

Design, Synthesis and Biological Evaluation of a Series of 5- and 7-hydroxycoumarin Derivatives as 5-HT_{1A} Serotonin Receptor Antagonists

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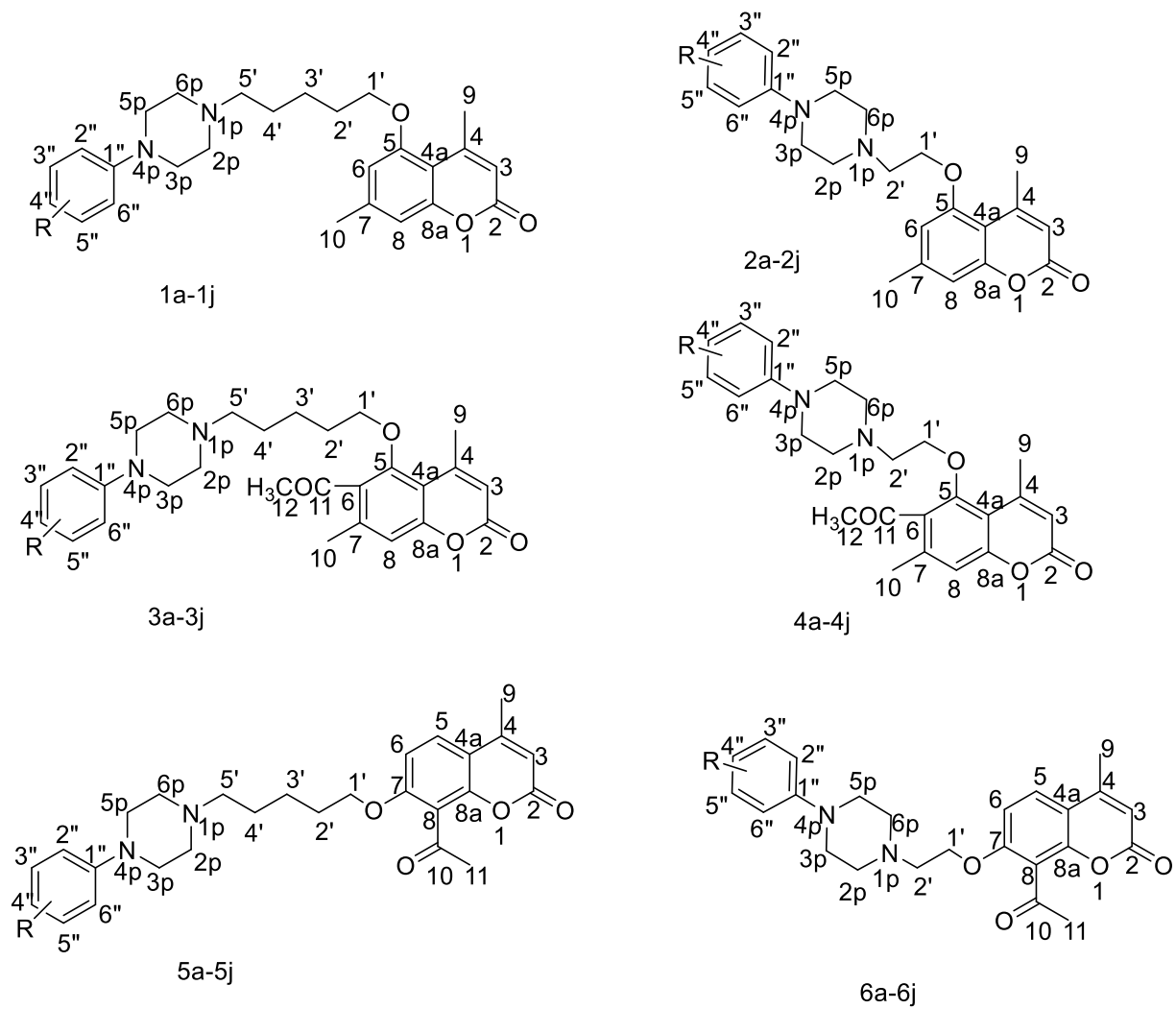
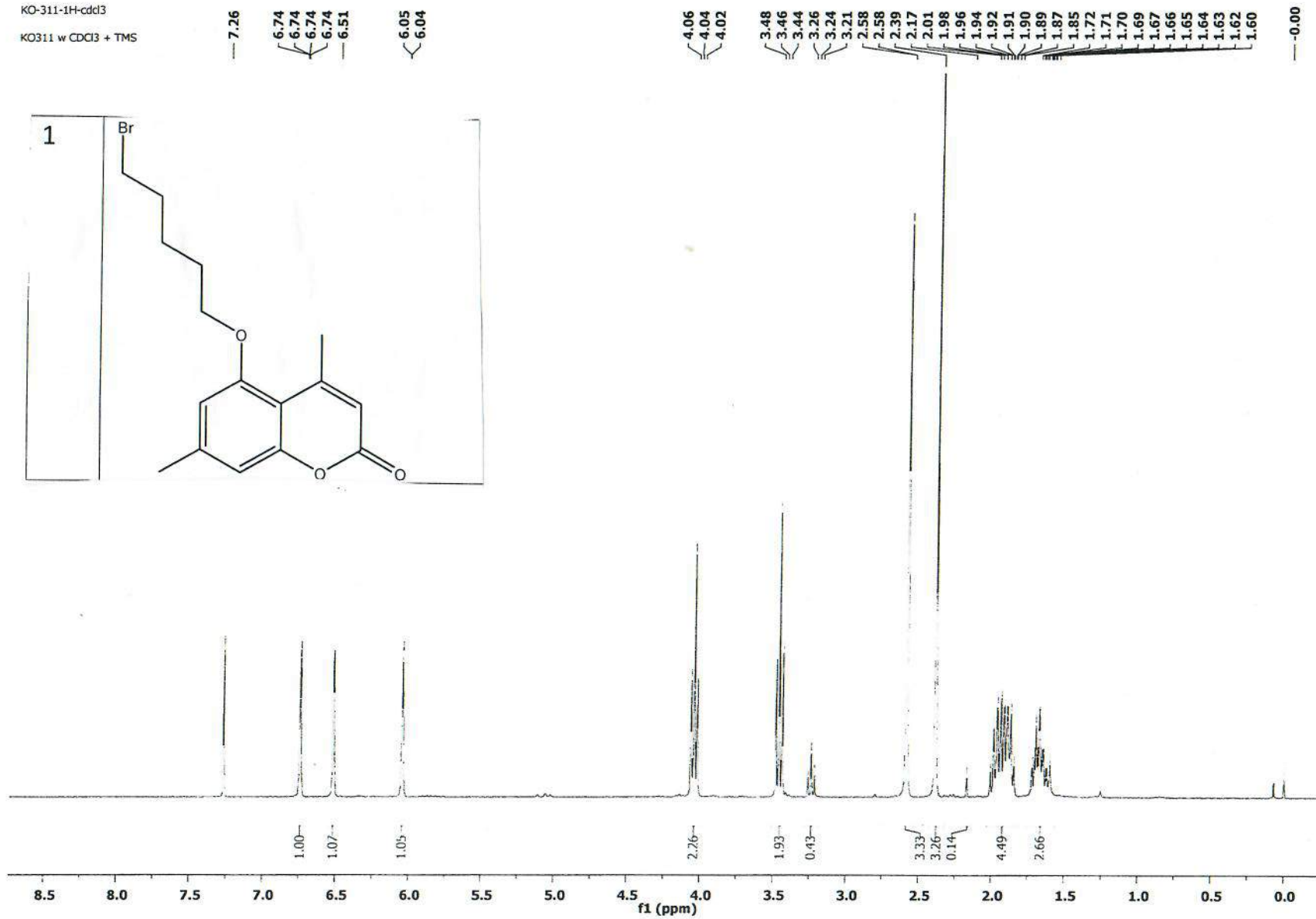
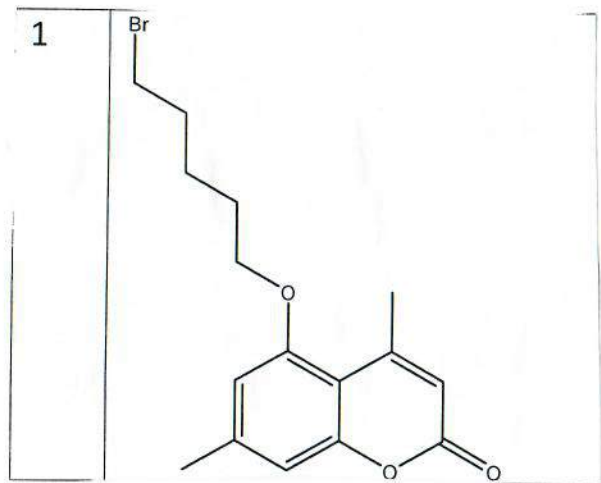


