Supplementary Data

O-Aminoalkyl-*O*-Trimethyl-2,3-Dehydrosilybins: Synthesis and *in vitro* Effects toward Prostate Cancer Cells

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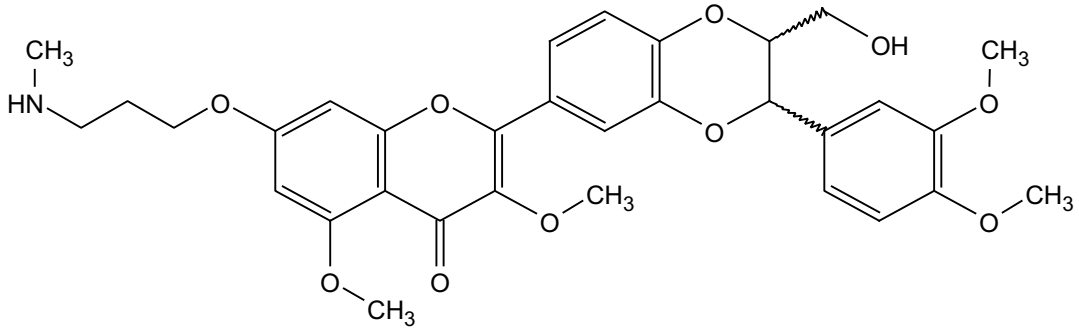
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Corresponding author.

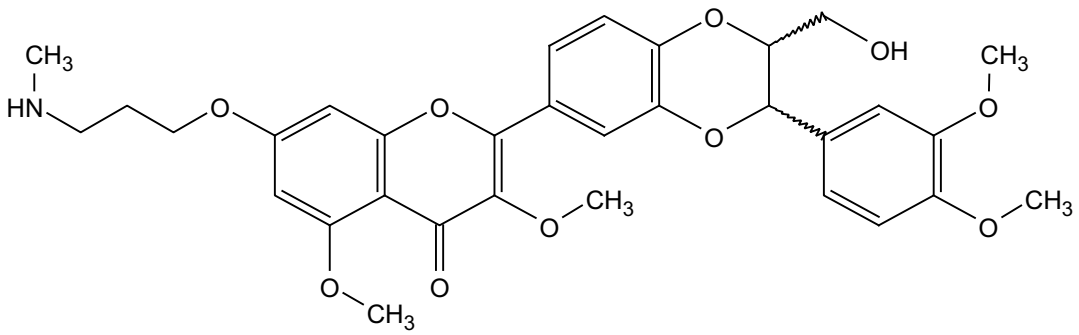
*E-mail: qchen@csufresno.edu. Phone: (+1)5592782394. Fax: (+1)5592784402.

NMR
SZ-208-4 CDCl3 HNMR 300MHZ



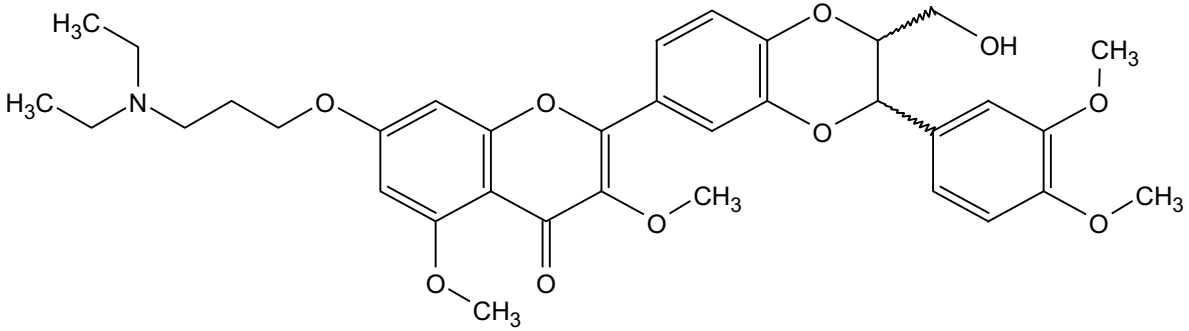
^{1}H NMR spectrum for compound 9
$CDCl_3$, 300 MHz

NMR
SZ-208-4 CDCl3 CNMR 75MHZ



^{13}C NMR spectrum for compound 9
$CDCl_3$, 75 MHz

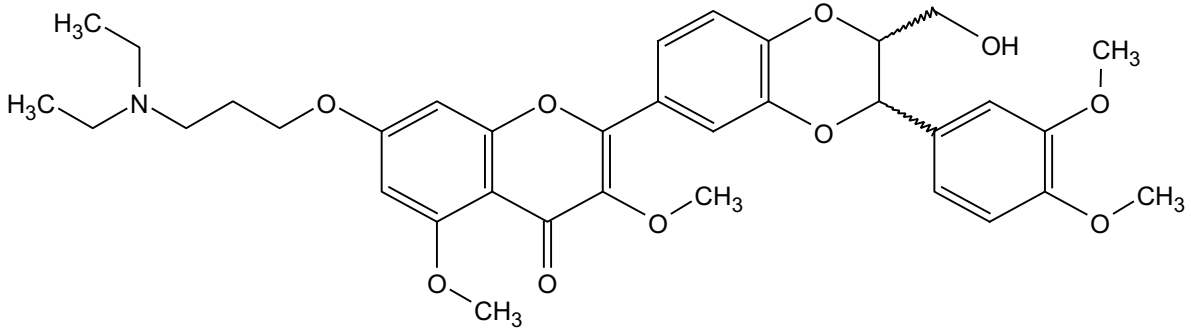
NMR
SZ-19-138 MeOD 1HNMR 300MHz



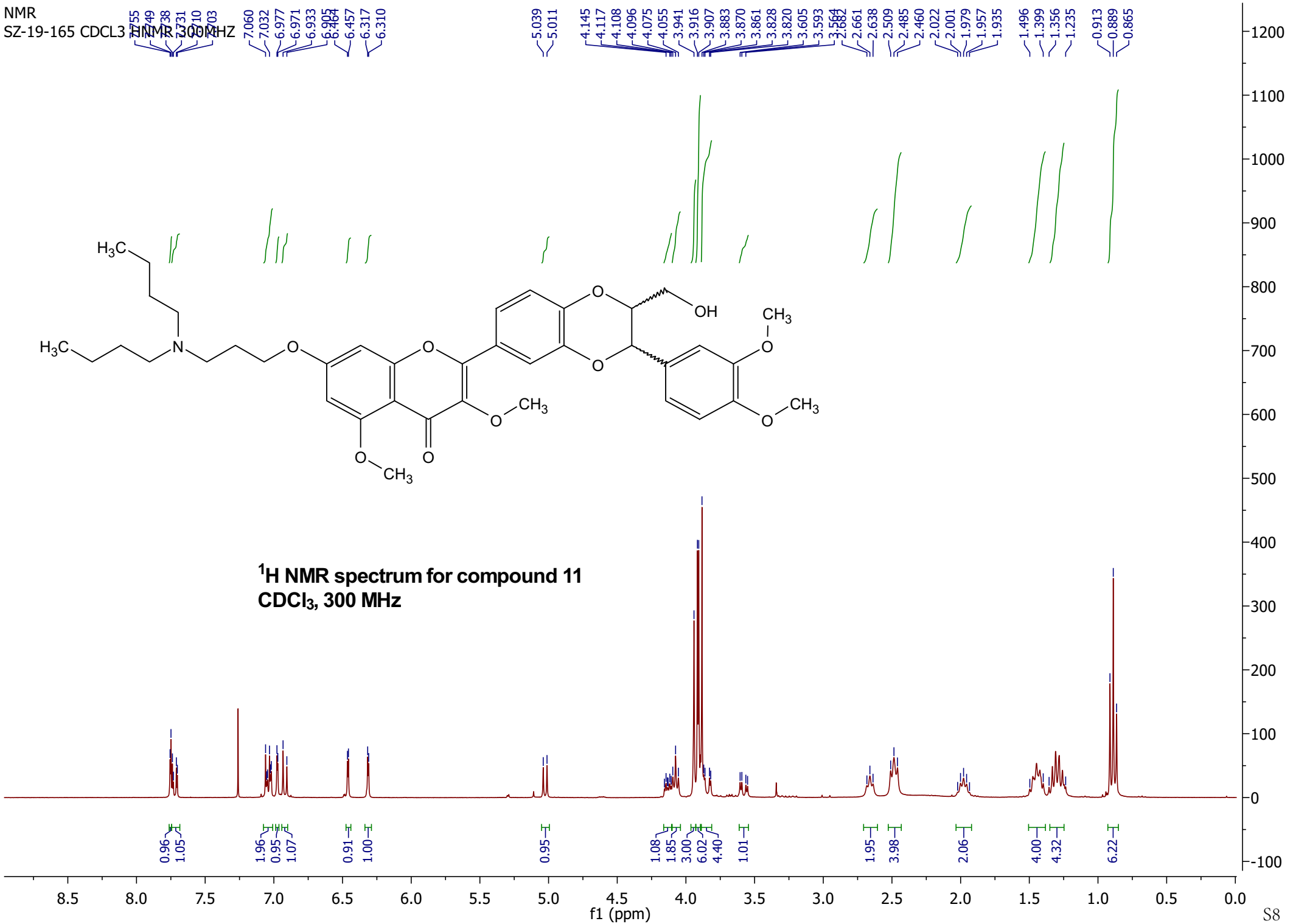
^{1}H NMR spectrum for Compound 10
MeOD, 300 MHz

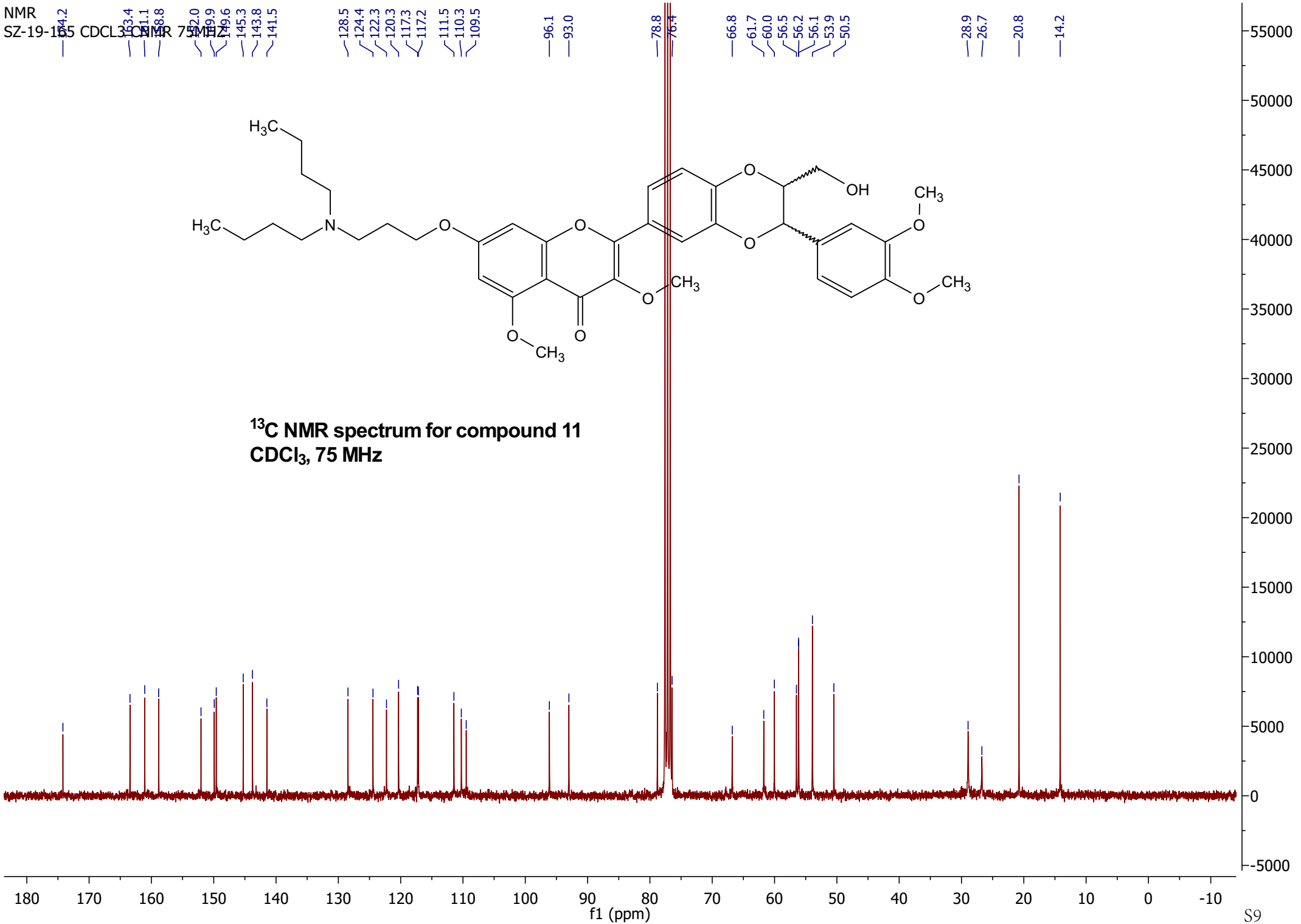
f1 (ppm)

NMR
SZ-19-138 MeOD CNMR 75MHz

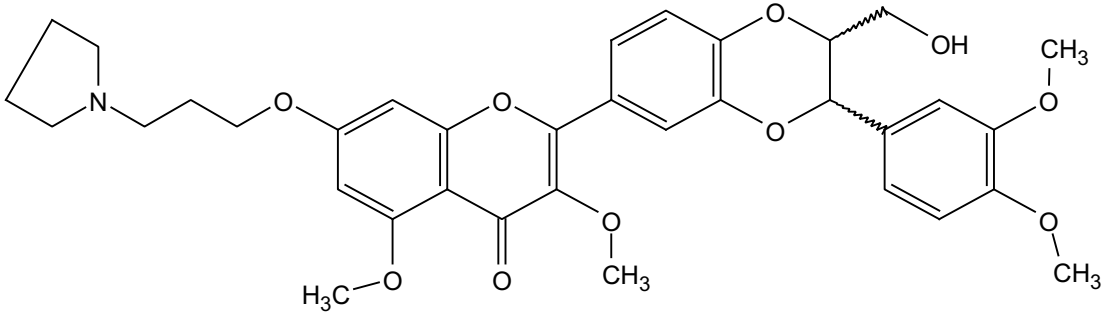


^{13}C NMR spectrum for compound 10
MeOD, 75 MHz

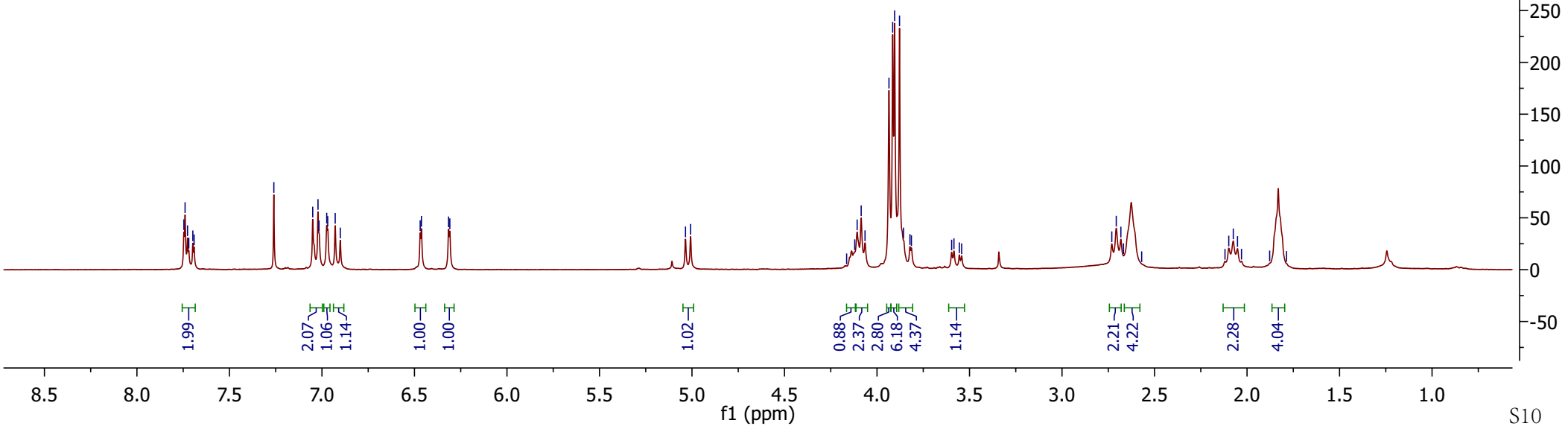

NMR
SZ-19-165 CDCL3 1HNMR 300MHZ
7.755 7.749 7.738 7.731 7.710 7.703 7.060 7.032 6.977 6.971 6.933 6.905 6.464 6.457 6.317 6.310
5.039 5.011
4.145 4.117 4.108 4.096 4.075 4.055 3.941 3.916 3.907 3.883 3.870 3.861 3.828 3.820 3.605 3.593 3.564 2.882 2.661 2.638 2.509 2.485 2.460 2.022 2.001 1.979 1.957 1.935
1.496 1.399 1.356 1.235
0.913 0.889 0.865
H3C
N
O
OH
CH3
O
O
O
O
O
O
O
CH3
CH3
CH3
O
O
1H NMR spectrum for compound 11
CDCl3, 300 MHz
0.96 1.05 1.96 0.95 1.07 0.91 1.00 0.95 1.08 1.85 3.00 6.02 4.40 1.01 1.95 3.98 2.06 4.00 4.32 6.22
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)
1200 1100 1000 900 800 700 600 500 400 300 200 100 0 -100


NMR
SZ-19-165 CDCL3 CNMR 75MHZ
164.2
163.4
161.1
158.8
152.0
149.9
149.6
145.3
143.8
141.5
128.5
124.4
122.3
120.3
117.3
117.2
111.5
110.3
109.5
96.1
93.0
78.8
76.4
66.8
61.7
60.0
56.5
56.2
56.1
53.9
50.5
28.9
26.7
20.8
14.2
H3C
H3C
N
O
O
O
O
O
OH
CH3
O
CH3
O
CH3
O
O
O
CH3
13C NMR spectrum for compound 11
CDCl3, 75 MHz
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

