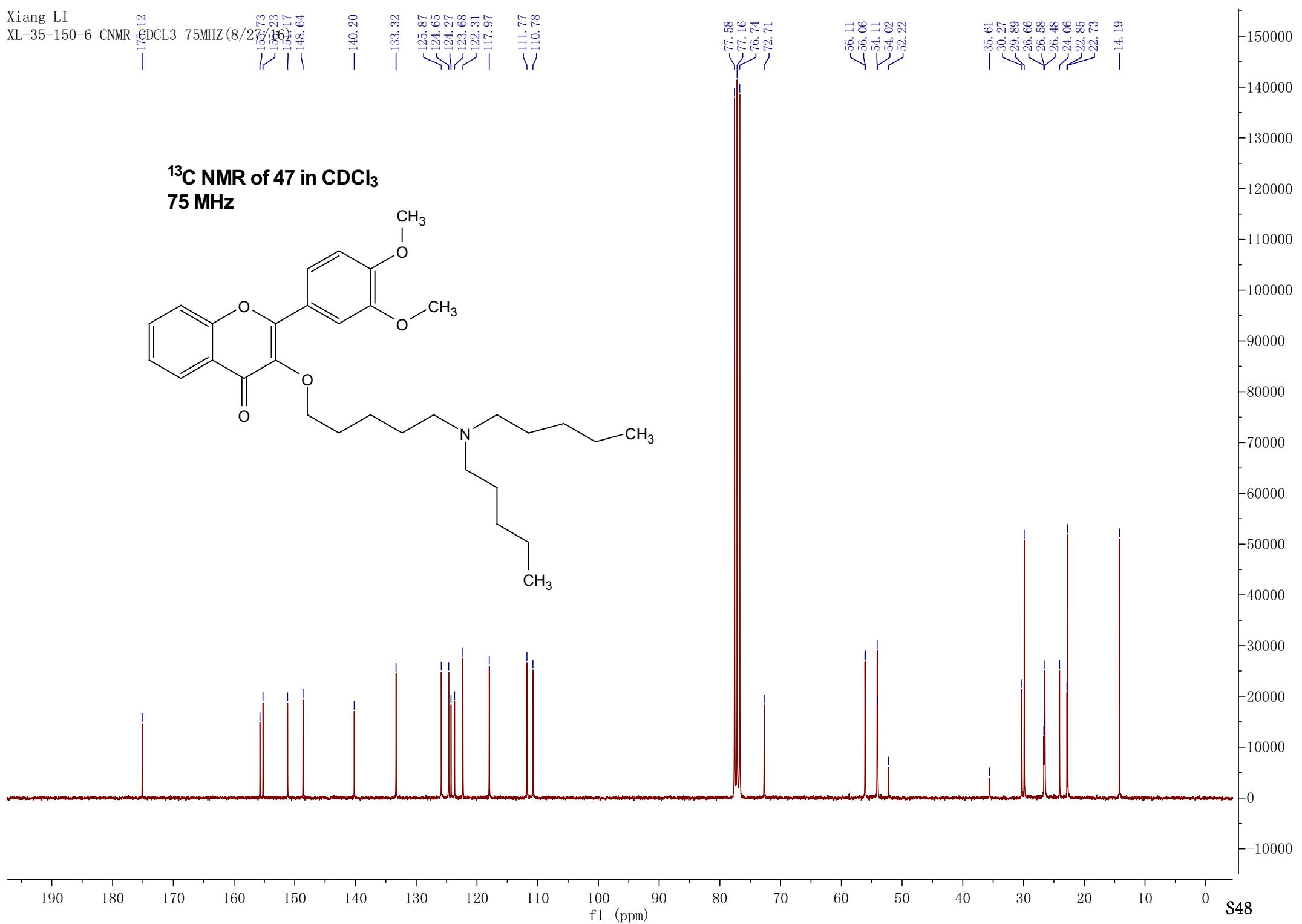
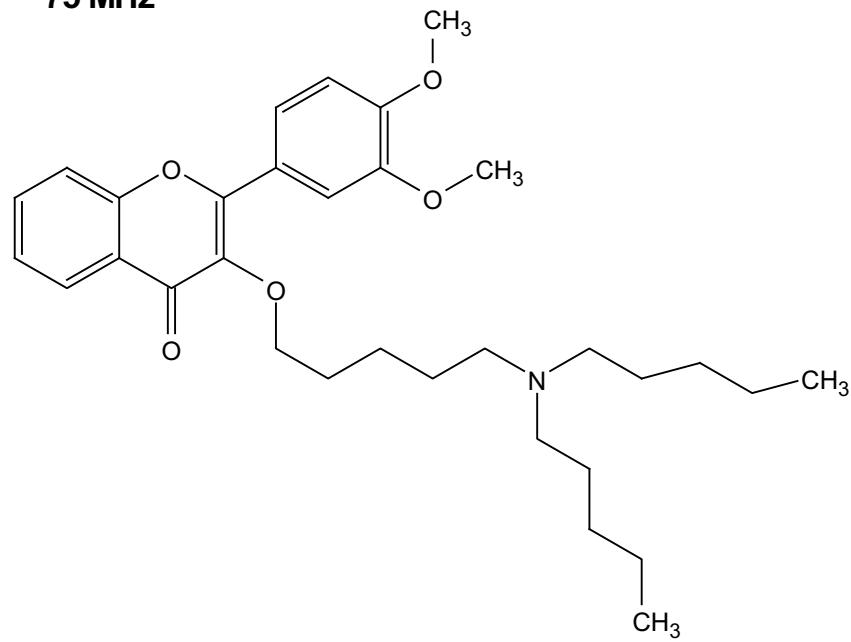
—157.73  
—155.23  
—152.17  
—148.64

—140.20

—133.32  
—125.87  
—124.65  
—124.27  
—123.68  
—122.31  
—117.97—111.77  
—110.78—77.58  
—77.16  
—76.74  
—72.71—56.11  
—56.06  
—54.11  
—54.02  
—52.22—35.61  
—30.27  
—29.89  
—26.66  
—26.58  
—26.48  
—24.06  
—22.85  
—22.73

—14.19

**<sup>13</sup>C NMR of 47 in CDCl<sub>3</sub>**  
**75 MHz**

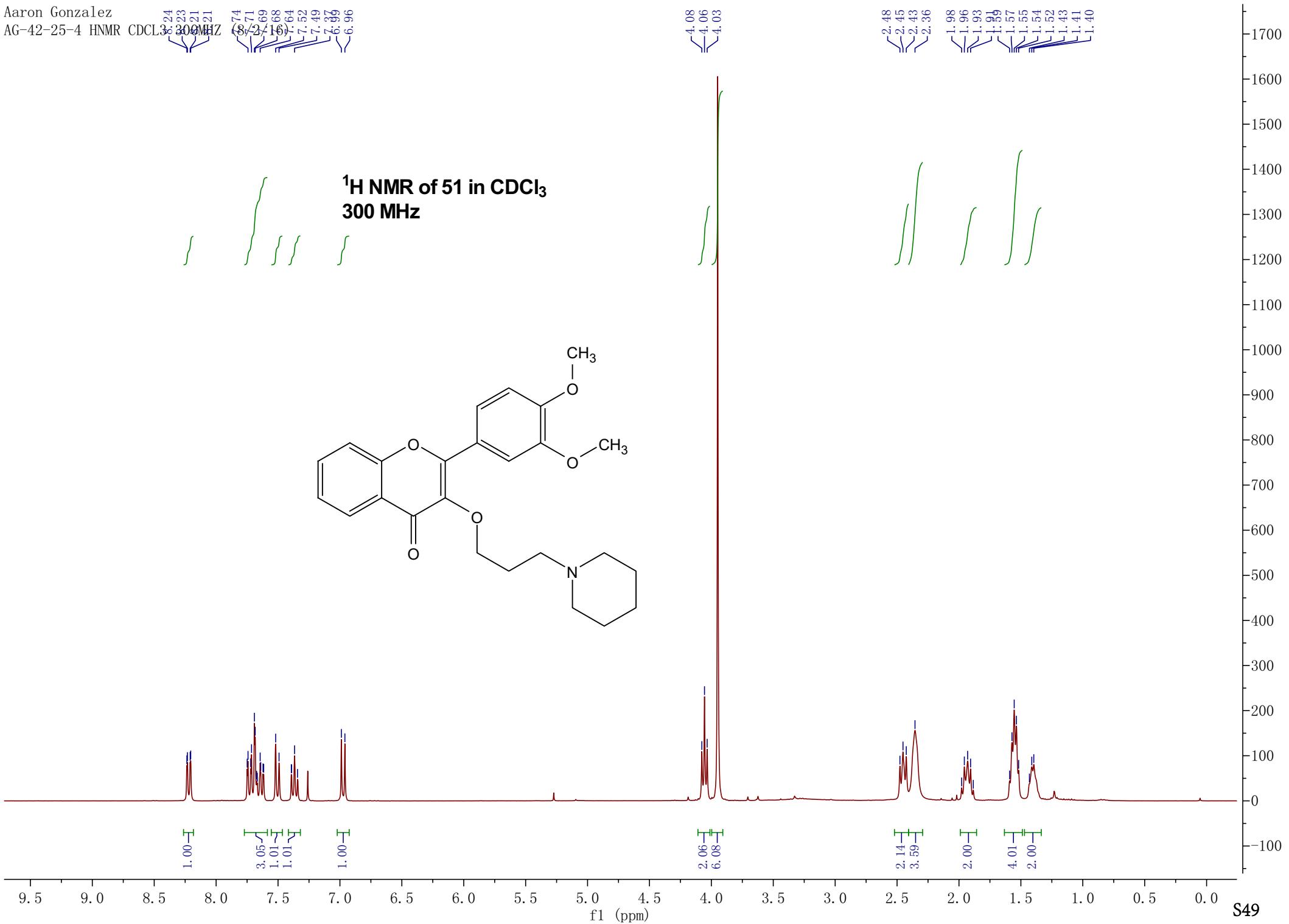
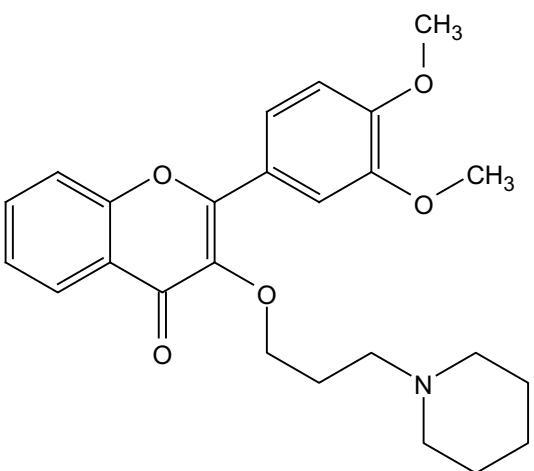


3.24  
3.21  
3.21  
7.74  
(8.71, 2.69)  
(8.71, 1.68)  
(8.71, 1.64)  
7.52  
7.49  
7.37  
6.96  
6.96

4.08  
4.06  
4.03

2.48  
2.45  
2.43  
2.36  
1.98  
1.96  
1.93  
1.91  
1.57  
1.55  
1.54  
1.52  
1.43  
1.41  
1.40

**<sup>1</sup>H NMR of 51 in CDCl<sub>3</sub>  
300 MHz**

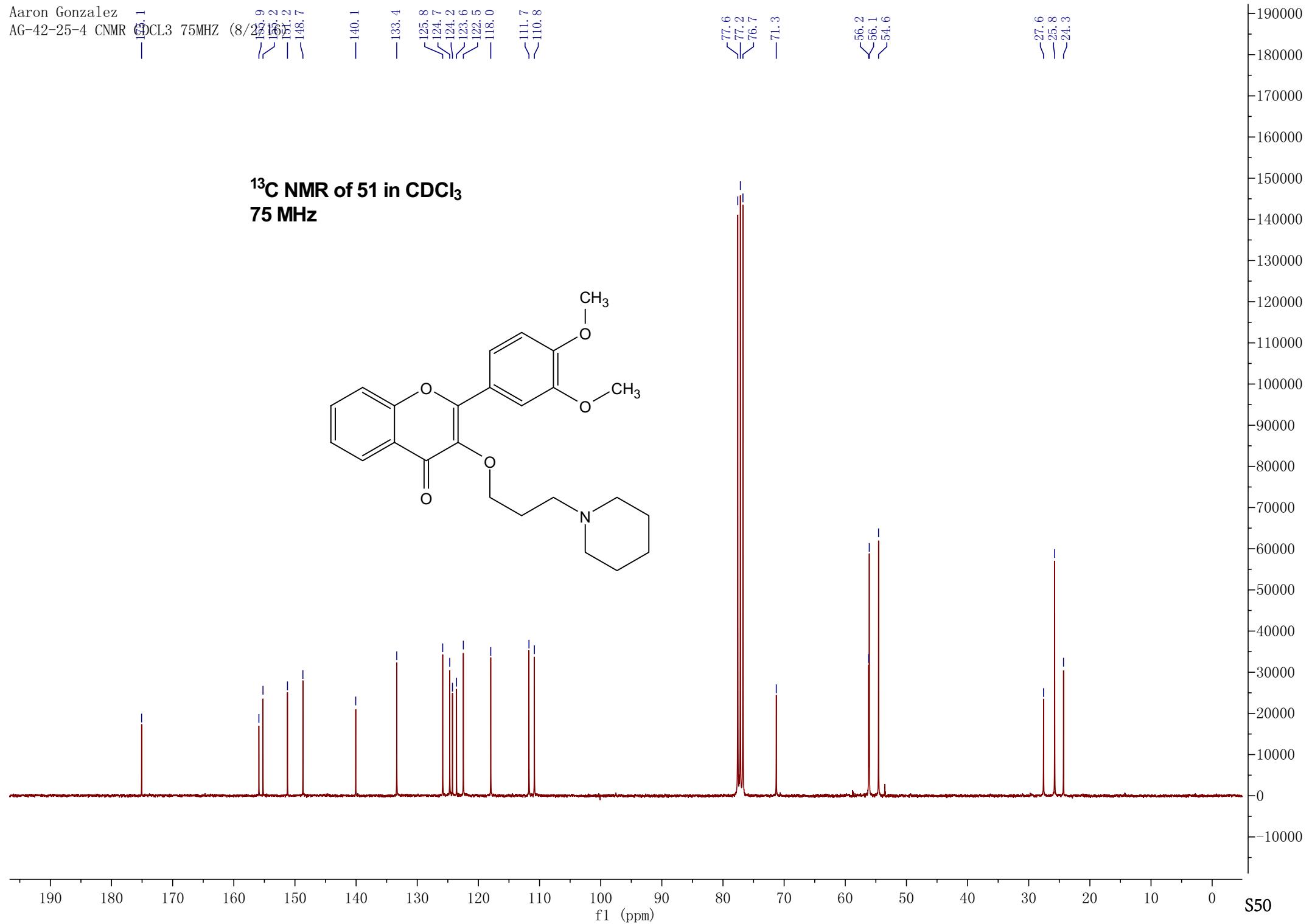
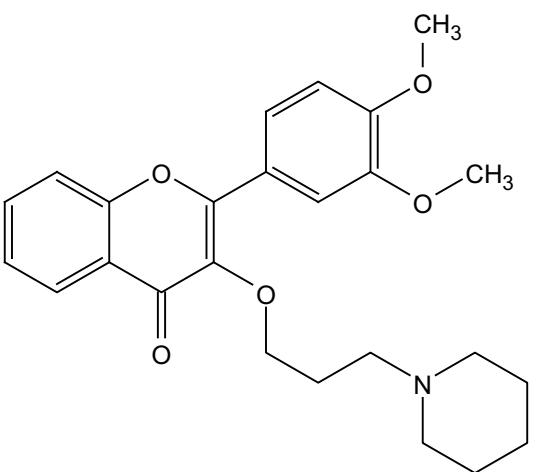


— 140.1  
— 133.4  
— 125.8  
— 124.7  
— 124.2  
— 123.6  
— 122.5  
— 118.0  
— 111.7  
— 110.8

— 77.6  
— 77.2  
— 76.7  
— 71.3

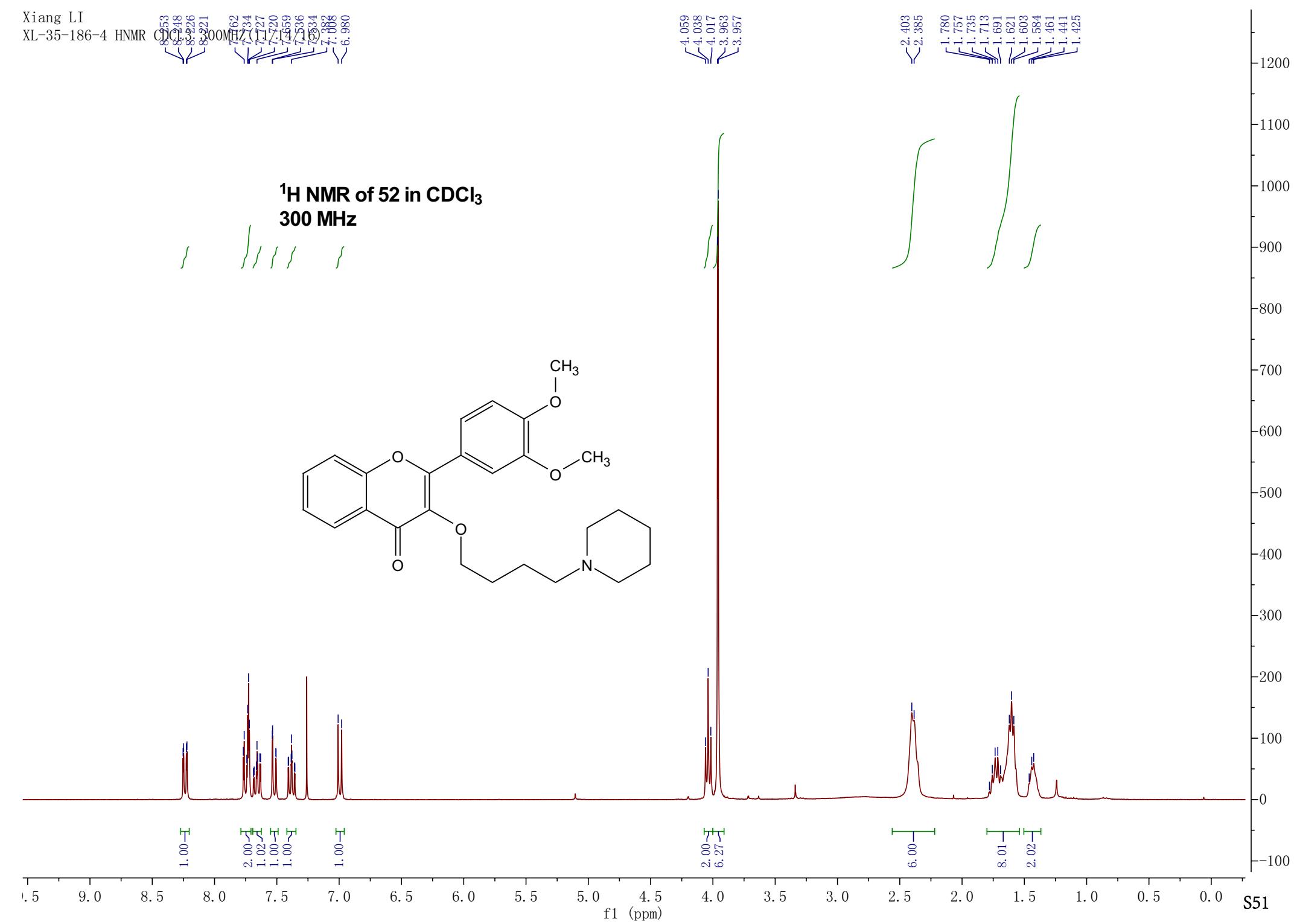
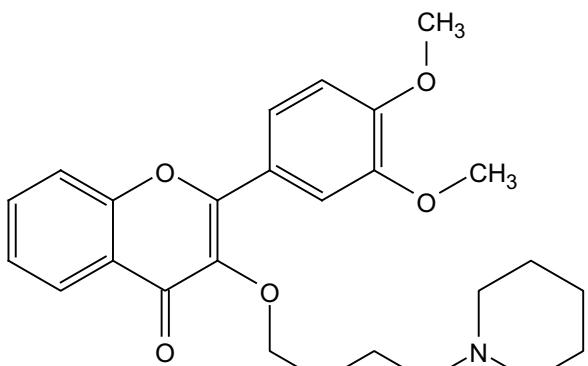
— 56.2  
— 56.1  
— 54.6  
— 27.6  
— 25.8  
— 24.3

**<sup>13</sup>C NMR of 51 in CDCl<sub>3</sub>**  
**75 MHz**



8.553  
8.448  
8.326  
8.321  
7.662  
7.334  
7.227  
7.159  
7.136  
7.034  
7.008  
6.980

**<sup>1</sup>H NMR of 52 in CDCl<sub>3</sub>**  
**300 MHz**



Xiang LI

XL-35-186-4 CNMR14  
CDCl<sub>3</sub> 75MHz (0.1)

154.92  
154.27  
156.29  
145.74

-140.09

-133.42

125.85  
124.73  
124.27  
123.58  
122.46  
-118.04

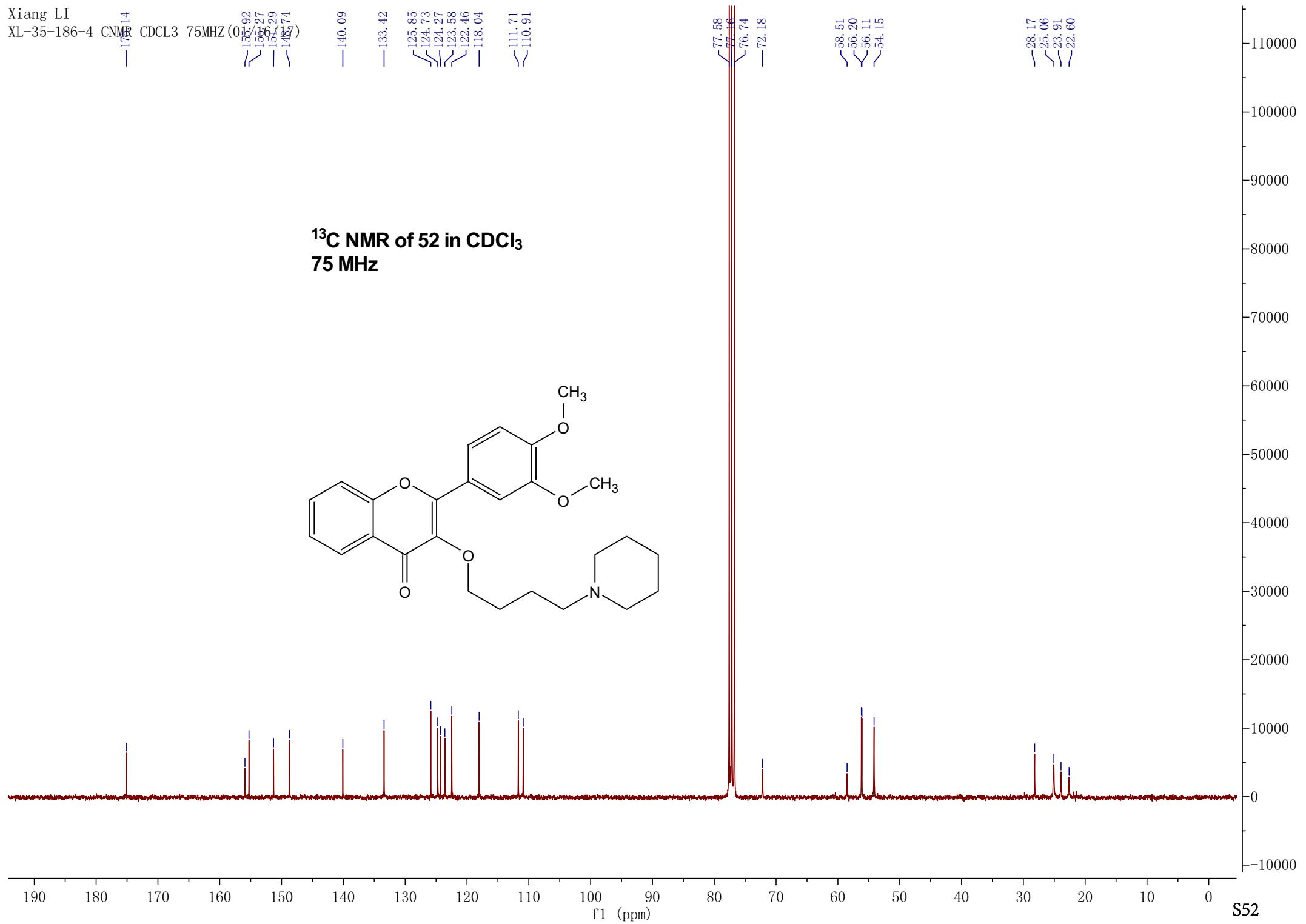
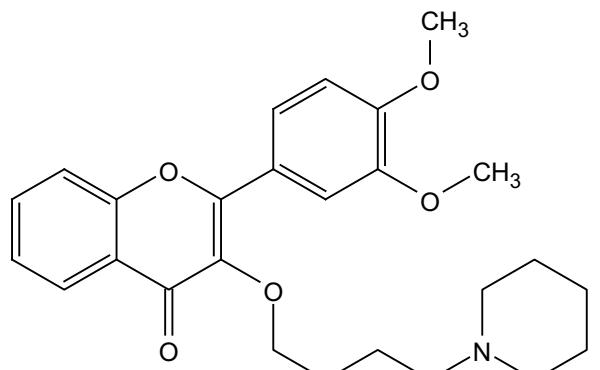
-111.71  
-110.91

77.58  
77.16  
76.74  
-72.18

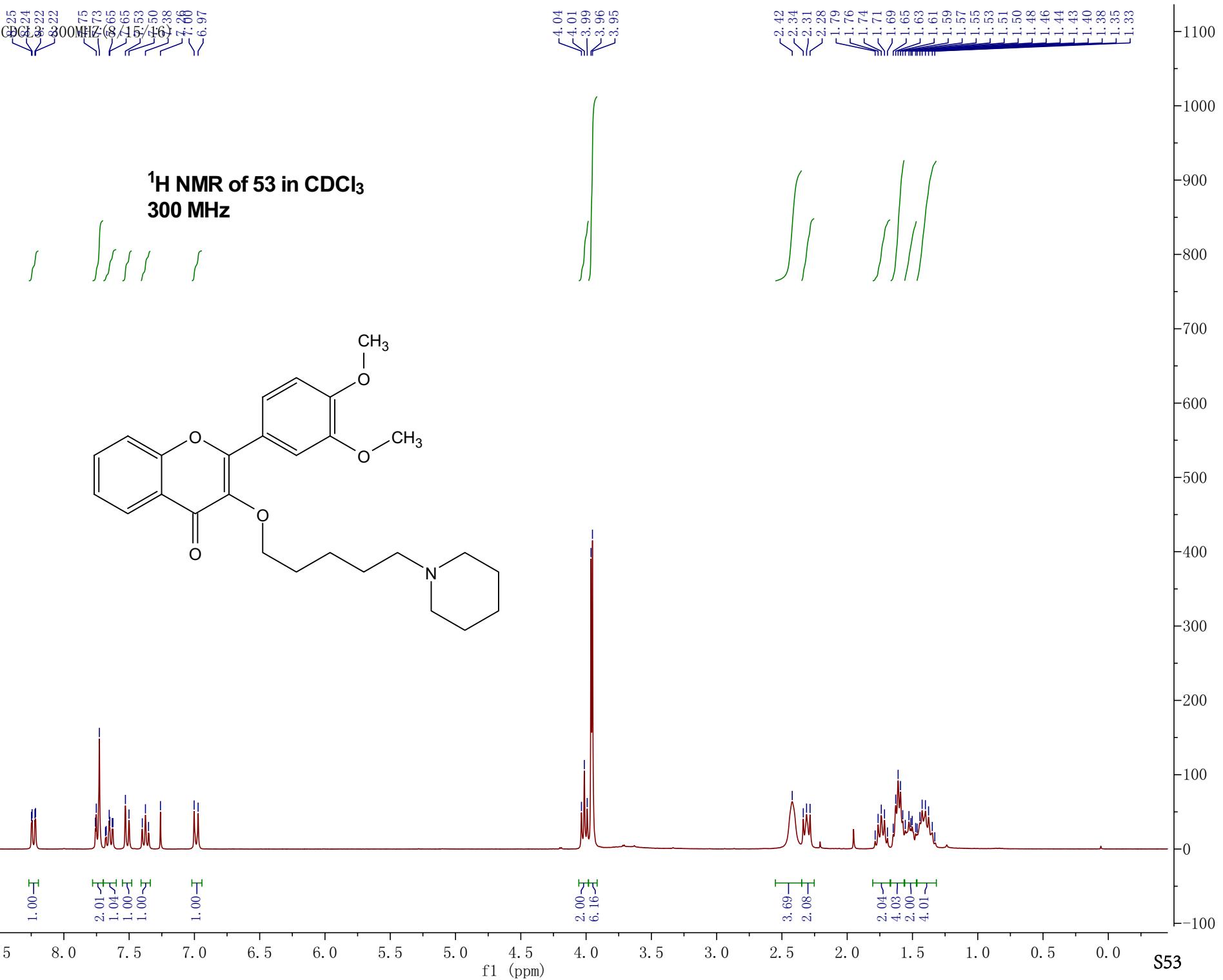
58.51  
56.20  
56.11  
-54.15

-28.17  
-25.06  
-23.91  
-22.60

**<sup>13</sup>C NMR of 52 in CDCl<sub>3</sub>  
75 MHz**



S52



-174.13  
 ~154.82  
 ~154.26  
 -154.20  
 -148.66

-140.19

-133.35

~125.88  
 ~124.68  
 ~124.28  
 ~123.68  
 ~122.37  
 -118.00

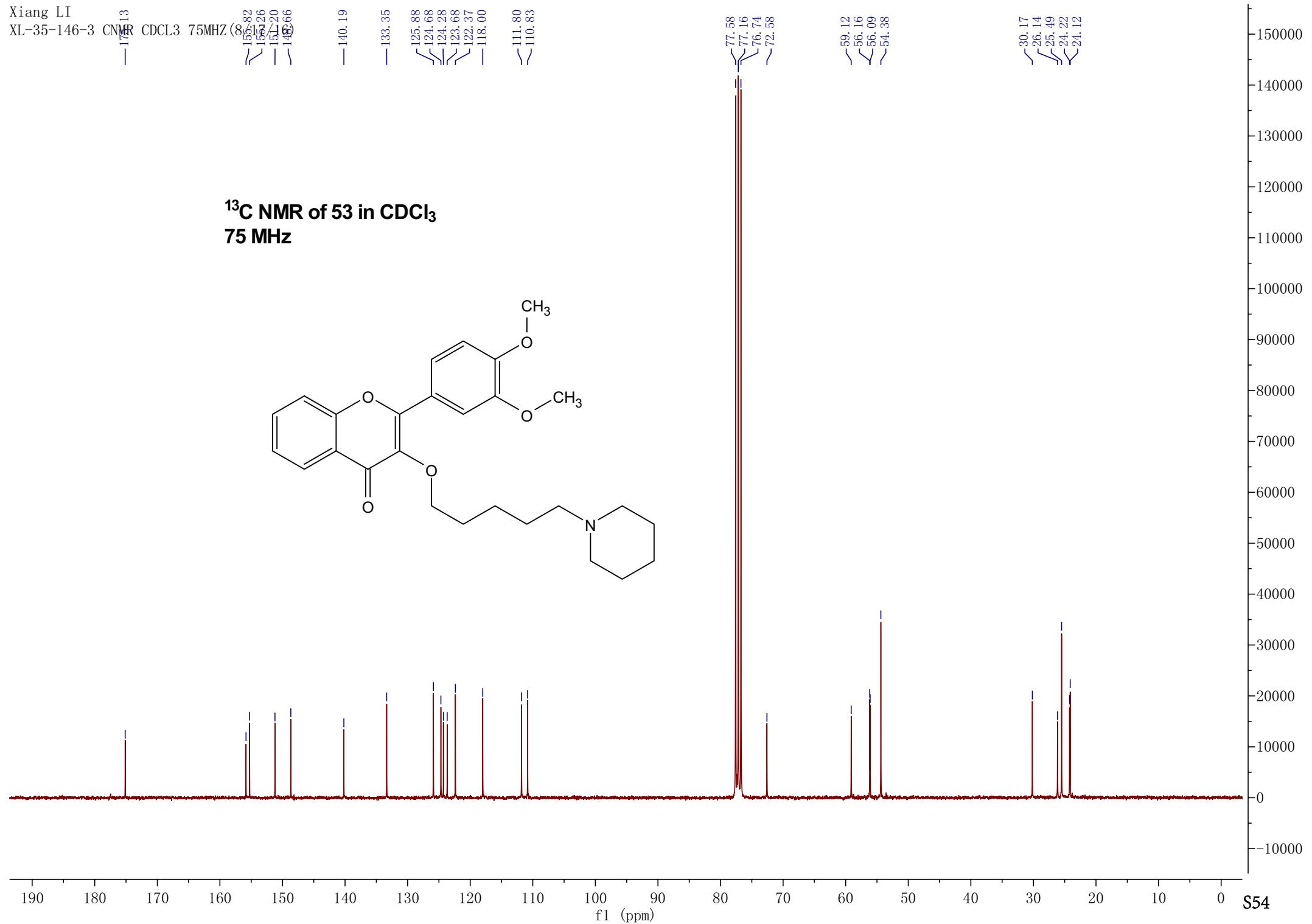
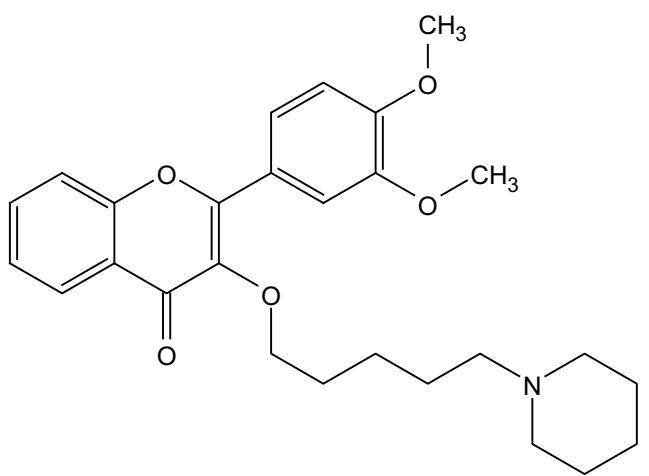
~111.80  
 ~110.83