Figure 1S. Atom Numbering of compounds 1a-1j, 2a-2j, 3a-3j, 4a-4j, 5a-5j, 6a-6j.

^1H NMR and ^{13}C NMR Spectra

KO-311-1H-cdcl3
KO311 w CDCl3 + TMS



4

KO-311-13C-cdd3
KO 311 13C in CDCl3

161.16
157.40
155.55
154.27
143.19

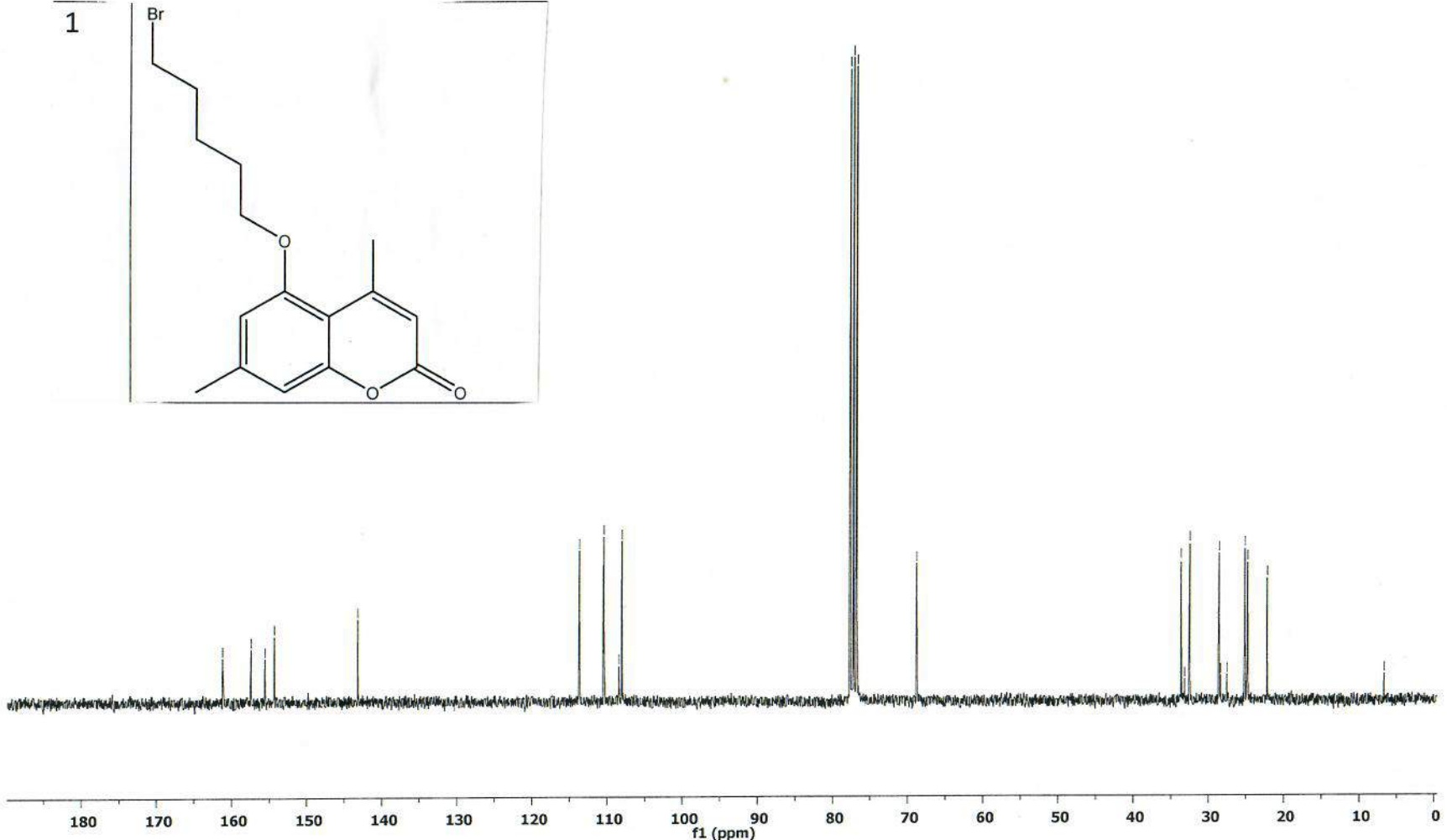
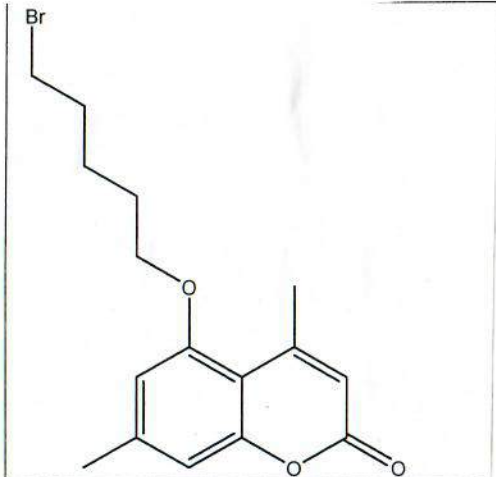
113.69
110.41
108.42
108.01