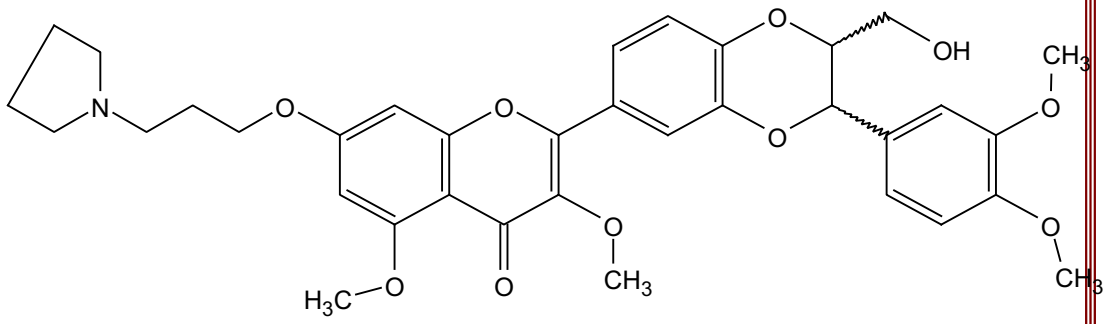
NMR
SZ-19-177-2 CDCl3 HNMR 300MHZ



^{1}H NMR spectrum for compound 12
$CDCl_3$, 300 MHz



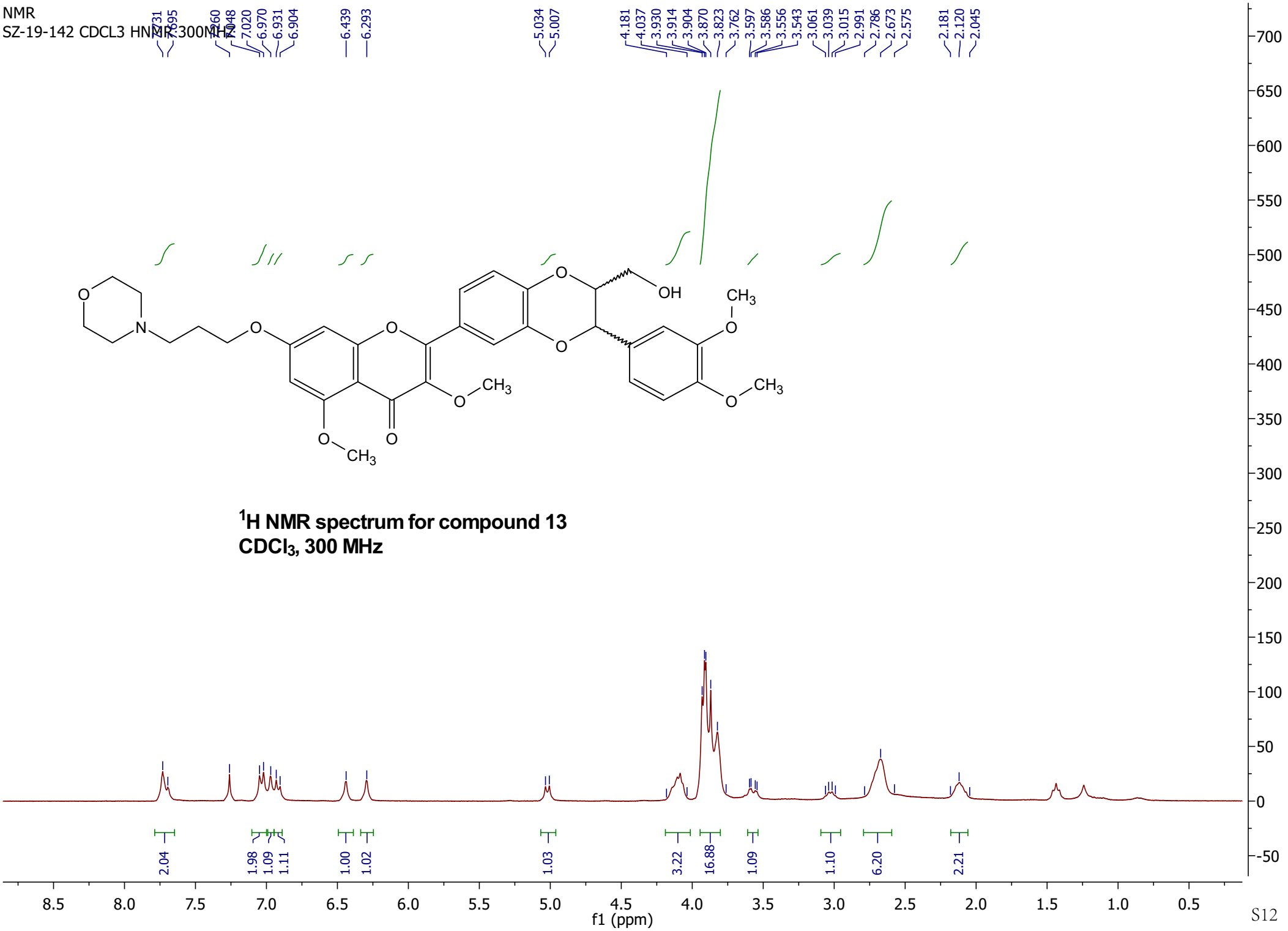
NMR
SZ-177-2 CDCL3 CNMR 75MHZ



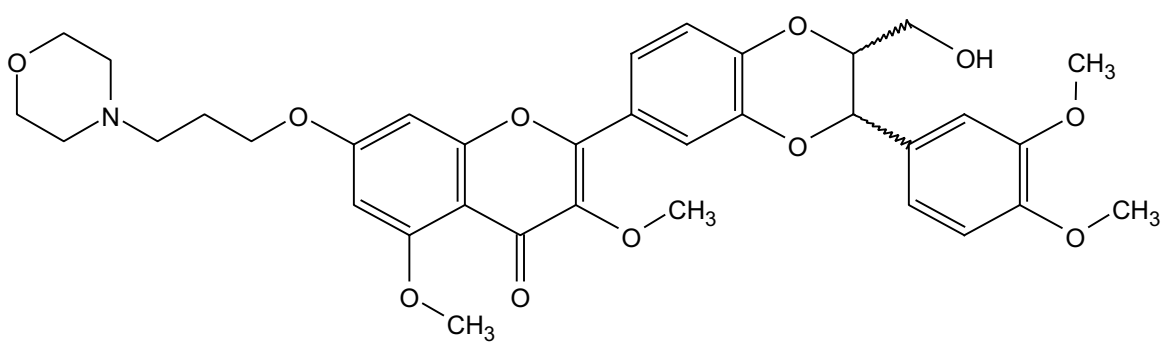
^{13}C NMR spectrum for compound 12
$CDCl_3$, 75 MHz