~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

**<sup>13</sup>C NMR of 53 in CDCl<sub>3</sub>**  
**75 MHz**

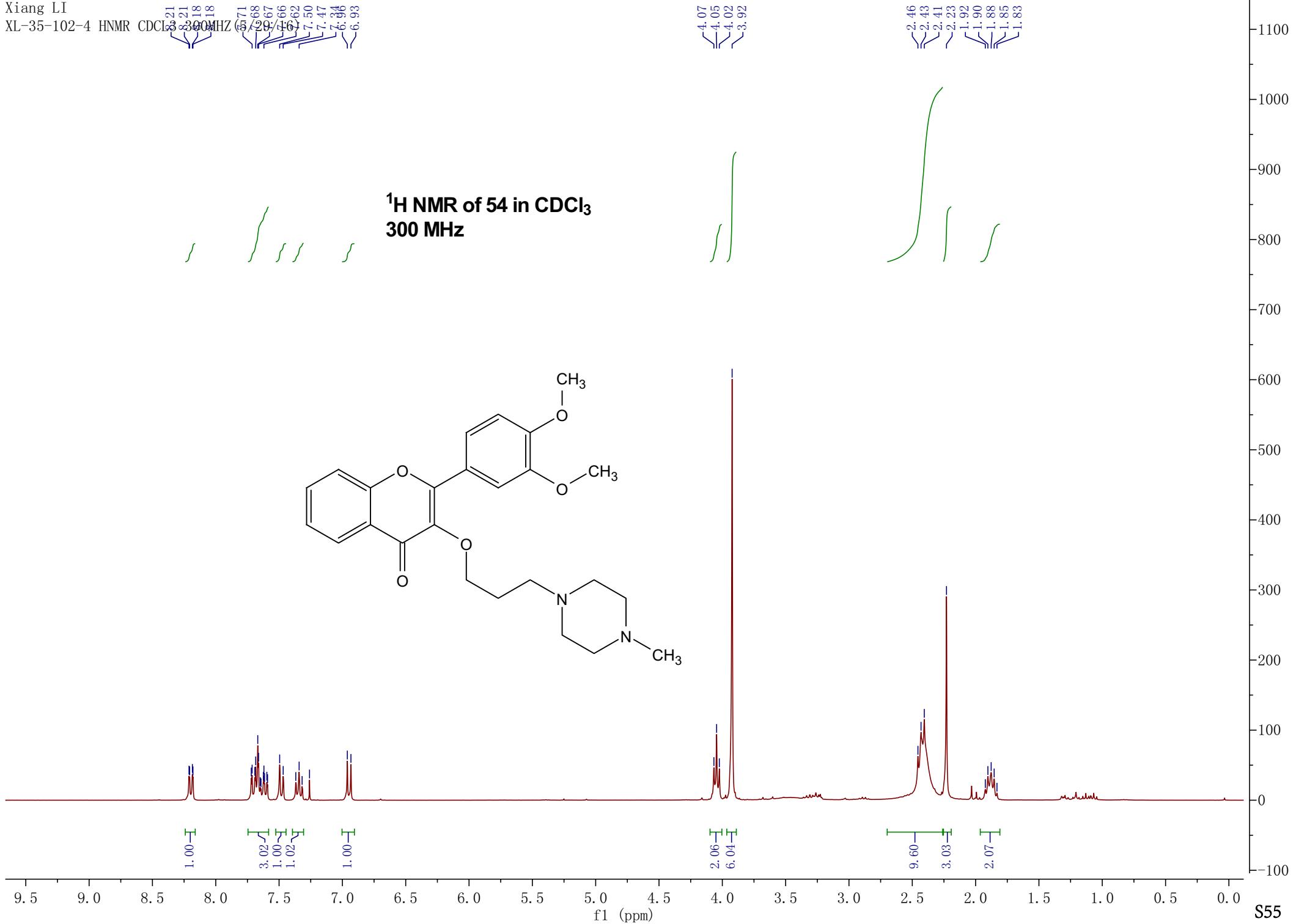
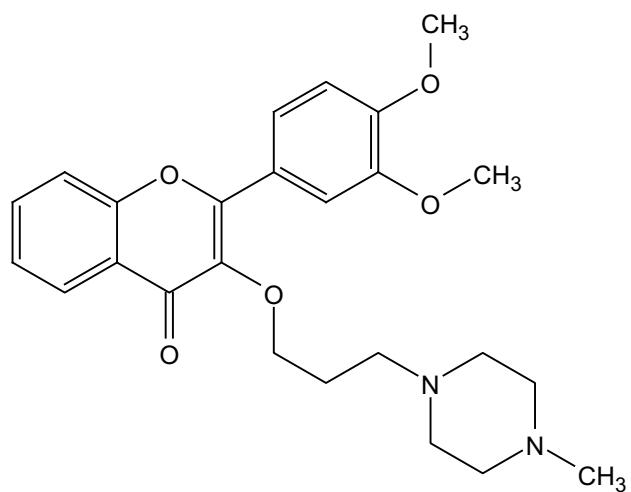


3.21  
3.18  
1.18  
5.71  
5.68  
2.67  
2.66  
1.62  
1.61  
7.50  
7.47  
7.34  
6.93

4.07  
4.05  
4.02  
3.92

2.46  
2.43  
2.41  
2.23  
1.92  
1.90  
1.88  
1.85  
1.83

**<sup>1</sup>H NMR of 54 in CDCl<sub>3</sub>**  
**300 MHz**



—175.01

—159.80  
—155.18  
—154.19  
—148.66

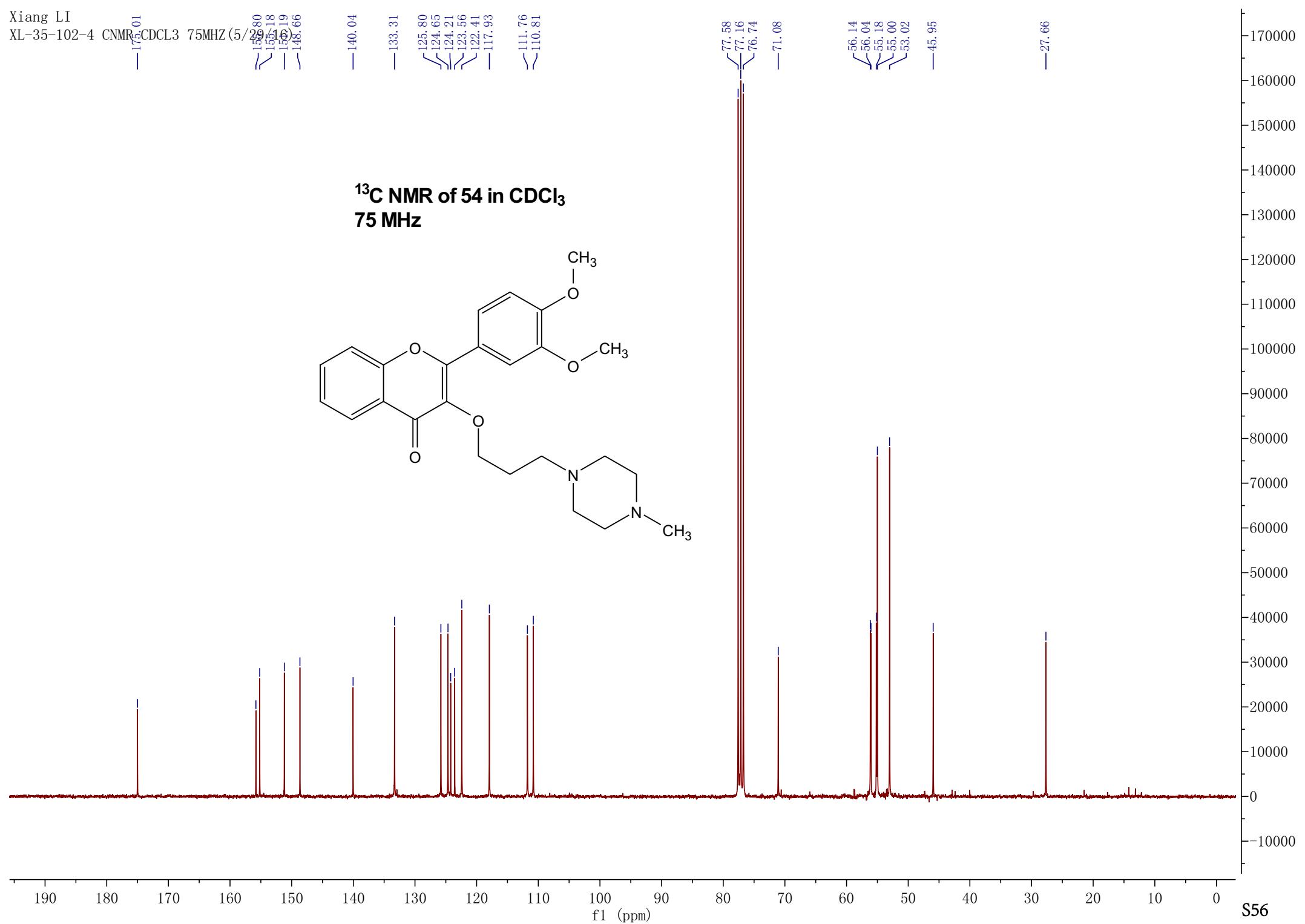
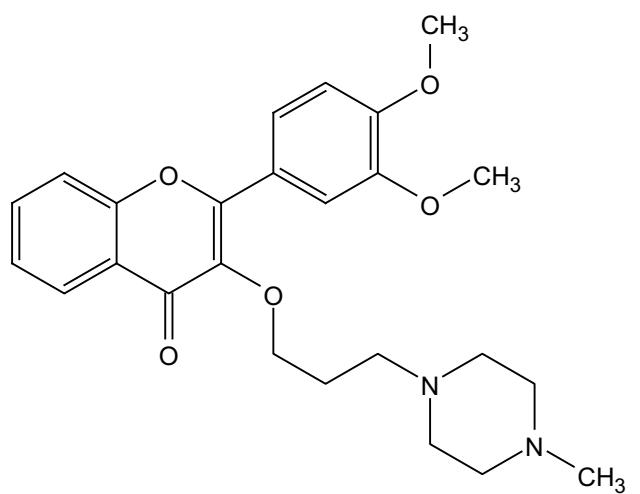
—140.04

—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

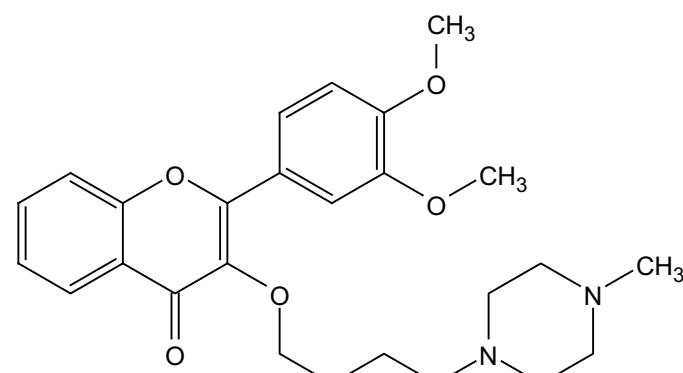
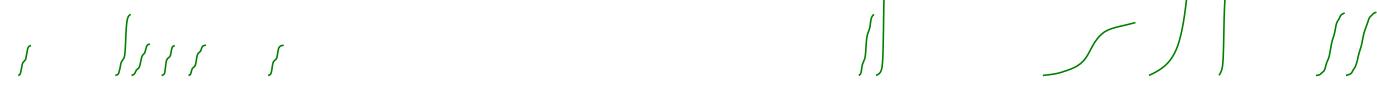
—27.66

**<sup>13</sup>C NMR of 54 in CDCl<sub>3</sub>**  
**75 MHz**



19 20 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95

**<sup>1</sup>H NMR of 55 in CDCl<sub>3</sub>**  
**300 MHz**



— 156.75  
 — 156.20  
 — 151.18  
 — 148.64

— 140.11  
 — 133.31  
 125.83  
 124.65  
 124.23  
 123.63  
 122.36  
 — 117.94

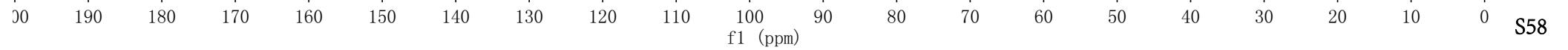
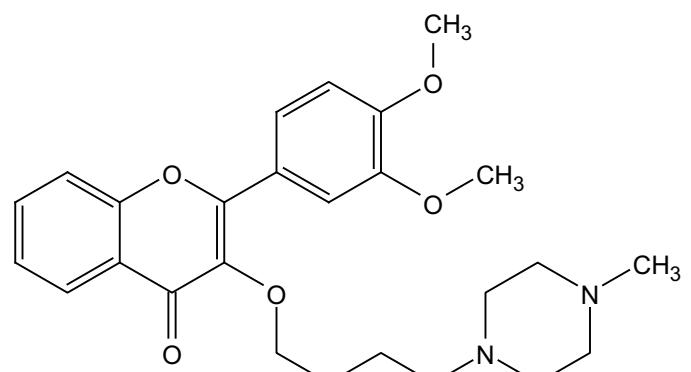
~ 111.79  
 ~ 110.79

77.58  
 77.16  
 76.74  
 ~ 72.49

58.18  
 56.12  
 56.04  
 55.03  
 53.03

— 45.99

— 28.24  
 — 23.31



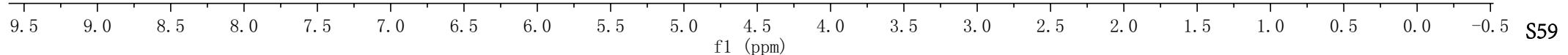
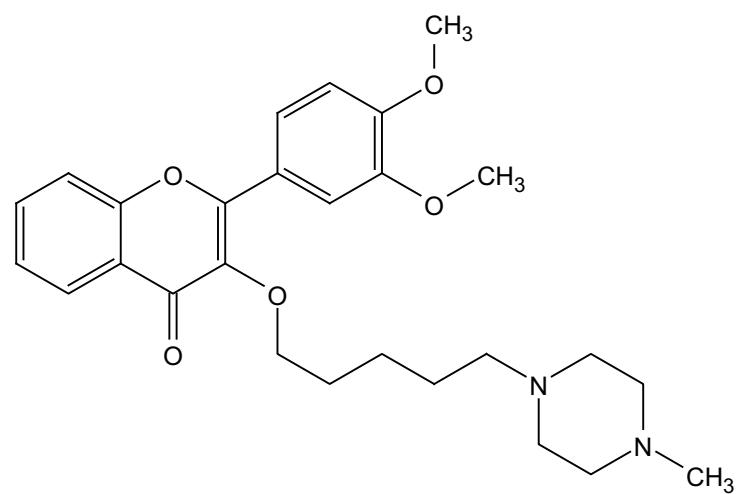
123  
73  
72  
71  
63  
51  
48  
35  
26  
96  
95

4.02  
4.00  
3.98  
3.94  
3.93

2.44  
2.30  
2.27  
2.25

1.74  
1.72  
1.70  
1.46  
1.45  
1.42  
1.39  
1.36  
1.35

**<sup>1</sup>H NMR of 56 in CDCl<sub>3</sub>**  
**300 MHz**



—174.09

 $\sim$ 157.74  
 $\sim$ 156.22  
 $\sim$ 155.18  
 $\sim$ 146.64

—140.17

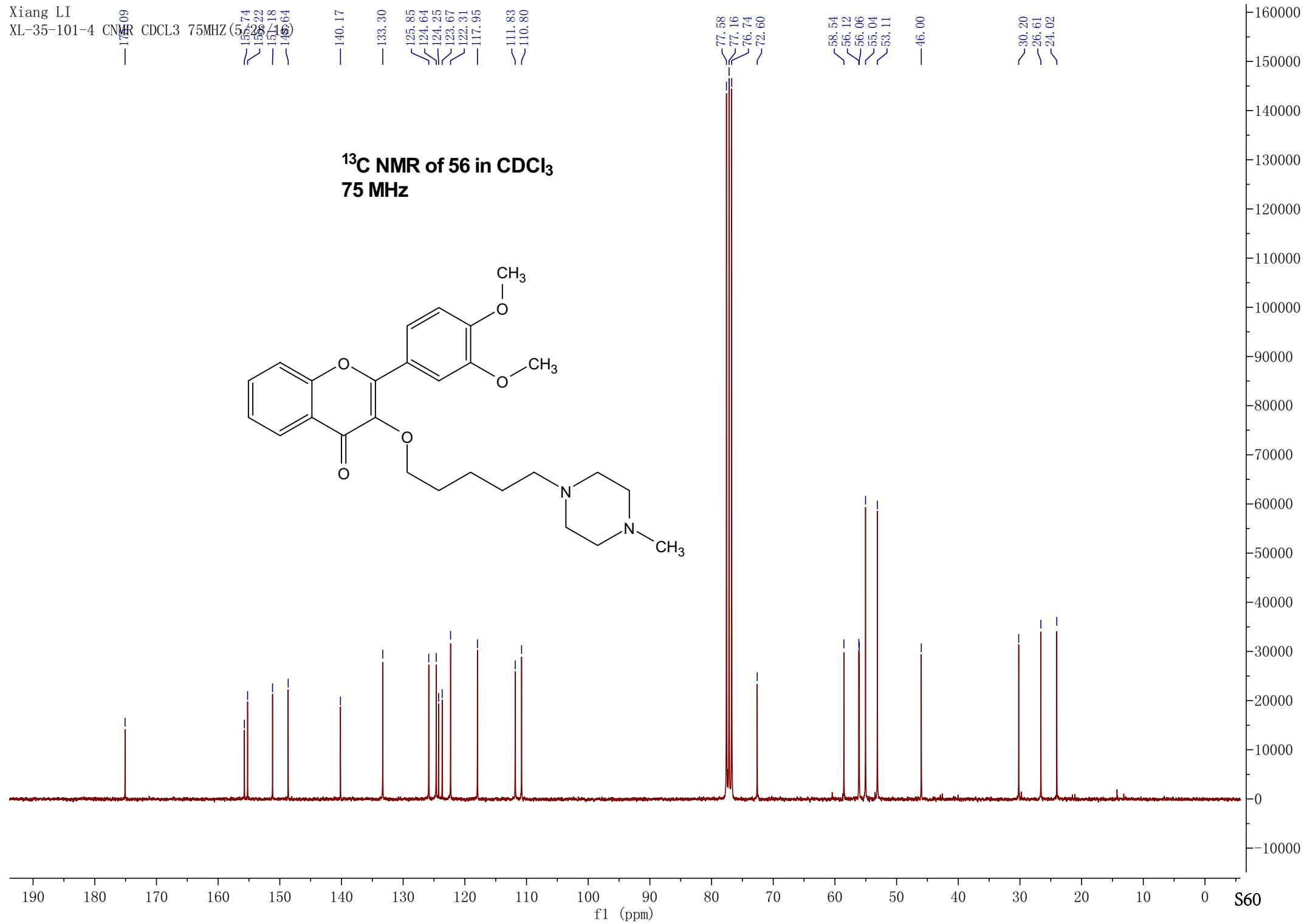
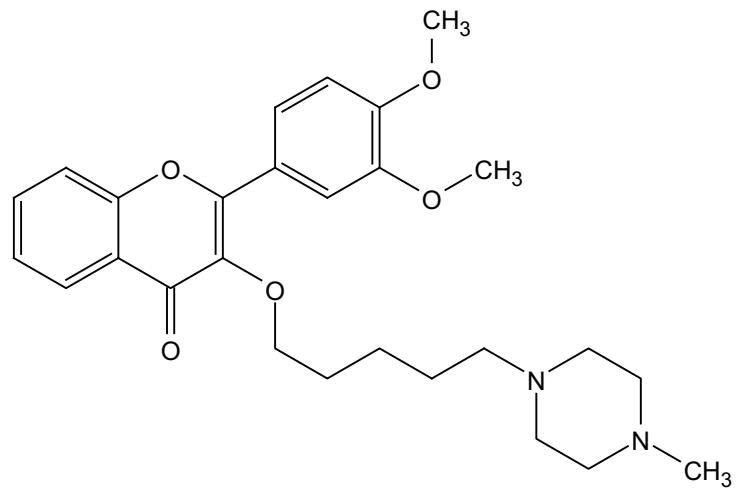
—133.30

125.85  
124.64  
124.25  
123.67  
122.31  
—117.95 $\sim$ 111.83  
 $\sim$ 110.8077.58  
77.16  
76.74  
72.6058.54  
56.12  
56.06  
55.04  
53.11

—46.00

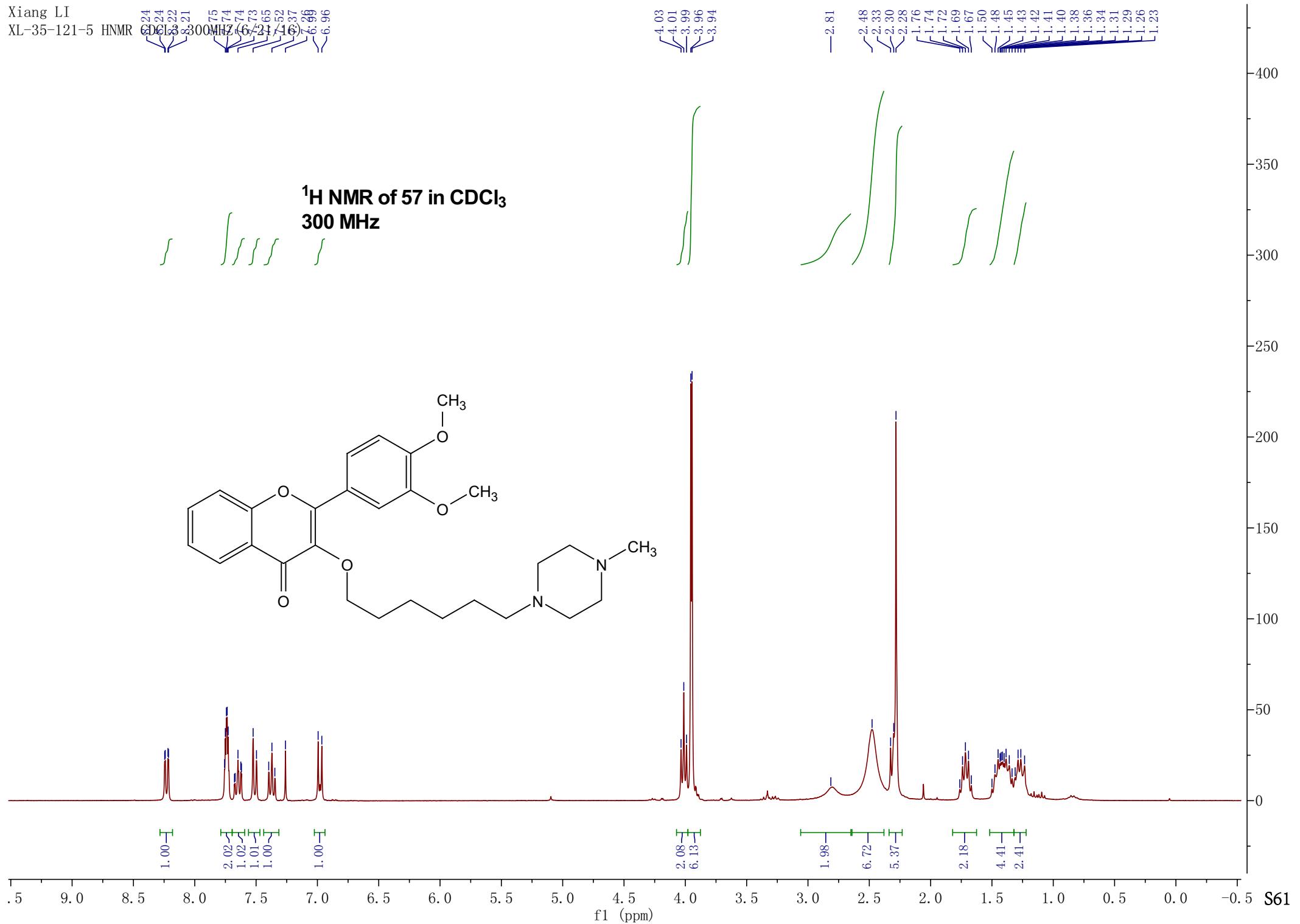
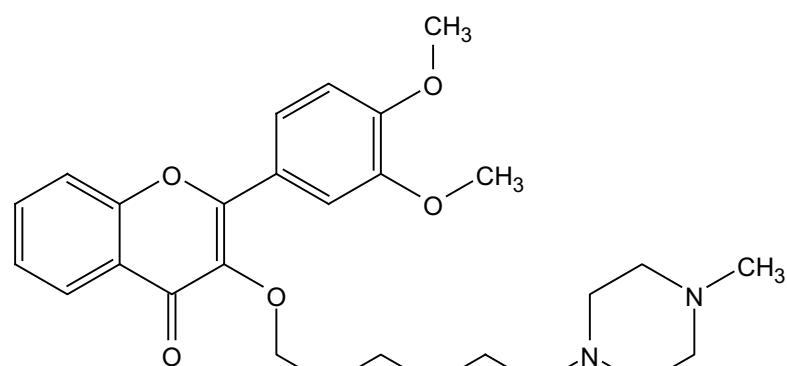
 $\sim$ 30.20  
 $\sim$ 26.61  
 $\sim$ 24.02