77.65
77.23
76.81
68.82

33.62
33.16
32.49
28.60
28.40
27.51
25.16
24.87
24.80
22.20

6.67

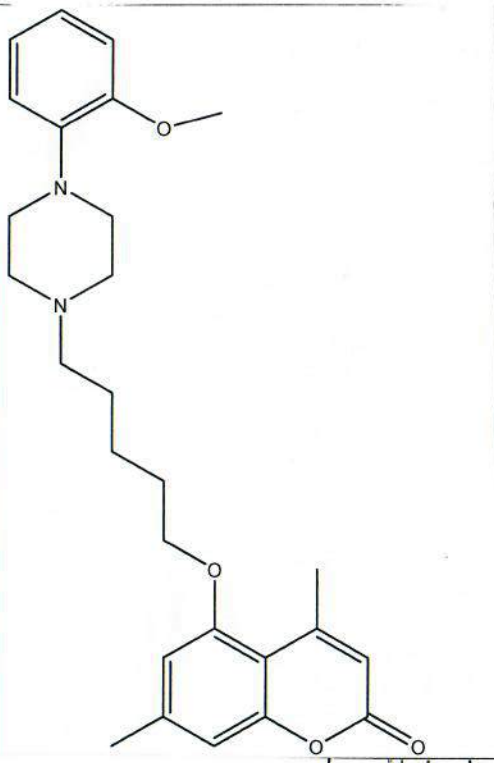
1



U

KO-312-1H-cdd3
KO312 w CDCl3 + TMS

1a



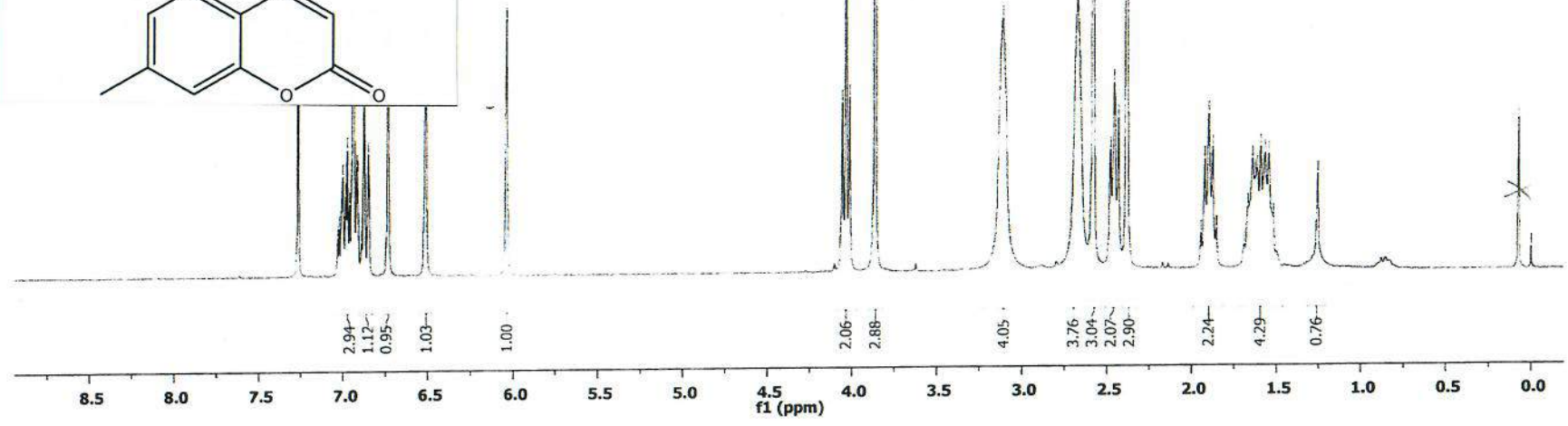
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6.97
6.94
6.94
6.92
6.91
6.88
6.85
6.73
6.64
6.04