NMR
SZ-19-142 CDCL3 HNMR 300MHz

^{1}H NMR spectrum for compound 13
$CDCl_3$, 300 MHz

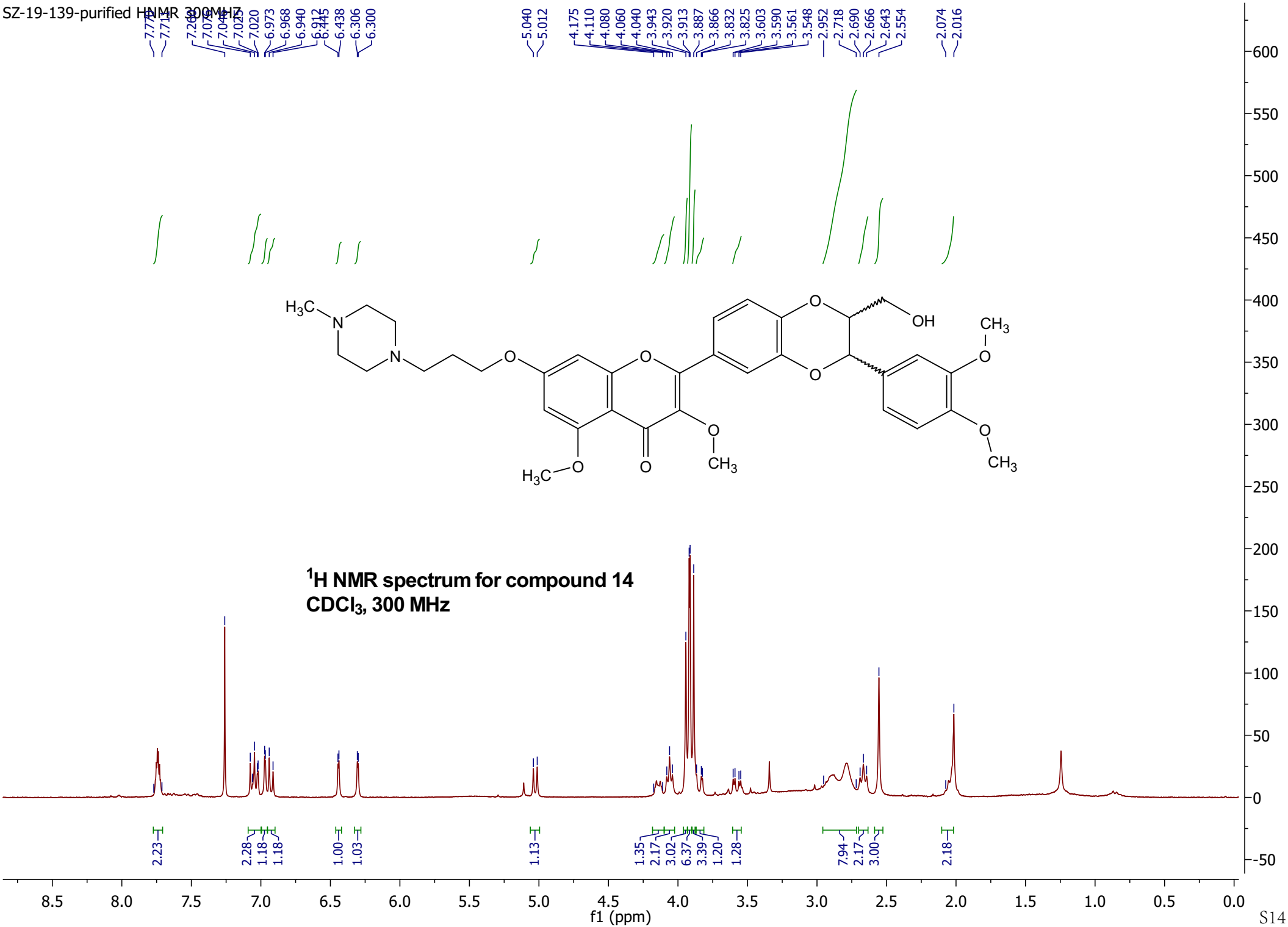


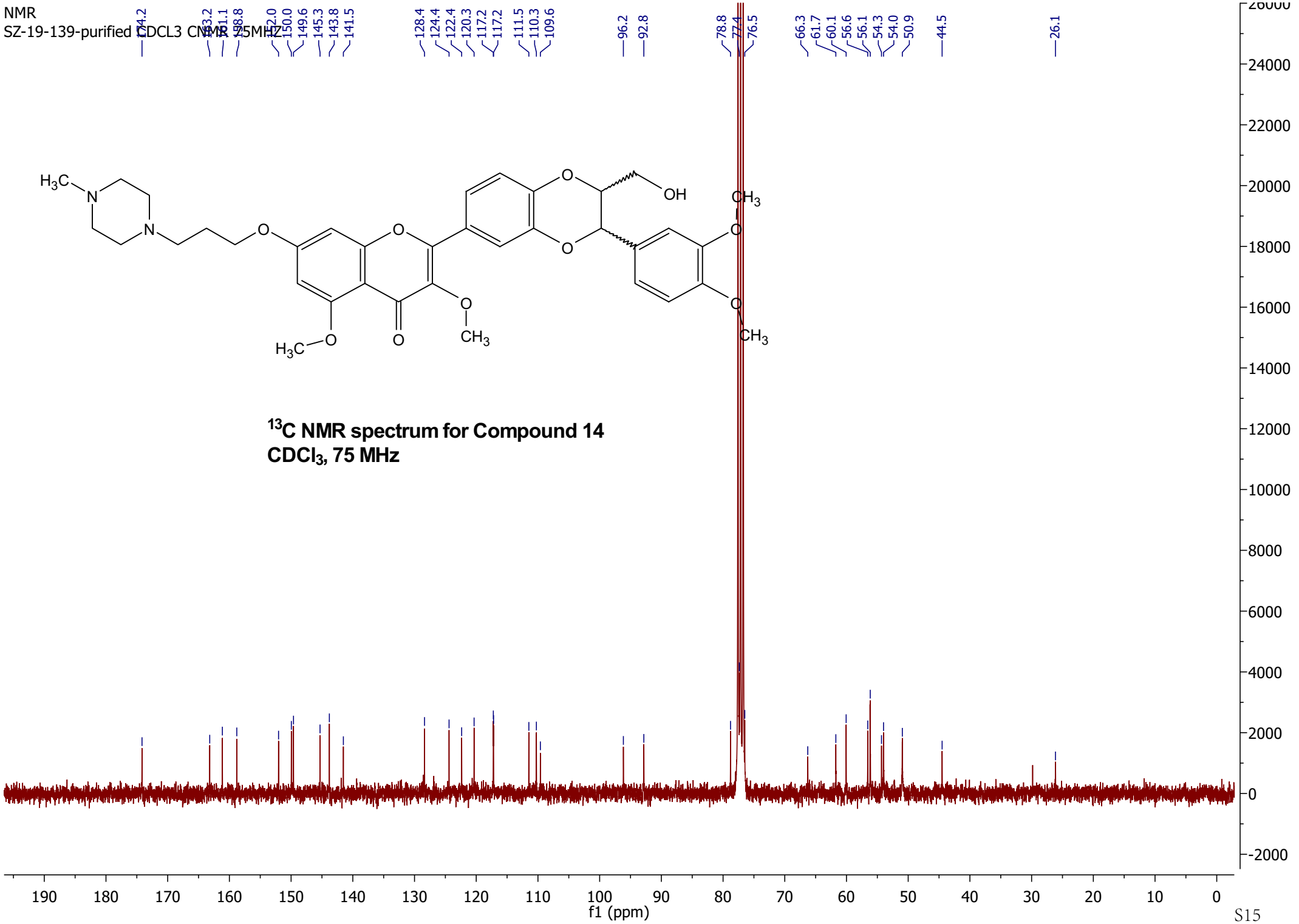
NMR
SZ-19-142 CDCL3 CNMR 75MHZ



^{13}C NMR spectrum for compound 13
$CDCl_3$, 75 MHz

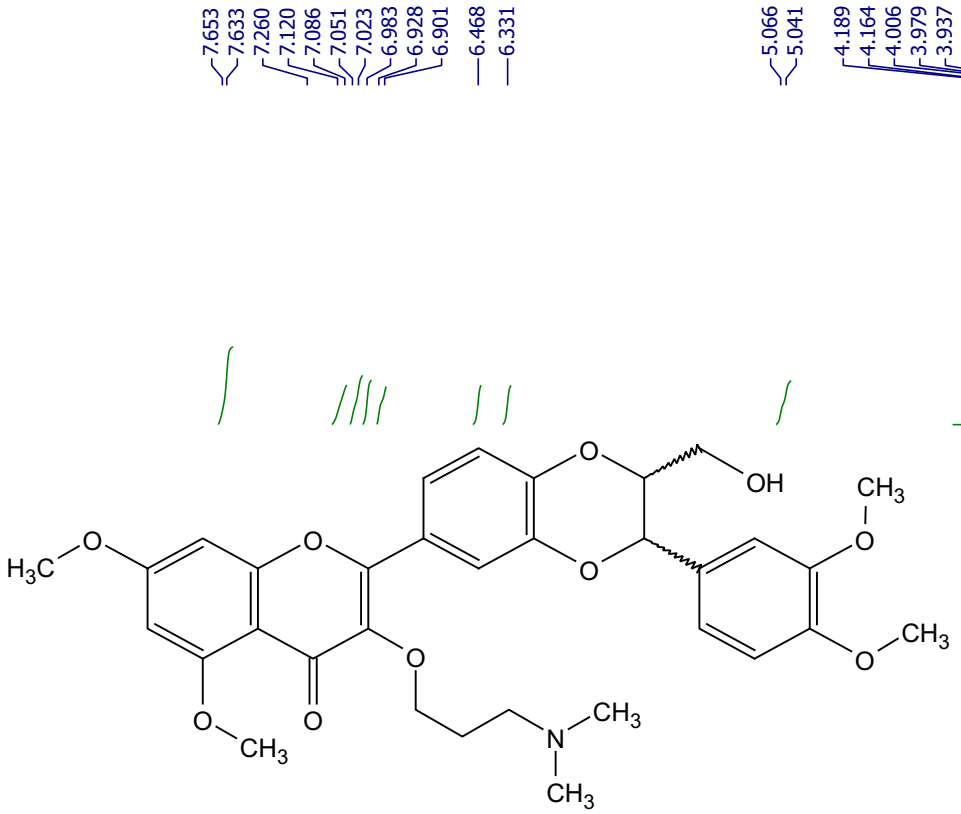
SZ-19-139-purified HNMR 300MHZ



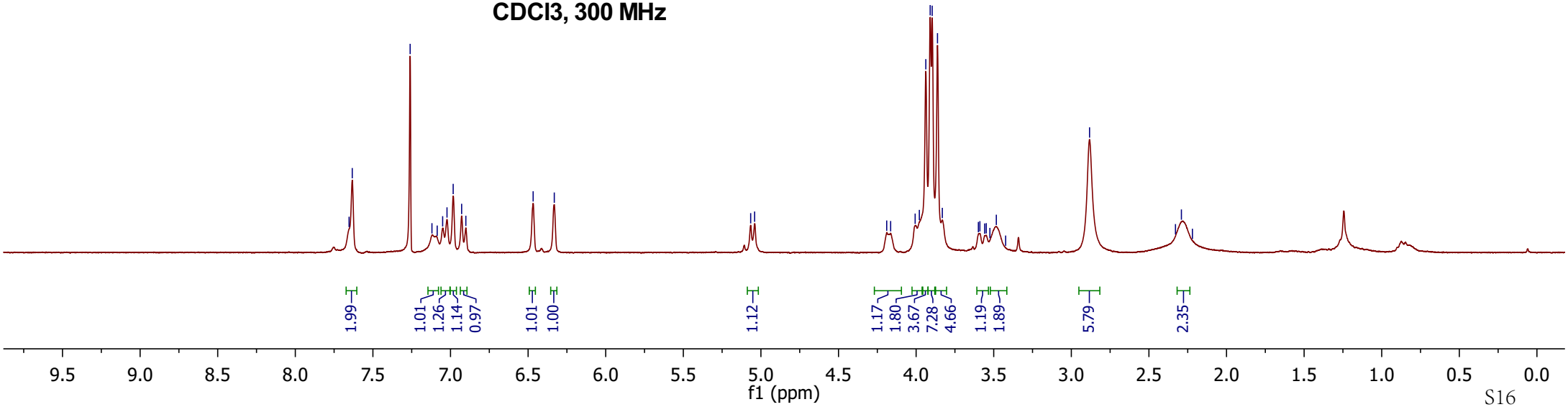


^{13}C NMR spectrum for Compound 14
$CDCl_3$, 75 MHz

E:
BV-48-23-R2-CDCL3

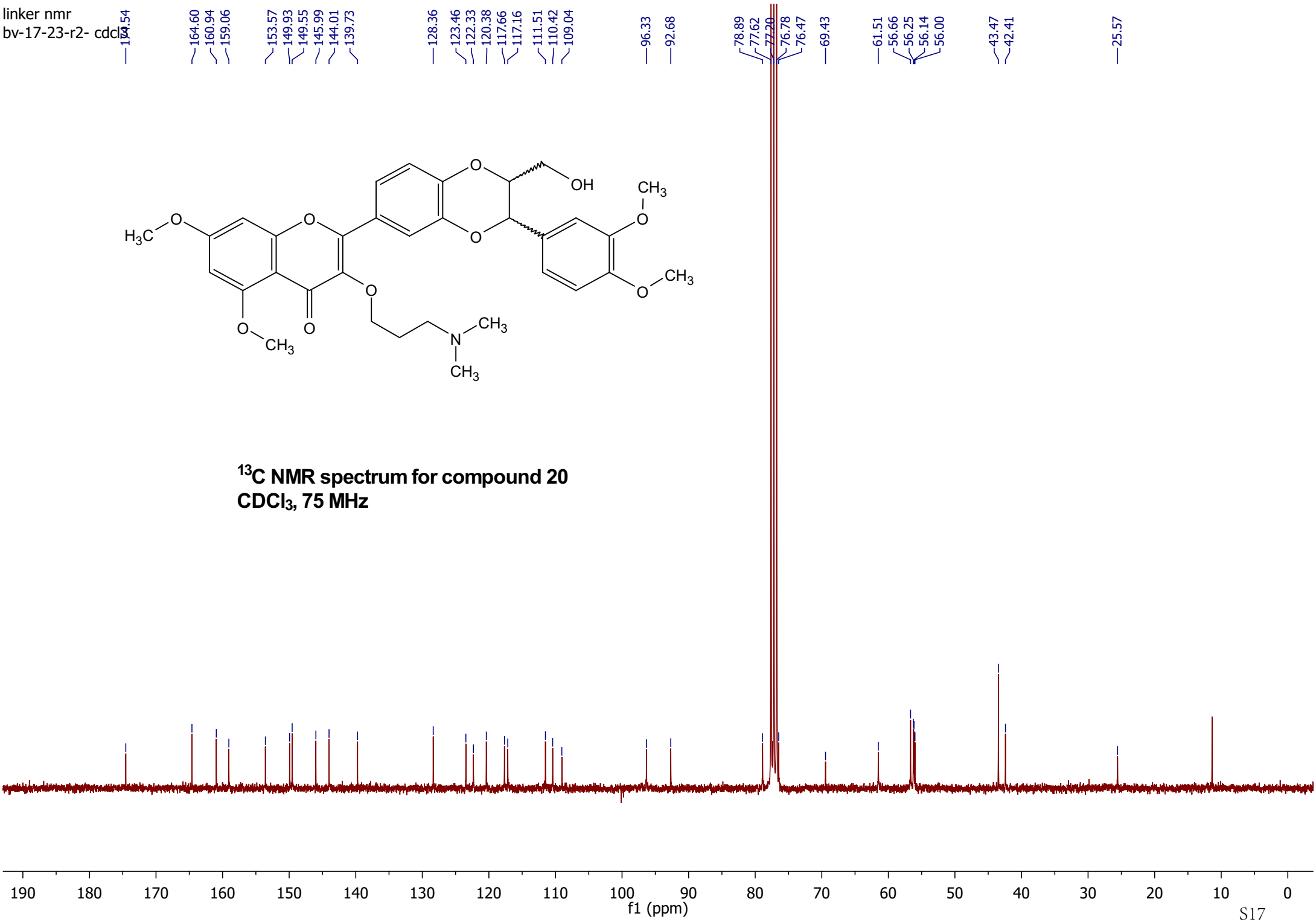


1H NMR spectrum for compound 20
CDCl3, 300 MHz

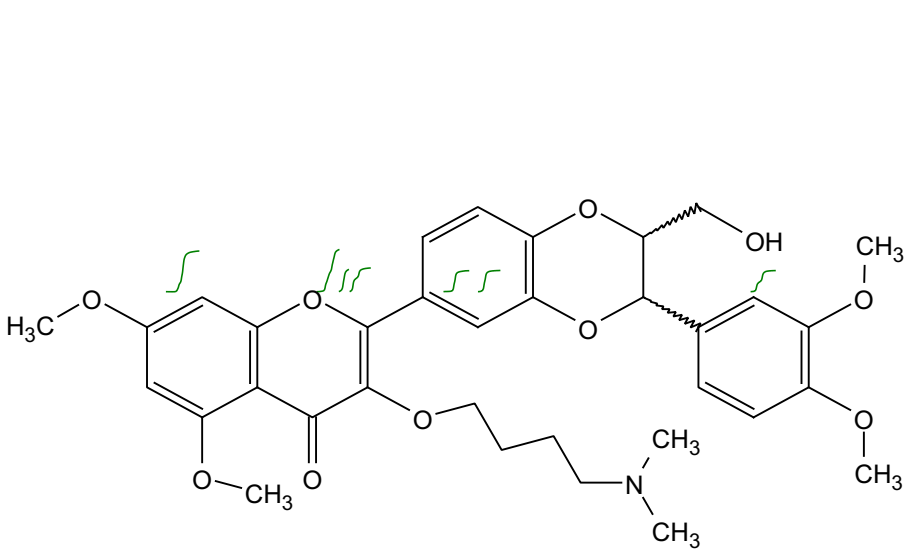


linker nmr
bv-17-23-r2- cdcl3

^{13}C NMR spectrum for compound 20
$CDCl_3$, 75 MHz

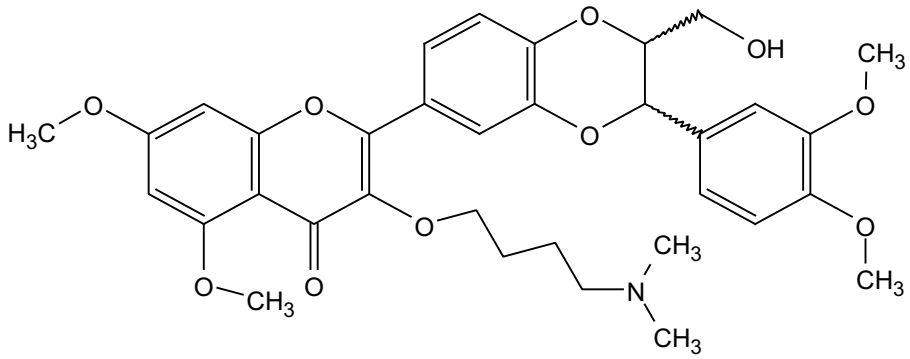


andre vignau
av 39-36 dimethylamaine 55



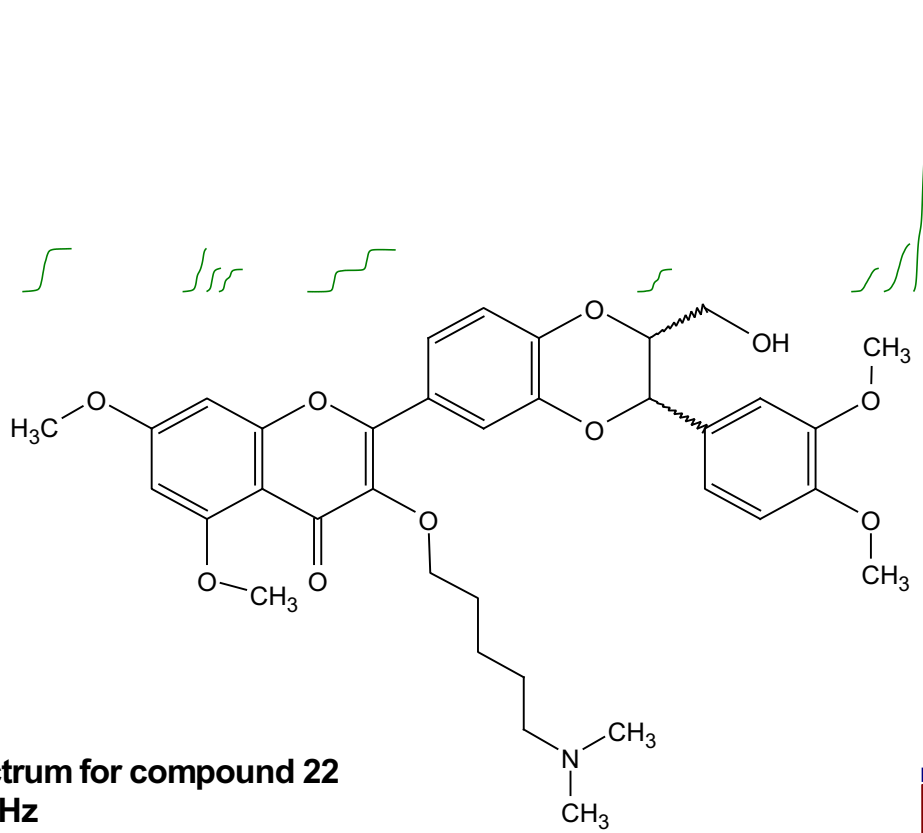
^{1}H NMR spectrum for compound 21
$CDCl_3$, 300 MHz

andre vignau
av 39-36 dimethylamine 5c c13



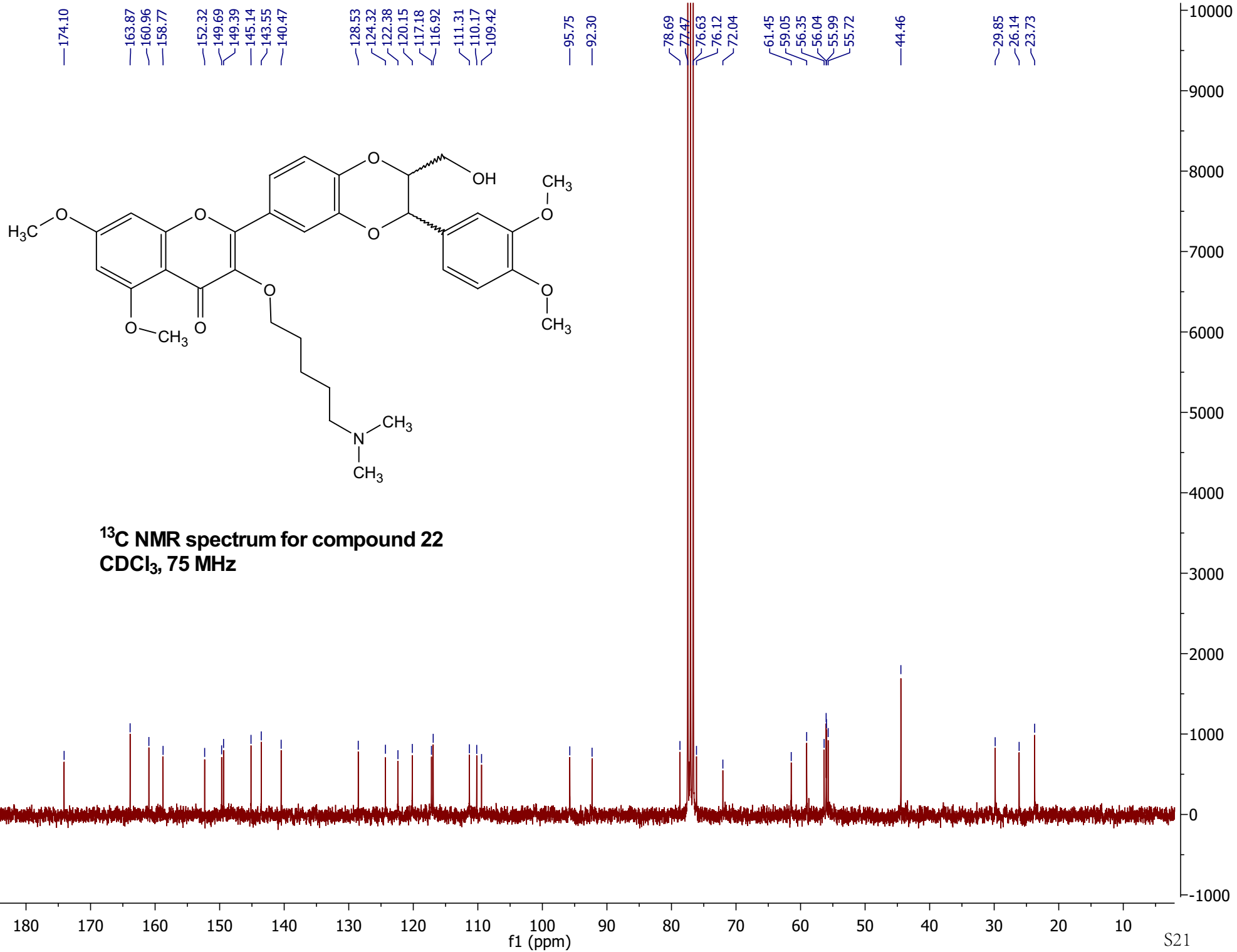
^{13}C NMR spectrum for compound 21
$CDCl_3$, 75 MHz

andre vignau
av 37-30



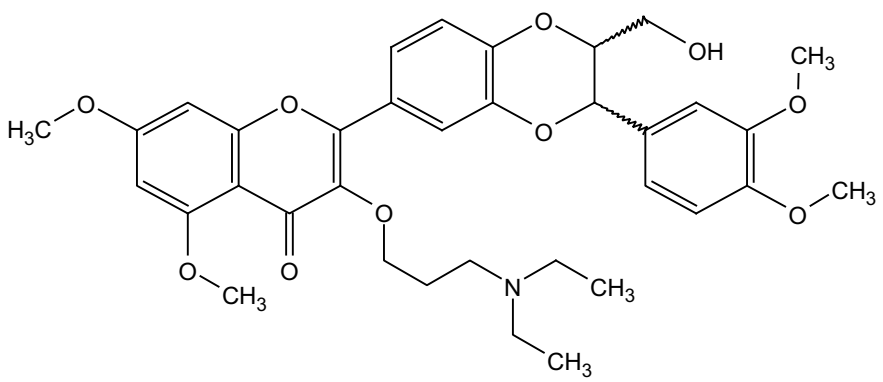
^{1}H NMR sepctrum for compound 22
$CDCl_3$, 300 MHz