**<sup>13</sup>C NMR of 56 in CDCl<sub>3</sub>**  
**75 MHz**





<sup>1</sup>H NMR of 57 in CDCl<sub>3</sub>  
300 MHz

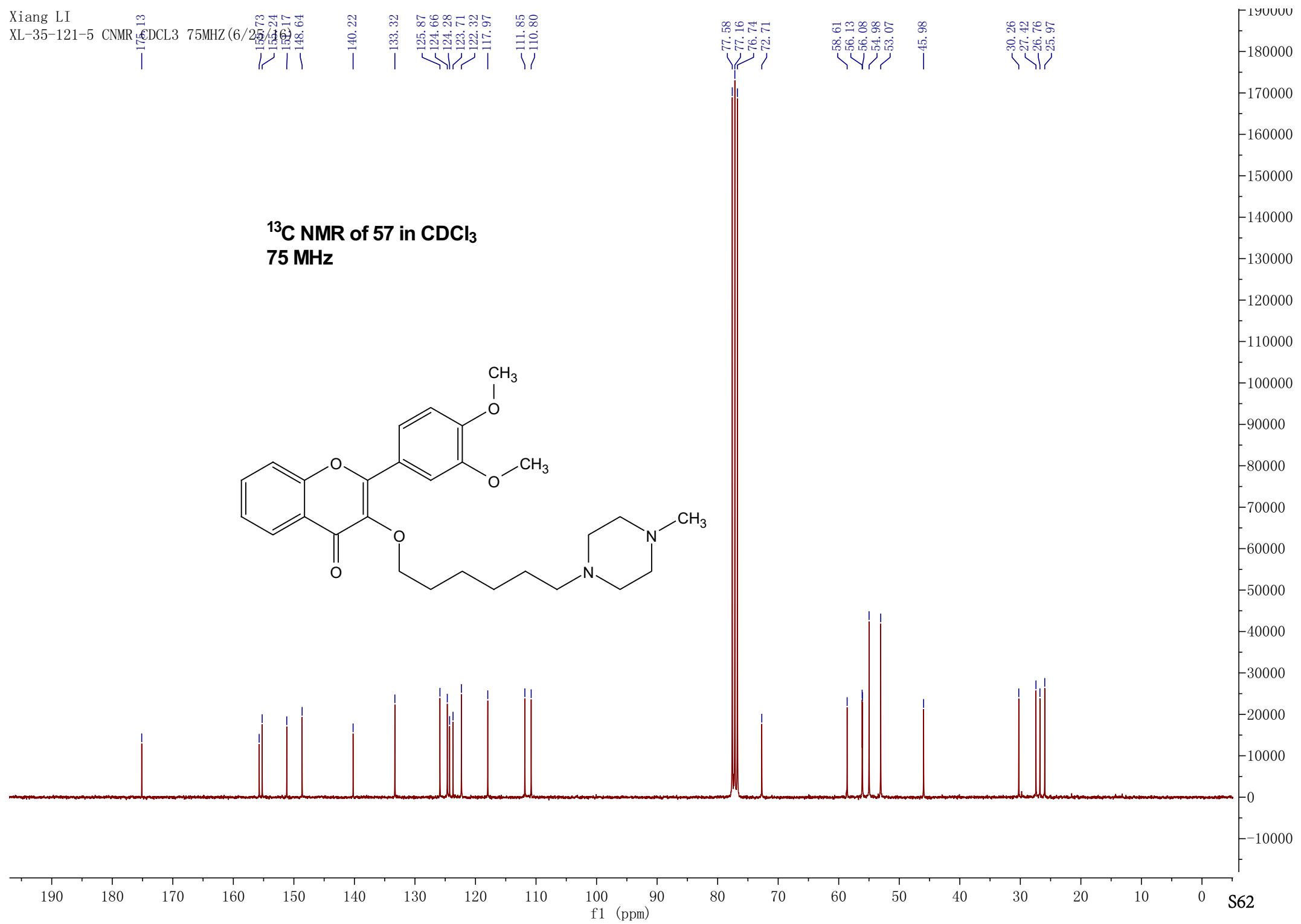
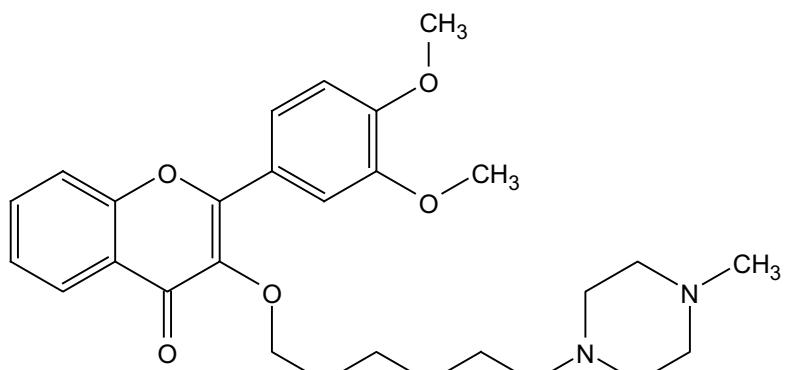


— 176.13  
— 159.73  
— 155.24  
— 152.17  
— 148.64

— 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

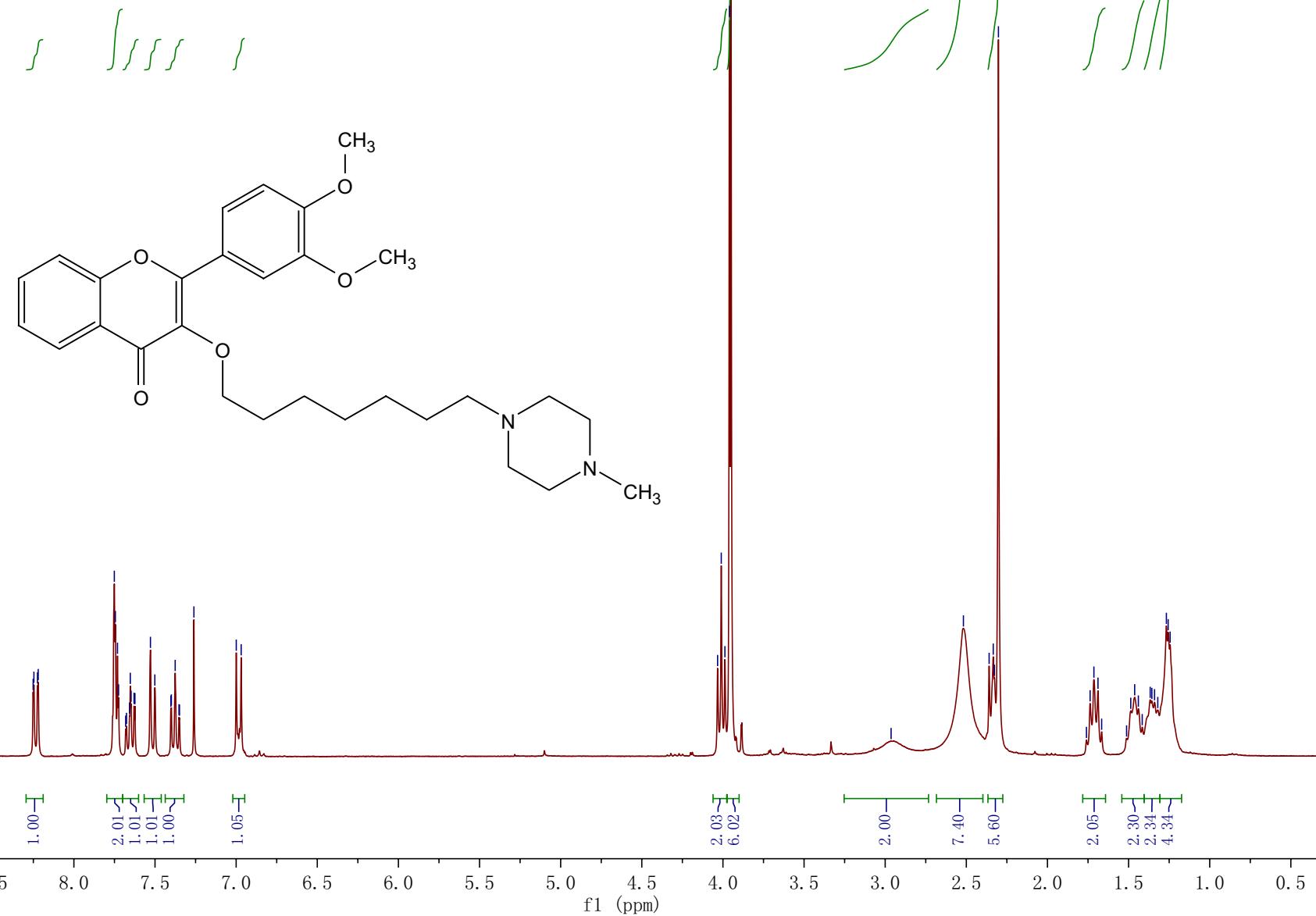
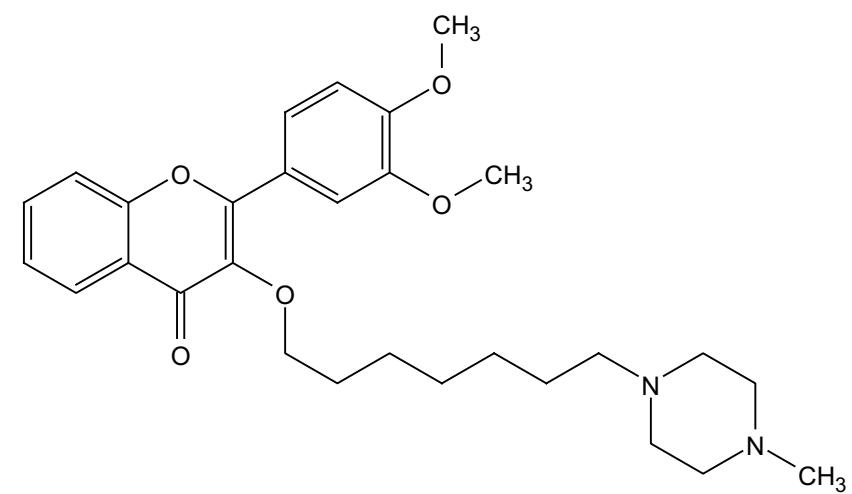
**<sup>13</sup>C NMR of 57 in CDCl<sub>3</sub>**  
**75 MHz**



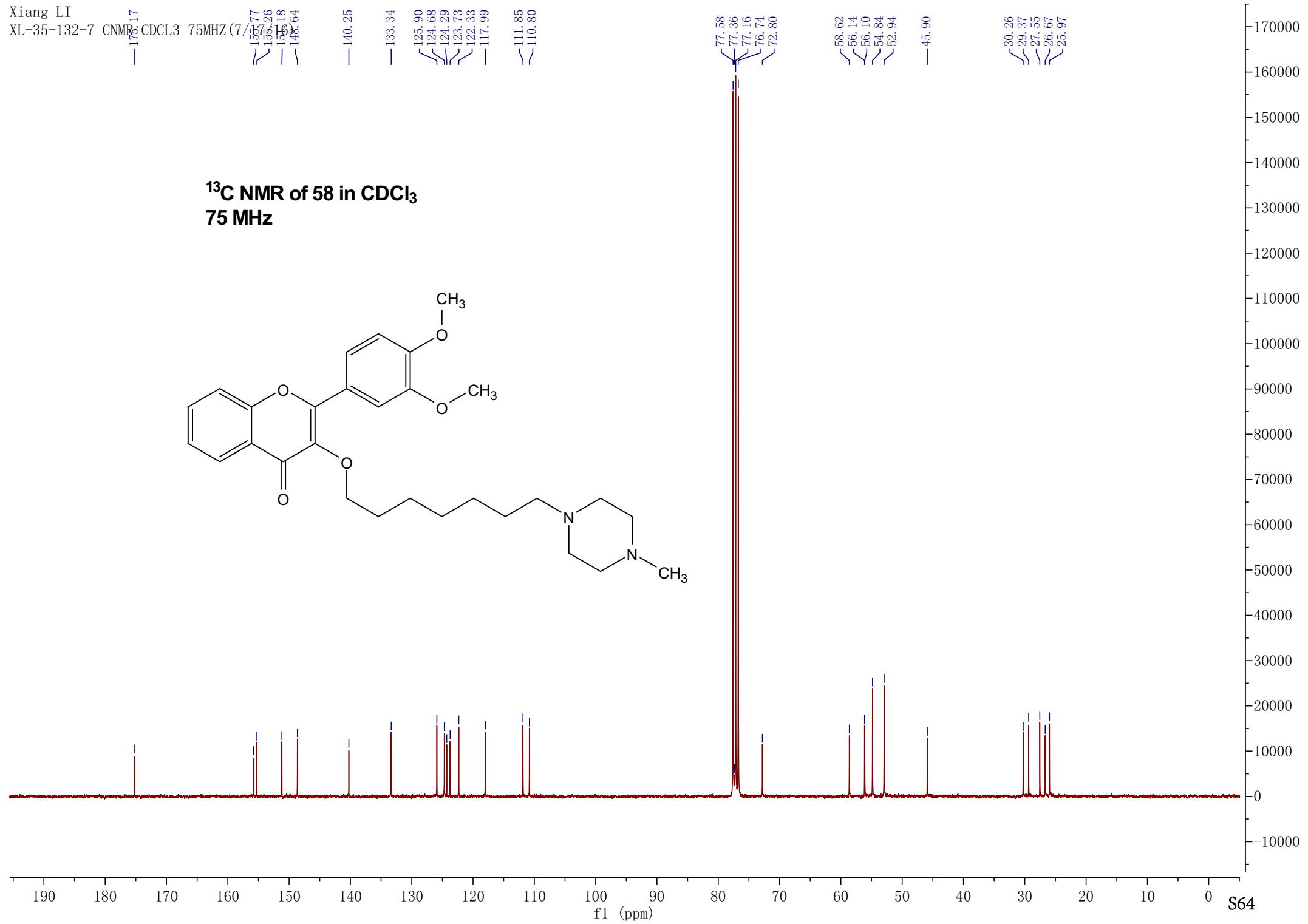
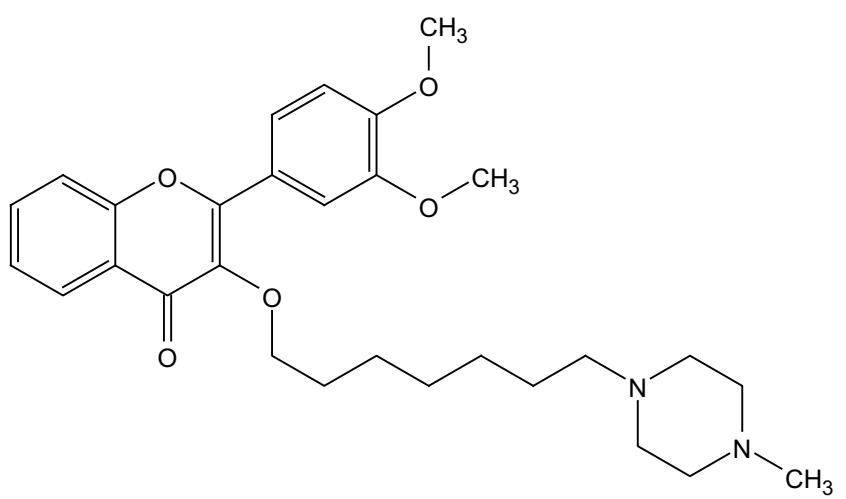
1.25  
1.25  
3.22  
3.22  
7.75  
7.74  
7.73  
7.65  
7.53  
7.50  
7.47  
7.46  
7.38  
7.26  
7.16  
6.97



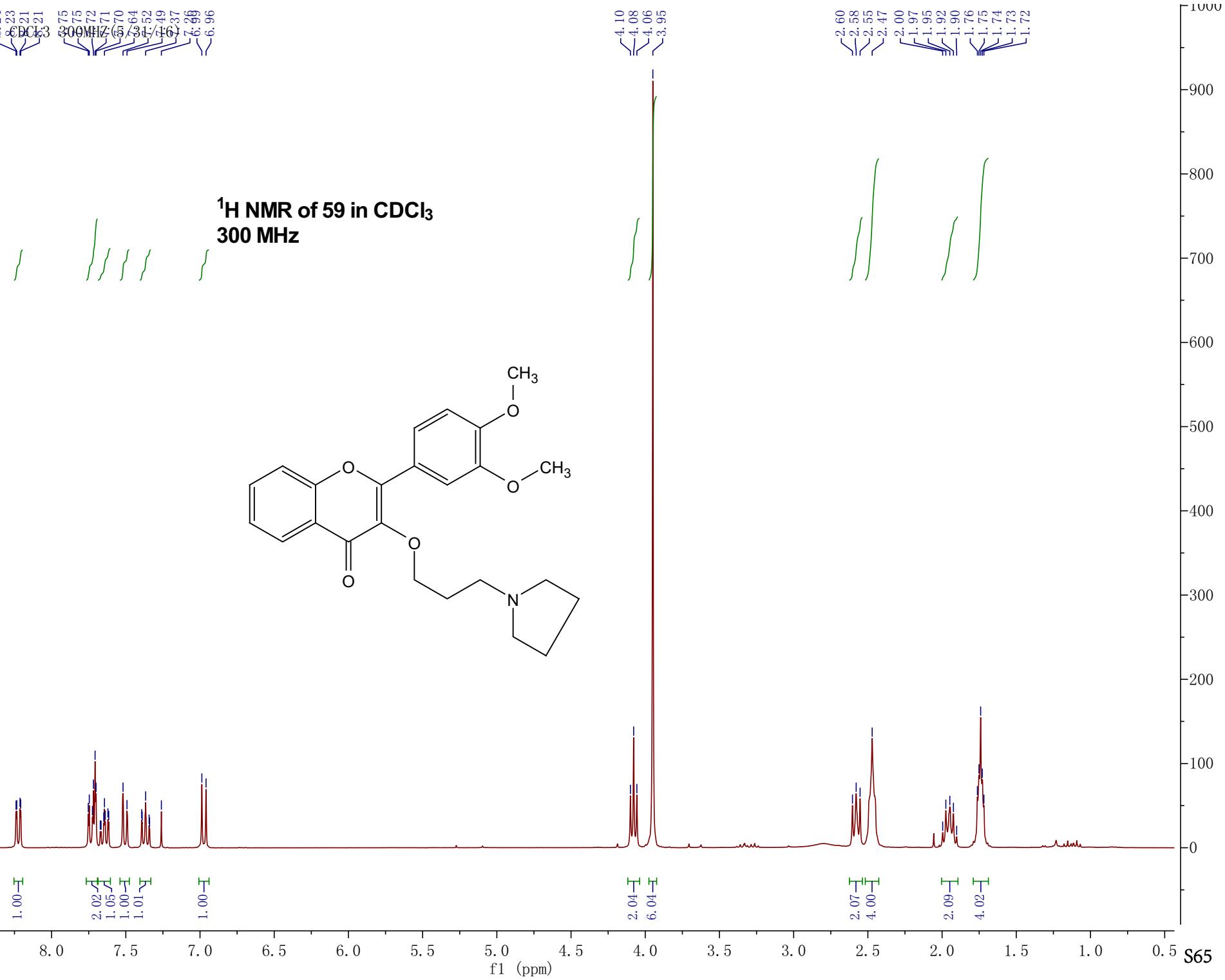
**<sup>1</sup>H NMR of 58 in CDCl<sub>3</sub>**  
**300 MHz**



**<sup>13</sup>C NMR of 58 in CDCl<sub>3</sub>**  
**75 MHz**



XL-35-104-4 HNMR  $\delta$  ppm CDCl<sub>3</sub> 300MHz (5/31/16)



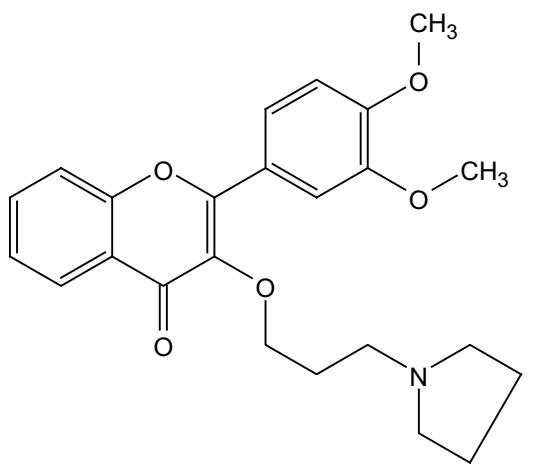
—178.09  
 —153.89  
 —152.24  
 —152.23  
 —148.71

—140.08  
 —133.35  
 125.85  
 124.69  
 124.26  
 123.61  
 122.44  
 —117.98  
 —111.78  
 —110.84

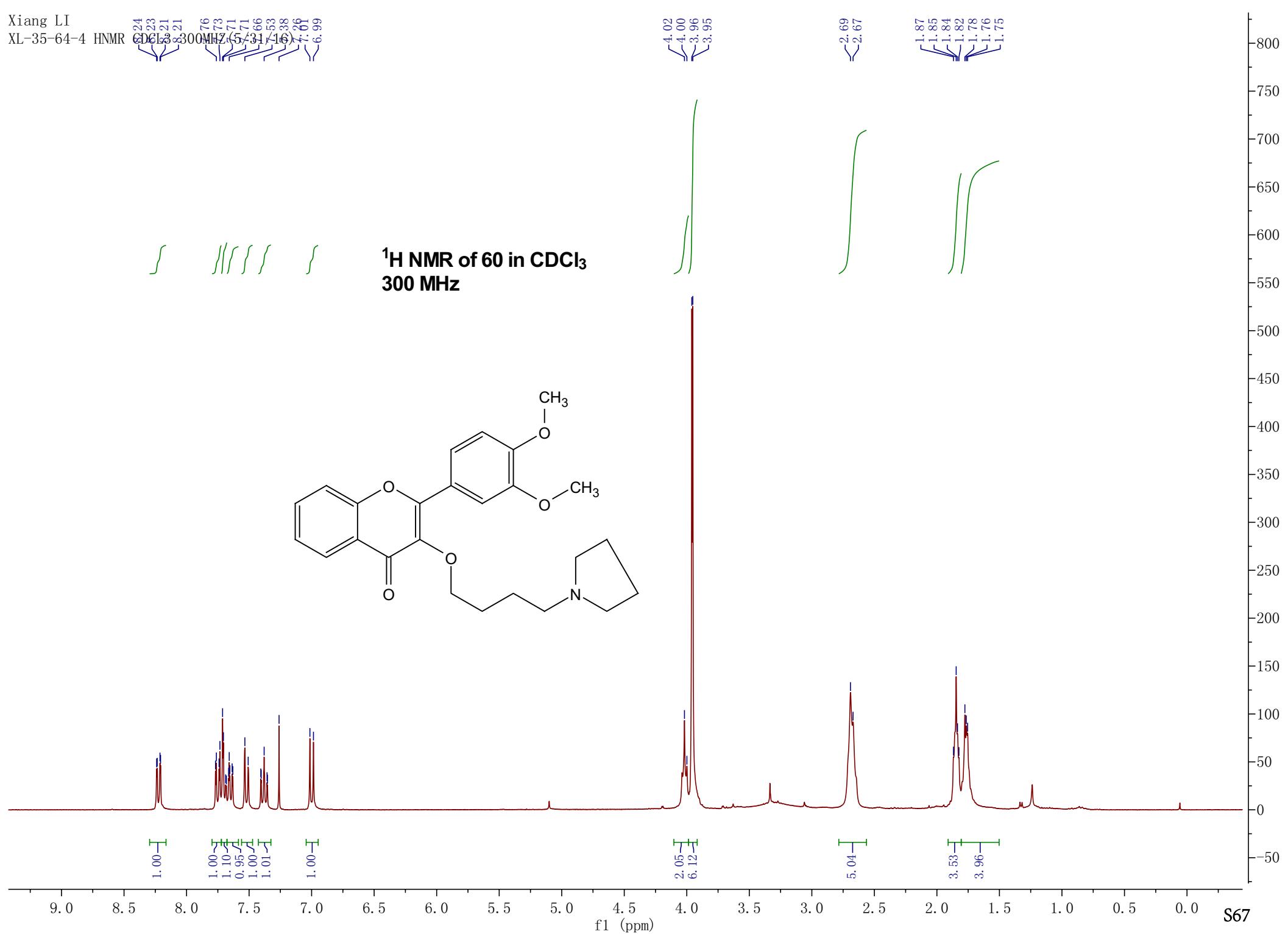
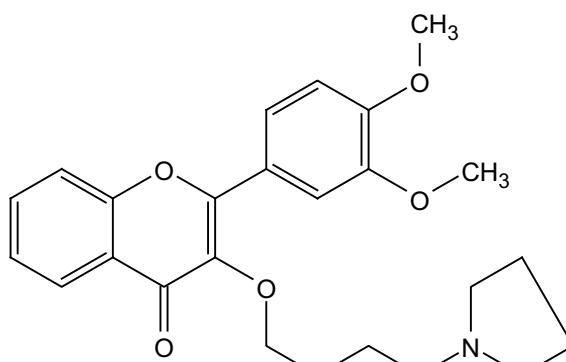
77.58  
 77.16  
 76.74  
 —71.22  
 56.18  
 56.09  
 54.24  
 53.29

—29.73  
 —23.51

**<sup>13</sup>C NMR of 59 in CDCl<sub>3</sub>**  
**75 MHz**



**<sup>1</sup>H NMR of 60 in CDCl<sub>3</sub>**  
**300 MHz**



—176.14

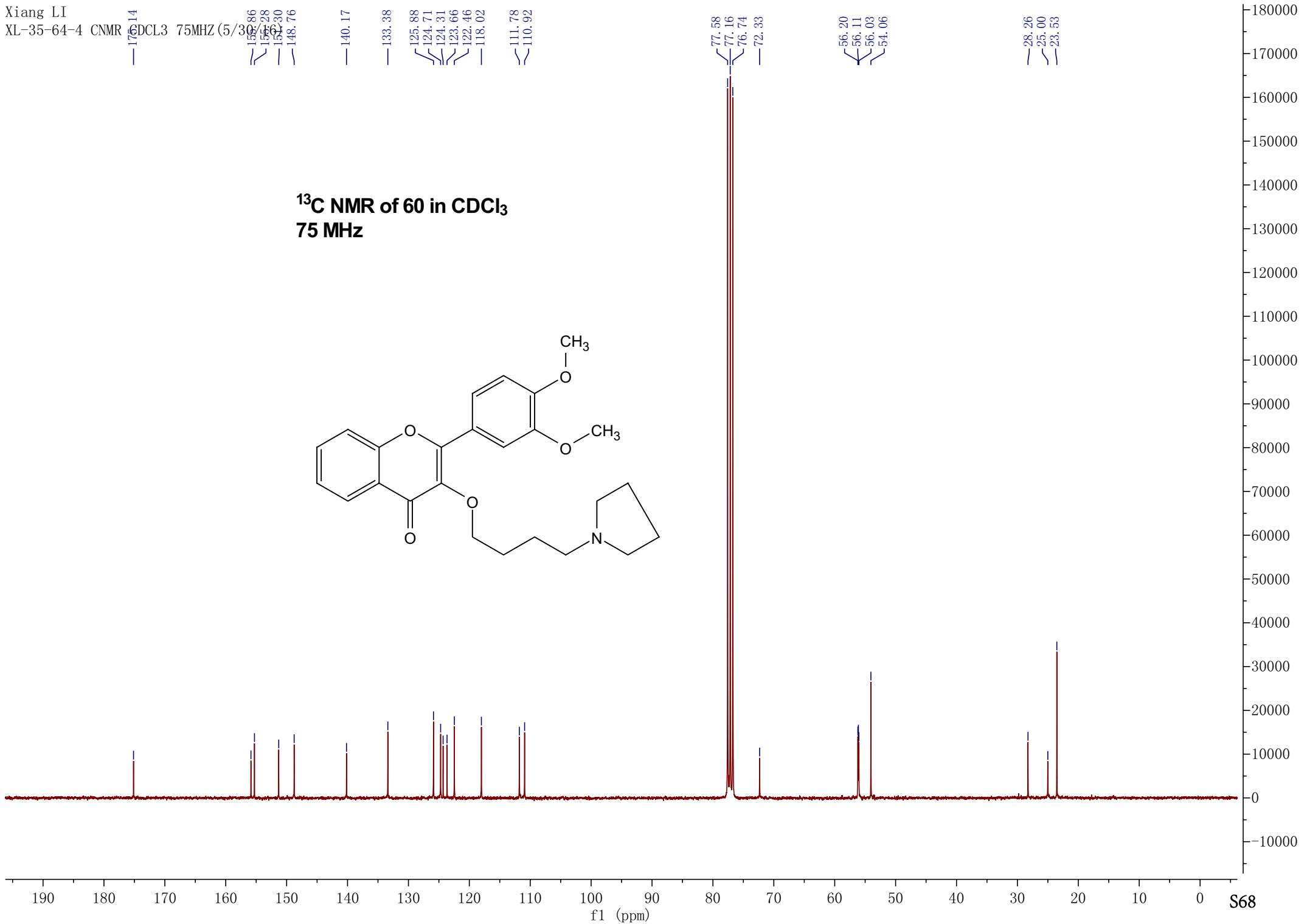
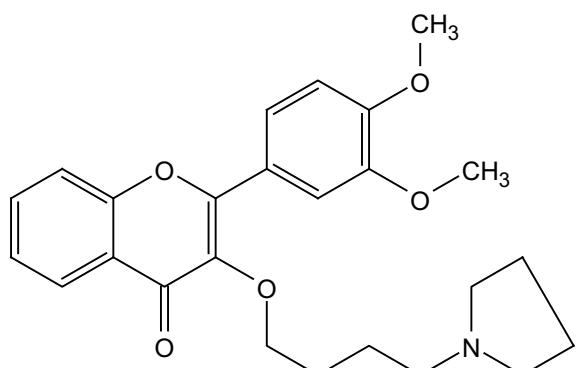
 $\begin{cases} -150.86 \\ -152.28 \\ -152.30 \\ -148.76 \end{cases}$ 

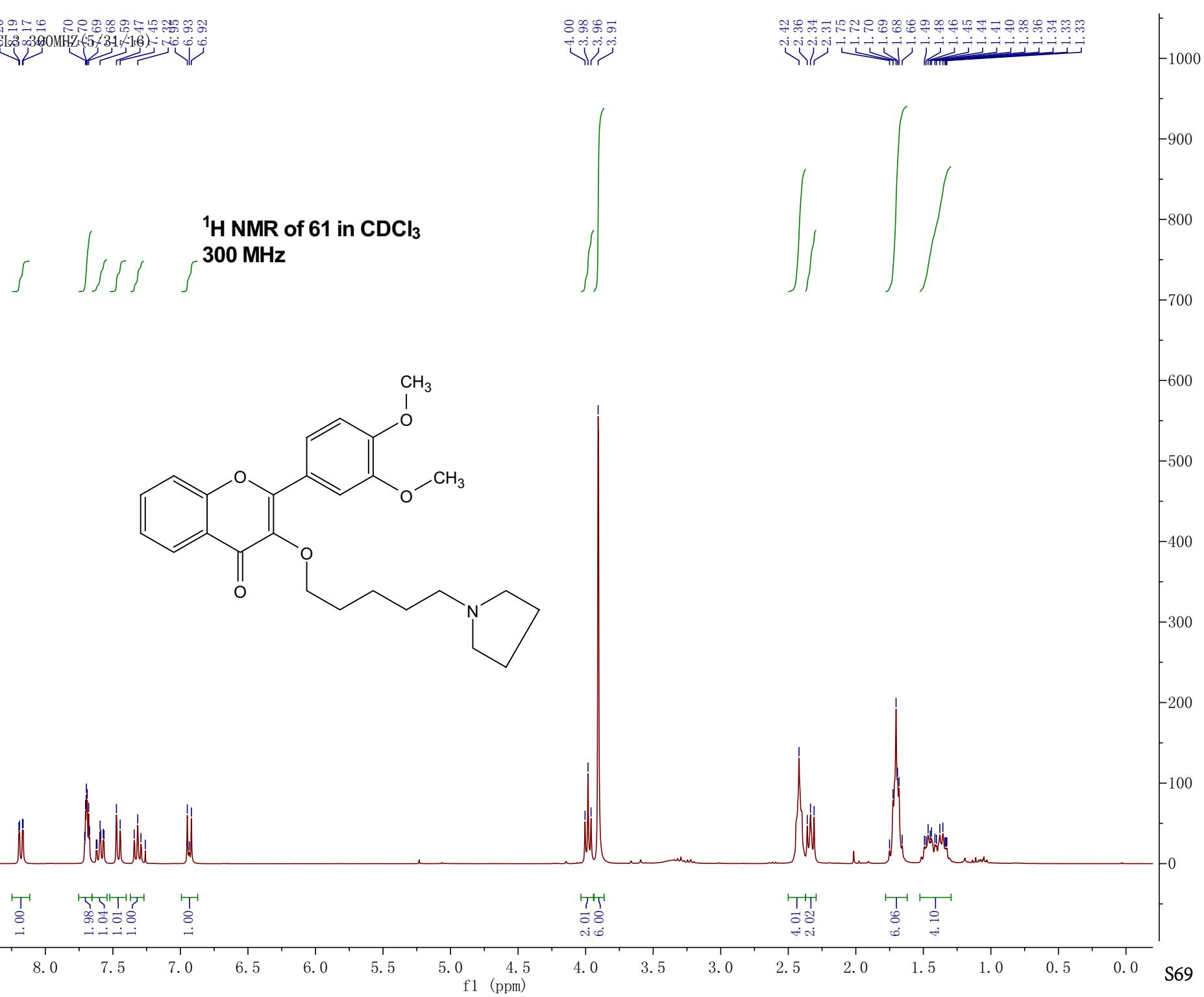
—140.17

—133.38

 $\begin{cases} 125.88 \\ 124.71 \\ 124.31 \\ 123.66 \\ 122.46 \\ -118.02 \end{cases}$  $\sim 111.78$  $\sim 110.92$  $\begin{cases} 77.58 \\ 77.16 \\ 76.74 \\ -72.33 \end{cases}$  $\begin{cases} 56.20 \\ 56.11 \\ 56.03 \\ 54.06 \end{cases}$  $\begin{cases} -28.26 \\ -25.00 \\ -23.53 \end{cases}$ 