4.06
4.03
4.01
3.86

3.11
2.67
2.58
2.58
2.48
2.46
2.43
2.38
1.92
1.90
1.88
1.64
1.59
1.57
1.55

0.07
-0.00

1a



1a

KO-312-13C
KO 312 13C

161.17
157.45
155.52
154.29
152.40

143.21

123.45
121.25
118.54
113.62
111.39
110.31
108.39
108.05

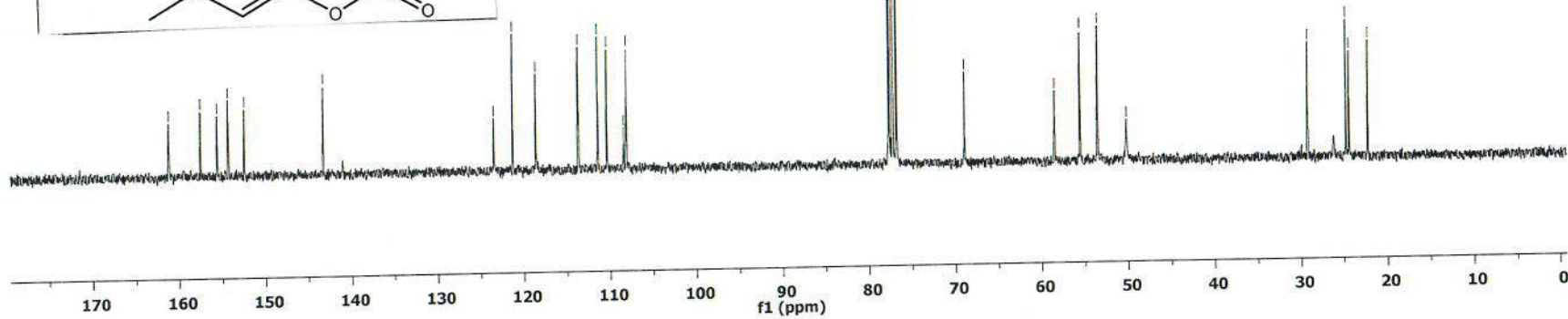
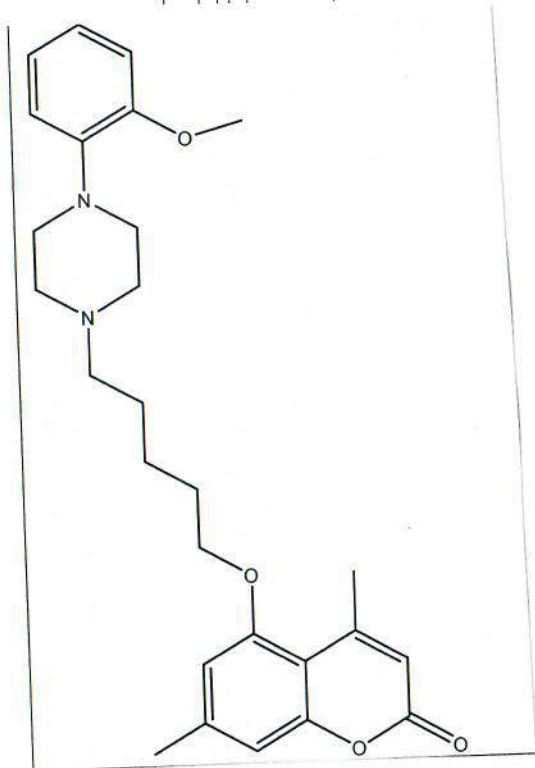
77.65
77.23
76.81

68.93

58.49
55.58
53.50
50.19

29.21
24.77
24.40
22.19

1a



KO-313-1H-cdd3

KO313 w CDCl3 + TM

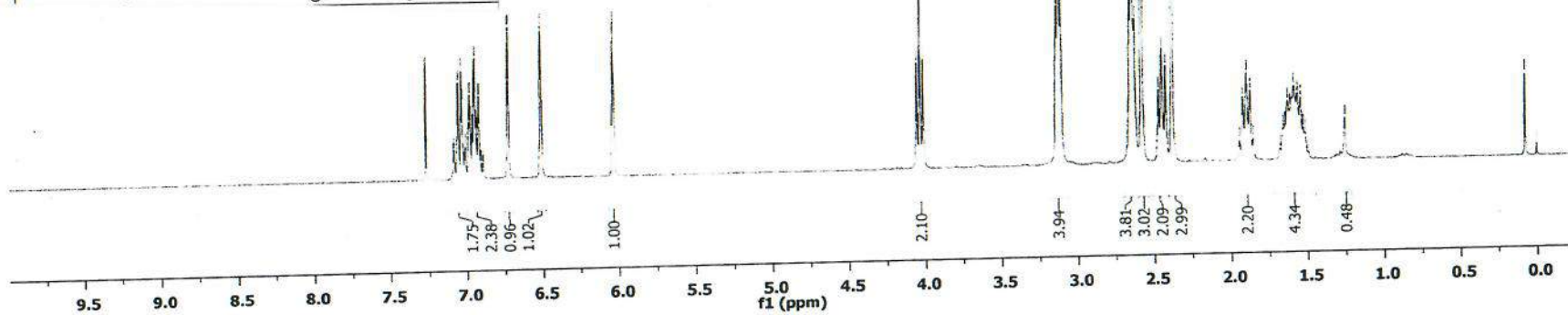
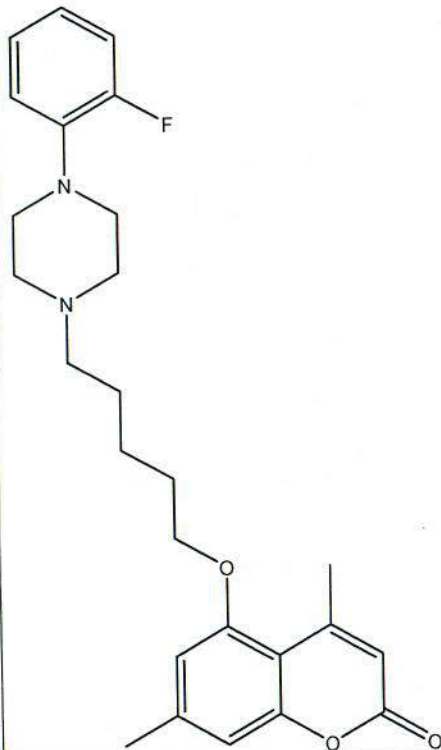
7.27
7.09
7.08
7.06
7.05
7.04
7.03
7.03
7.01
6.99
6.98
6.97
6.96
6.94
6.94
6.92
6.92
6.91
6.90
6.89
6.73
6.73
6.51
6.04
6.03