andre vignau
av 37-30 c13

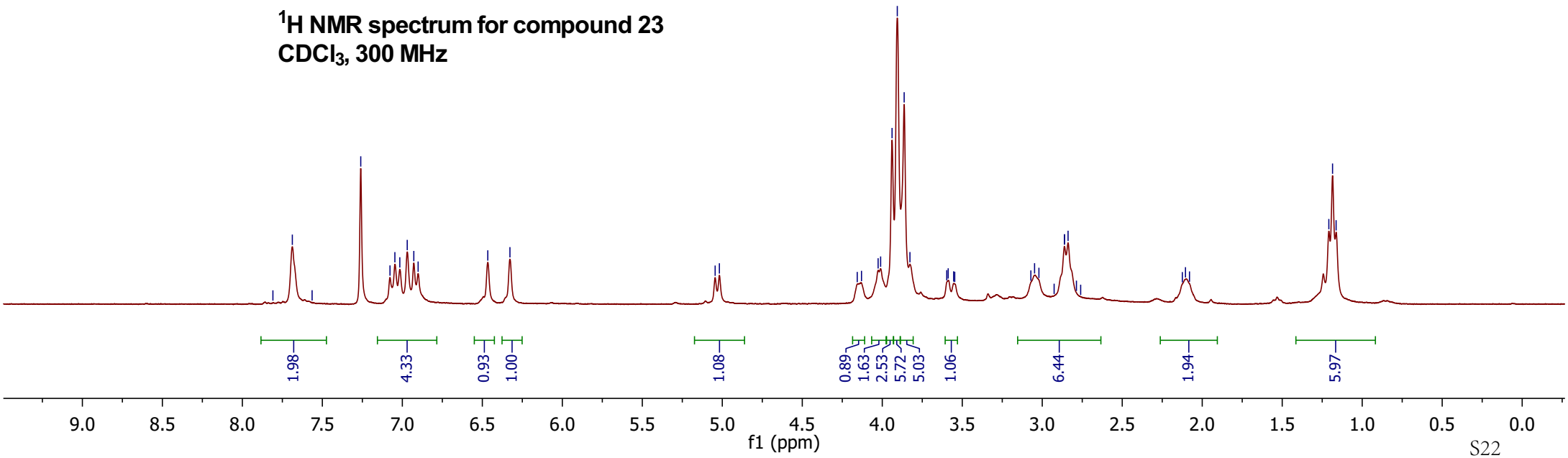


^{13}C NMR spectrum for compound 22
$CDCl_3$, 75 MHz

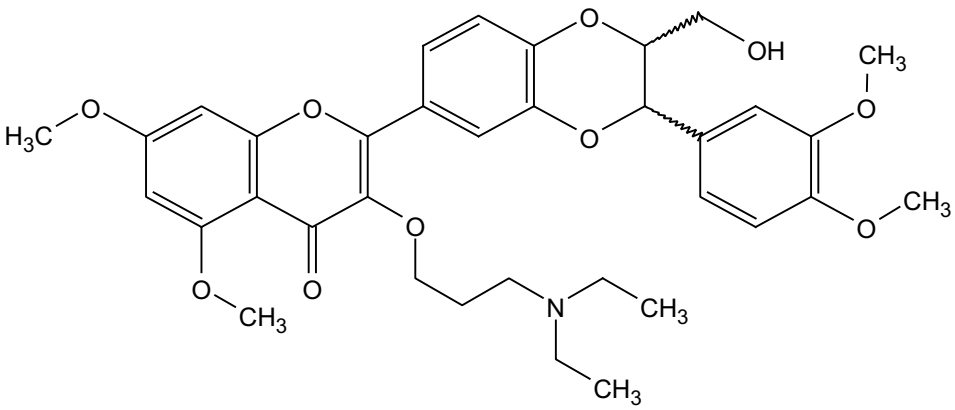
linker nmr
bv-17-232 cdcl3



^{1}H NMR spectrum for compound 23
$CDCl_3$, 300 MHz

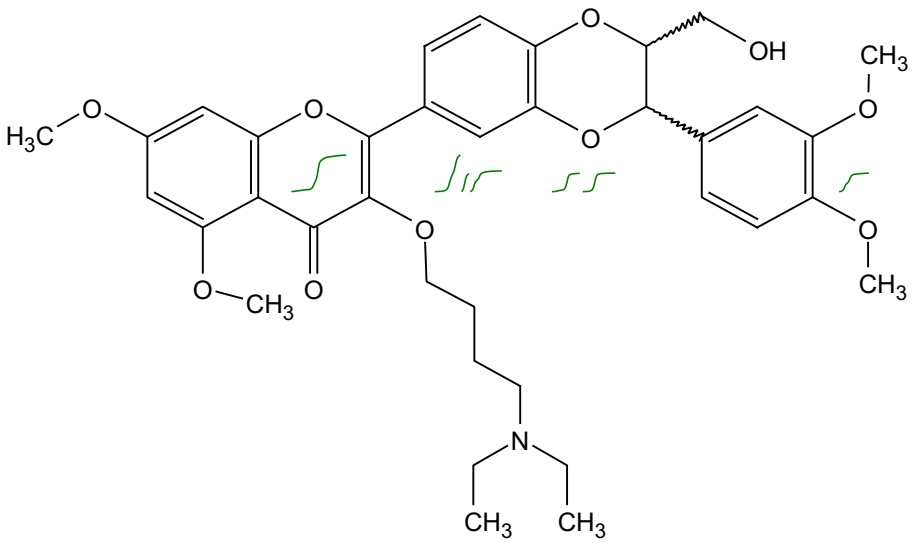


linker nmr
bv-17-232 cdcl3



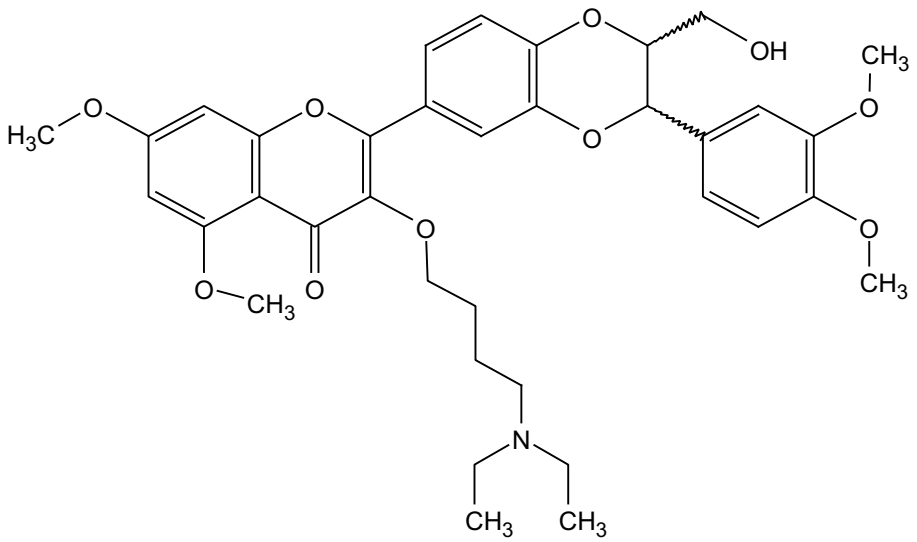
^{13}C NMR spectrum for compound 23
$CDCl_3$, 75 MHz

Andre
AV-39-35-R2 HNMR CDCl3 300MHZ



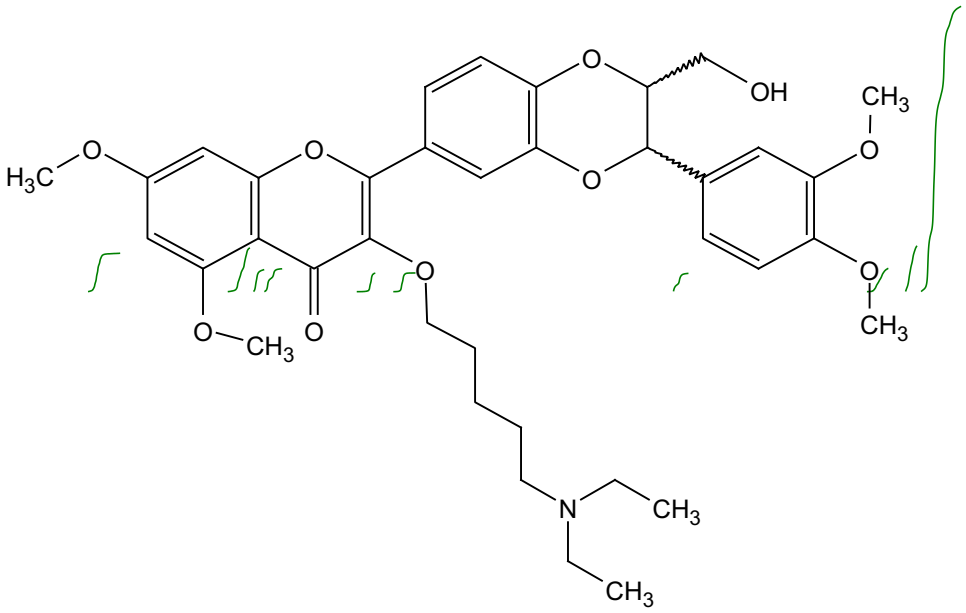
^{1}H NMR spectrum for compound 24
$CDCl_3$, 300 MHz

Andre
AV-39-35-R2 CNMR CDCL3 75MHZ



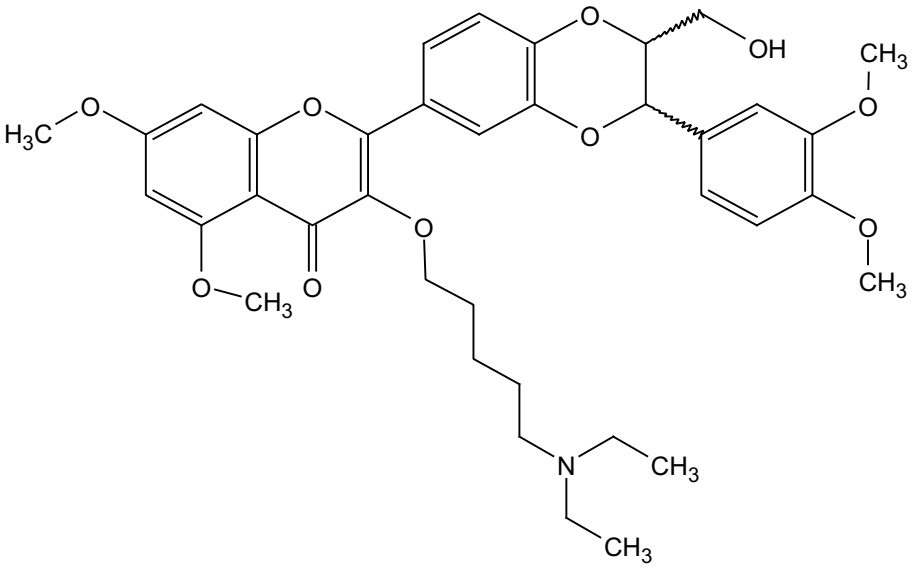
^{13}C NMR spectrum for compound 24
$CDCl_3$, 75 MHz

andre vignau
av 37-16 diethylamine



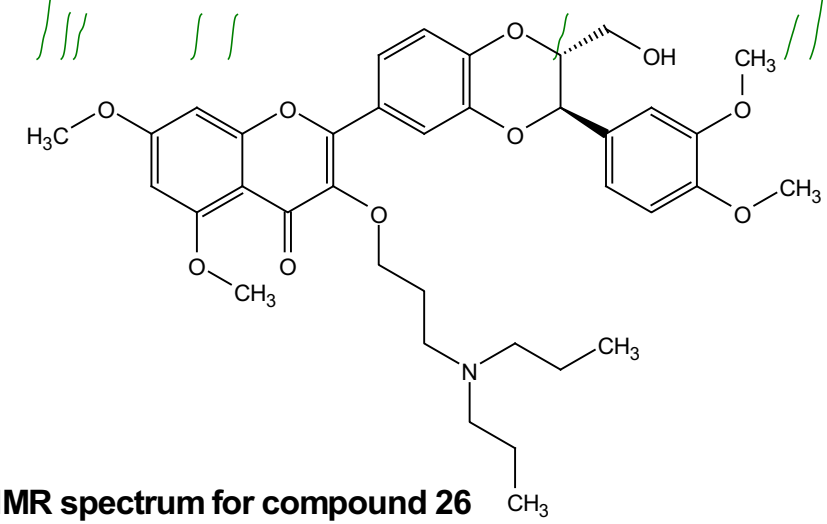
^{1}H NMR spectrum for compound 25
$CDCl_3$, 300 MHz

andre vignau
av 39-16 c13



^{13}C NMR spectrum for compound 25
$CDCl_3$, 75 MHz

linker nmr
bv-48-52-r1 cdcl3

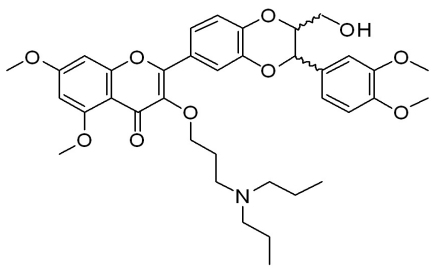


^{1}H NMR spectrum for compound 26
$CDCl_3$, 300 MHz

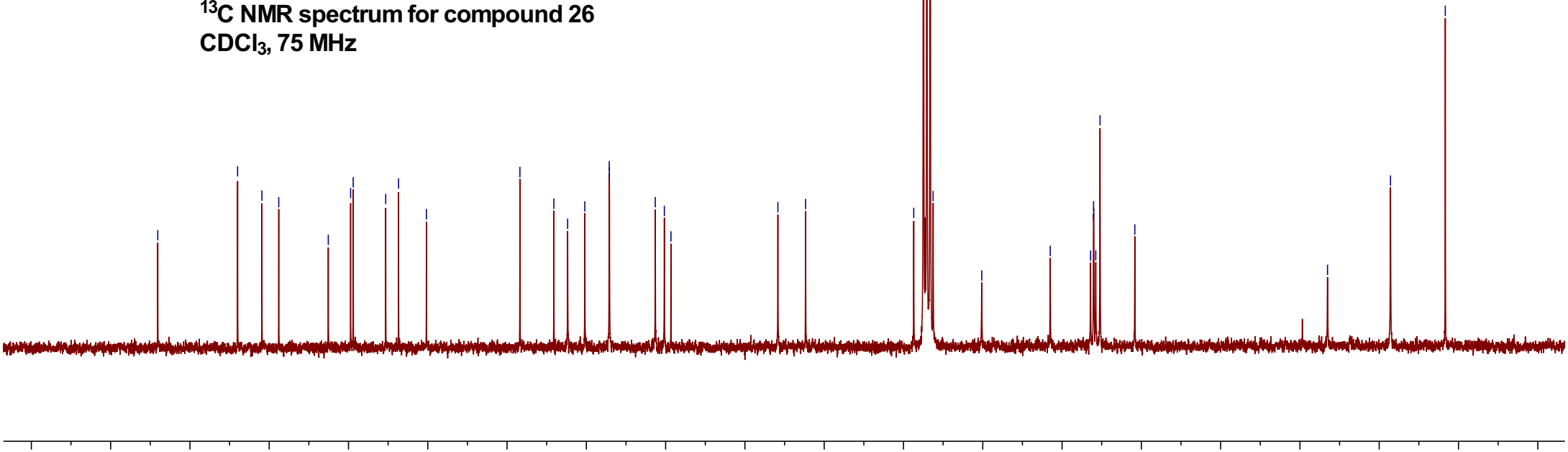
f1 (ppm)

linker nmr
bv-48-52-r1 cdcl3

174.06
163.99
160.92
158.80
152.55
149.73
149.40
145.30
143.69
140.17
128.38
124.10
122.36
120.19
117.11
117.09
111.31
110.16
109.33
95.84
92.35
78.71
76.26
70.13
61.49
56.40
56.03
56.00
55.75
55.21
50.82
26.52
18.58
11.66

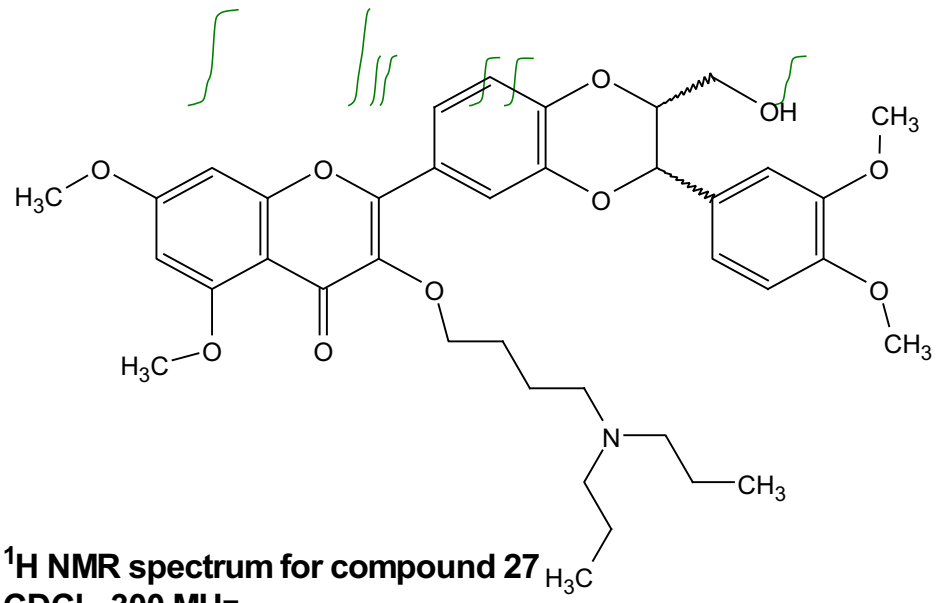


^{13}C NMR spectrum for compound 26
$CDCl_3$, 75 MHz



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

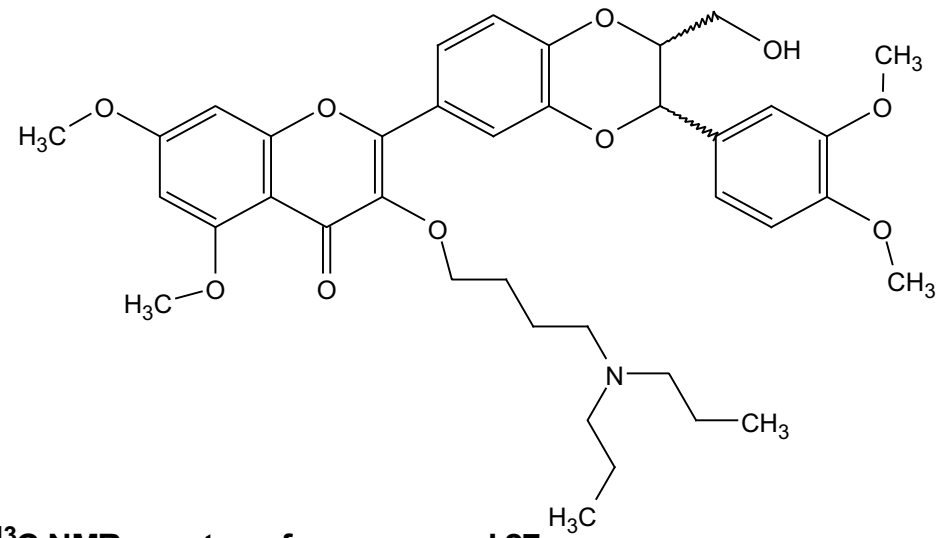
Andre
AV-39-41-R2 HNMR CDCl3 300MHz



^{1}H NMR spectrum for compound 27
$CDCl_3$, 300 MHz

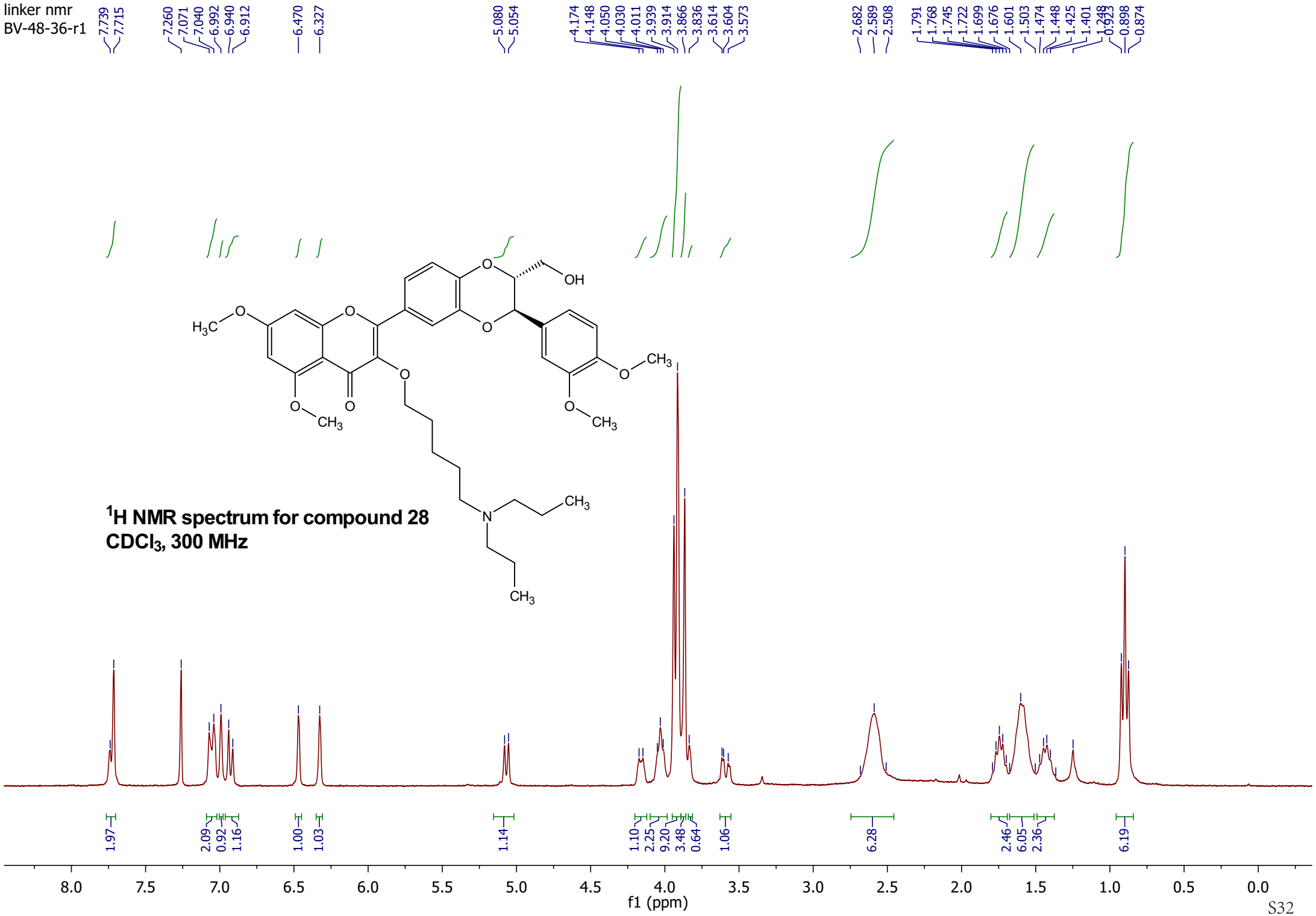
f1 (ppm)