**$^{13}\text{C}$  NMR of 60 in  $\text{CDCl}_3$**   
**75 MHz**





— 155.63  
— 155.11  
— 155.07  
— 148.54

— 140.08

— 133.20

— 125.72

— 124.53

— 124.15

— 123.56

— 122.23

— 117.87

— 111.72

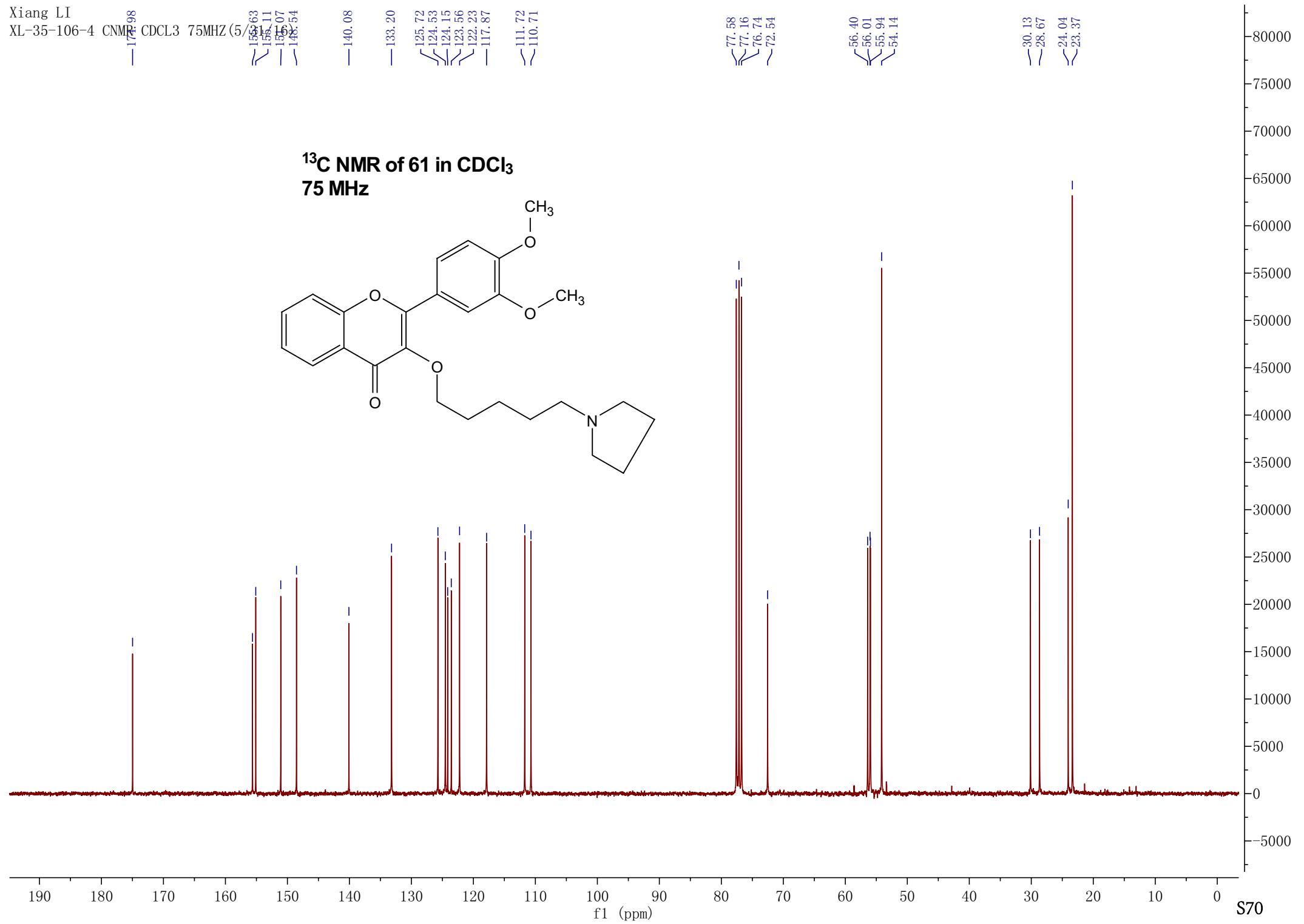
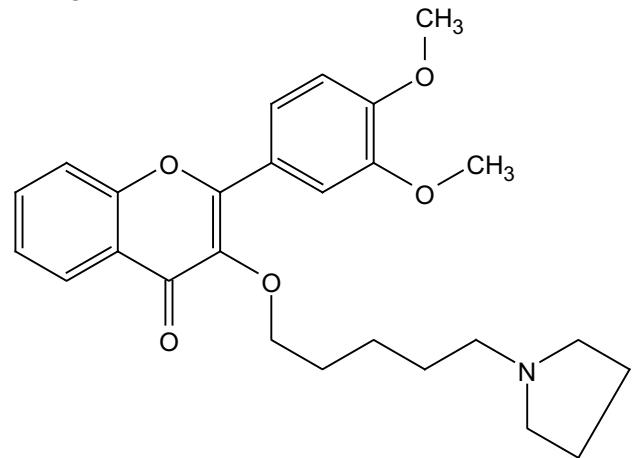
— 110.71

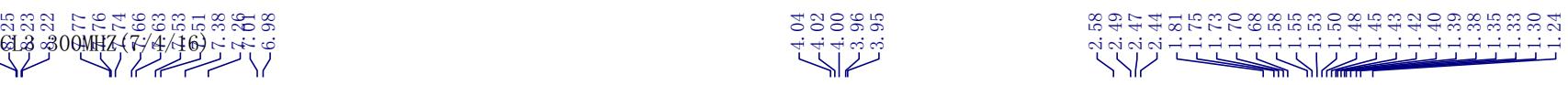
— 77.58  
— 77.16  
— 76.74  
— 72.54

— 56.40  
— 56.01  
— 55.94  
— 54.14

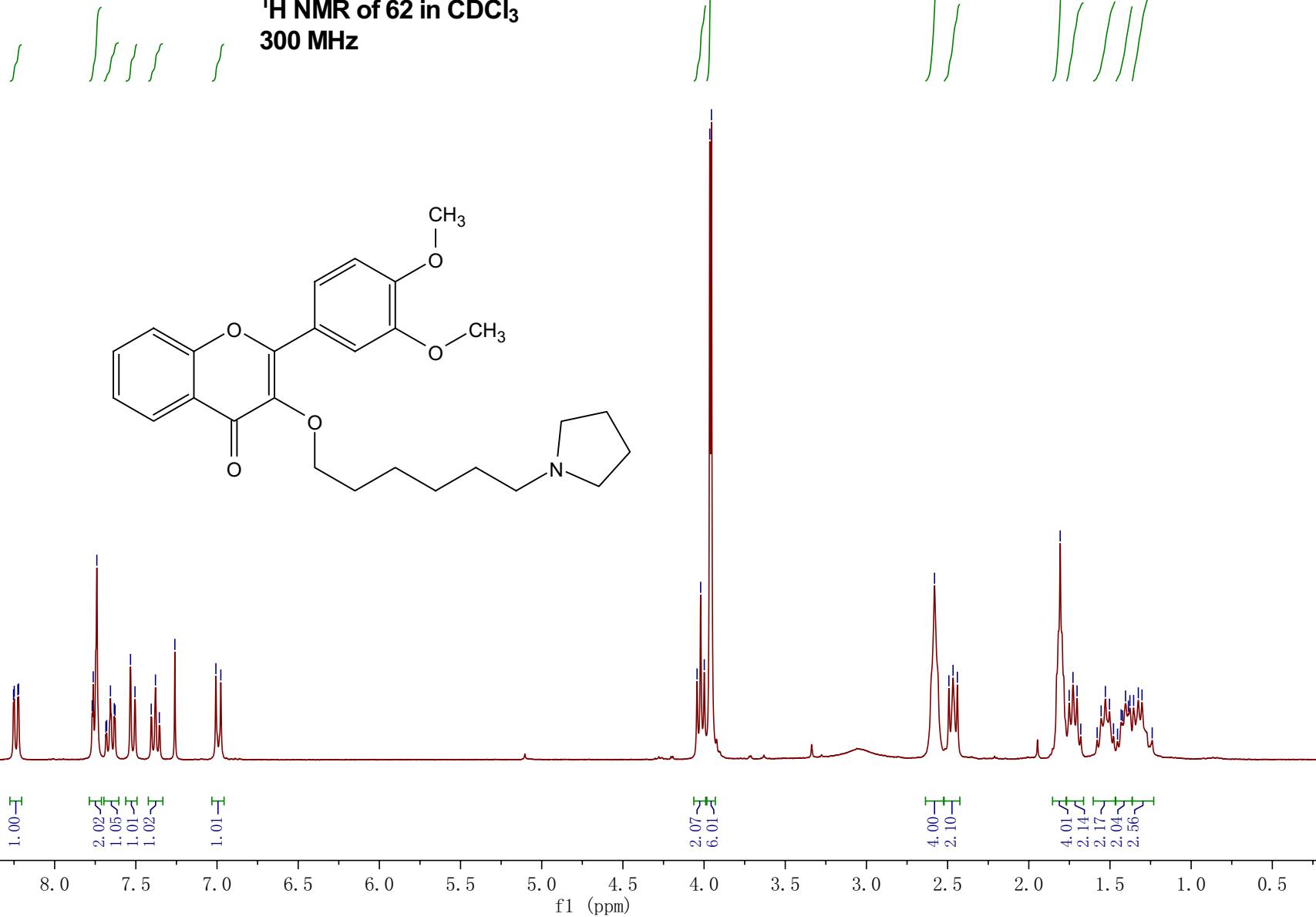
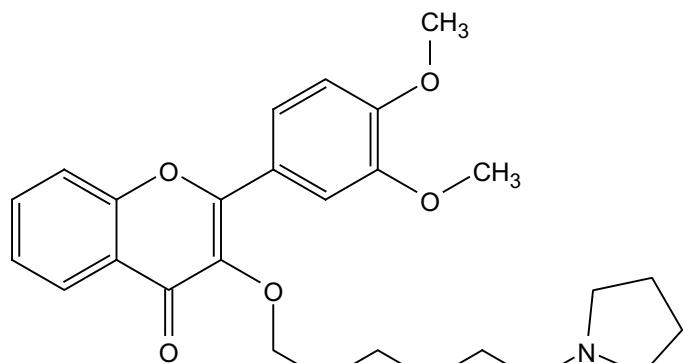
— 30.13  
— 28.67  
— 24.04  
— 23.37

**<sup>13</sup>C NMR of 61 in CDCl<sub>3</sub>**  
**75 MHz**





**<sup>1</sup>H NMR of 62 in CDCl<sub>3</sub>  
300 MHz**



— 154.80  
— 154.27  
— 152.20  
— 148.66

— 140.24

— 133.35

— 125.90  
— 124.69  
— 124.30  
— 123.72  
— 122.38  
— 118.01

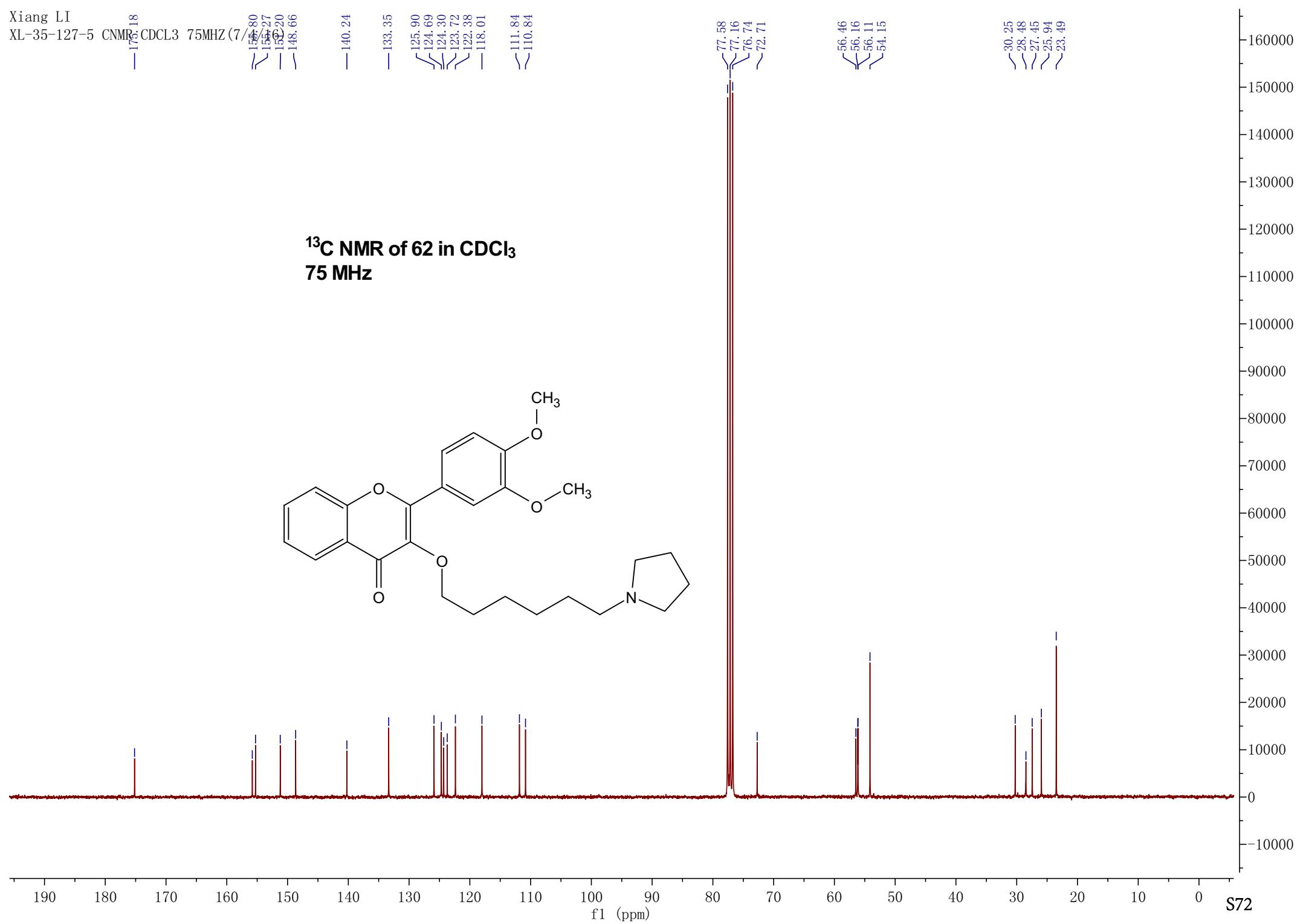
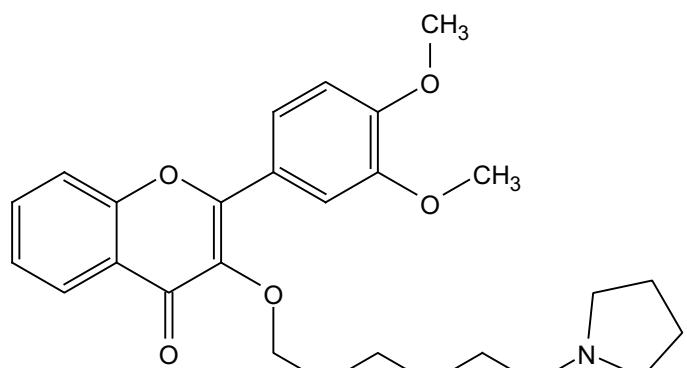
— 111.84  
— 110.84

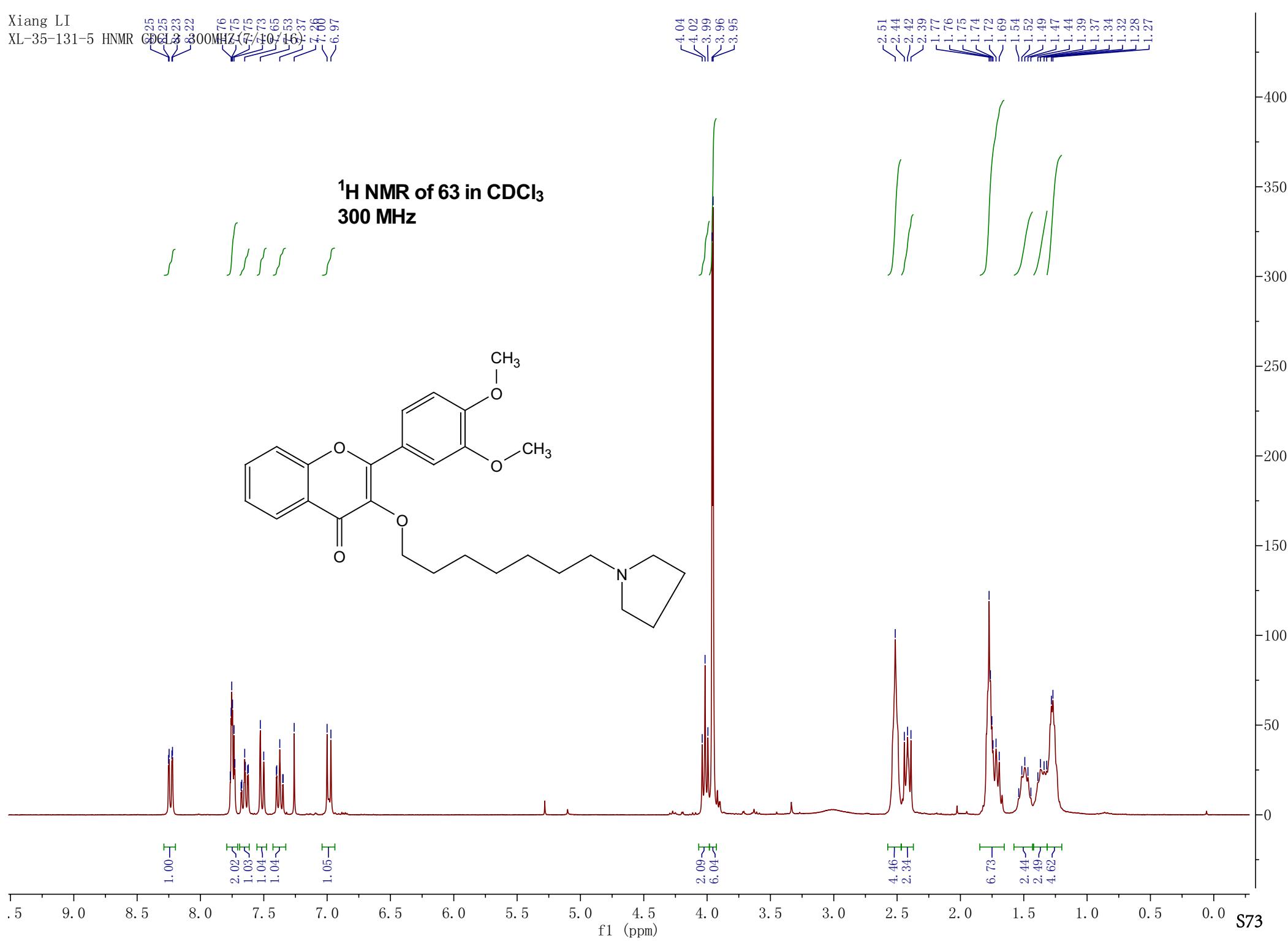
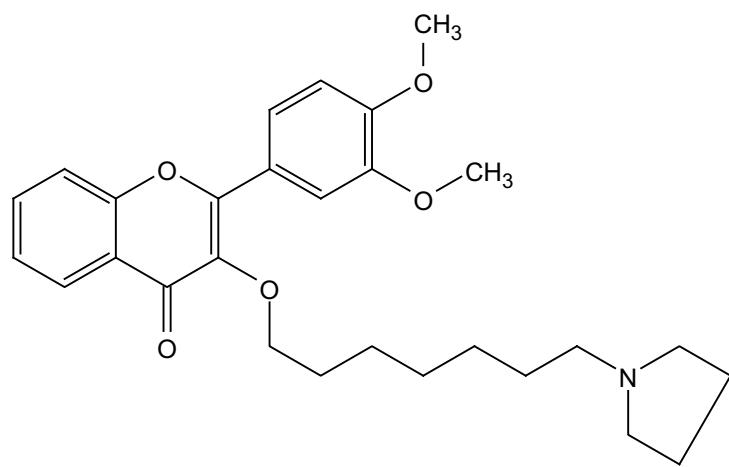
— 77.58  
— 77.16  
— 76.74  
— 72.71

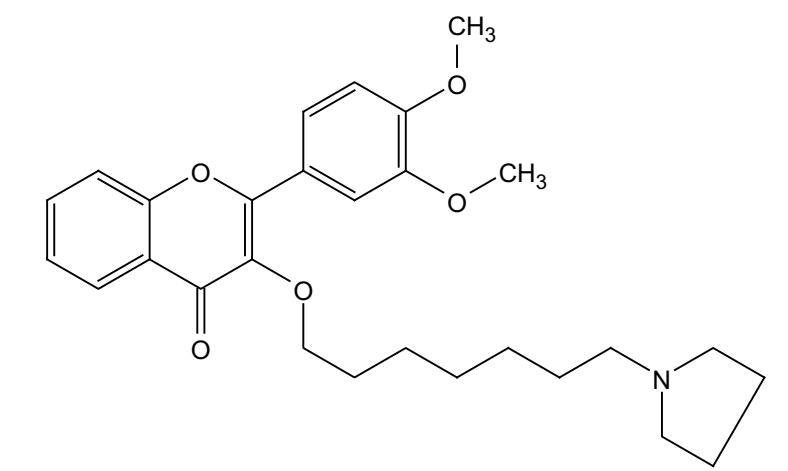
— 56.46  
— 56.16  
— 56.11  
— 54.15

— 30.25  
— 28.48  
— 27.45  
— 25.94  
— 23.49

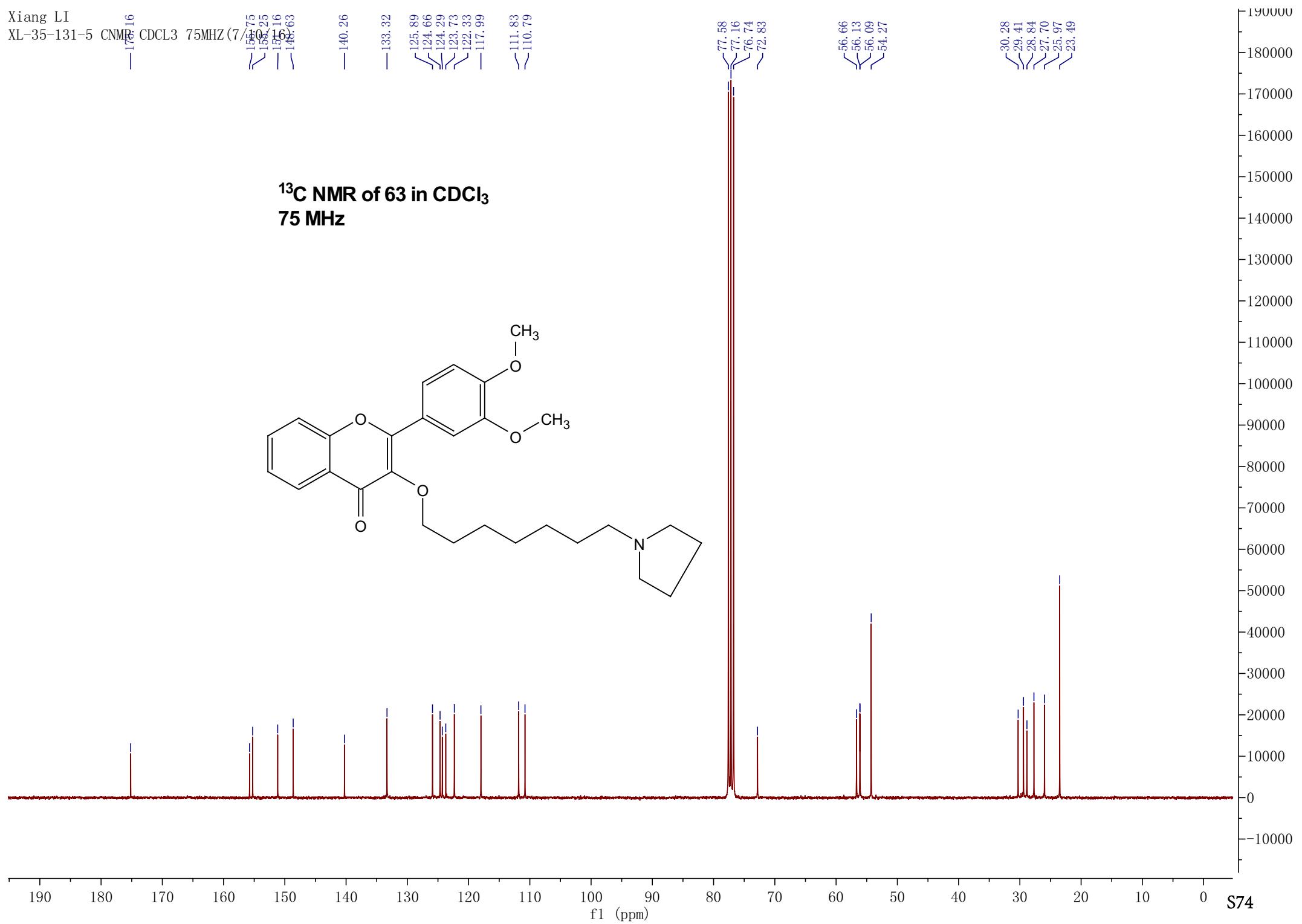
**<sup>13</sup>C NMR of 62 in CDCl<sub>3</sub>  
75 MHz**







**<sup>13</sup>C NMR of 63 in CDCl<sub>3</sub>**  
**75 MHz**

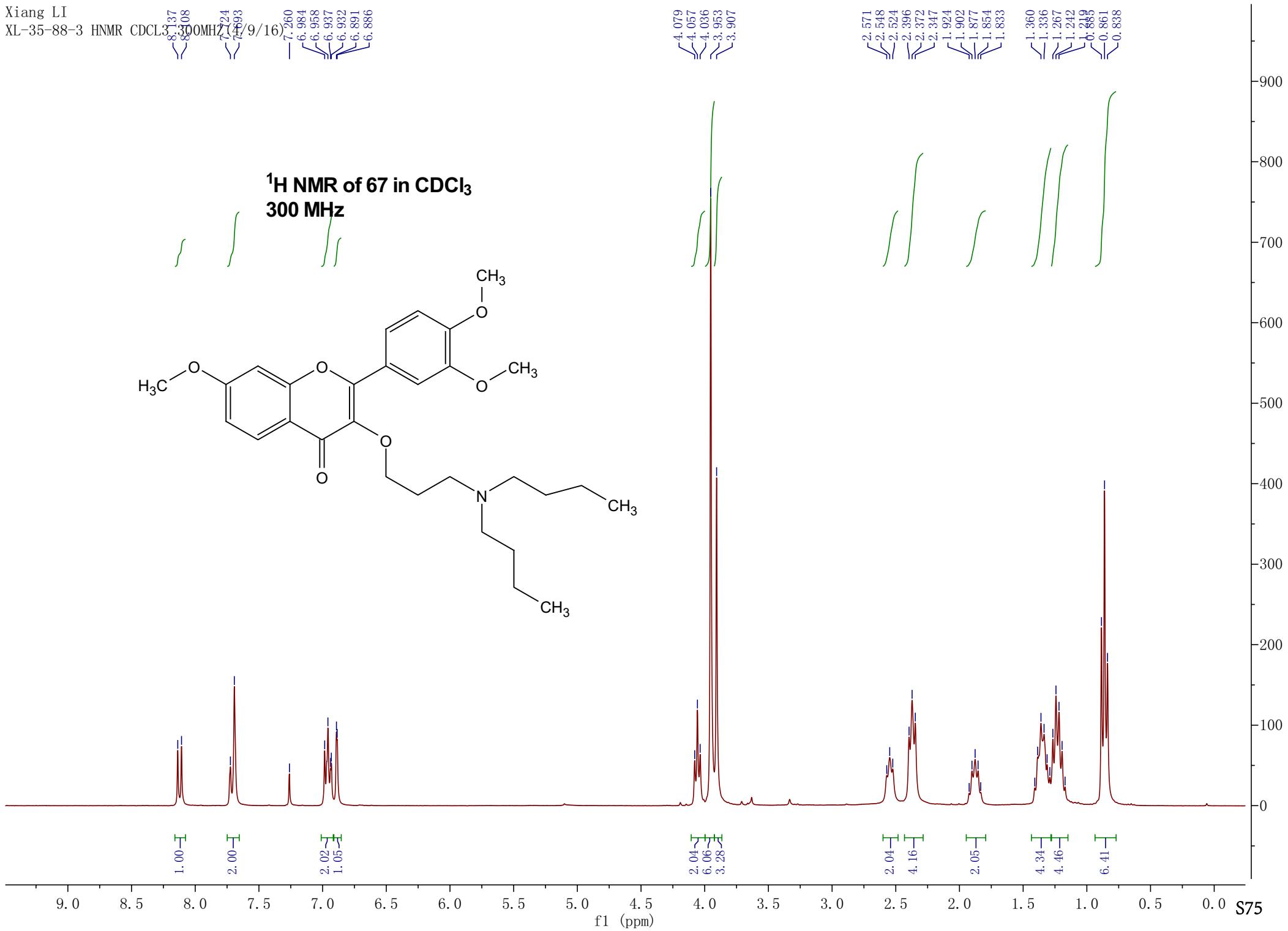
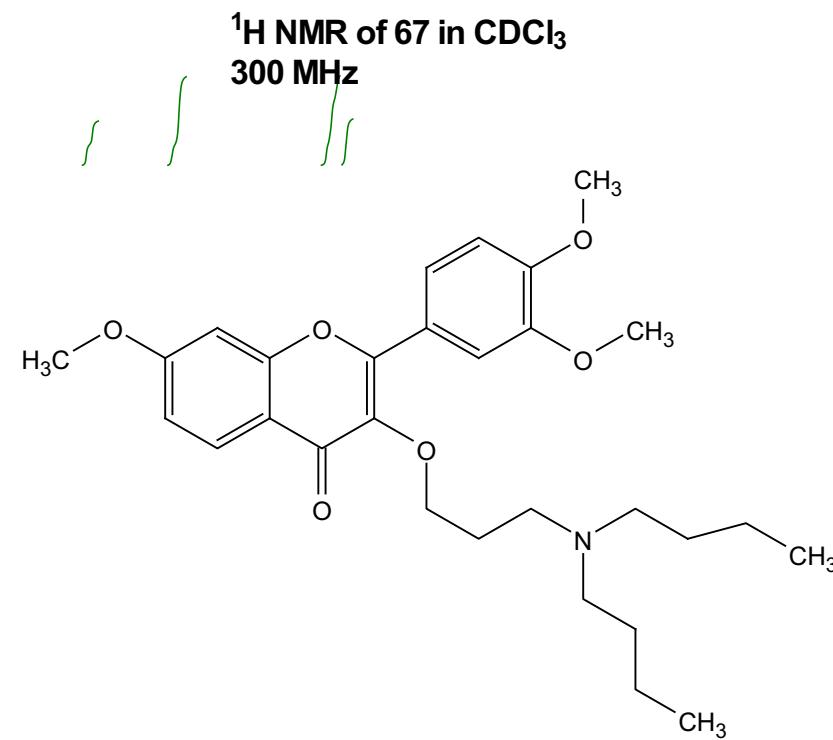