4.05
4.03
4.01

3.14
3.12
3.11
2.66
2.64
2.63
2.58
2.58
2.58

1.94
1.92
1.90
1.87
1.85
1.66
1.63
1.62
1.59
1.57
1.55
1.53
1.52
0.77
-0.00

1b



16

16

KO-313-13C
KO 313 13C

161.15
157.52
157.46
155.50
154.29
154.26

143.19
140.11
140.01

124.70
124.66
122.86
122.76
119.16
119.12
116.43
116.16
113.59
110.27
108.36
108.01

77.65
77.23
76.81

68.96

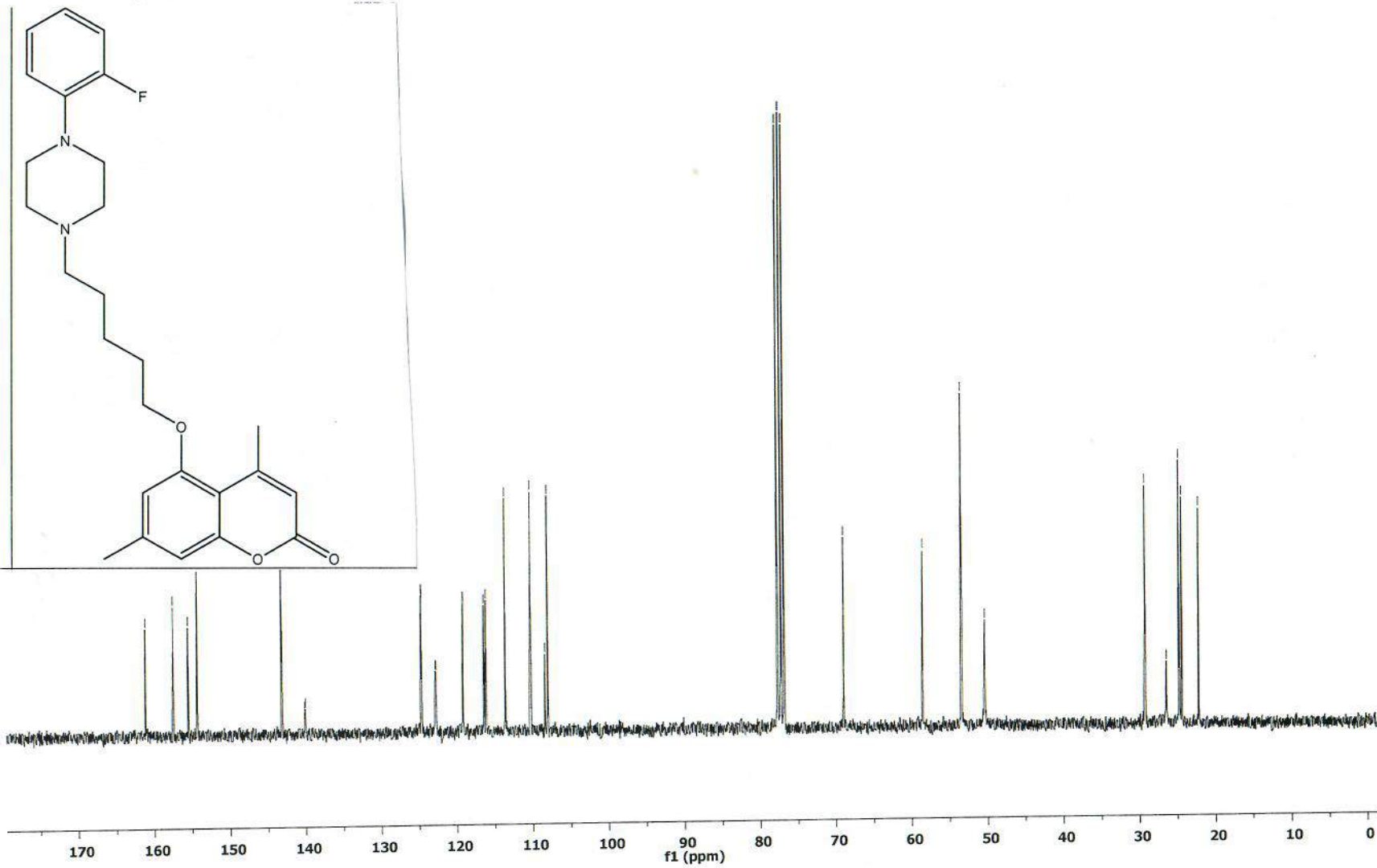
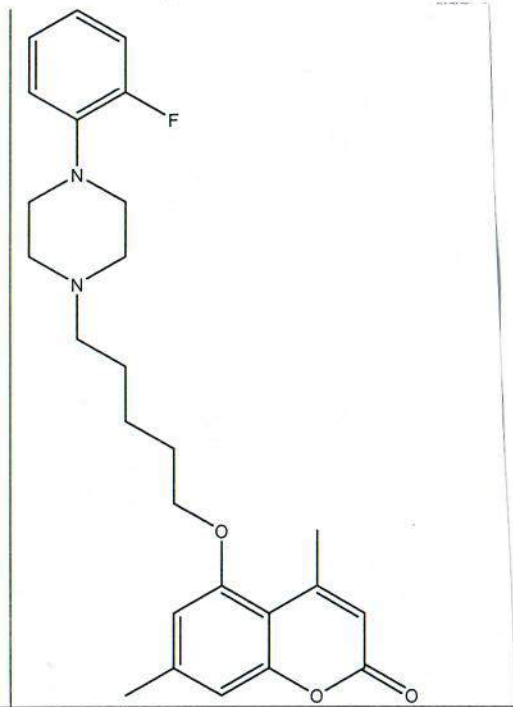
58.52