Andre
AV-39-41-R2 CNMR CDCL3 75MHZ

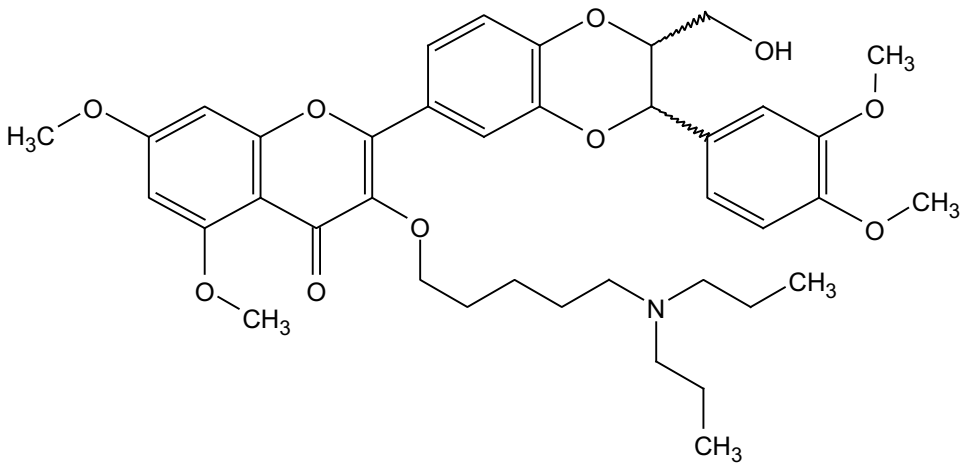


^{13}C NMR spectrum for compound 27
$CDCl_3$, 75 MHz

linker nmr
BV-48-36-r1

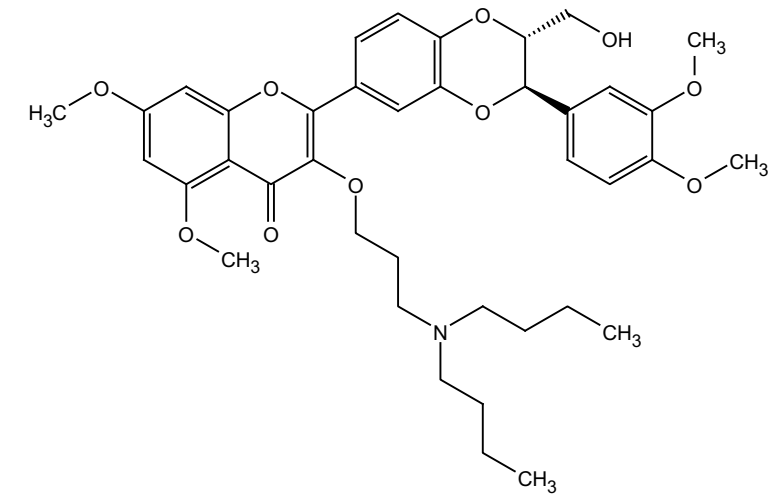


linker nmr
BV-48-36-r1 cdcl3



^{13}C NMR spectrum for compound 28
75 MHz, $CDCl_3$

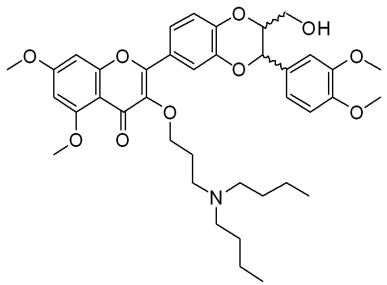
linker nmr
bv-48-13-r2 cdcl3



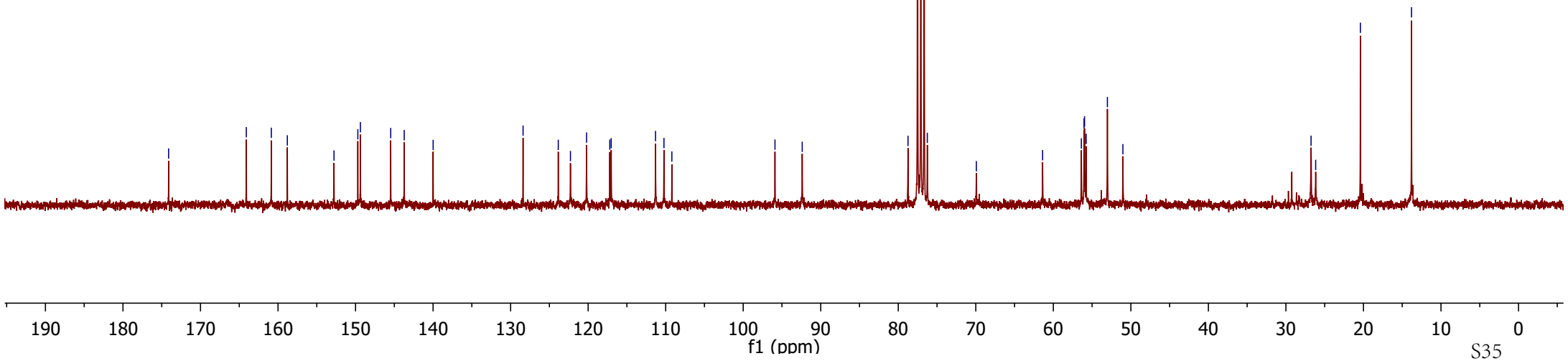
^{1}H NMR spectrum for compound 29
$CDCl_3$, 300 MHz

linker nmr
bv-48-13-r2 cdcl3

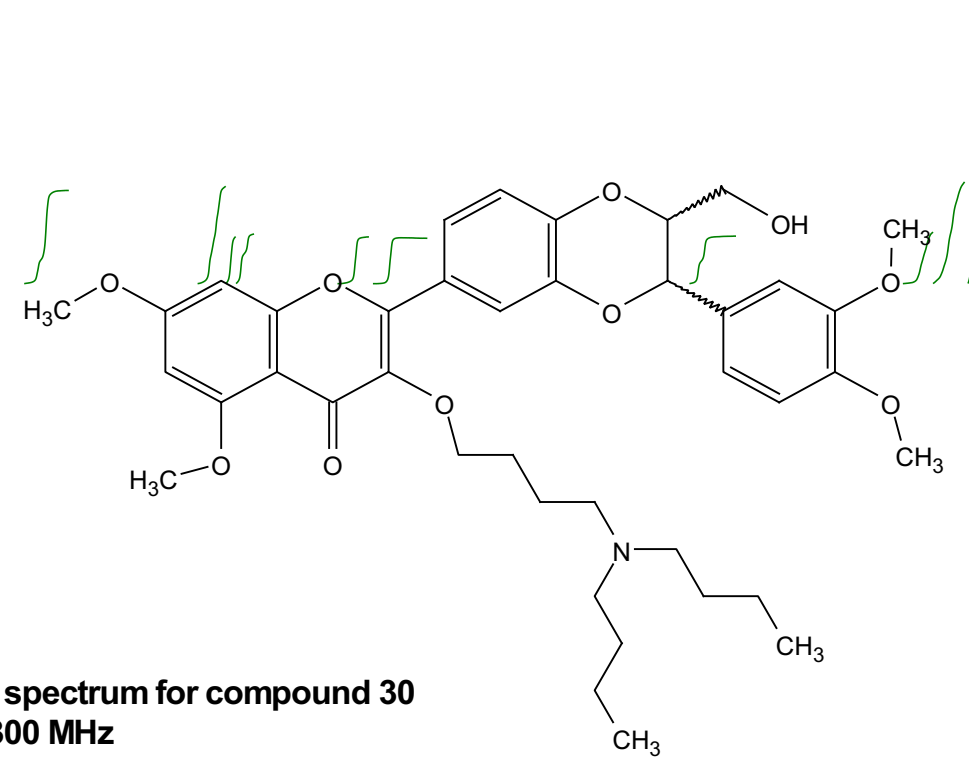
174.11
164.09
160.87
158.80
152.78
149.71
149.37
145.46
143.72
139.99
128.39
123.85
122.28
120.20
117.21
117.03
111.31
110.22
109.20
95.90
92.39
78.74
76.25
69.93
61.38
56.39
56.04
55.98
55.77
53.02
51.03
26.76
26.16
20.40
13.80



^{13}C NMR spectrum for compound 29
$CDCl_3$, 75 MHz

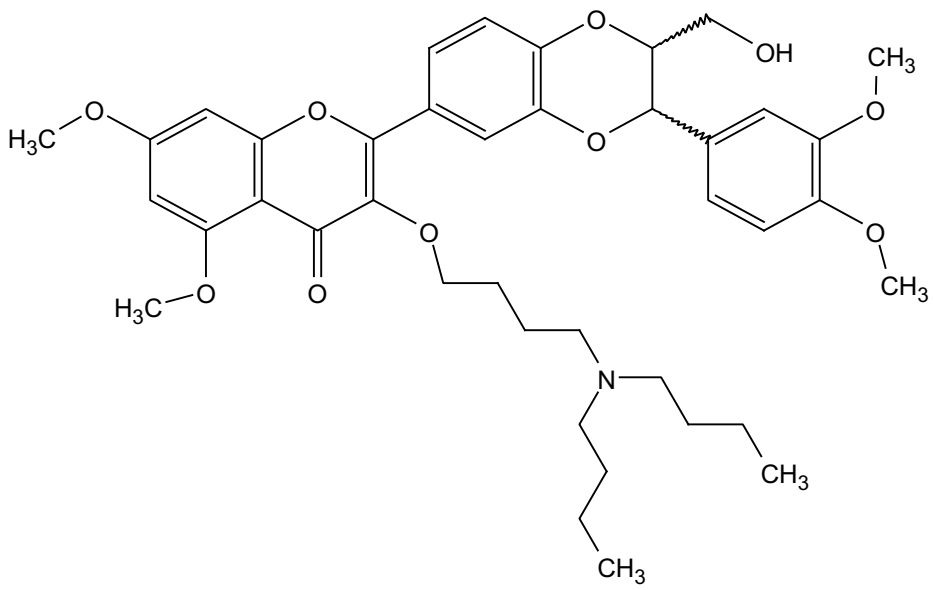


andre vignau
av 39-40-R2



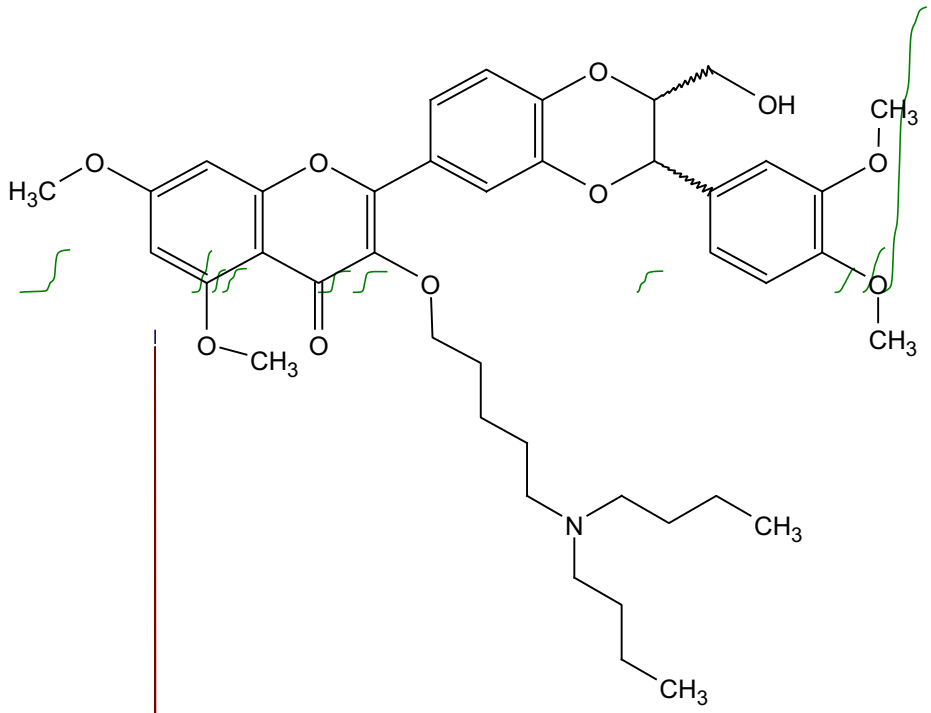
^{1}H NMR spectrum for compound 30
$CDCl_3$, 300 MHz

andre vignau
av 39-40-R2 C13



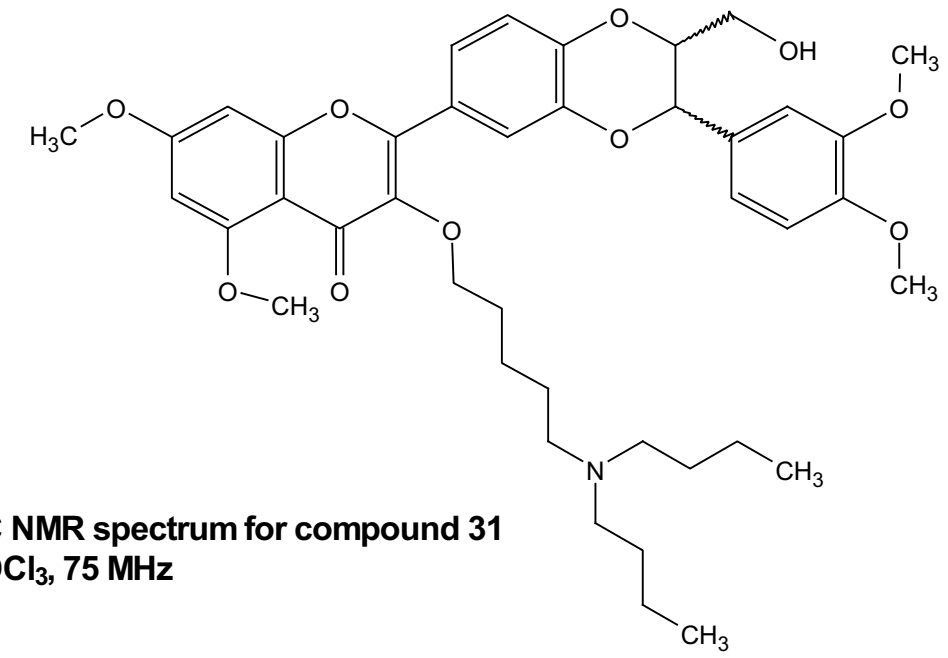
^{13}C NMR spectrum for compound 30
$CDCl_3$, 75 MHz

andre vignau
av-39-26



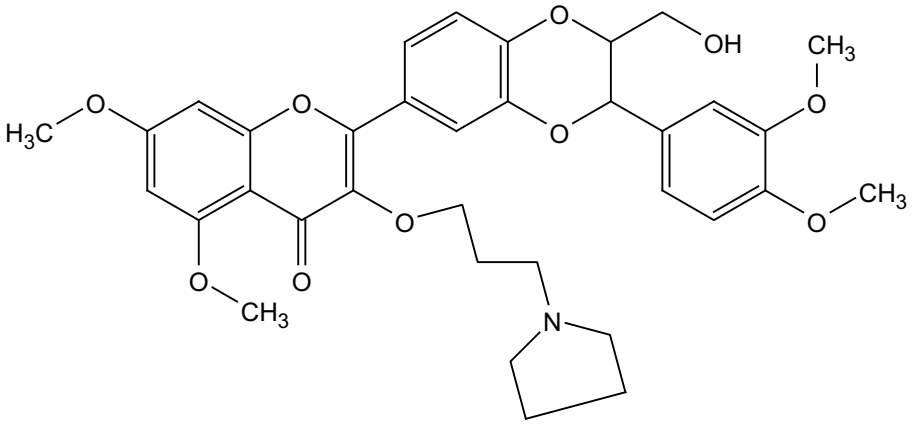
^{1}H NMR spectrum for compound 31
$CDCl_3$, 300 MHz