8.37  
 8.08  
 7.93  
 7.24  
 7.00  
 6.984  
 6.958  
 6.937  
 6.932  
 6.891  
 6.886

-7.260  
 4.079  
 4.057  
 4.036  
 3.953  
 3.907

2.571  
 2.548  
 2.524  
 2.396  
 2.372  
 2.347  
 1.924  
 1.902  
 1.877  
 1.854  
 1.833

1.360  
 1.336  
 1.267  
 1.242  
 1.219  
 1.085  
 0.861  
 0.838



—179.60  
—169.02  
—154.00  
—154.37  
—154.37  
—152.05  
—148.68

—139.93

~127.20  
~123.75  
~122.22  
~118.17  
~114.36  
~111.65  
~110.78

—100.03

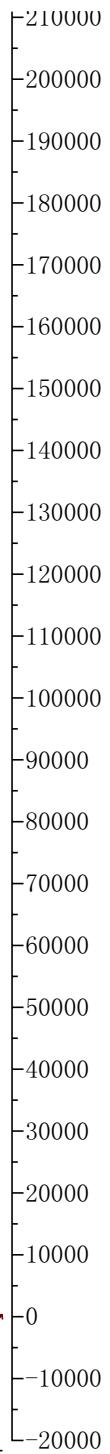
77.58  
77.16  
76.74  
—71.43

56.17  
56.05  
55.95  
53.83  
51.09

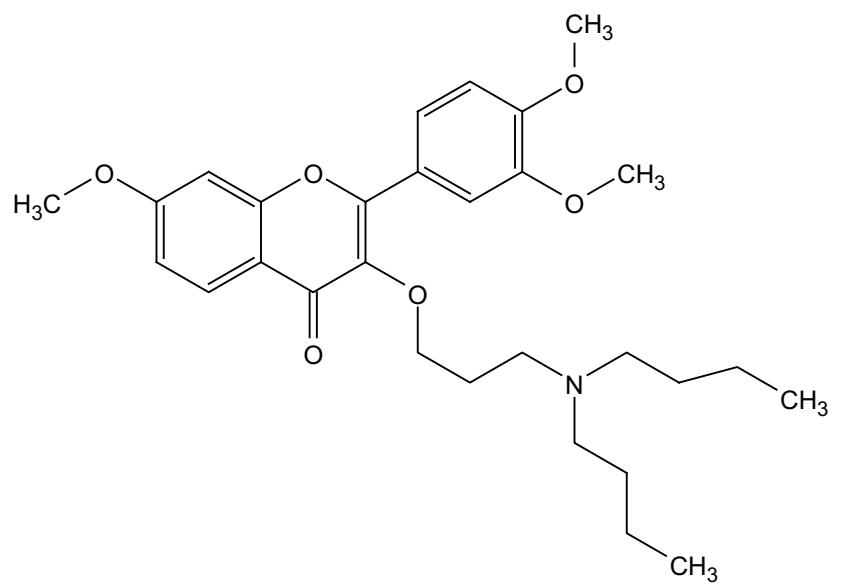
~28.91  
~27.92

—20.78

—14.14



**<sup>13</sup>C NMR of 67 in CDCl<sub>3</sub>**  
**75 MHz**

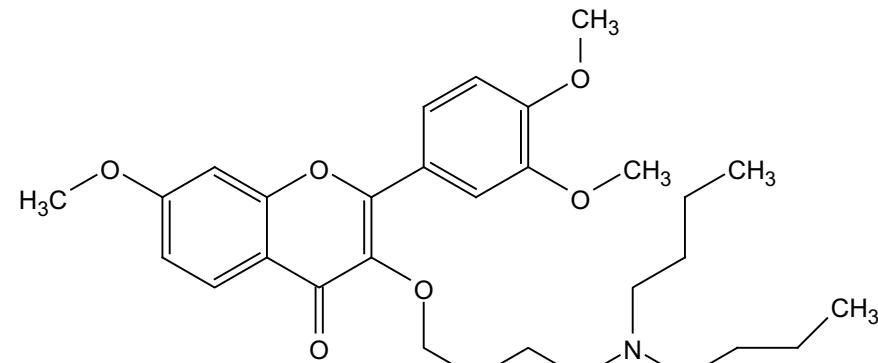


15  
12  
73  
26  
7.00  
6.97  
6.94  
6.90

4.06  
4.03  
4.01  
3.96  
3.92

2.40  
2.37  
2.35  
1.75  
1.73  
1.71  
1.55  
1.53  
1.38  
1.36  
1.29  
1.27  
1.24  
0.90  
0.88  
0.85

**<sup>1</sup>H NMR of 68 in CDCl<sub>3</sub>**  
**300 MHz**



1.00  
2.00  
2.00  
1.04

2.01  
6.15  
3.28

6.03  
2.16  
2.11  
4.41  
4.53  
6.35

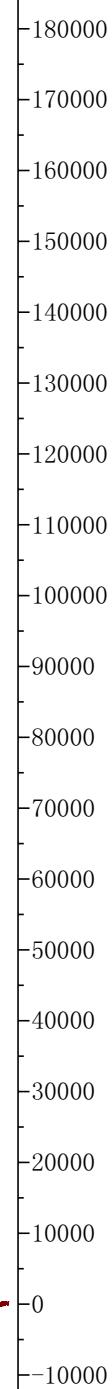
CDCl<sub>3</sub> 75MHz (4/100)  
—176.64  
—168.02  
~155.27  
~155.02  
~148.67

—140.02

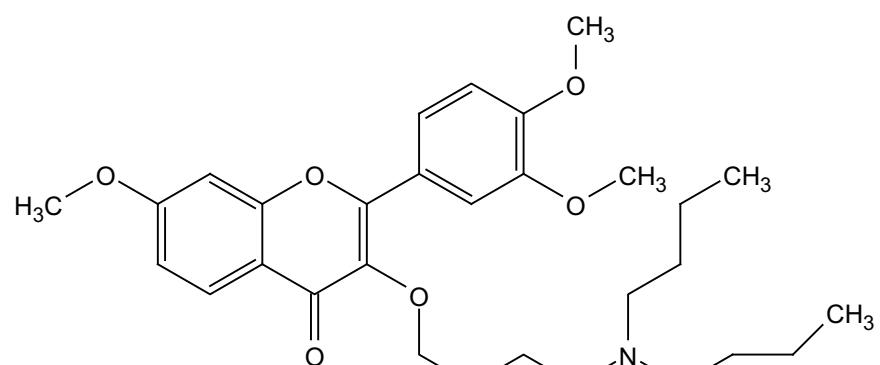
~127.23  
~123.83  
~122.13  
~118.21  
~114.33  
~111.68  
~110.78

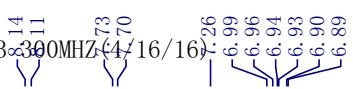
—100.04

77.58  
77.16  
76.74  
~72.74  
~56.17  
~56.07  
~55.96  
~53.82  
~29.15  
~28.38  
—23.35  
—20.82  
—14.20

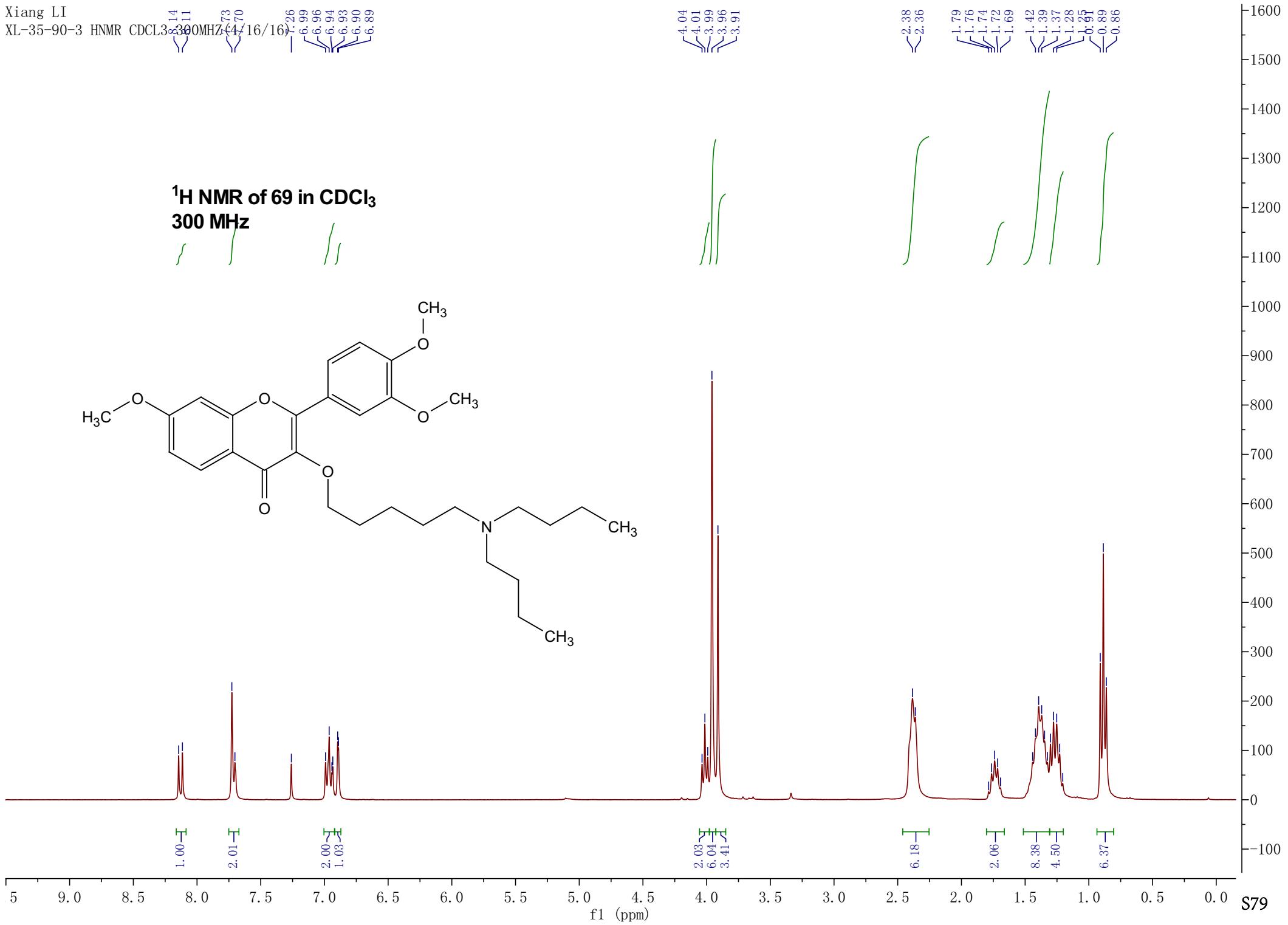
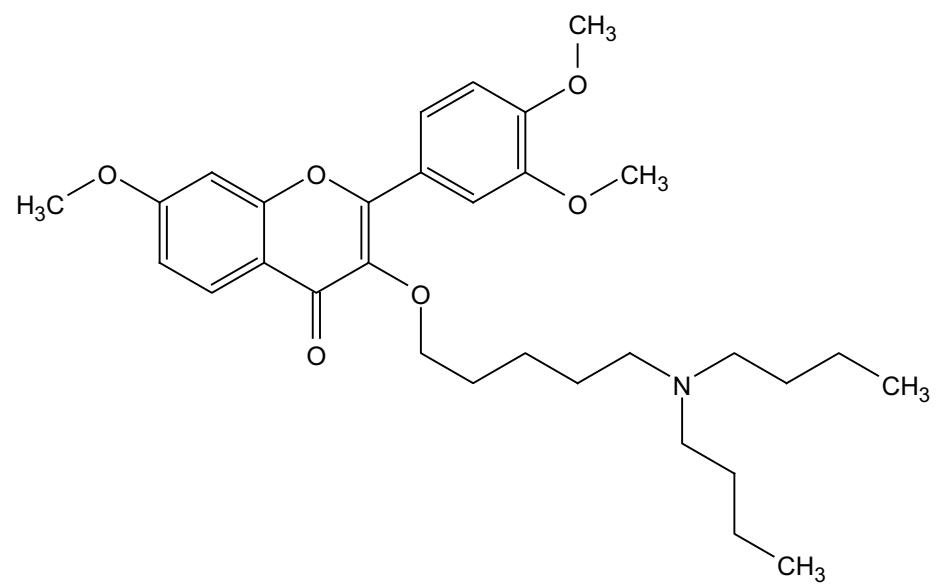


**<sup>13</sup>C NMR of 68 in CDCl<sub>3</sub>  
75 MHz**





**<sup>1</sup>H NMR of 69 in CDCl<sub>3</sub>**  
**300 MHz**



-176.63  
 -160.01  
 -154.00  
 -154.28  
 -154.16  
 -152.02  
 -148.65

-140.03

~127.23  
 ~123.85  
 ~122.10  
 ~118.22  
 ~114.32  
 ~111.75  
 ~110.78

-100.05

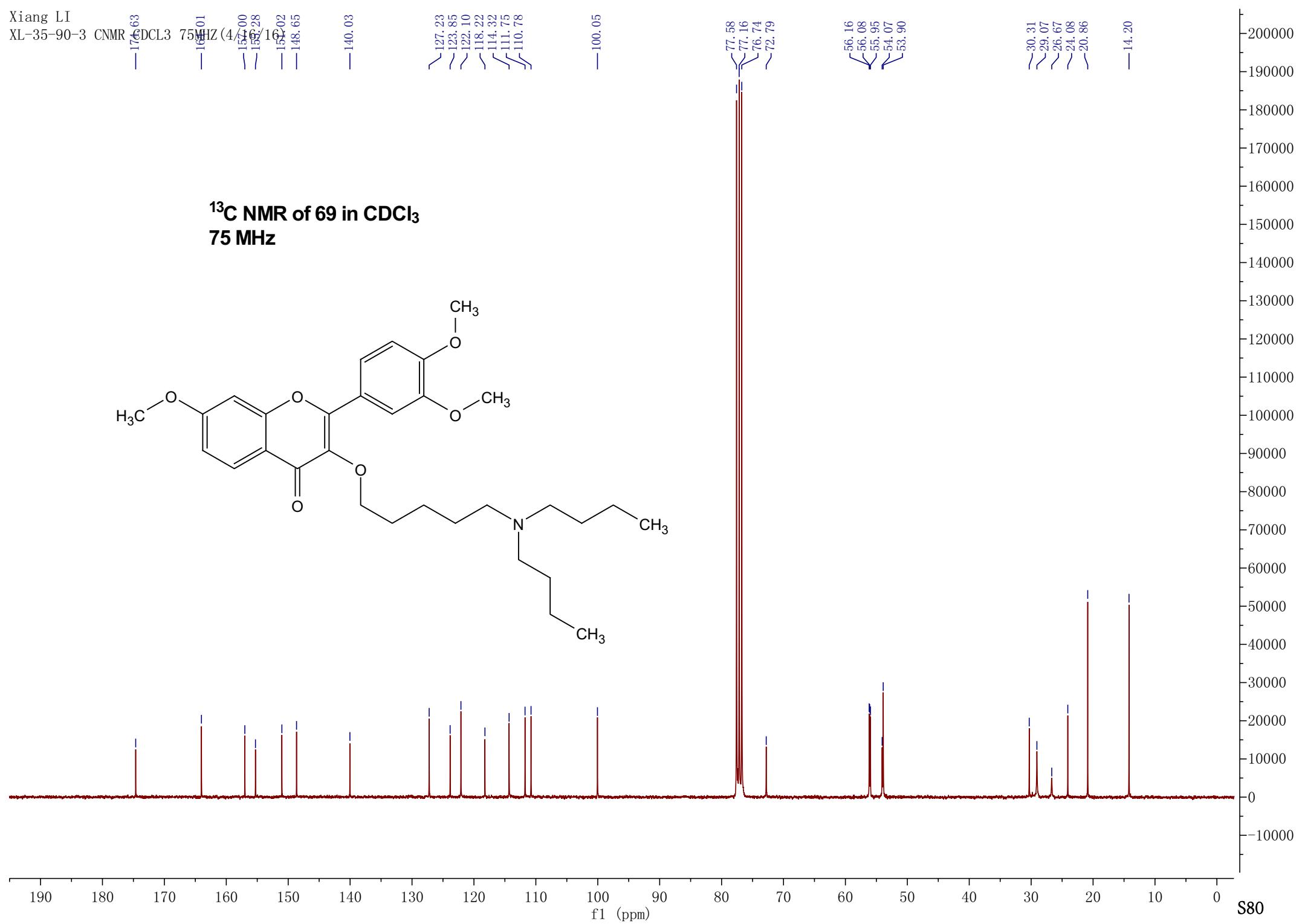
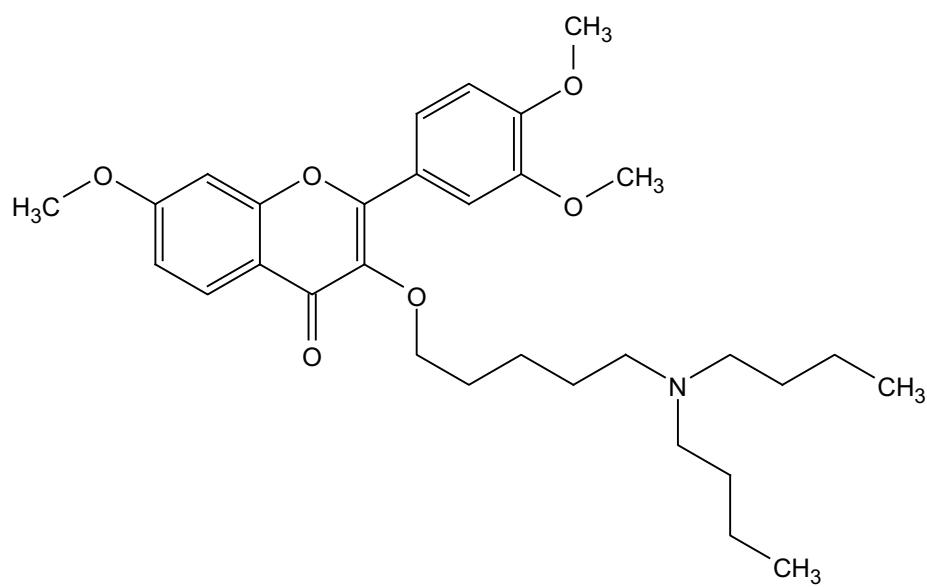
77.58  
 77.16  
 76.74  
 ~72.79

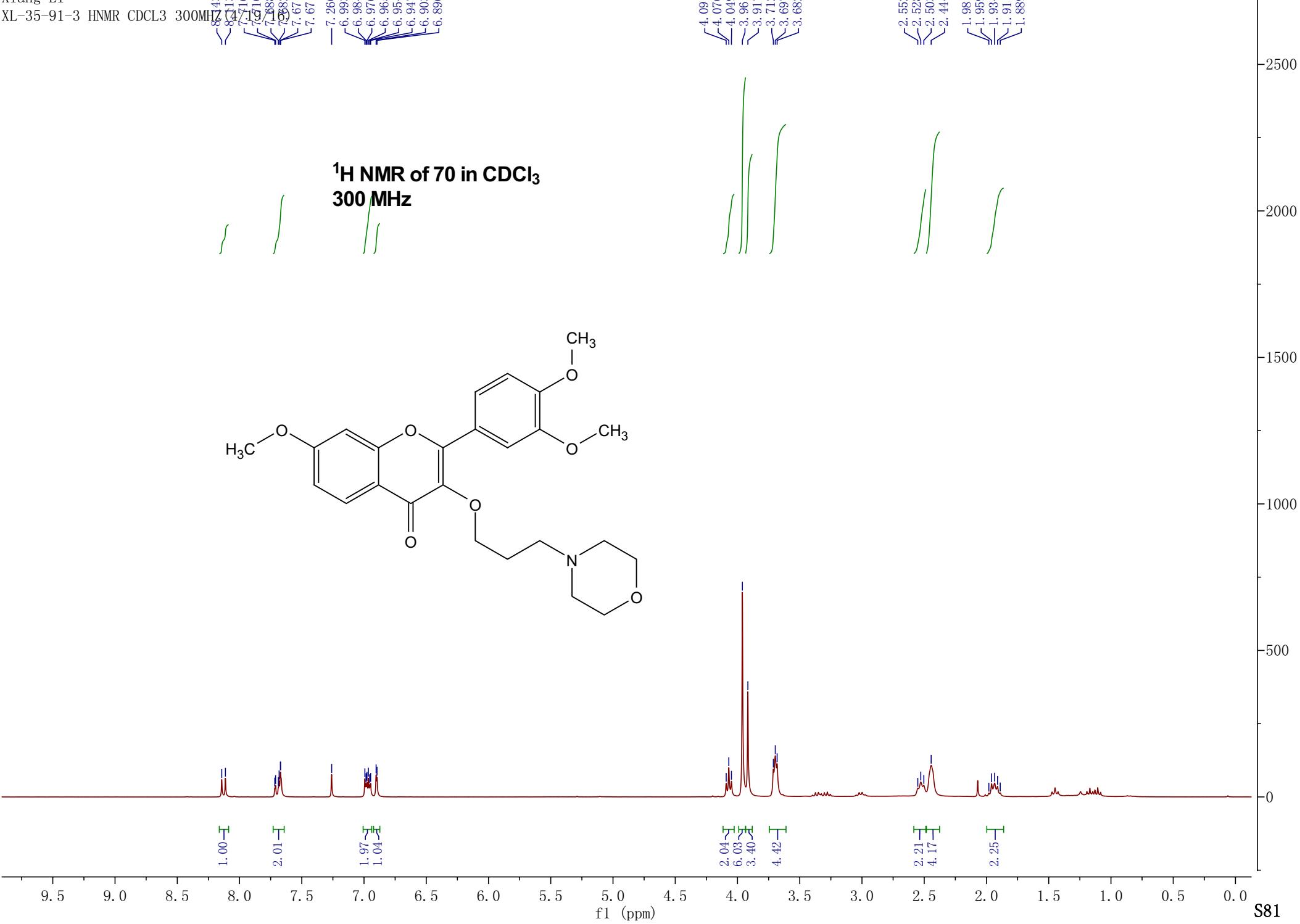
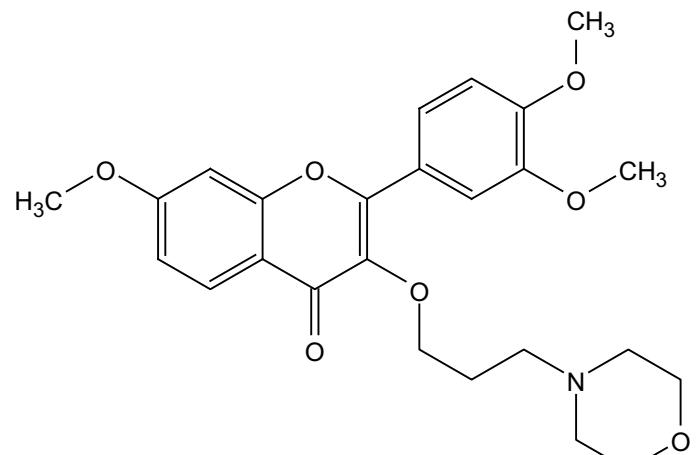
56.16  
 56.08  
 55.95  
 54.07  
 53.90

~30.31  
 ~29.07  
 ~26.67  
 ~24.08  
 ~20.86

-14.20

**<sup>13</sup>C NMR of 69 in CDCl<sub>3</sub>**  
**75 MHz**





— 176.60  
 — 168.11  
 — 157.05  
 — 157.52  
 — 152.14  
 — 148.75

— 139.87

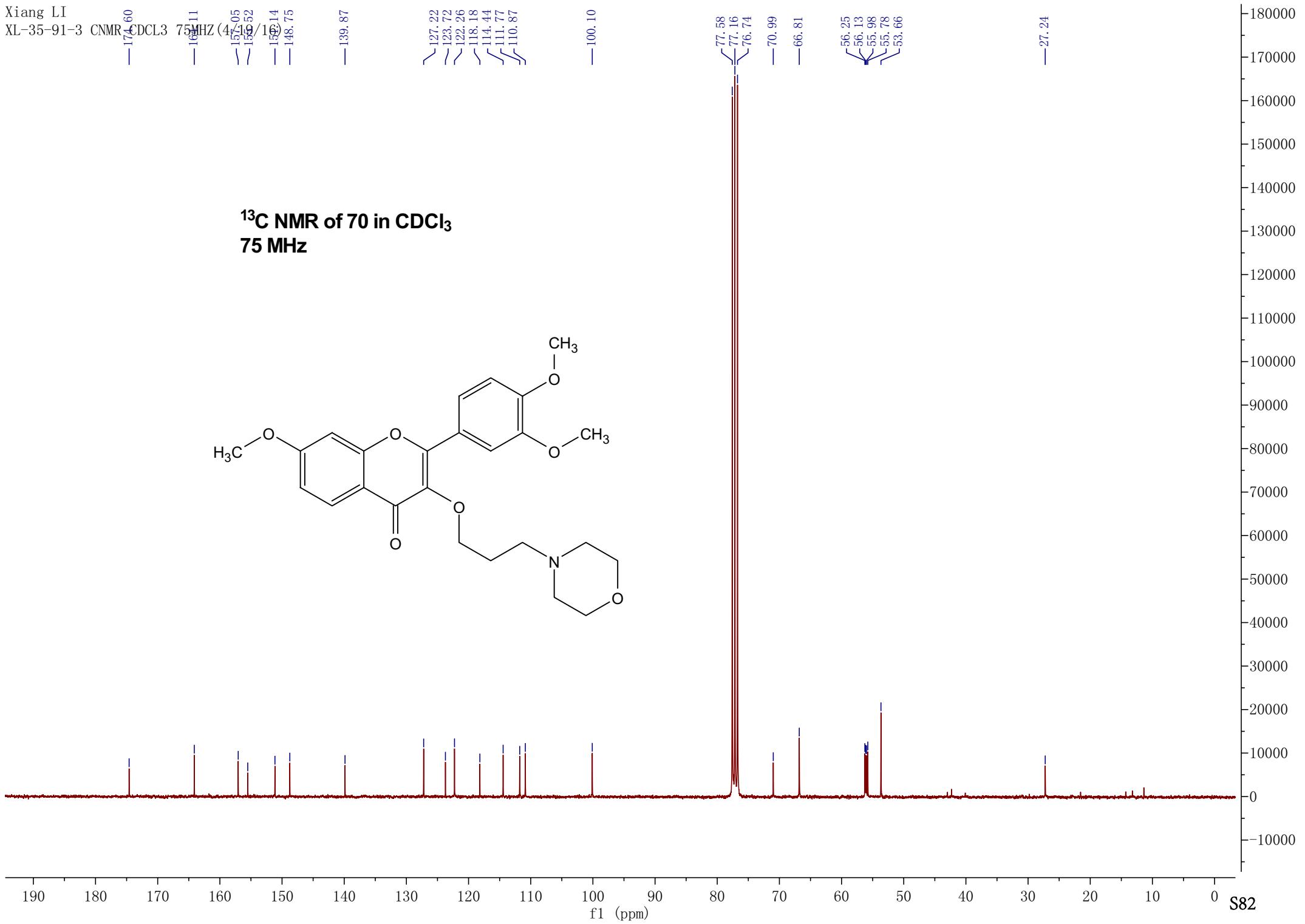
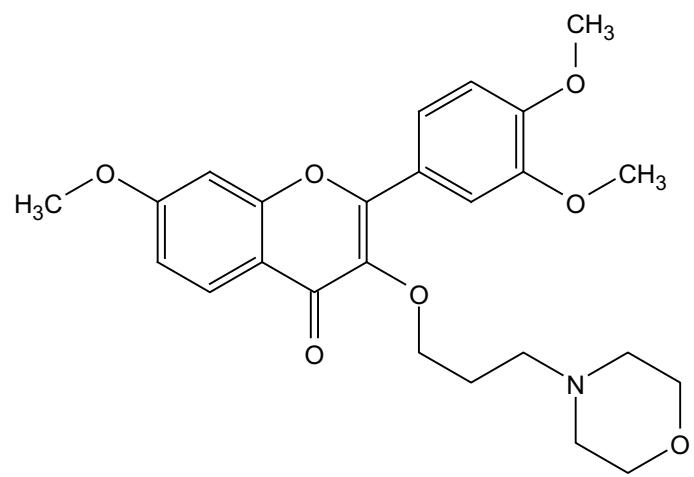
— 127.22  
 — 123.72  
 — 122.26  
 — 118.18  
 — 114.44  
 — 111.77  
 — 110.87

— 100.10

— 77.58  
 — 77.16  
 — 76.74  
 — 70.99  
 — 66.81  
 — 56.25  
 — 56.13  
 — 55.98  
 — 55.78  
 — 53.66