53.43

50.38

29.24
26.45
24.75
24.41
22.18

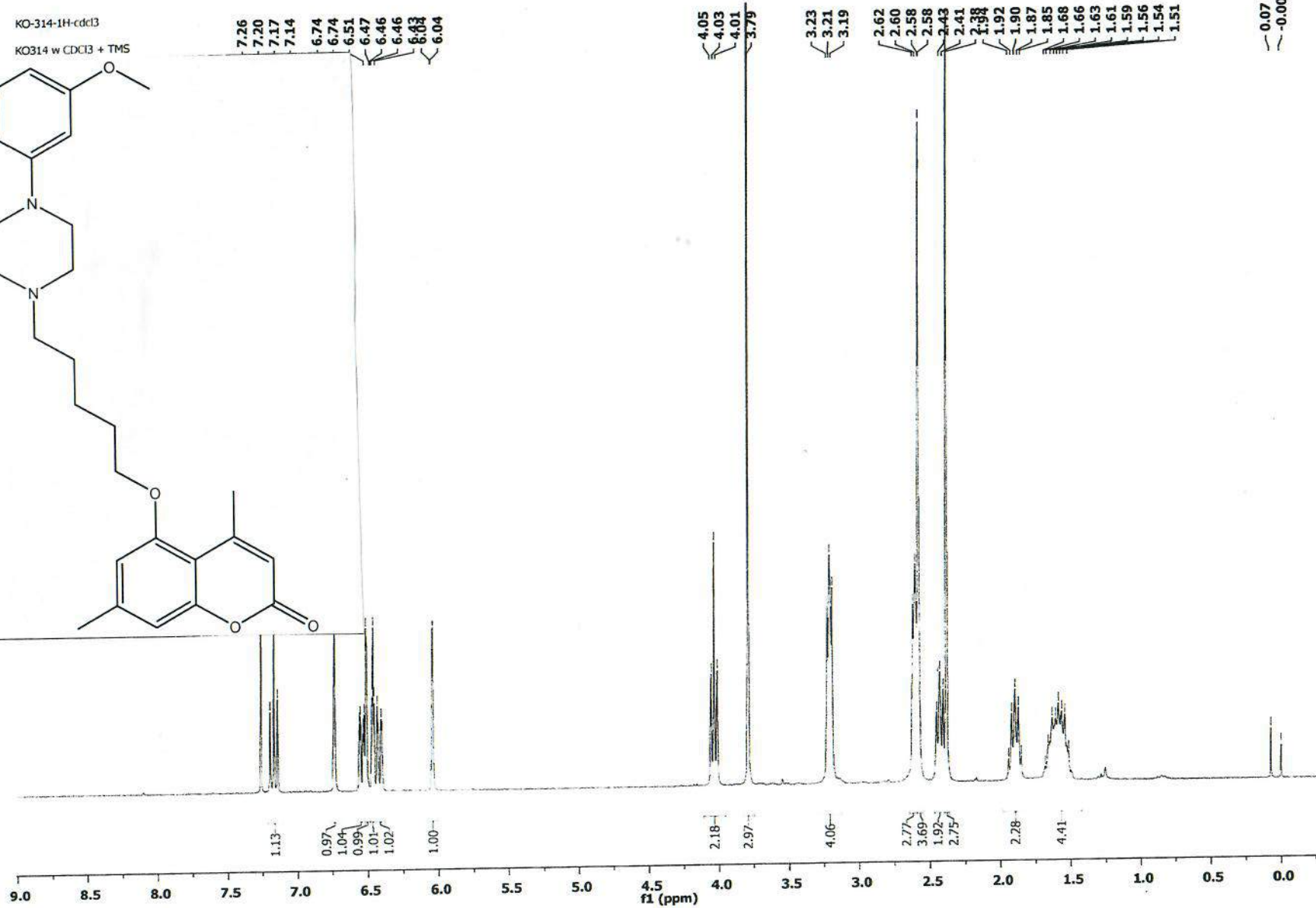
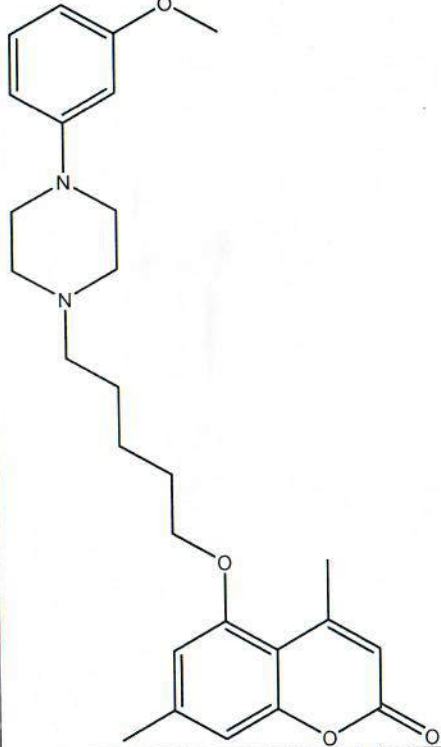
1b