Andre
AV-39-26 CNMR CDCL3 75MHZ



^{13}C NMR spectrum for compound 31
$CDCl_3$, 75 MHz

linker nmr
bv-17-37-r1- cdcl3



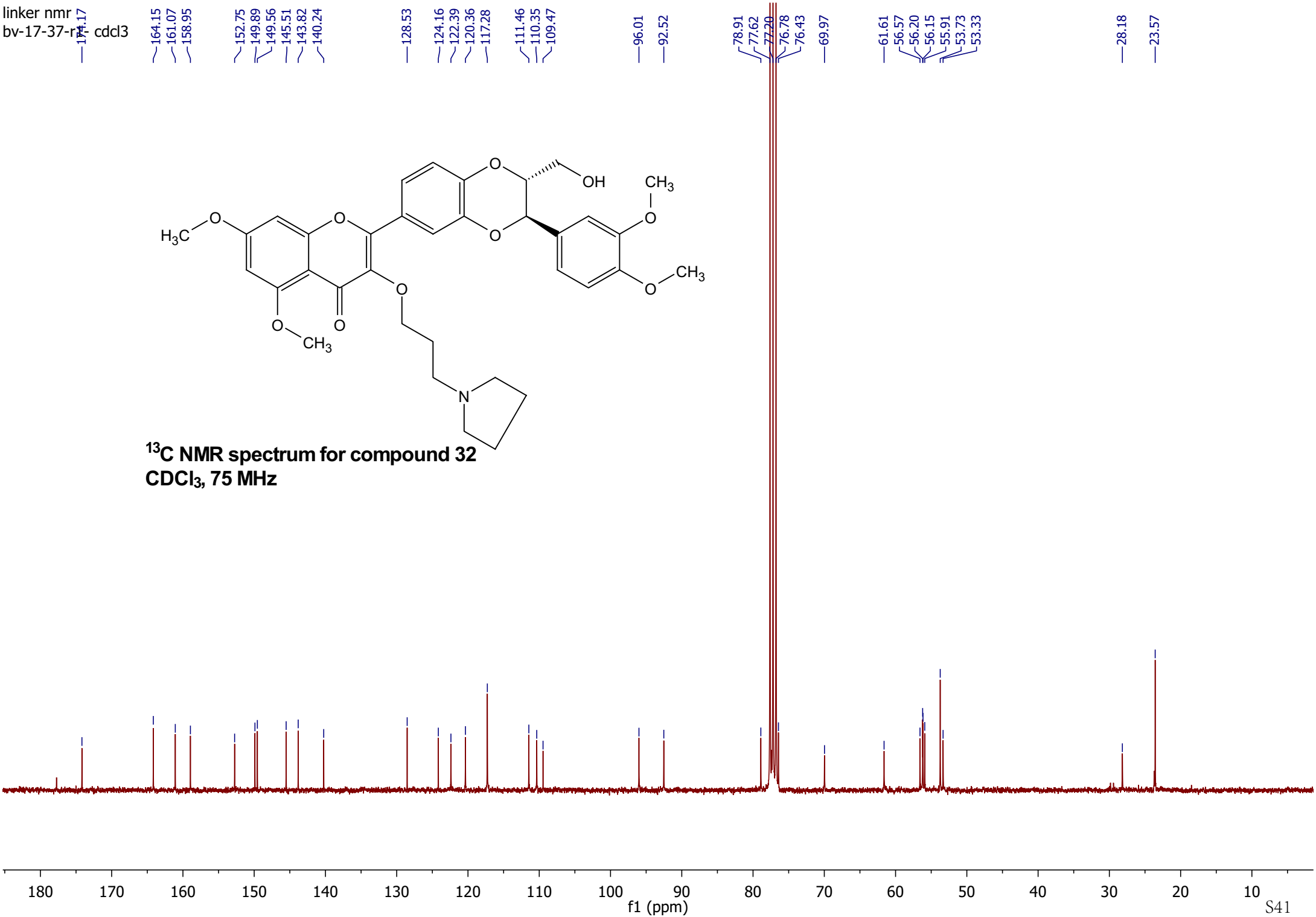
^{1}H NMR spectrum for compound 32
$CDCl_3$, 300 MHz

f1 (ppm)

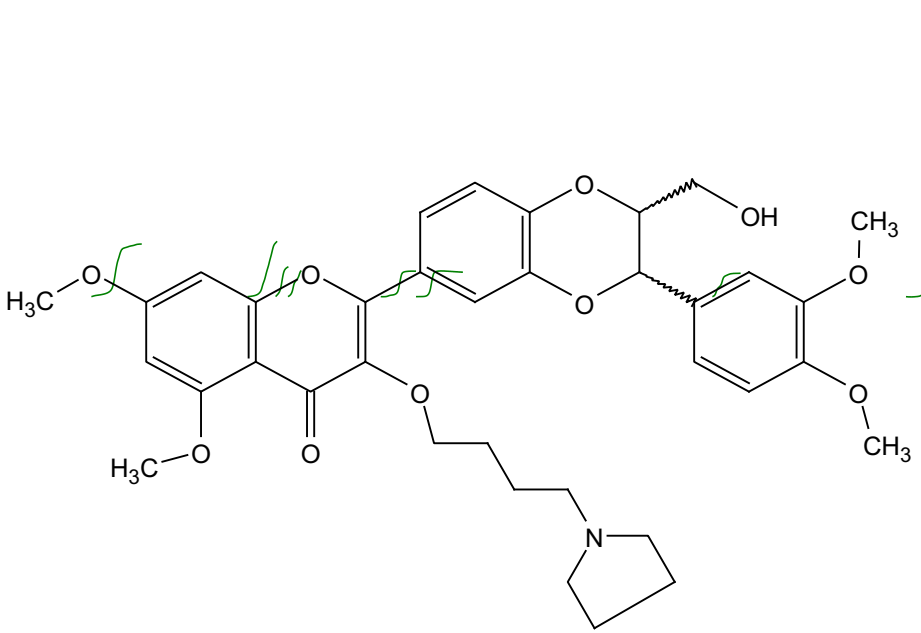
linker nmr
bv-17-37-r1 - cdcl3

177.17
164.15
161.07
158.95
152.75
149.89
149.56
145.51
143.82
140.24
128.53
124.16
122.39
120.36
117.28
111.46
110.35
109.47
96.01
92.52
78.91
77.62
77.20
76.78
76.43
69.97
61.61
56.57
56.20
56.15
55.91
53.73
53.33
28.18
23.57

^{13}C NMR spectrum for compound 32
$CDCl_3$, 75 MHz

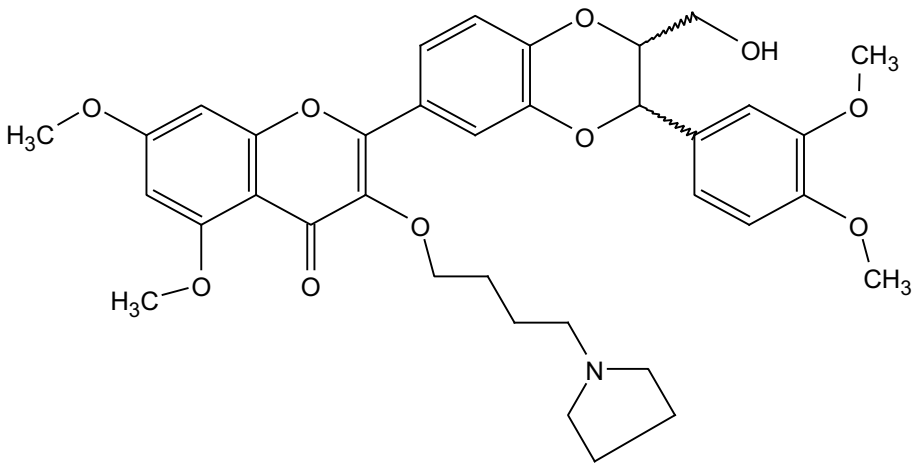


Andre
AV-39-41-R1 HNMR CDCl3 300MHz



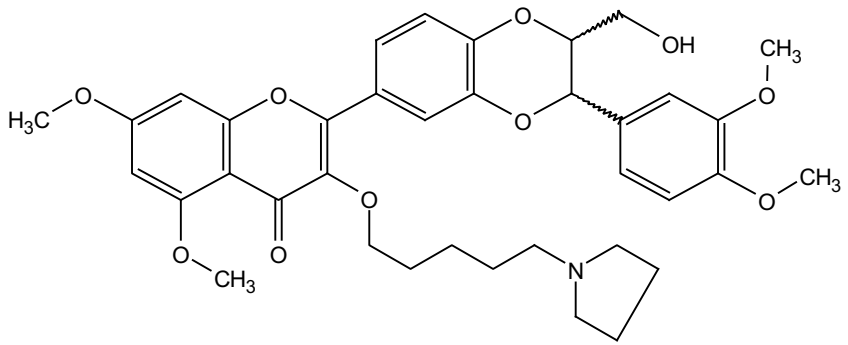
^{1}H NMR spectrum for compound 33
$CDCl_3$, 300 MHz

Andre
AV-39-41-R1 CNMR CDCL3 75MHZ



^{13}C NMR spectrum for compound 33
$CDCl_3$, 75 MHz

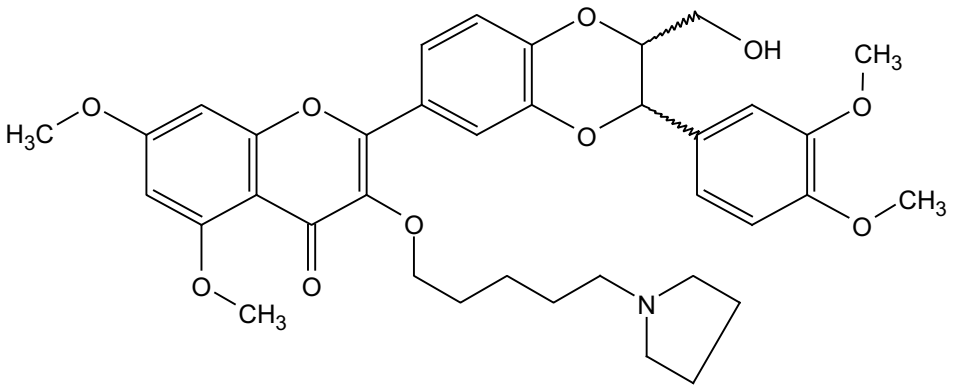
linker nmr
bv-17-36-r2- cdcl3



^{1}H NMR spectrum for compound 34
$CDCl_3$, 300 MHz

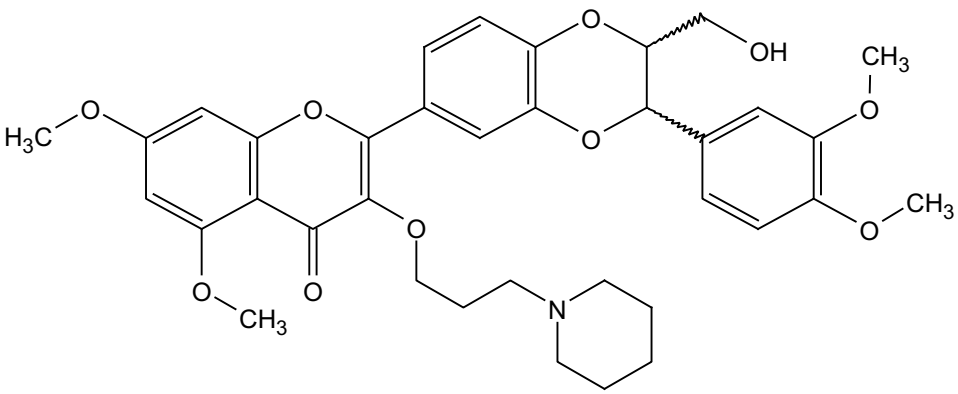
f1 (ppm)

linker nmr
bv-17-36-r2- cdcl3



^{13}C NMR spectrum for compound 34
$CDCl_3$, 75 MHz

BV-48-32-R2_CNMR CDCl3

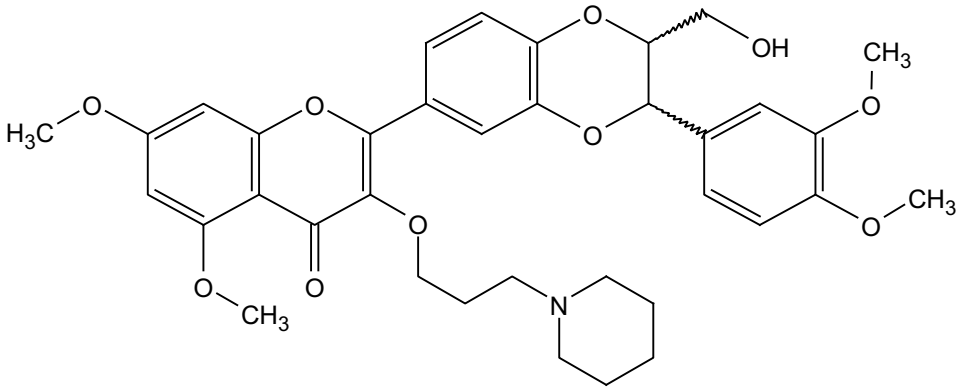


^{1}H NMR spectrum for compound 35
$CDCl_3$, 300 MHz

f1 (ppm)

linker nmr
bv-17-32-r2- cdcl3

174.06
164.02
160.93
158.80
152.60
149.76
149.42
145.33
143.68
140.09
128.34
124.04
122.28
120.20
117.15
111.32
110.18
109.30
95.87
92.36
78.71
77.45
76.61
76.29
70.07
61.51
56.42
56.05
56.01
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55.76
53.87
26.21
24.34
23.36

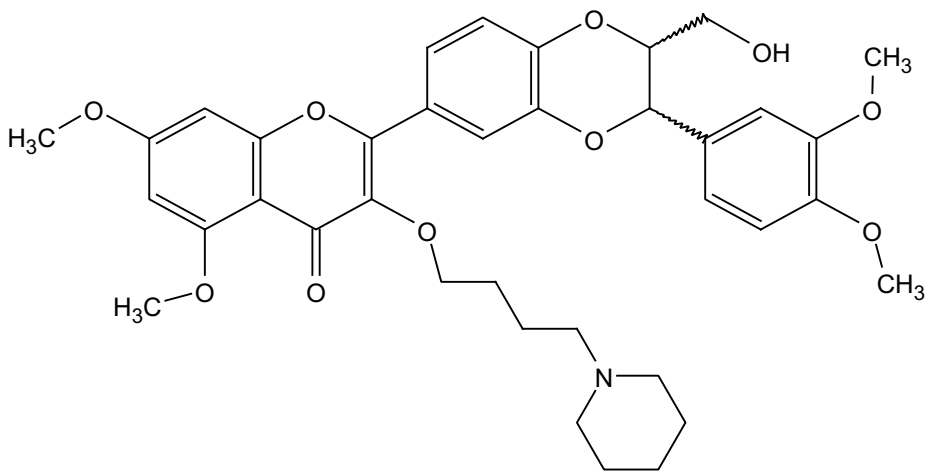


^{13}C NMR spectrum for compound 35
$CDCl_3$, 75 MHz

22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000

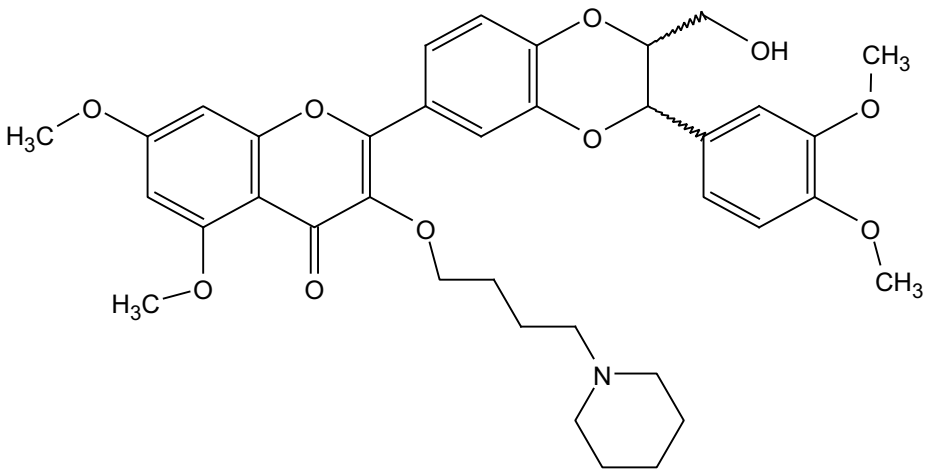
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Andre
AV-39-42-R1 HNMR CDCl3 300MHz



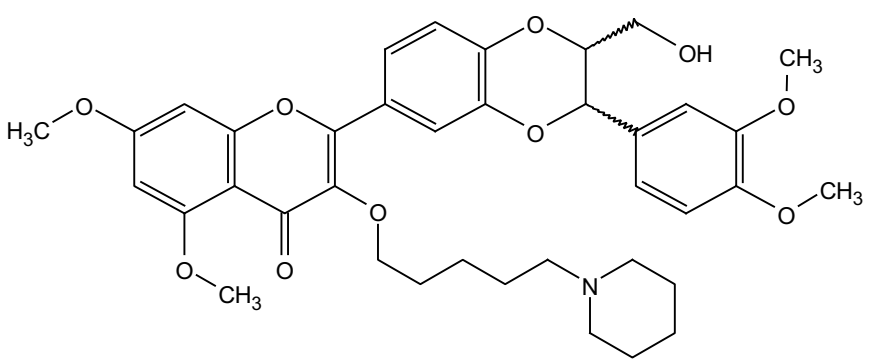
^{1}H NMR spectrum for compound 36
$CDCl_3$, 300 MHz