— 27.24

**<sup>13</sup>C NMR of 70 in CDCl<sub>3</sub>**  
**75 MHz**

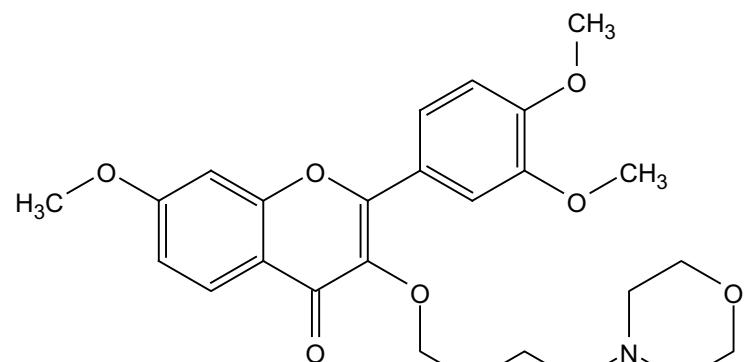


8.14  
8.11  
7.71  
7.70  
7.69  
7.26  
6.98  
6.97  
6.96  
6.94  
6.93  
6.89  
6.88

4.06  
4.03  
4.01  
3.95  
3.91  
3.69  
3.67  
3.66

2.38  
2.33  
2.30  
1.78  
1.76  
1.73  
1.71  
1.69  
1.62  
1.60  
1.57  
1.55  
1.53

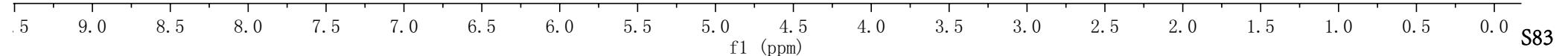
<sup>1</sup>H NMR of 71 in CDCl<sub>3</sub>  
300 MHz



1.00  
2.00  
2.02  
1.03

2.02  
6.06  
3.43  
4.01

6.04  
2.10  
2.23



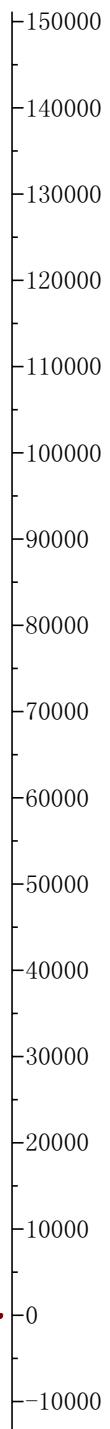
—139.94

~127.19  
~123.80  
~122.13  
~118.18  
~114.35  
~111.76  
~110.77

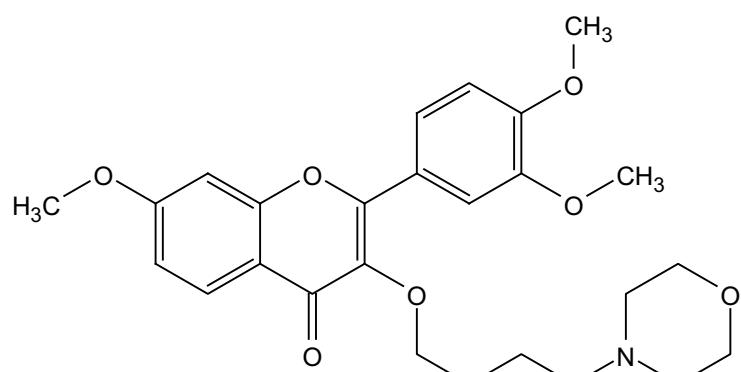
—100.05

77.58  
77.16  
76.74  
~72.49  
—67.00

—28.20  
—23.01



**<sup>13</sup>C NMR of 71 in CDCl<sub>3</sub>**  
**75 MHz**



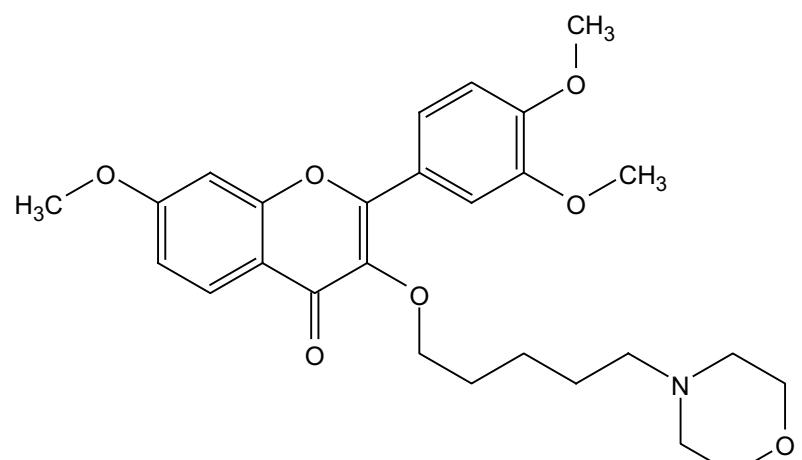
~8.039  
 ~8.009  
 ~7.212  
 ~7.286

-7.260  
 6.987  
 6.969  
 6.962  
 6.940  
 6.933  
 6.894  
 6.887

4.030  
 4.008  
 3.985  
 3.956  
 3.951  
 3.908  
 3.706  
 3.691  
 3.676

2.403  
 2.301  
 2.278  
 2.252  
 1.779  
 1.756  
 1.732  
 1.709  
 1.687  
 1.526  
 1.478  
 1.452  
 1.431  
 1.407  
 1.385

**<sup>1</sup>H NMR of 72 in CDCl<sub>3</sub>**  
**300 MHz**



1.00  
2.01  
2.02  
1.00

2.01  
6.03  
3.37  
4.05

4.10  
2.13  
2.05  
4.49

-179.60  
 -167.03  
 -152.00  
 -152.33  
 -152.02  
 -148.64

-139.98

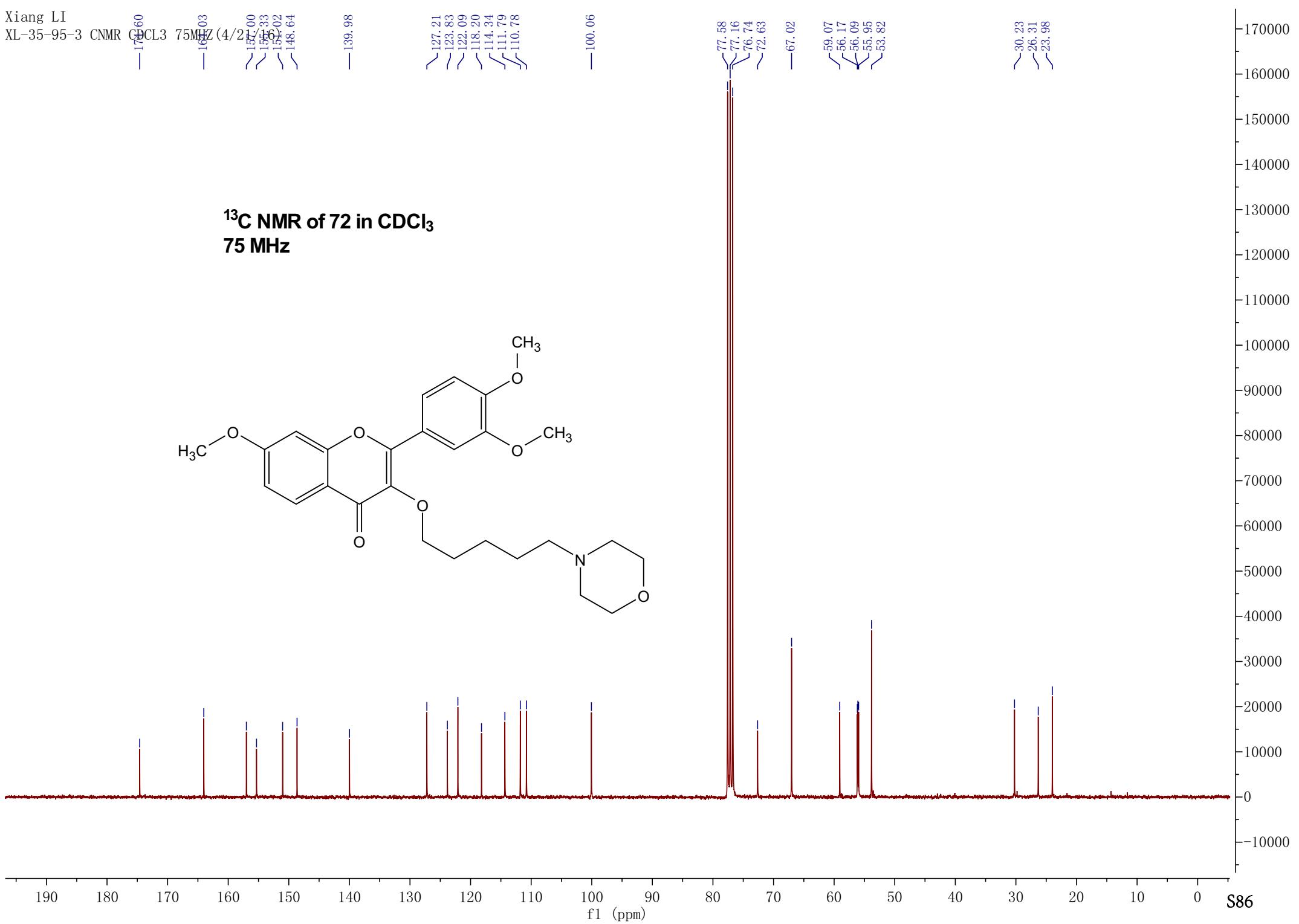
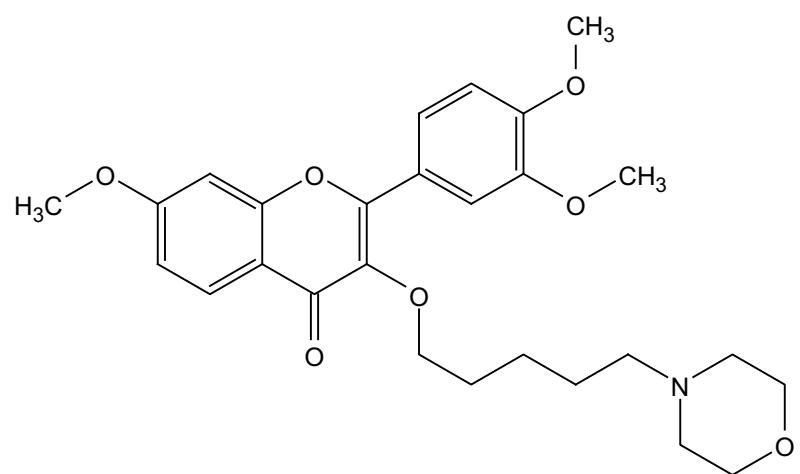
~127.21  
 ~123.83  
 ~122.09  
 ~118.20  
 ~114.34  
 ~111.79  
 ~110.78

-100.06

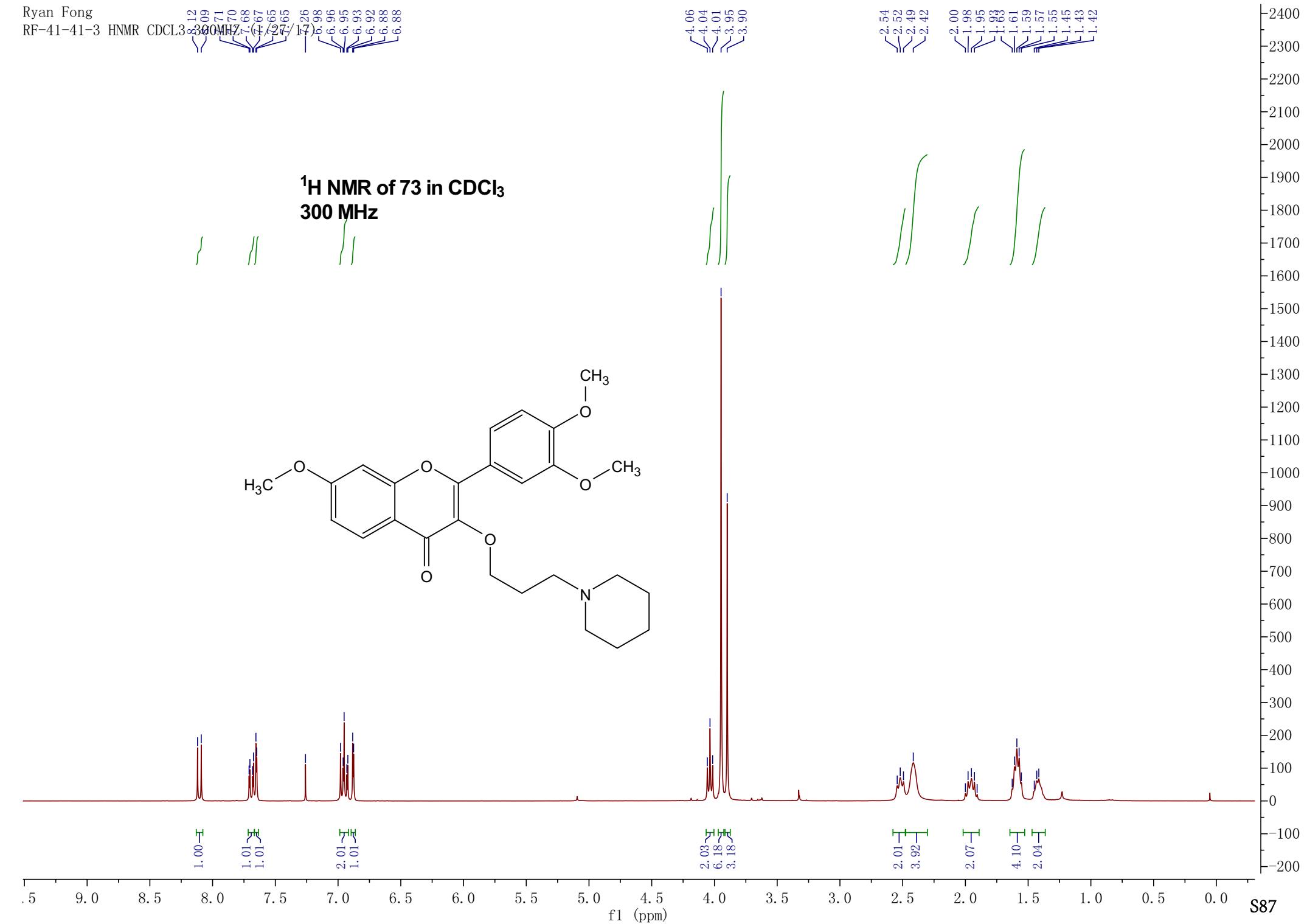
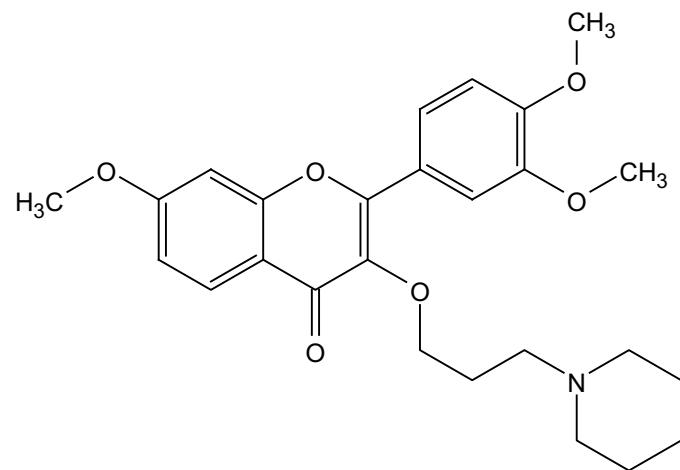
~77.58  
 ~77.16  
 ~76.74  
 ~72.63  
 -67.02  
 ~59.07  
 ~56.17  
 ~56.09  
 ~55.95  
 ~53.82

~30.23  
 ~26.31  
 ~23.98

**<sup>13</sup>C NMR of 72 in CDCl<sub>3</sub>**  
**75 MHz**



**<sup>1</sup>H NMR of 73 in CDCl<sub>3</sub>  
300 MHz**



—174.46  
—168.95  
—157.90 (90)  
—155.39 (27)  
—155.99 (7)  
—148.62

—139.71

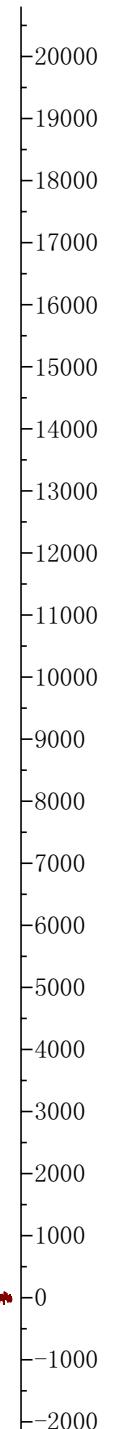
—127.05  
—123.55  
—122.16  
—118.02  
—114.29  
—111.54  
—110.76

—99.94

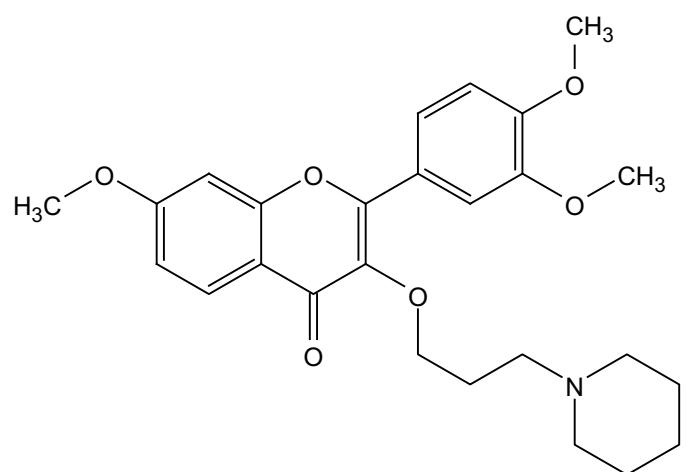
—77.49  
—77.07  
—76.64  
—71.09

—56.12  
—55.98  
—55.84  
—54.39

—27.27  
—25.45  
—24.06



**<sup>13</sup>C NMR of 73 in CDCl<sub>3</sub>  
75 MHz**



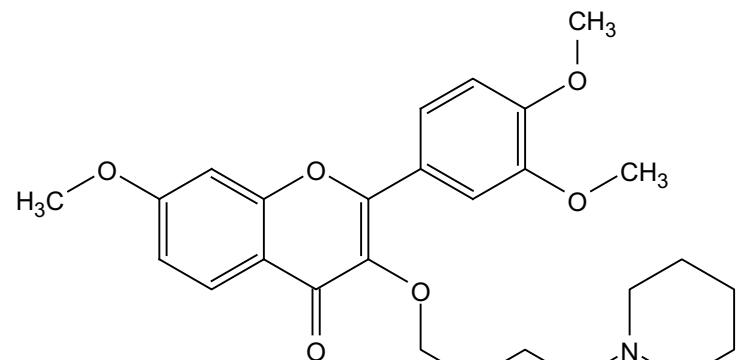
8.98  
8.00  
7.17  
7.10  
7.08  
7.06  
6.981  
6.957  
6.950  
6.928  
6.920  
6.883  
6.876

7.60  
7.58  
7.56  
7.54  
7.52  
7.50  
7.48  
7.46  
7.44  
7.42  
7.40  
7.38  
7.36  
7.34  
7.32  
7.30  
7.28  
7.26  
7.24  
7.22  
7.20  
7.18  
7.16  
7.14  
7.12  
7.10  
7.08  
7.06  
7.04  
7.02  
7.00  
6.98  
6.96  
6.94  
6.92  
6.90  
6.88  
6.86  
6.84  
6.82  
6.80  
6.78  
6.76  
6.74  
6.72  
6.70  
6.68  
6.66  
6.64  
6.62  
6.60  
6.58  
6.56  
6.54  
6.52  
6.50  
6.48  
6.46  
6.44  
6.42  
6.40  
6.38  
6.36  
6.34  
6.32  
6.30  
6.28  
6.26  
6.24  
6.22  
6.20  
6.18  
6.16  
6.14  
6.12  
6.10  
6.08  
6.06  
6.04  
6.02  
6.00  
5.98  
5.96  
5.94  
5.92  
5.90  
5.88  
5.86  
5.84  
5.82  
5.80  
5.78  
5.76  
5.74  
5.72  
5.70  
5.68  
5.66  
5.64  
5.62  
5.60  
5.58  
5.56  
5.54  
5.52  
5.50  
5.48  
5.46  
5.44  
5.42  
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5.36  
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5.28  
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5.24  
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5.14  
5.12  
5.10  
5.08  
5.06  
5.04  
5.02  
5.00  
4.98  
4.96  
4.94  
4.92  
4.90  
4.88  
4.86  
4.84  
4.82  
4.80  
4.78  
4.76  
4.74  
4.72  
4.70  
4.68  
4.66  
4.64  
4.62  
4.60  
4.58  
4.56  
4.54  
4.52  
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4.48  
4.46  
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4.38  
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4.08  
4.06  
4.04  
4.02  
4.00  
3.98  
3.96  
3.94  
3.92  
3.90  
3.88  
3.86  
3.84  
3.82  
3.80  
3.78  
3.76  
3.74  
3.72  
3.70  
3.68  
3.66  
3.64  
3.62  
3.60  
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3.56  
3.54  
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3.50  
3.48  
3.46  
3.44  
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3.16  
3.14  
3.12  
3.10  
3.08  
3.06  
3.04  
3.02  
3.00  
2.98  
2.96  
2.94  
2.92  
2.90  
2.88  
2.86  
2.84  
2.82  
2.80  
2.78  
2.76  
2.74  
2.72  
2.70  
2.68  
2.66  
2.64  
2.62  
2.60  
2.58  
2.56  
2.54  
2.52  
2.50  
2.48  
2.46  
2.44  
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2.40  
2.38  
2.36  
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2.32  
2.30  
2.28  
2.26  
2.24  
2.22  
2.20  
2.18  
2.16  
2.14  
2.12  
2.10  
2.08  
2.06  
2.04  
2.02  
2.00  
1.98  
1.96  
1.94  
1.92  
1.90  
1.88  
1.86  
1.84  
1.82  
1.80  
1.78  
1.76  
1.74  
1.72  
1.70  
1.68  
1.66  
1.64  
1.62  
1.60  
1.58  
1.56  
1.54  
1.52  
1.50  
1.48  
1.46  
1.44  
1.42  
1.40  
1.38  
1.36  
1.34  
1.32  
1.30  
1.28  
1.26  
1.24  
1.22  
1.20  
1.18  
1.16  
1.14  
1.12  
1.10  
1.08  
1.06  
1.04  
1.02  
1.00  
0.98  
0.96  
0.94  
0.92  
0.90  
0.88  
0.86  
0.84  
0.82  
0.80  
0.78  
0.76  
0.74  
0.72  
0.70  
0.68  
0.66  
0.64  
0.62  
0.60  
0.58  
0.56  
0.54  
0.52  
0.50  
0.48  
0.46  
0.44  
0.42  
0.40  
0.38  
0.36  
0.34  
0.32  
0.30  
0.28  
0.26  
0.24  
0.22  
0.20  
0.18  
0.16  
0.14  
0.12  
0.10  
0.08  
0.06  
0.04  
0.02  
0.00

4.036  
4.015  
3.993  
3.945  
3.898

2.328  
2.302  
2.276  
1.751  
1.728  
1.704  
1.681  
1.660  
1.622  
1.595  
1.574  
1.556  
1.539  
1.521  
1.430  
1.411  
1.395

1H NMR of 74 in CDCl<sub>3</sub>  
300 MHz



1.00  
2.02  
2.05  
2.03  
1.03

2.05  
6.03  
3.05

6.00  
2.11  
6.10  
2.04

-176.61  
-168.00  
~153.97  
~153.33  
~152.01  
~148.63

(8/23)

~127.18  
~123.75  
~122.17  
~118.15  
~114.33  
~111.67  
~110.76

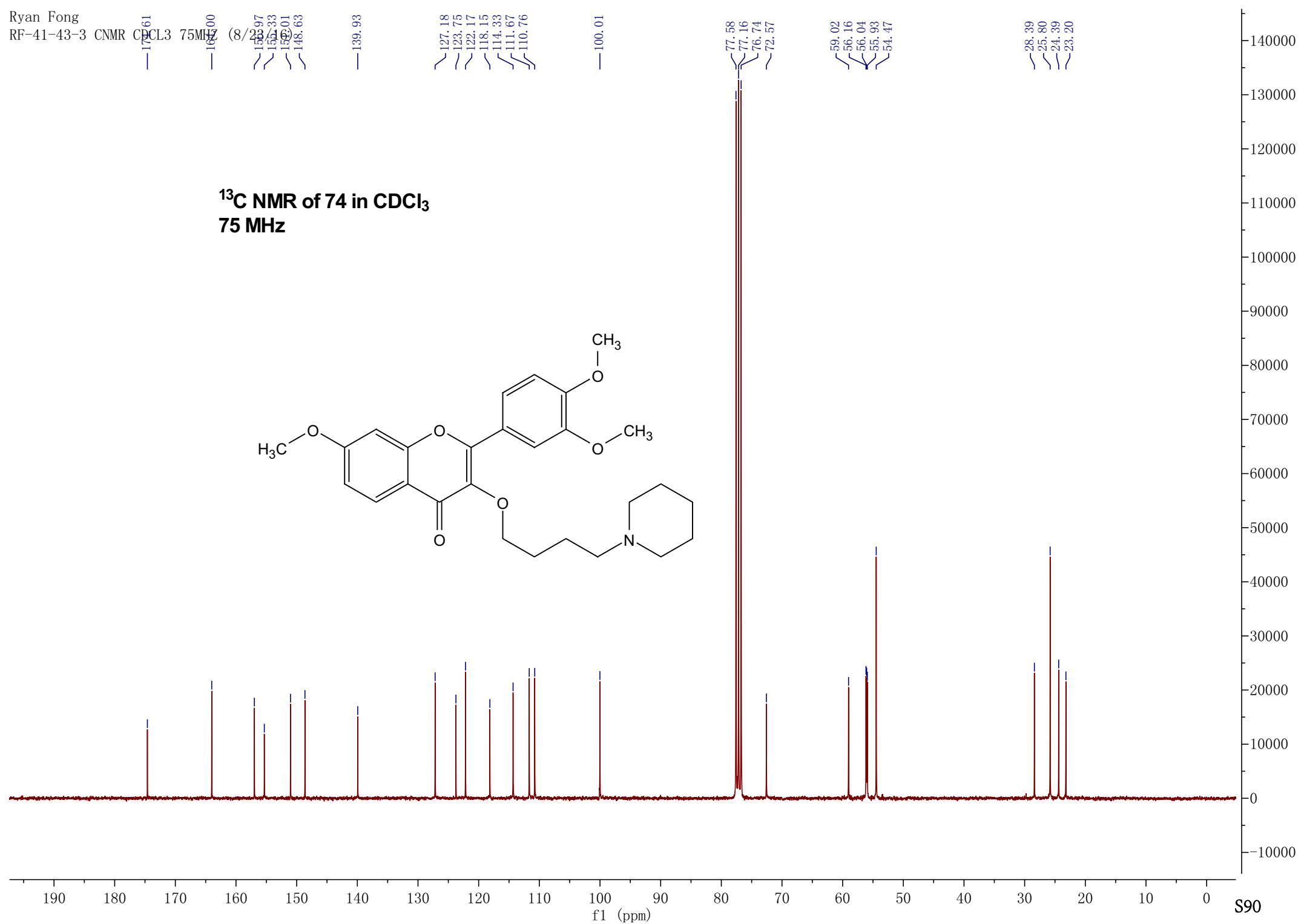
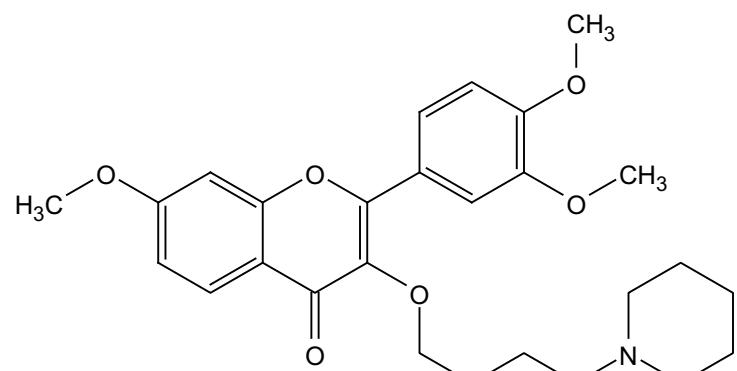
-139.93

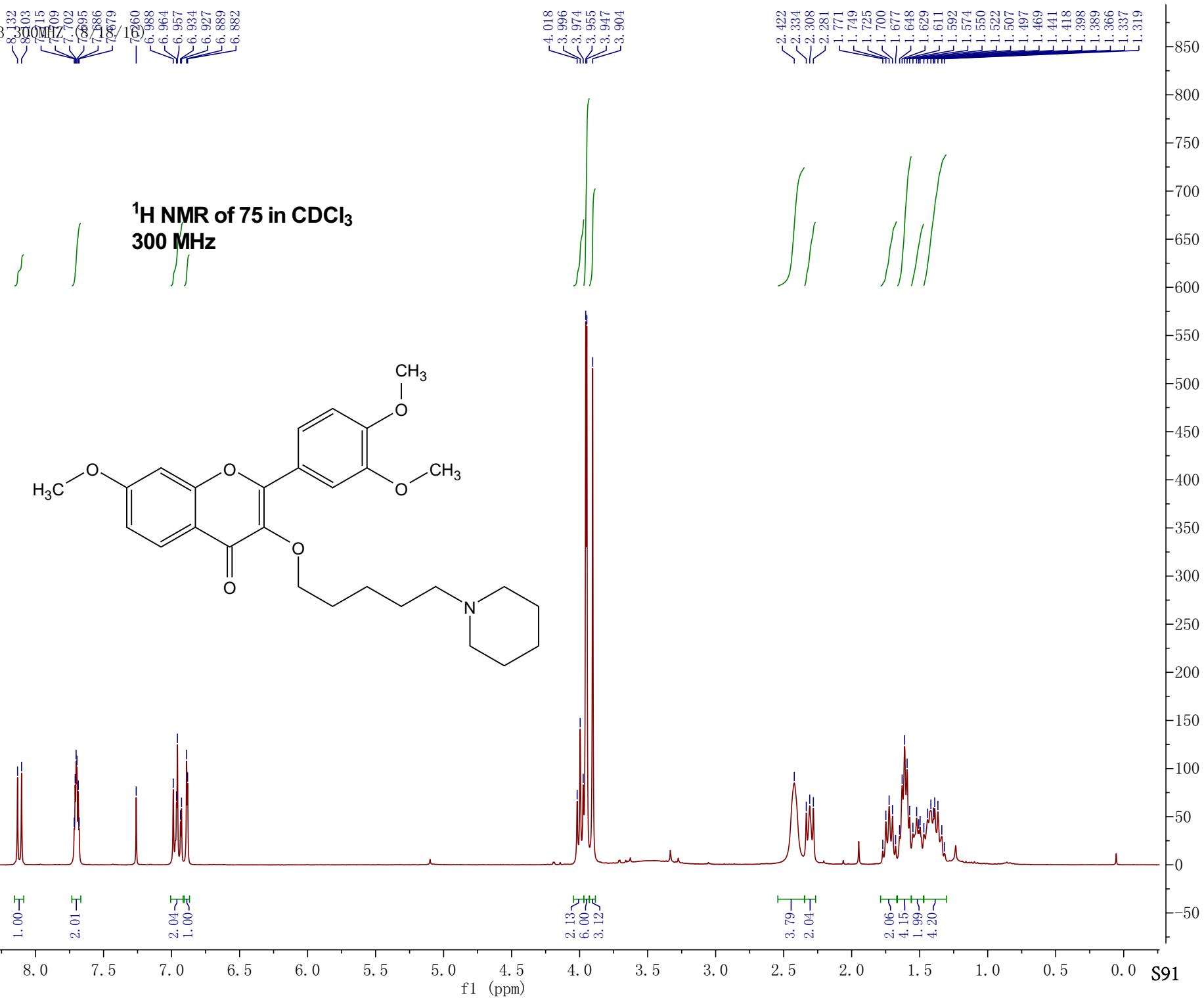
~77.58  
~77.16  
~76.74  
~72.57

59.02  
56.16  
56.04  
55.93  
54.47

~28.39  
~25.80  
~24.39  
~23.20

**<sup>13</sup>C NMR of 74 in CDCl<sub>3</sub>  
75 MHz**





Ryan Fong  
RF-41-45-3 CNMR CDCL<sub>3</sub> 75MHz

-174.61  
-165.02  
-158.00 (8.36)  
-155.36  
-154.88/02  
-148.64

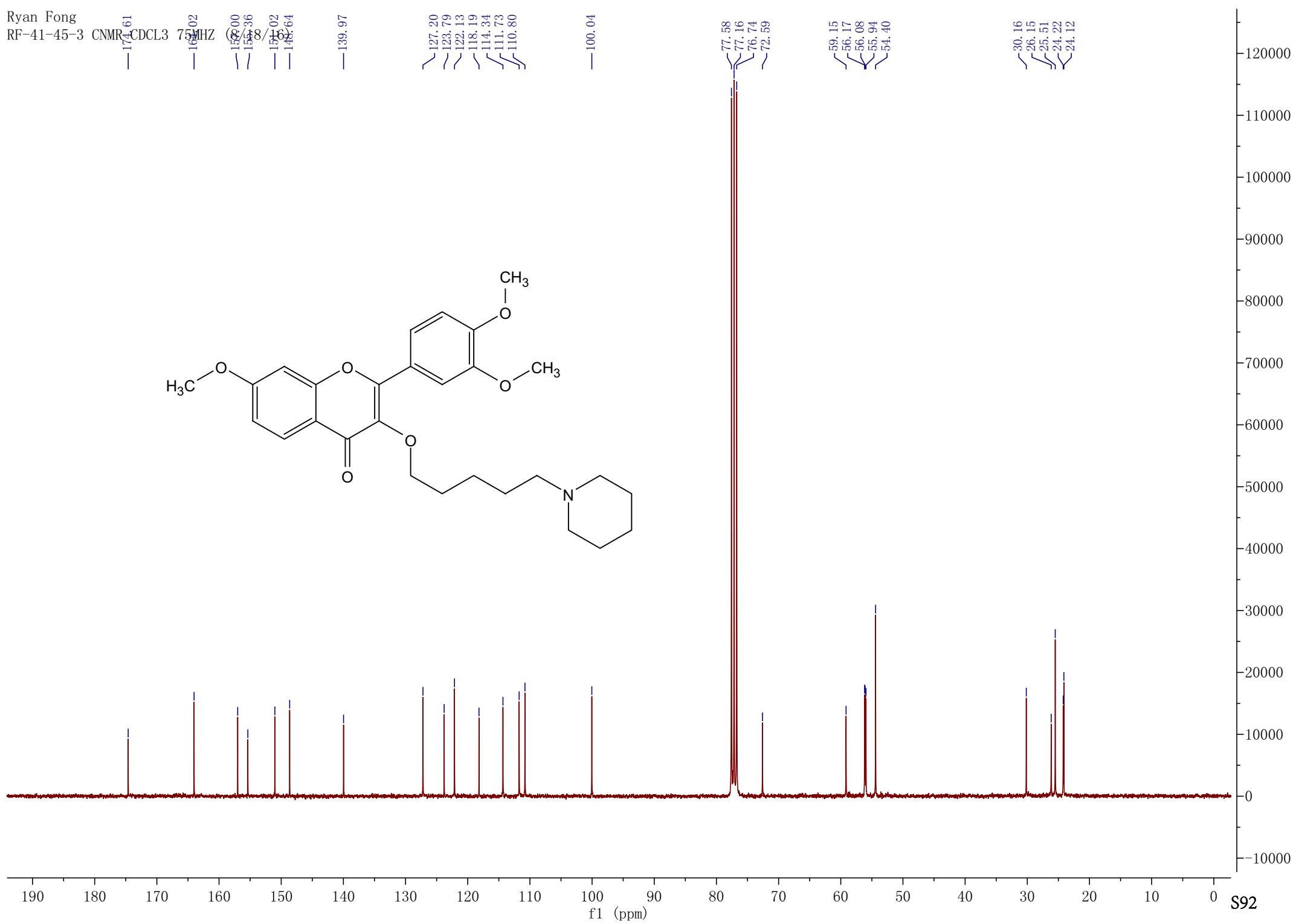
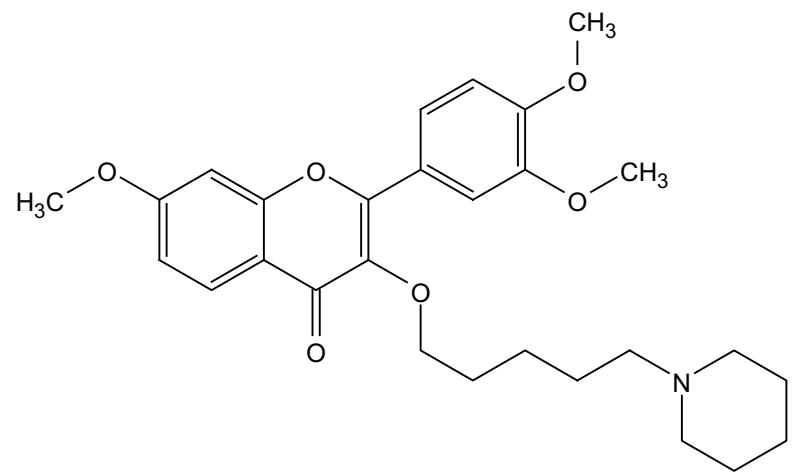
-139.97

~127.20  
~123.79  
~122.13  
~118.19  
~114.34  
~111.73  
~110.80

-100.04

77.58  
77.16  
76.74  
72.59  
59.15  
56.17  
56.08  
55.94  
54.40

30.16  
26.15  
25.51  
24.22  
24.12

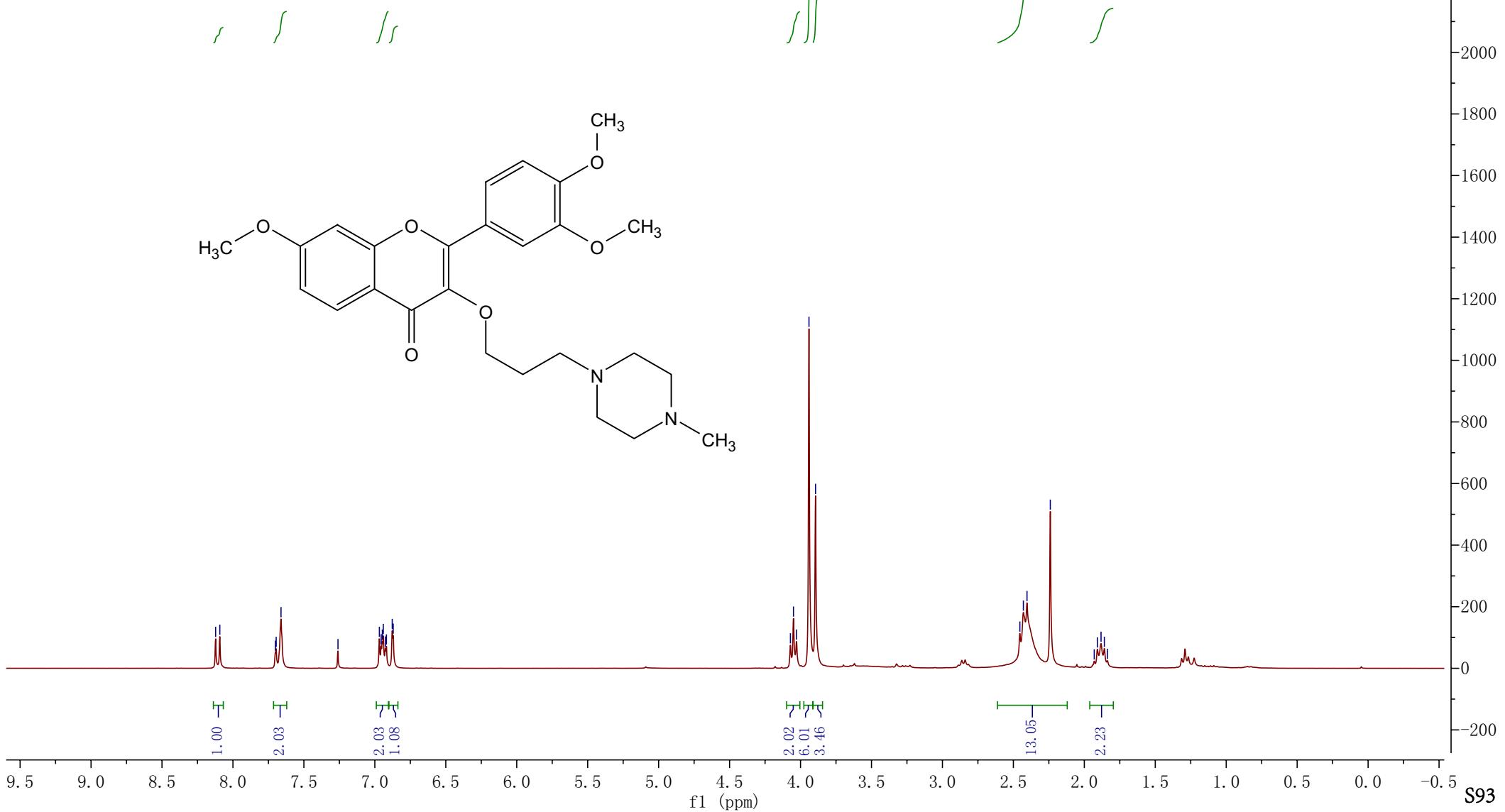
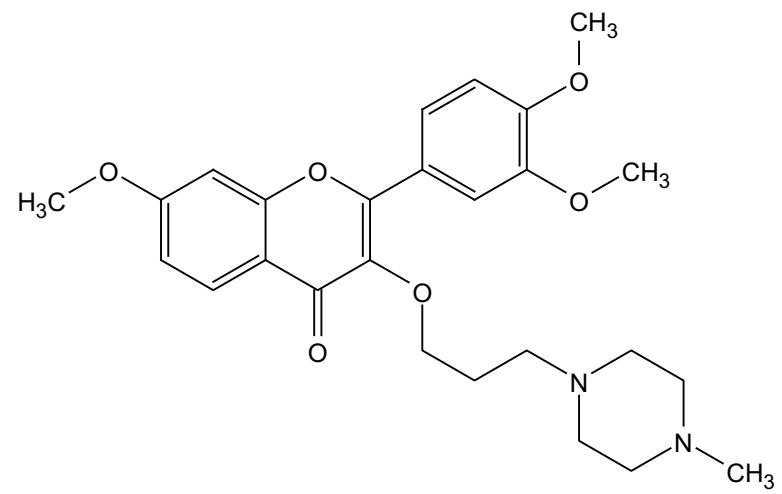


300MHz (4/26/16)  
 8.09 7.70 7.66 7.26  
 6.97 6.96 6.95 6.94 6.93 6.92 6.88 6.87

4.07 4.05 4.03 3.94 3.89

2.45 2.43 2.40 2.24 1.93 1.91 1.88 1.86 1.84

**<sup>1</sup>H NMR of 76 in CDCl<sub>3</sub>**  
**300 MHz**



—175.54  
 —160.01  
 —159.97  
 —158.38  
 —157.16  
 —157.03  
 —148.66

—139.87

~127.18  
 ~123.72  
 ~122.21  
 ~118.15  
 ~114.34  
 ~111.70  
 ~110.78

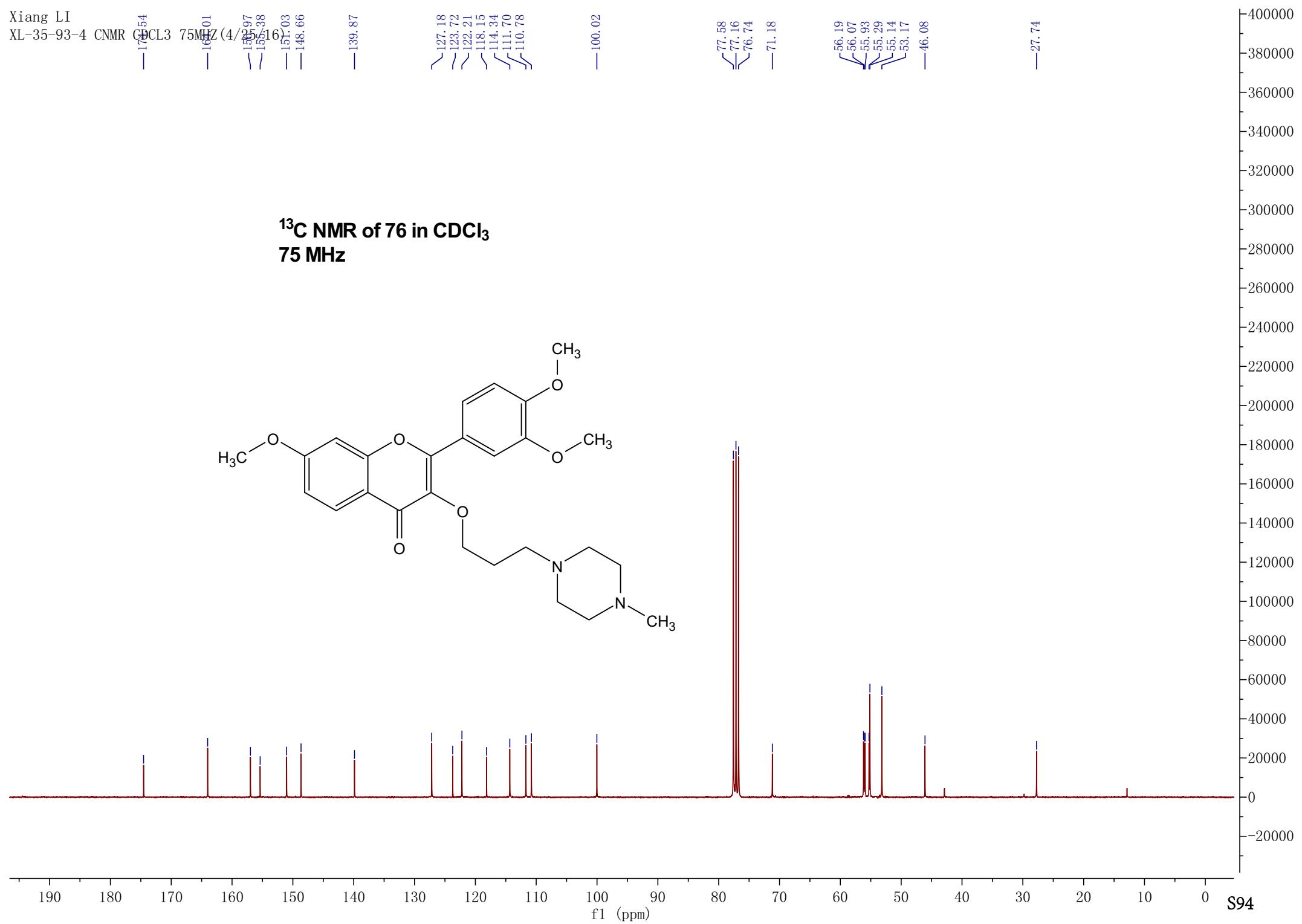
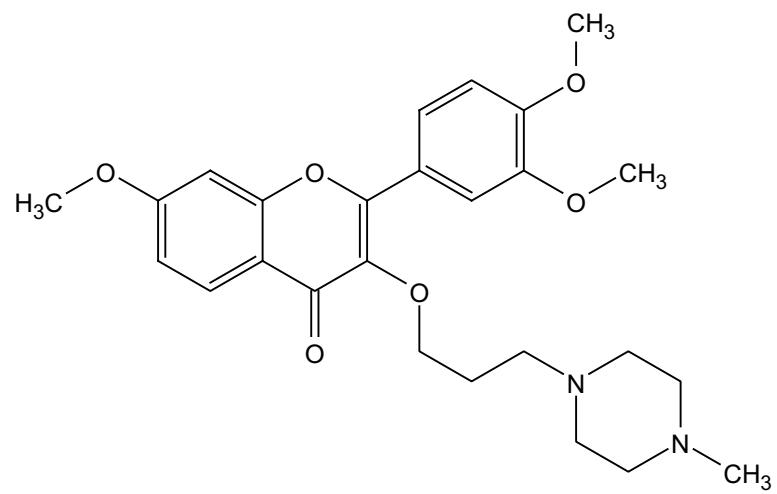
—100.02

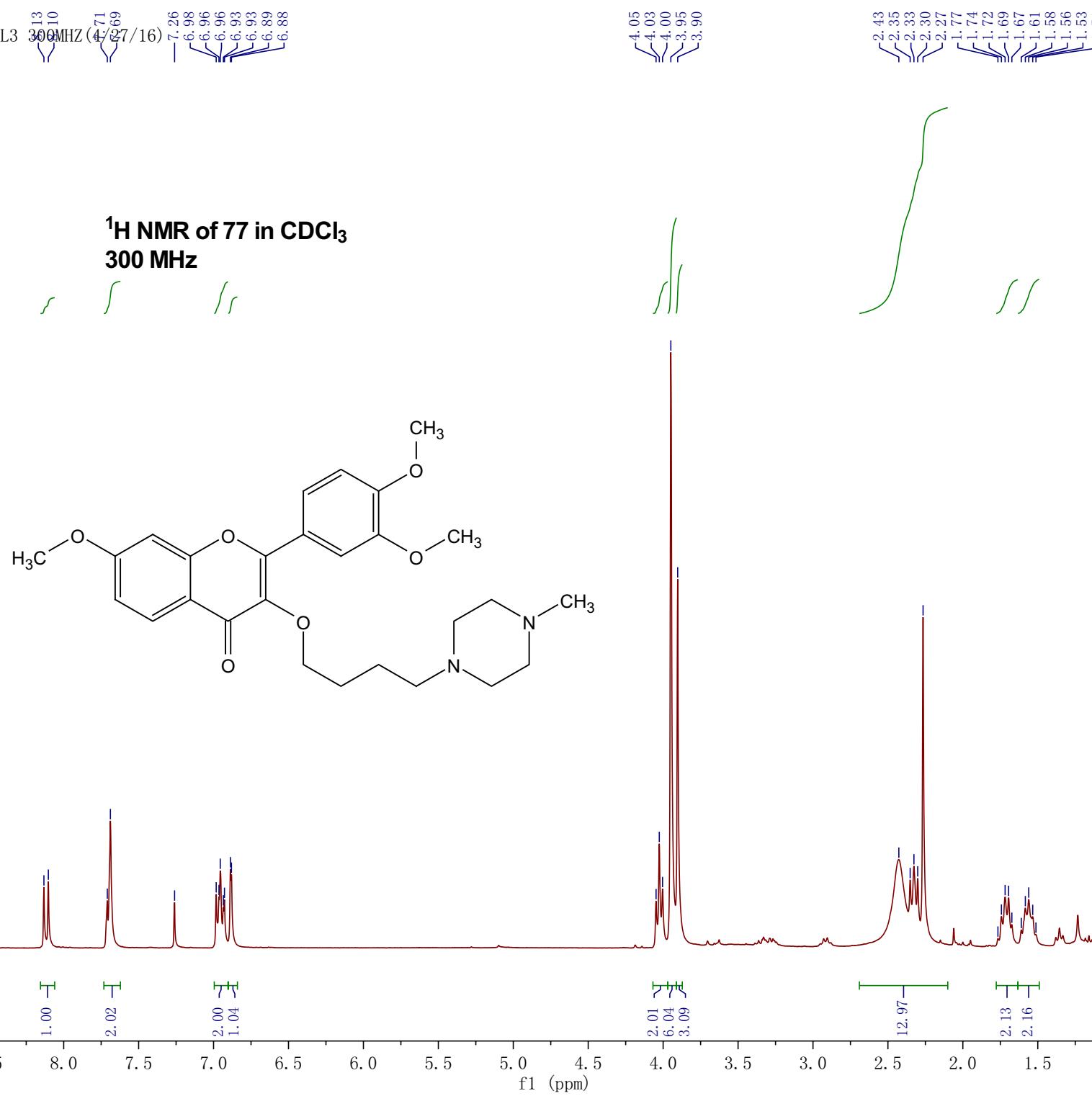
77.58  
 77.16  
 76.74  
 —71.18

56.19  
 56.07  
 55.93  
 55.29  
 55.14  
 53.17  
 —46.08

—27.74

**$^{13}\text{C}$  NMR of 76 in  $\text{CDCl}_3$**   
**75 MHz**





—176.60  
—167.02  
—152.99  
—152.31  
—152.02  
—148.65

—139.95

—127.21  
—123.80  
—122.16  
—118.19  
—114.33  
—111.73  
—110.78

—100.04

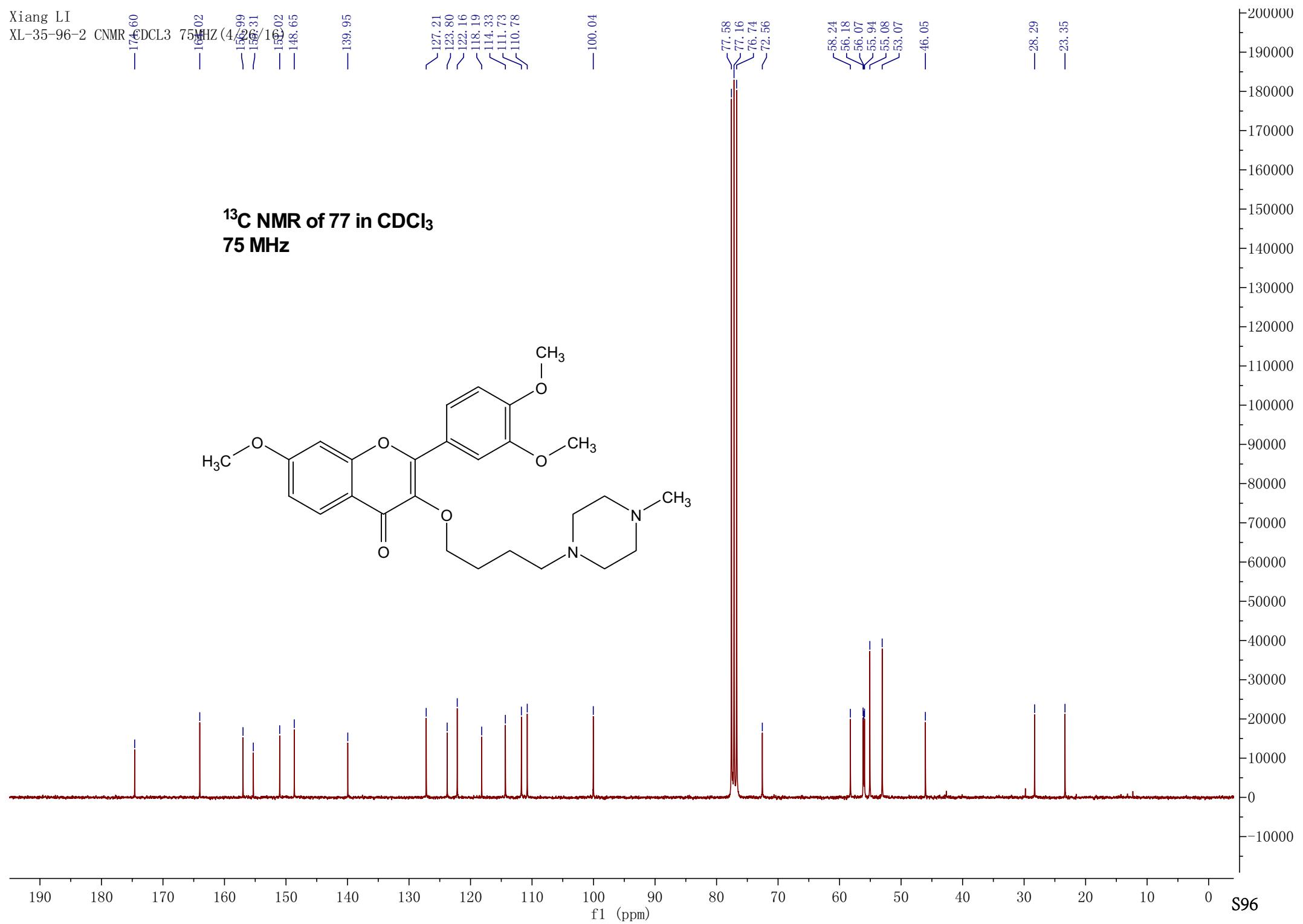
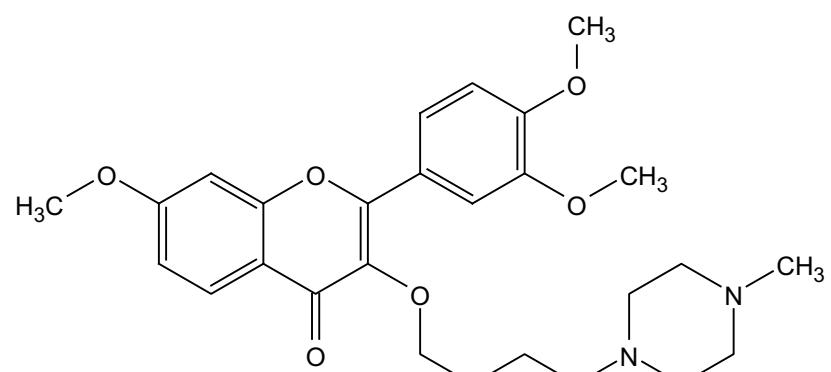
—77.58  
—77.16  
—76.74  
—72.56

—58.24  
—56.18  
—56.07  
—55.94  
—55.08  
—53.07

—46.05

—28.29  
—23.35

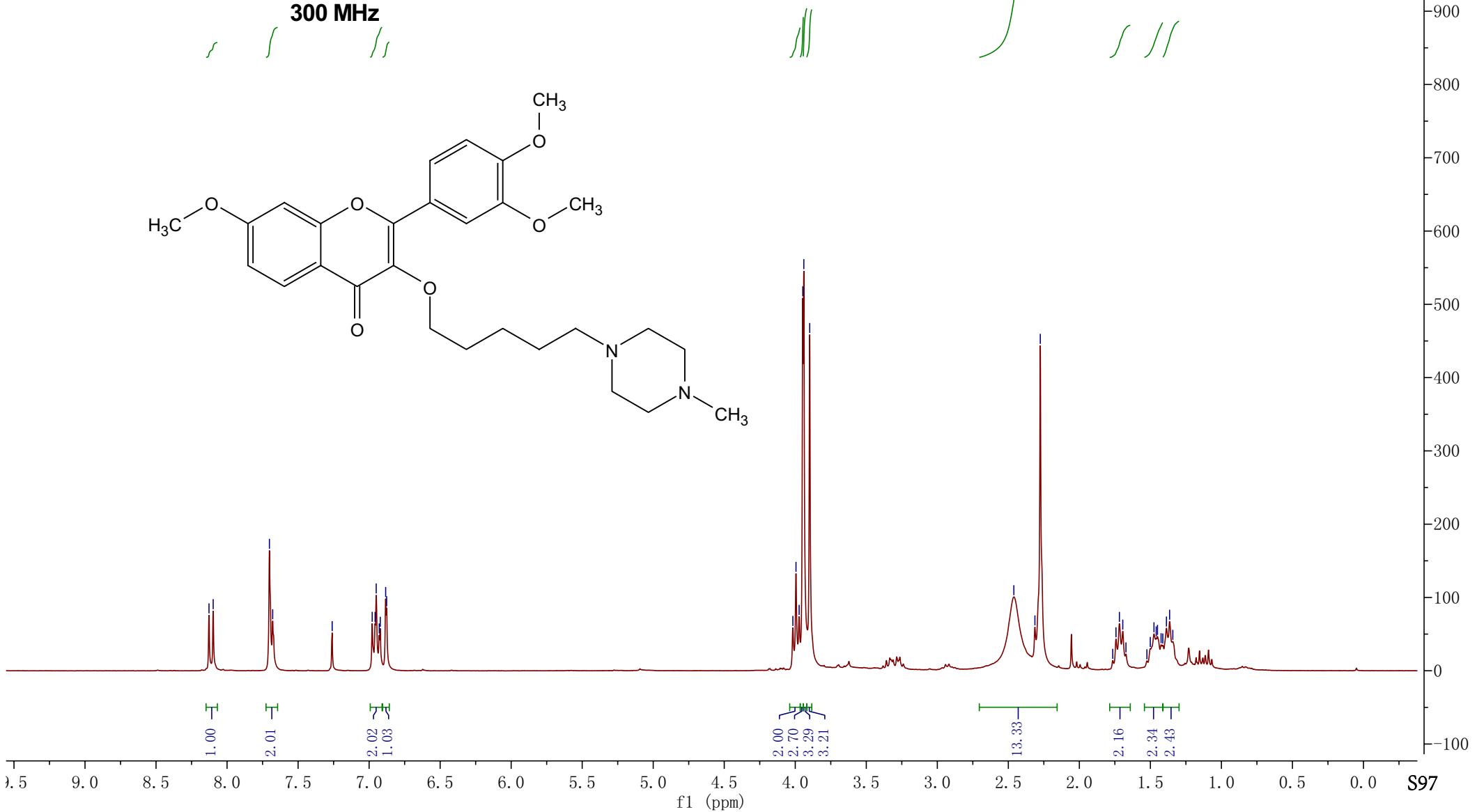
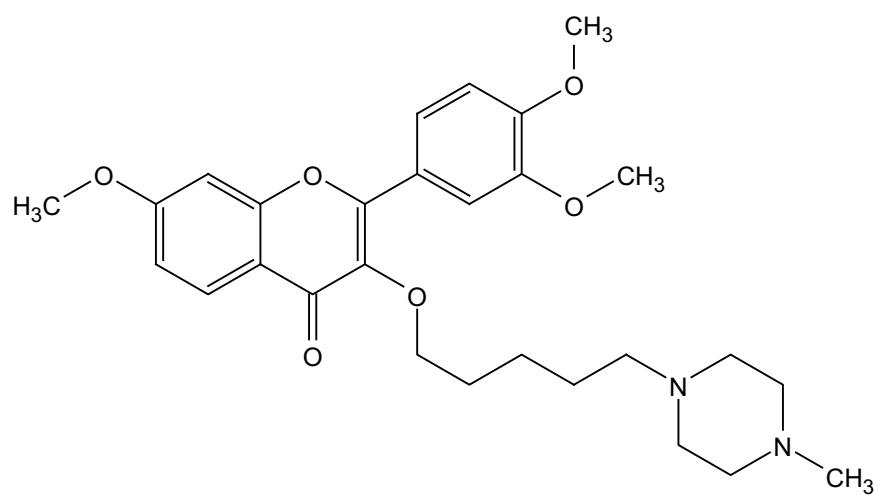
**<sup>13</sup>C NMR of 77 in CDCl<sub>3</sub>**  
**75 MHz**