Andre
AV-39-42-R1 CNMR CDCL3 75MHZ



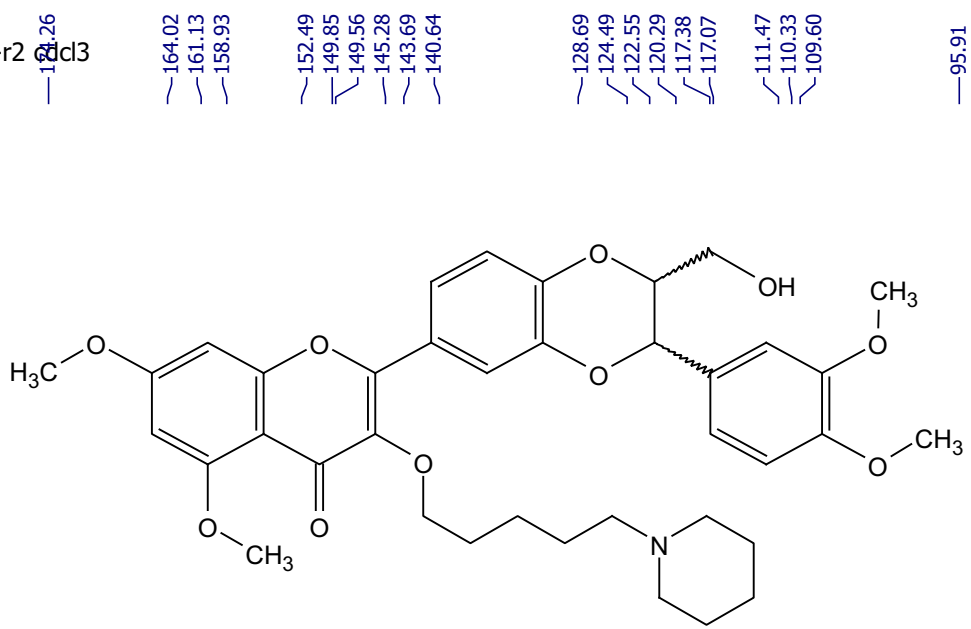
^{13}C NMR spectrum for compound 36
$CDCl_3$, 75 MHz

linker nmr
BV-48-37-r2 cdcl3



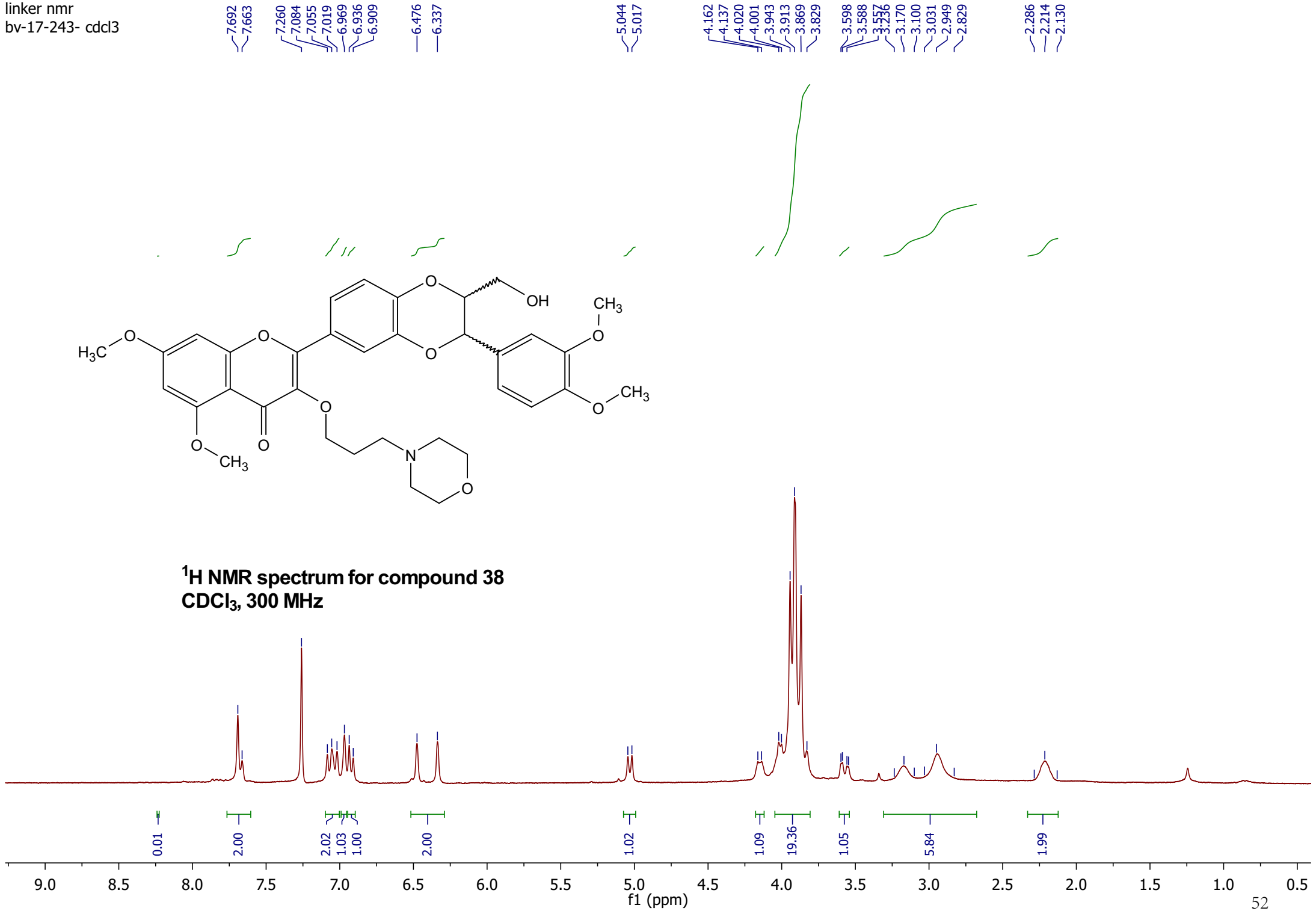
^{1}H NMR spectrum for compound 37
$CDCl_3$, 300 MHz

E:
BV-48-37-r2 cdcl3



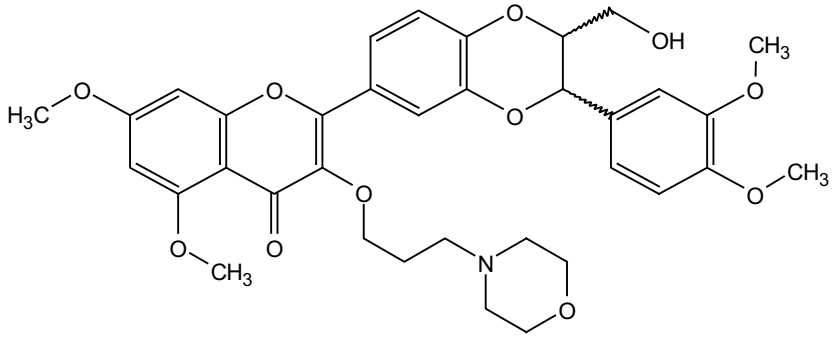
^{13}C NMR spectrum for compound 37
$CDCl_3$, 75 MHz

linker nmr
bv-17-243- cdcl3



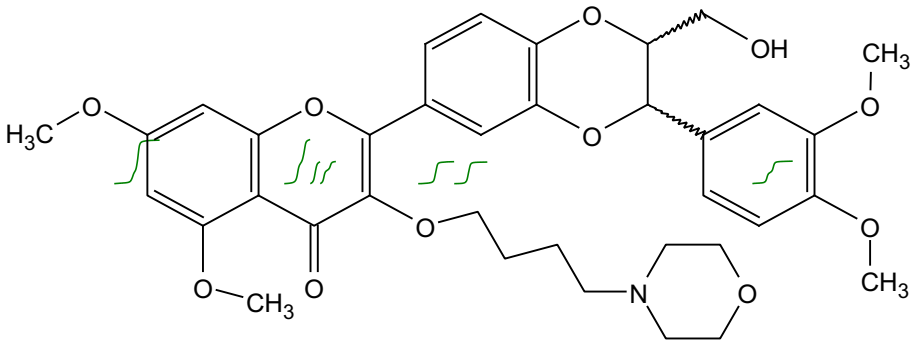
^{1}H NMR spectrum for compound 38
$CDCl_3$, 300 MHz

linker nmr
bv-17-243- cdcl3



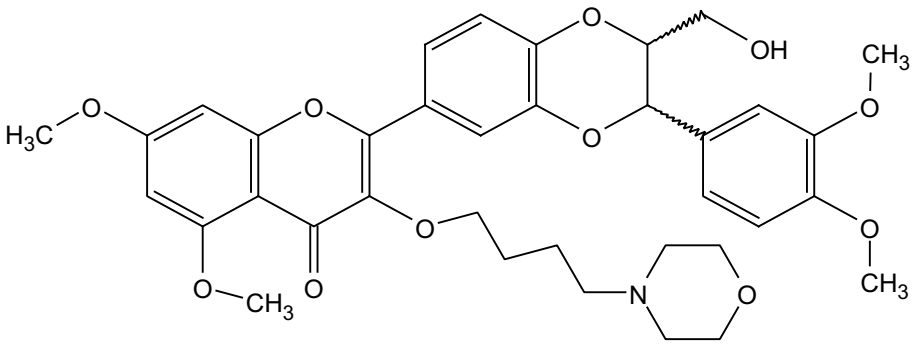
^{13}C NMR spectrum for compound 38
$CDCl_3$, 300 MHz

Andre
AV-39-40-R1 HNMR CDCl3 300MHZ



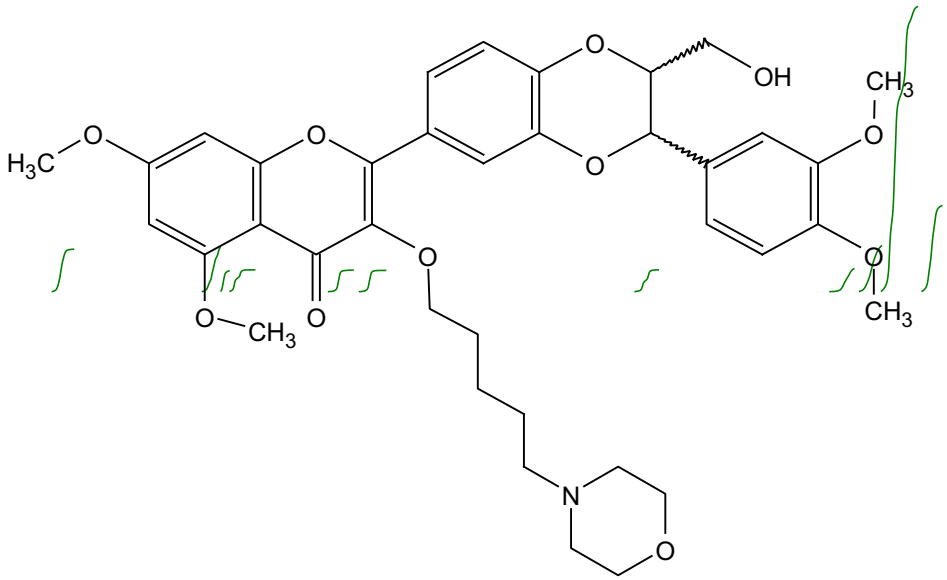
^{1}H NMR spectrum for compound 39
$CDCl_3$, 300 MHz

Andre
AV-39-40-R1 CNMR CDCL3 75MHZ



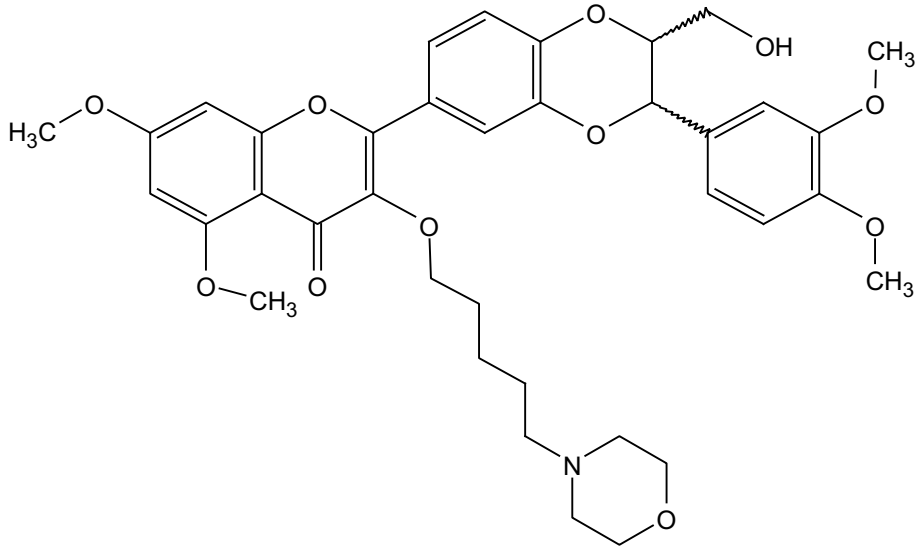
^{13}C NMR spectrum for compound 39
$CDCl_3$, 75 MHz

andre vignau
av 37-31



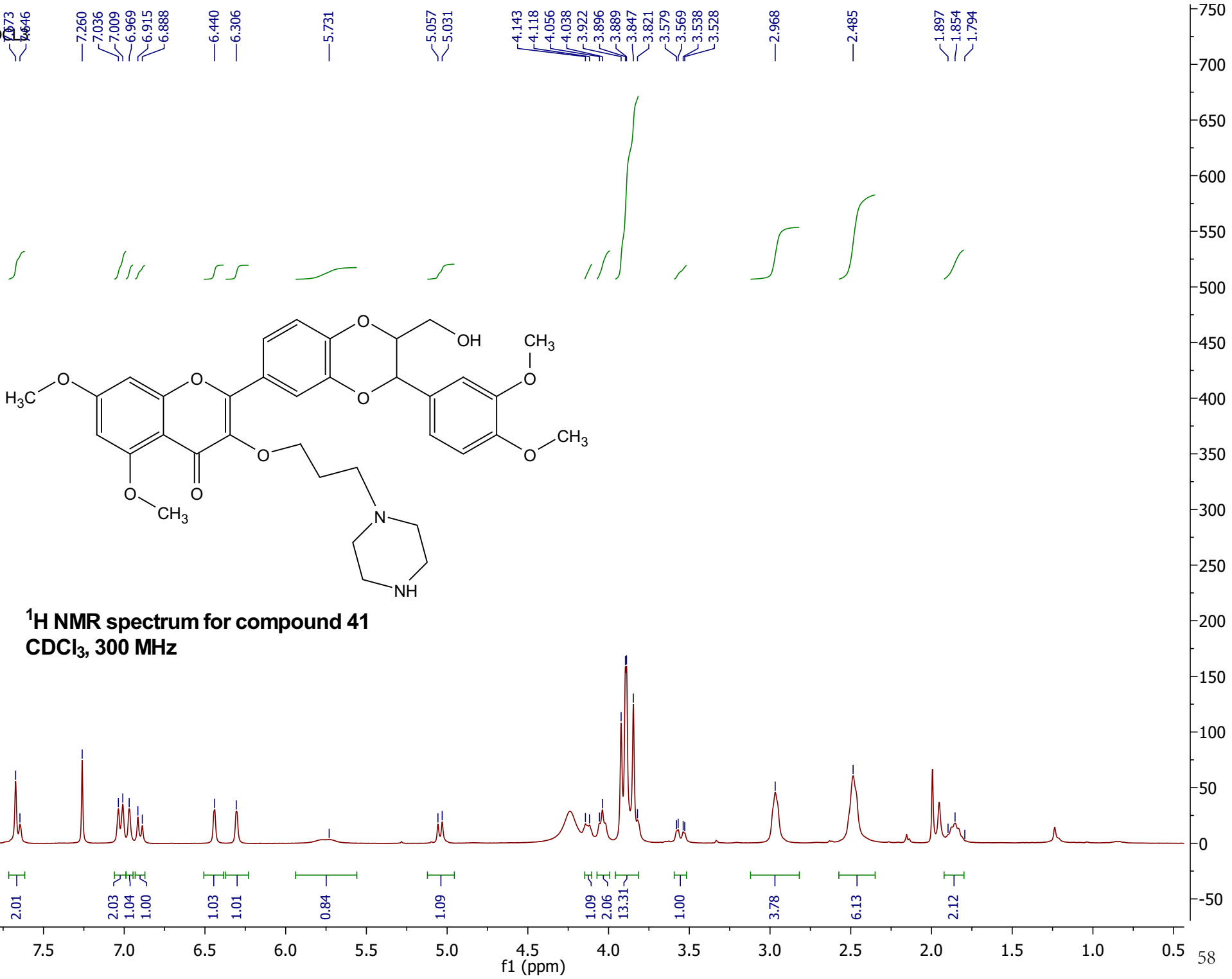
^{1}H NMR spectrum for compound 40
$CDCl_3$, 300 MHz