8.10  
7.70  
7.68  
7.26  
6.98  
6.96  
6.95  
6.93  
6.92  
6.88  
6.88  
6.88

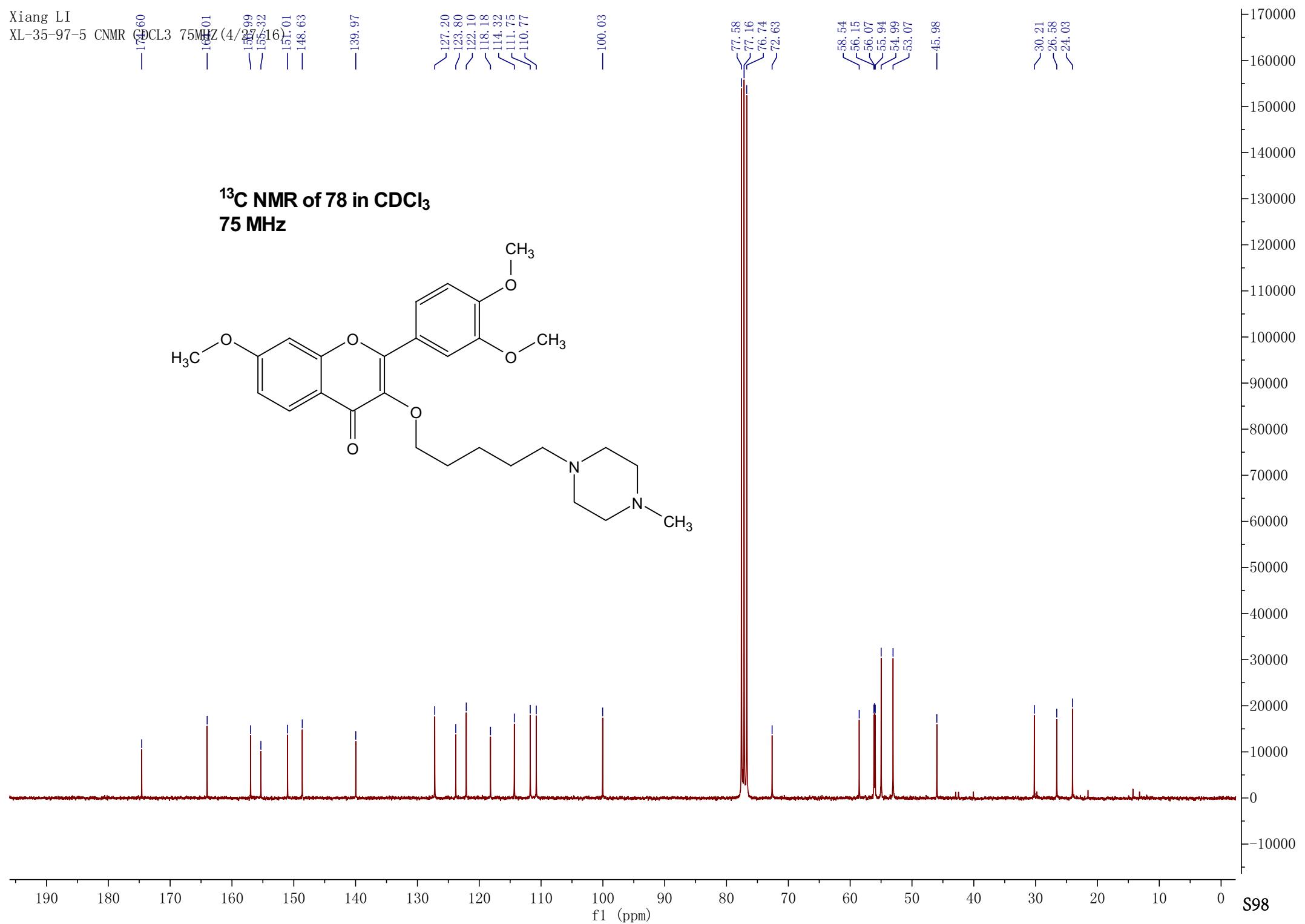
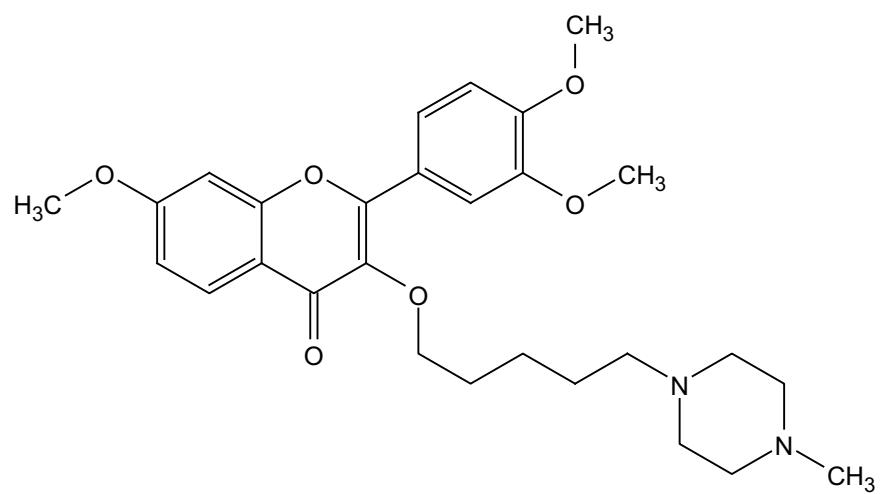
4.02  
3.99  
3.97  
3.95  
3.94  
3.90

2.46  
2.31  
2.28  
1.77  
1.74  
1.72  
1.69  
1.67  
1.52  
1.50  
1.47  
1.46  
1.45  
1.42  
1.41  
1.39  
1.36  
1.34

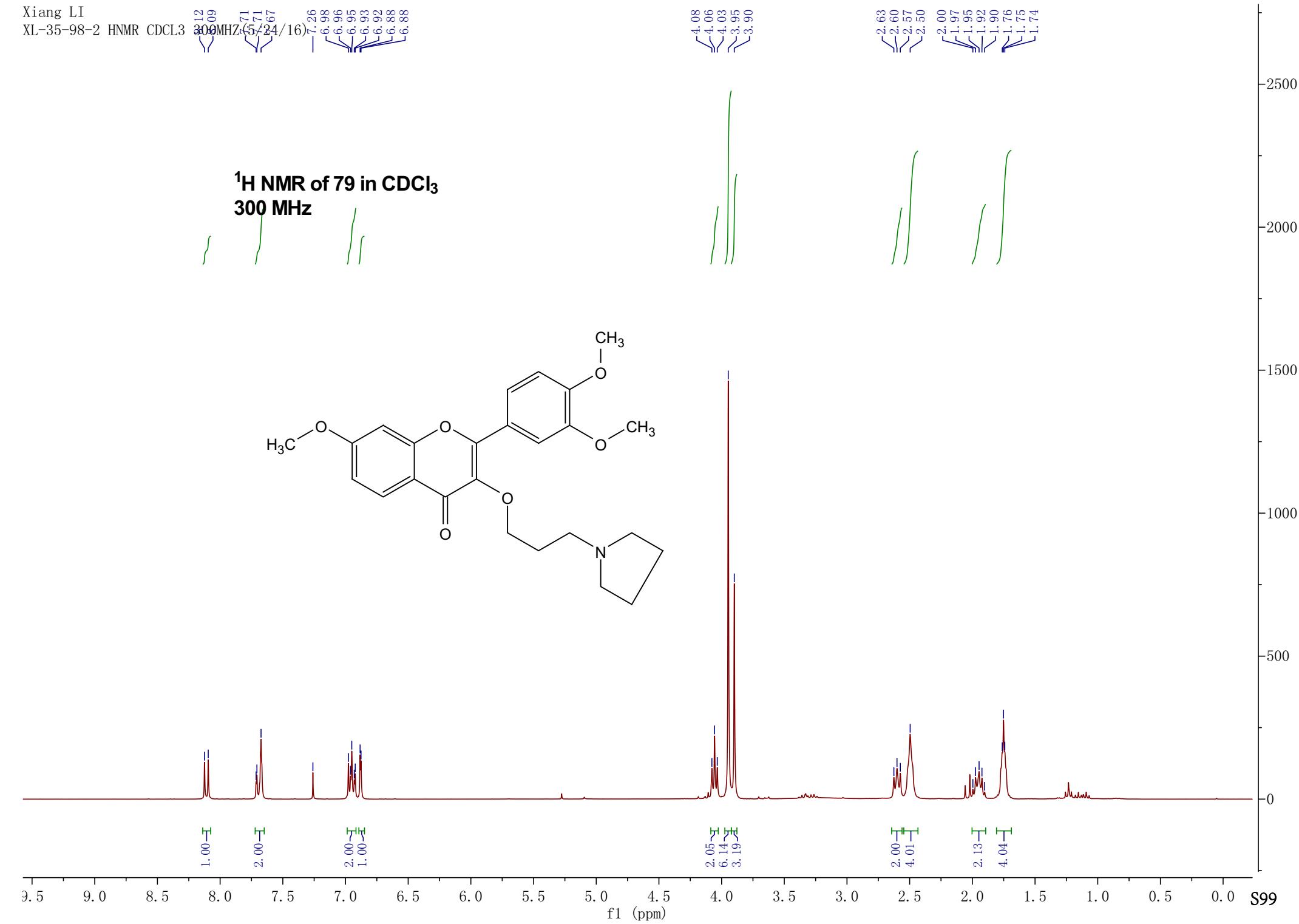
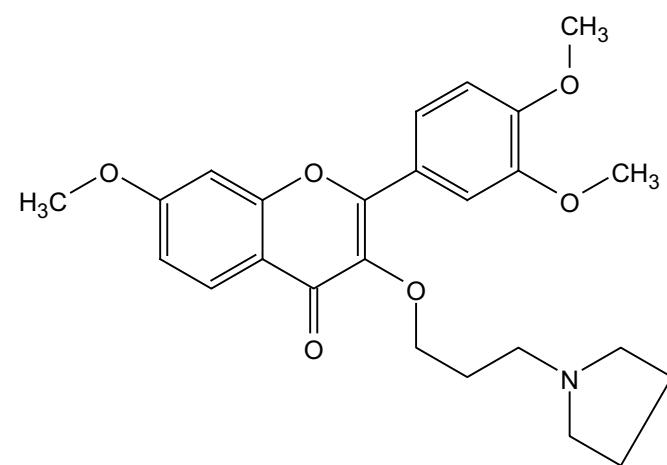
**<sup>1</sup>H NMR of 78 in CDCl<sub>3</sub>****300 MHz**

# <sup>13</sup>C NMR of 78 in CDCl<sub>3</sub>

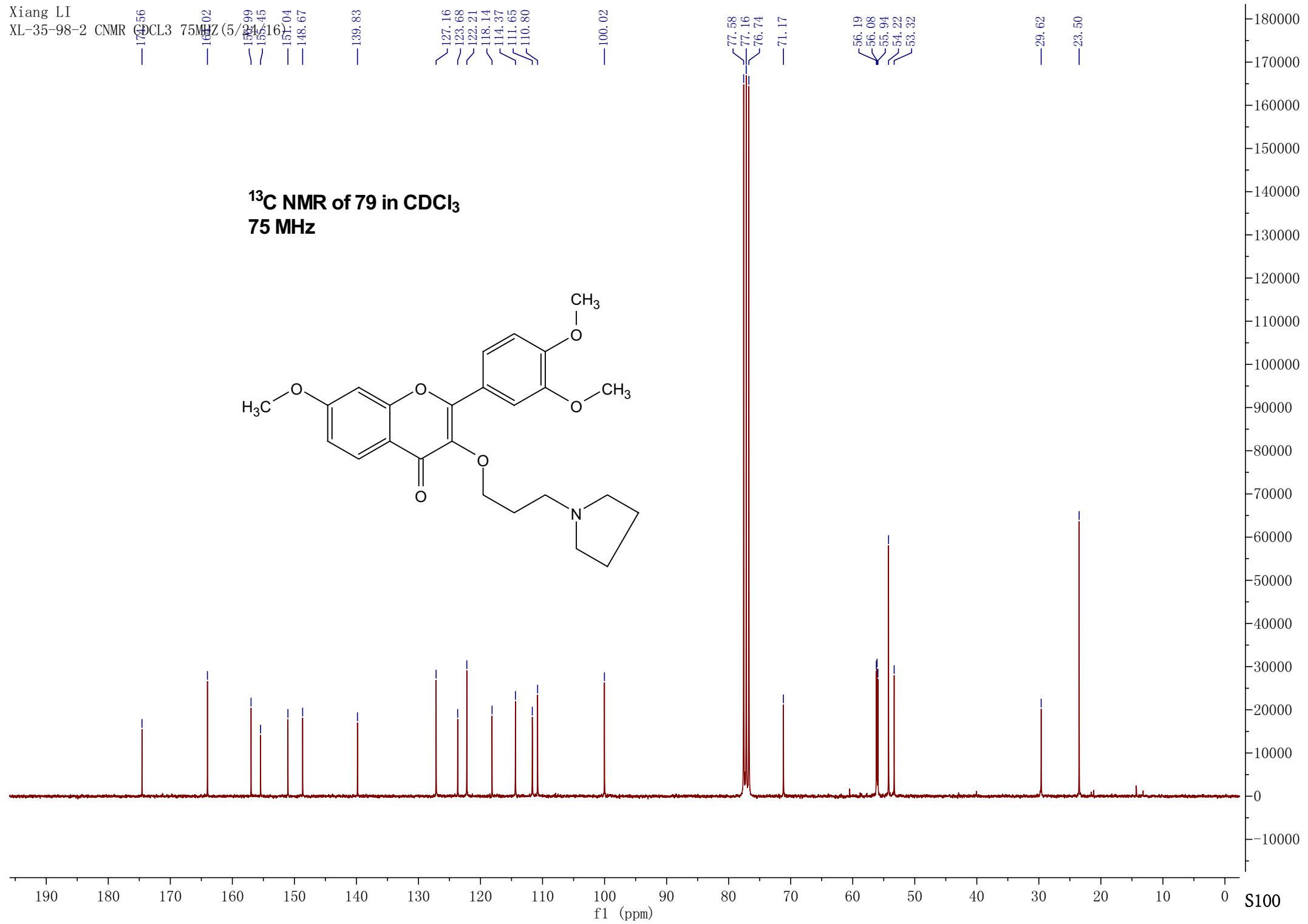
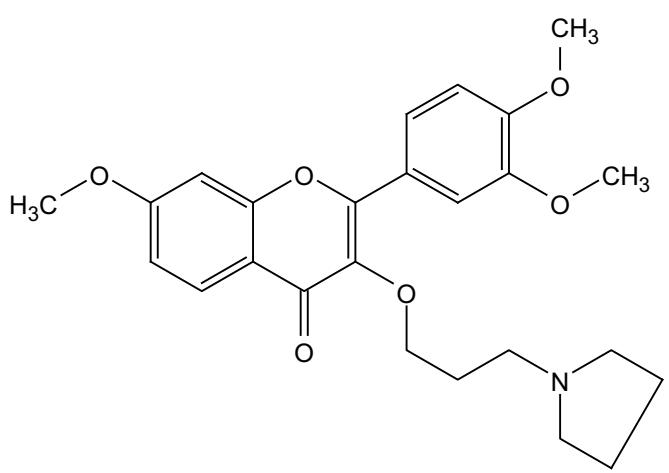
## 75 MHz



## <sup>1</sup>H NMR of 79 in CDCl<sub>3</sub>

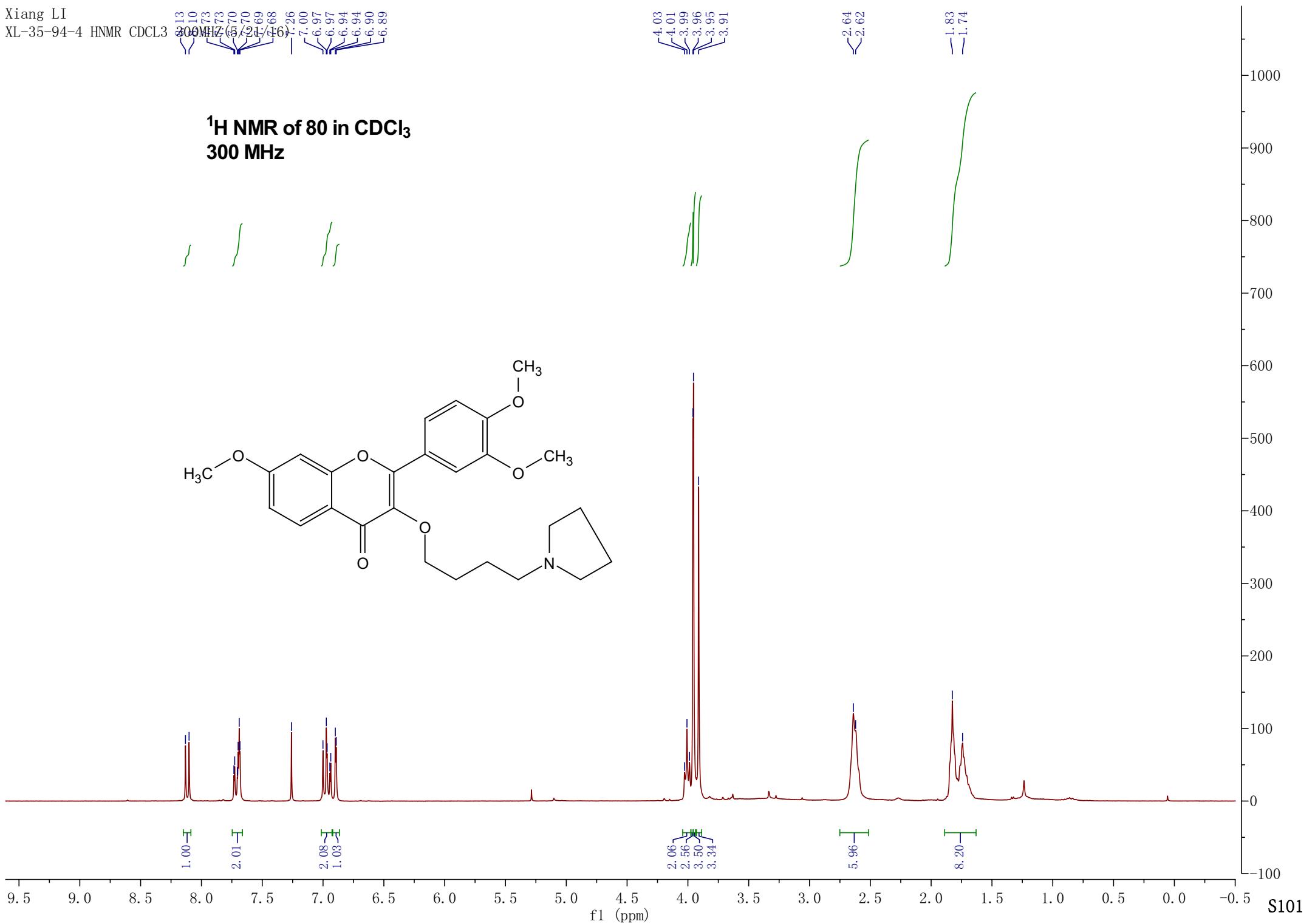
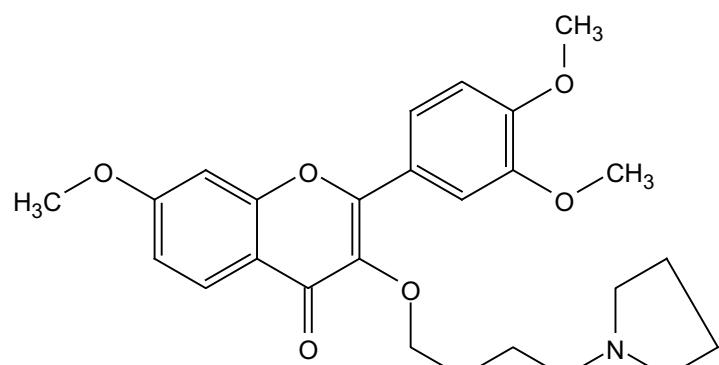


**$^{13}\text{C}$  NMR of 79 in CDCl<sub>3</sub>**  
**75 MHz**

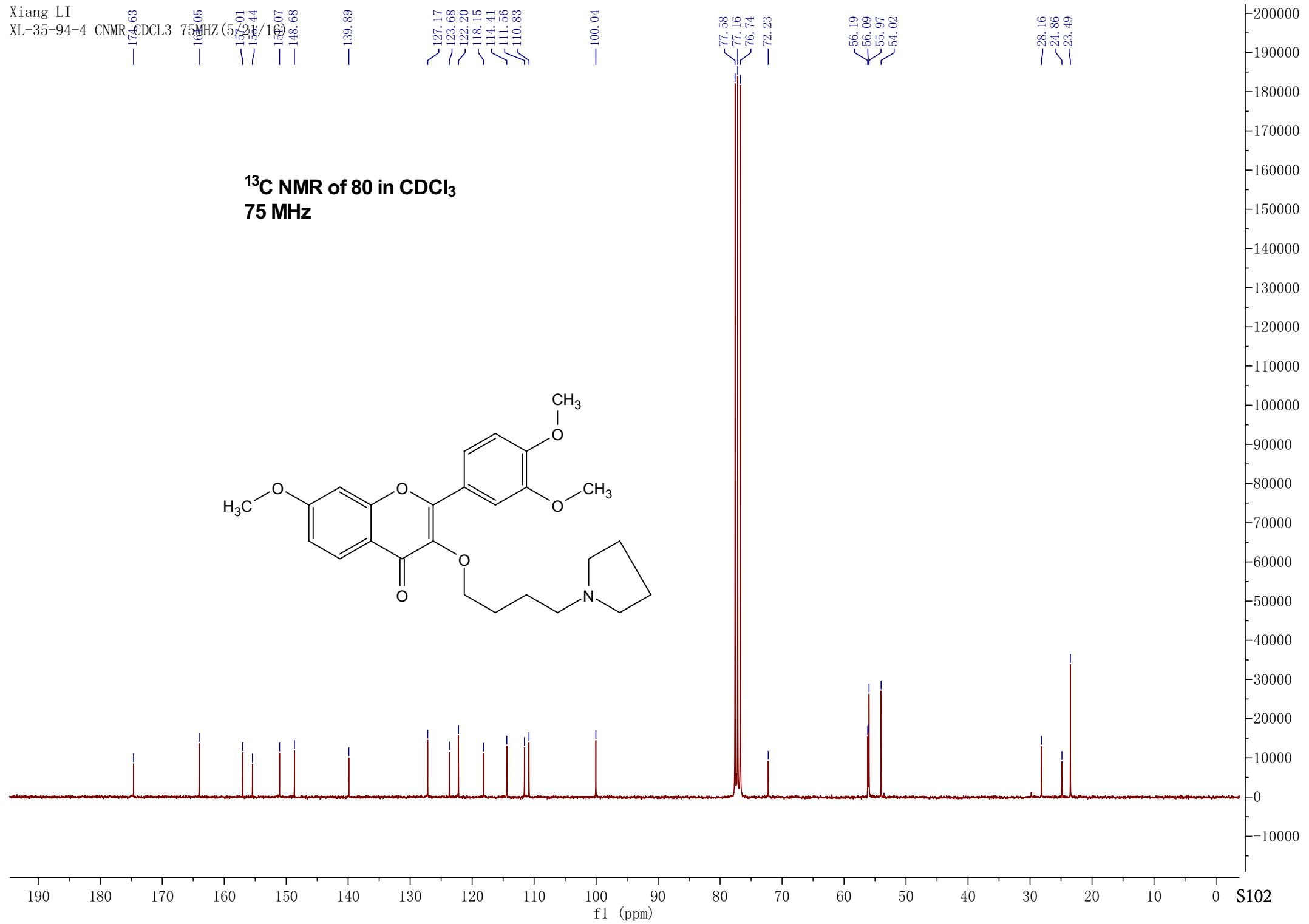
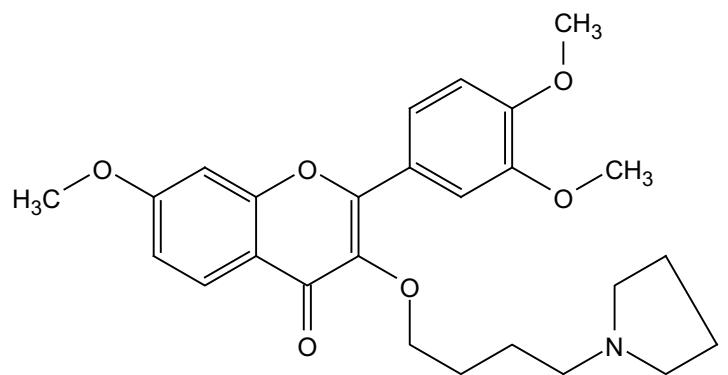


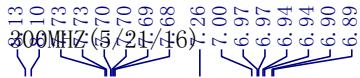


**<sup>1</sup>H NMR of 80 in CDCl<sub>3</sub>**  
**300 MHz**

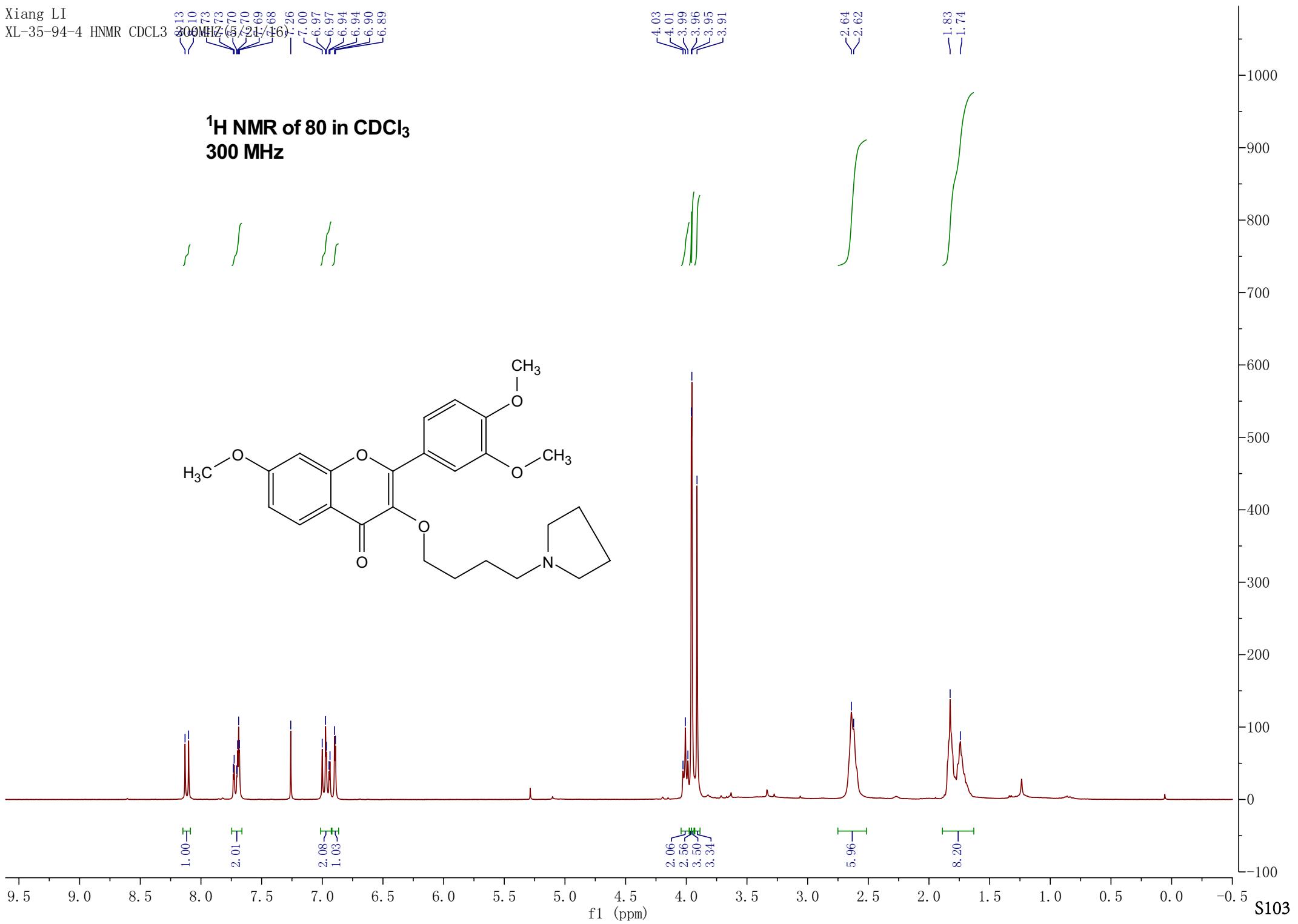
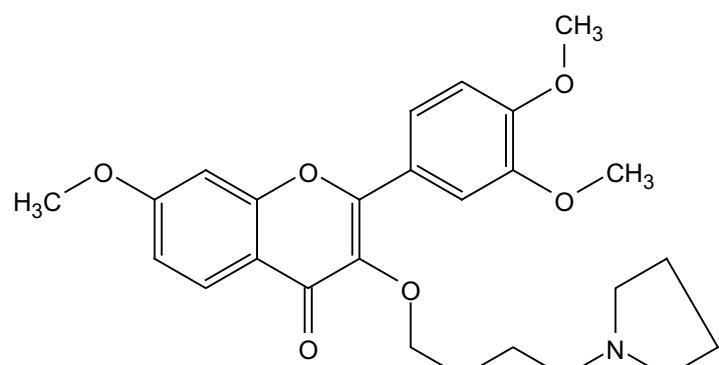


**<sup>13</sup>C NMR of 80 in CDCl<sub>3</sub>**  
**75 MHz**





**<sup>1</sup>H NMR of 80 in CDCl<sub>3</sub>**  
**300 MHz**



Xiang LI

XL-35-99-2 CNMR CDCl<sub>3</sub> 75MHz

—176.60  
—168.03  
—157.01  
—156.40  
—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

**<sup>13</sup>C NMR of 81 in CDCl<sub>3</sub>**  
**75 MHz**