andre vignau
av 37-31 c13

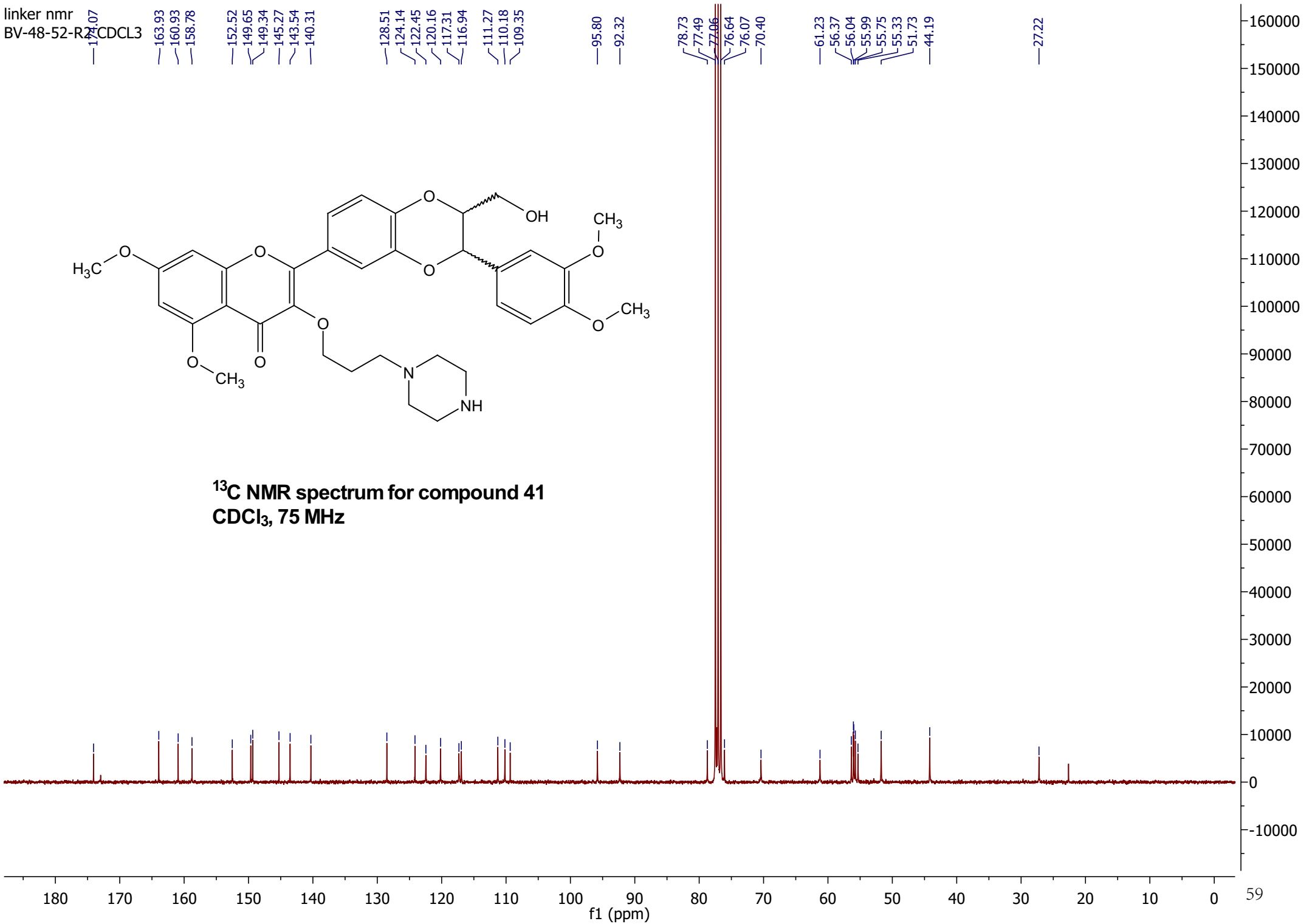


^{13}C NMR spectrum for compound 40
$CDCl_3$, 75 MHz

linker nmr
BV-48-52-R2 CDCL3

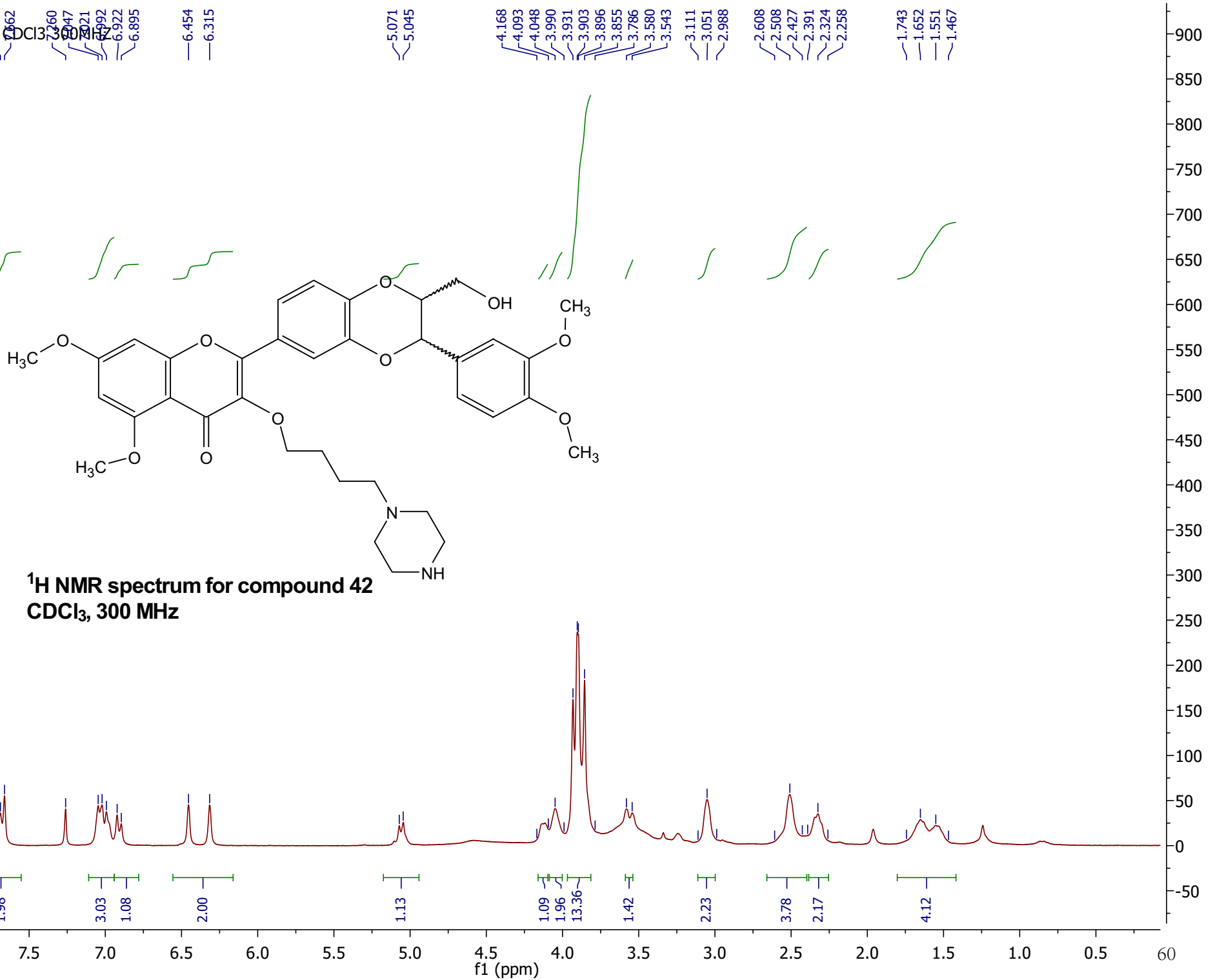


^{1}H NMR spectrum for compound 41
$CDCl_3$, 300 MHz



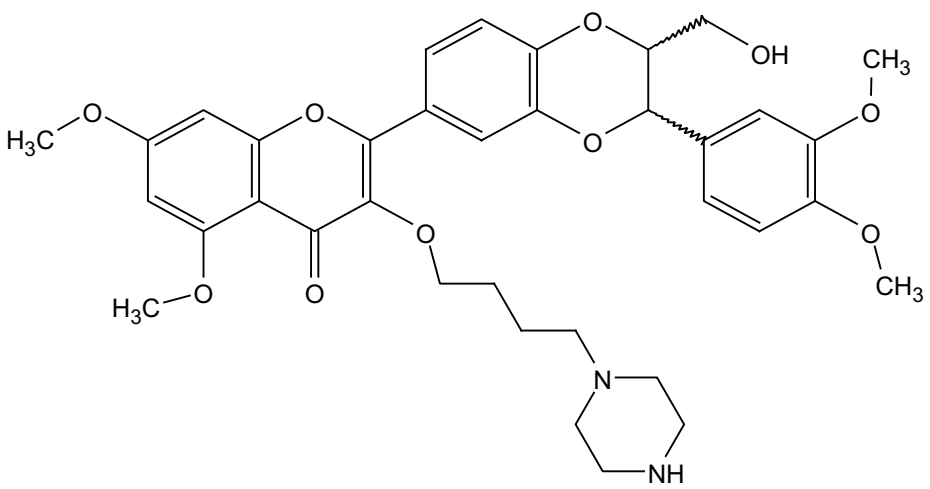
^{13}C NMR spectrum for compound 41
$CDCl_3$, 75 MHz

Andre
AV-39-42-R2 HNMR CDCl3 300MHz



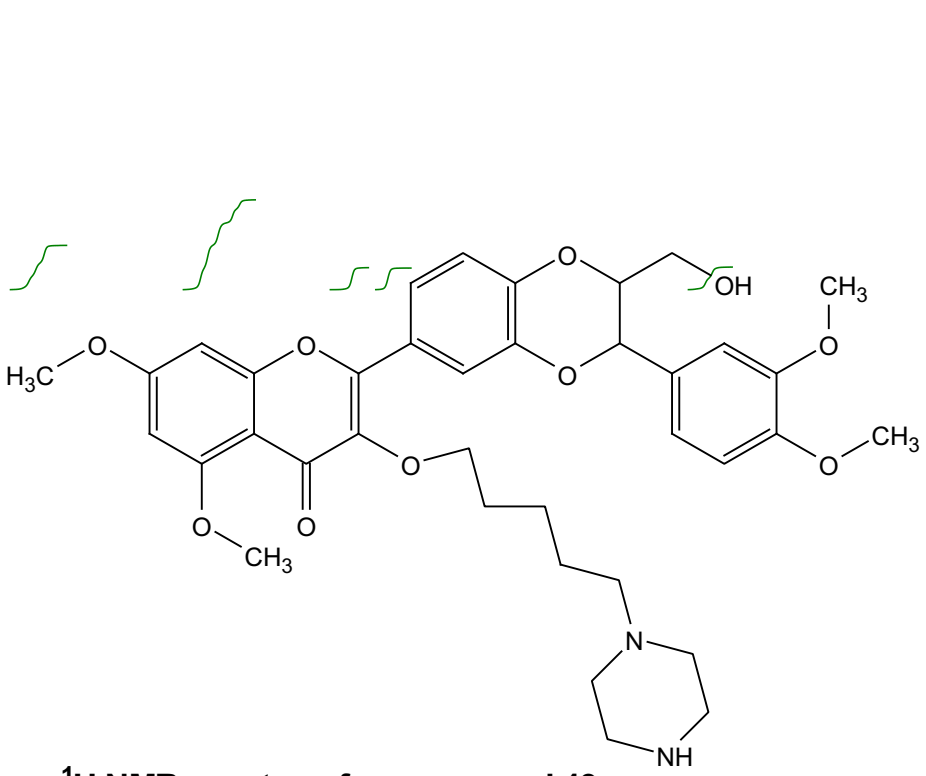
^{1}H NMR spectrum for compound 42
$CDCl_3$, 300 MHz

Andre
AV-39-42-R2 CNMR CDCL3 75MHZ



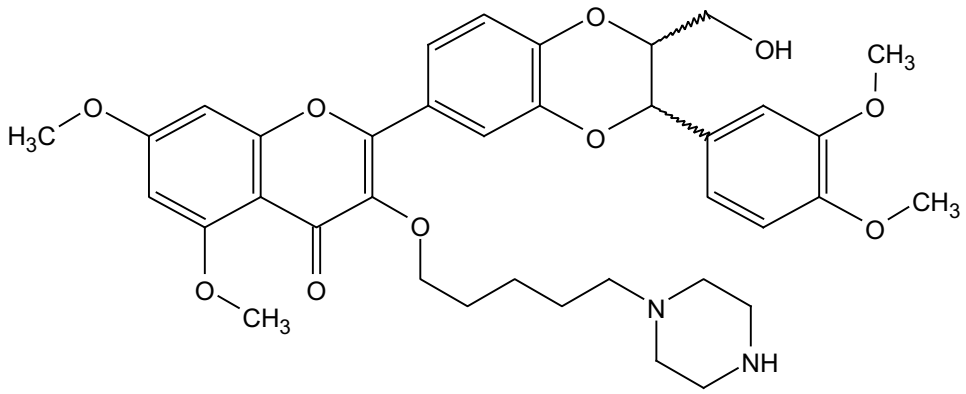
^{13}C NMR spectrum for compound 42
$CDCl_3$, 75 MHZ

linker nmr
BV-48-38-r1 cdcl3



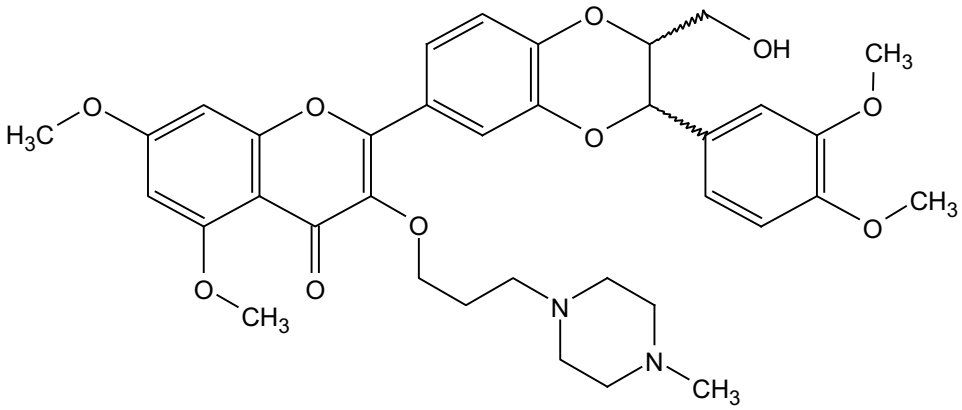
^{1}H NMR spectrum for compound 43
$CDCl_3$, 300 MHz

linker nmr
BV-48-38-r1 cdcl3



^{13}C NMR spectrum for compound 43
$CDCl_3$, 75 MHz

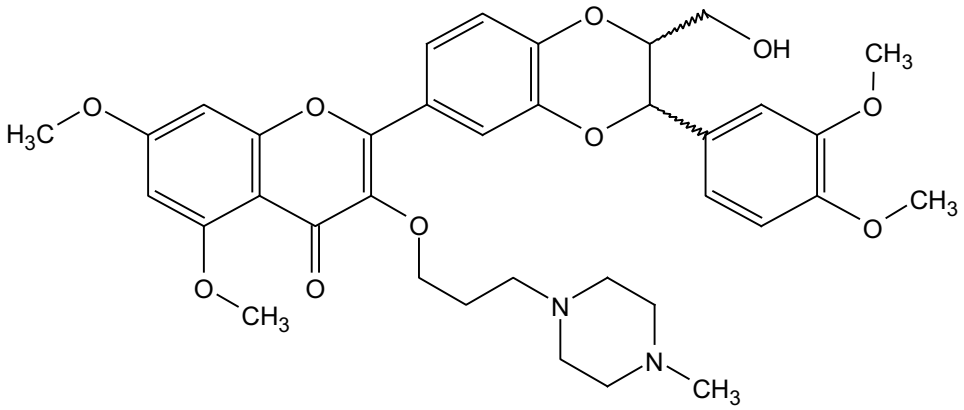
linker nmr
BV-48-32-r1 cdcl3



^{1}H NMR spectrum for compound 44
$CDCl_3$, 300 MHz

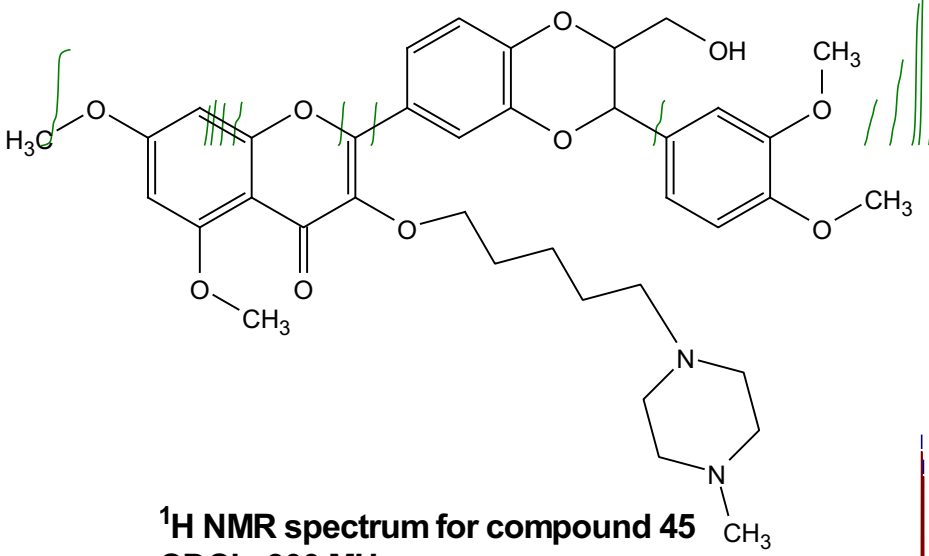
f1 (ppm)

linker nmr
BV-48-32-r1 cdcl3



^{13}C NMR spectrum for compound 44
75 MHz, $CDCl_3$

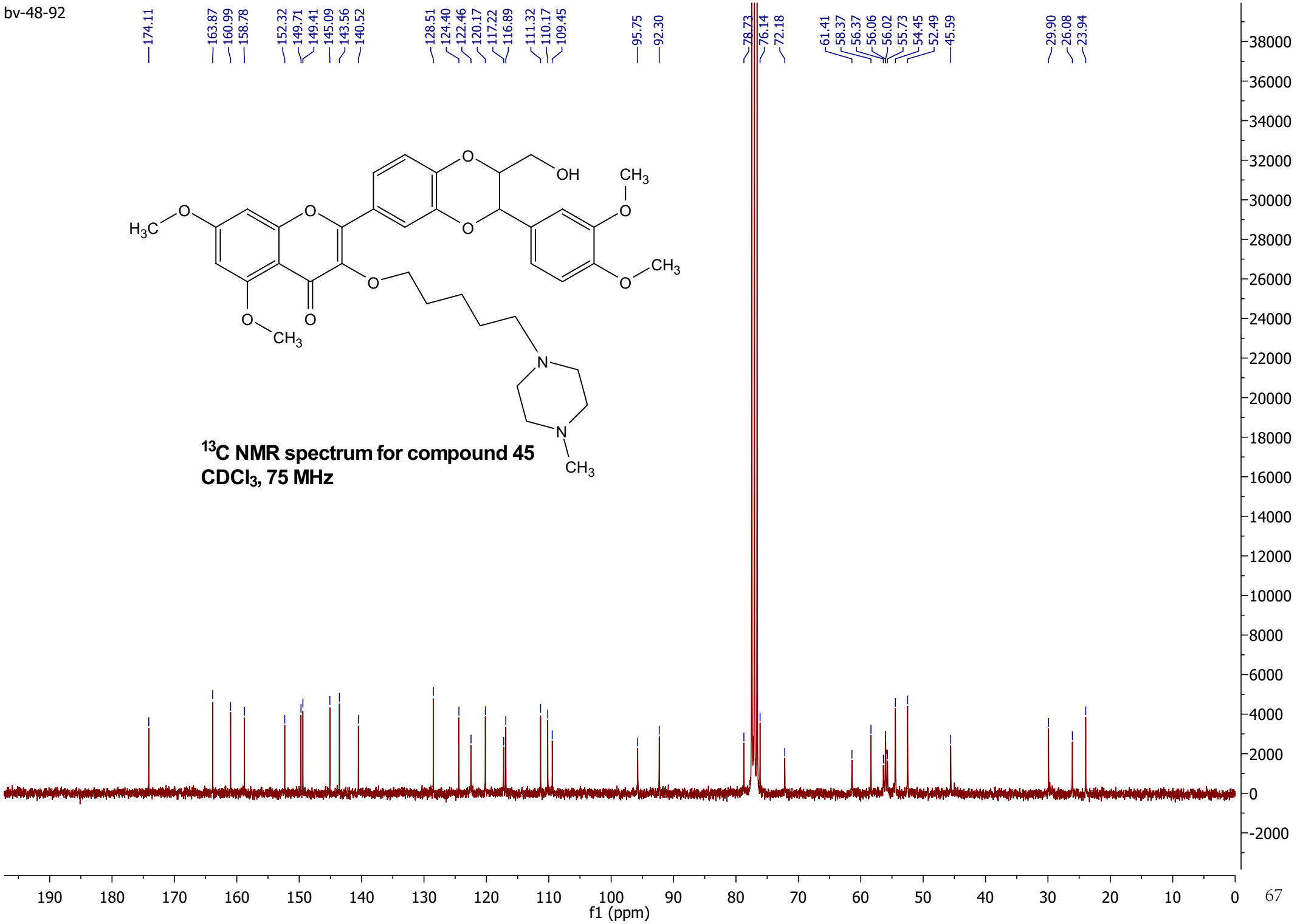
bv-48-92



^{1}H NMR spectrum for compound 45
$CDCl_3$, 300 MHz

f1 (ppm)

bv-48-92



^{13}C NMR spectrum for compound 45
$CDCl_3$, 75 MHz