1c

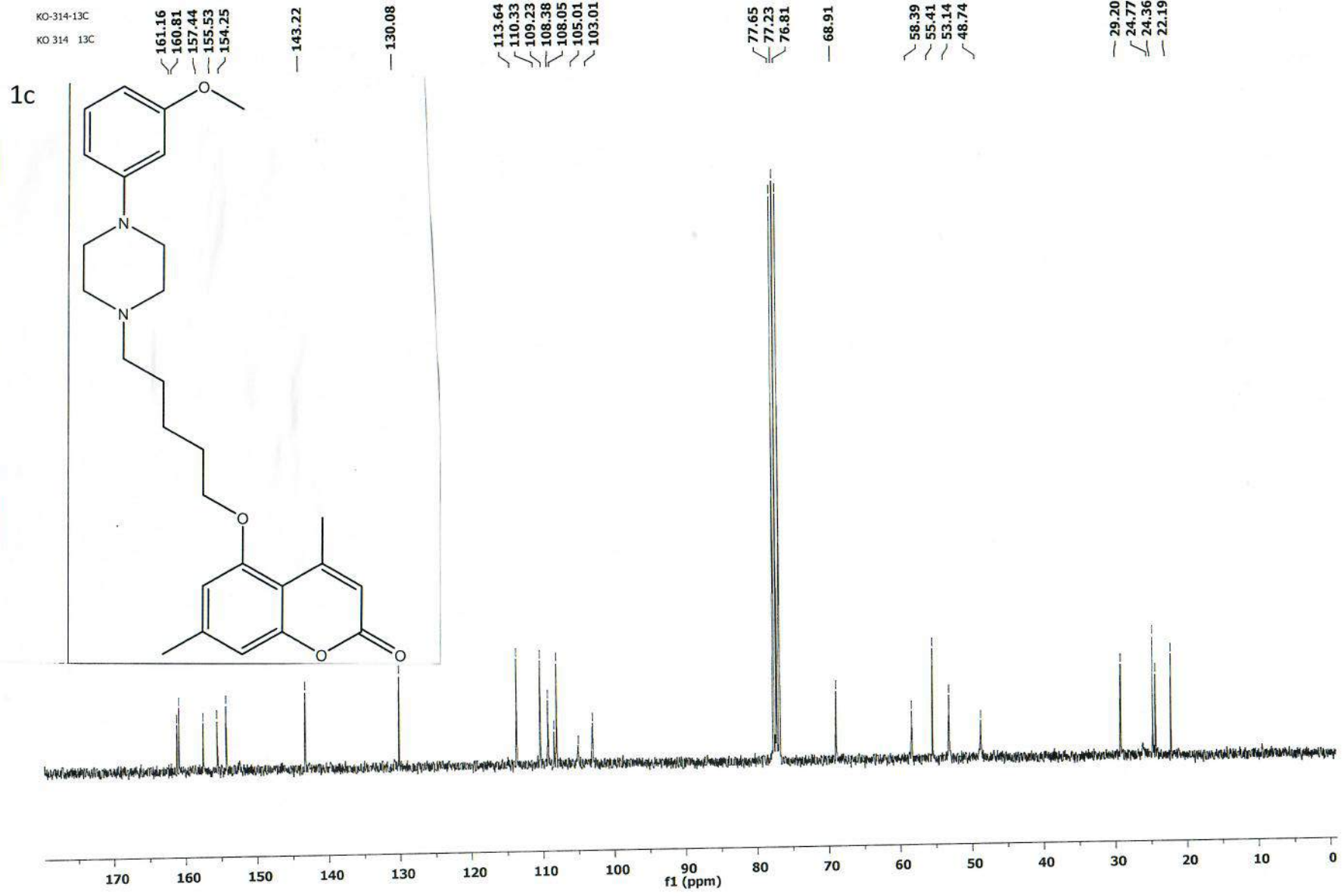
KO-314-1H-cdcl3

KO314 w CDCl3 + TMS

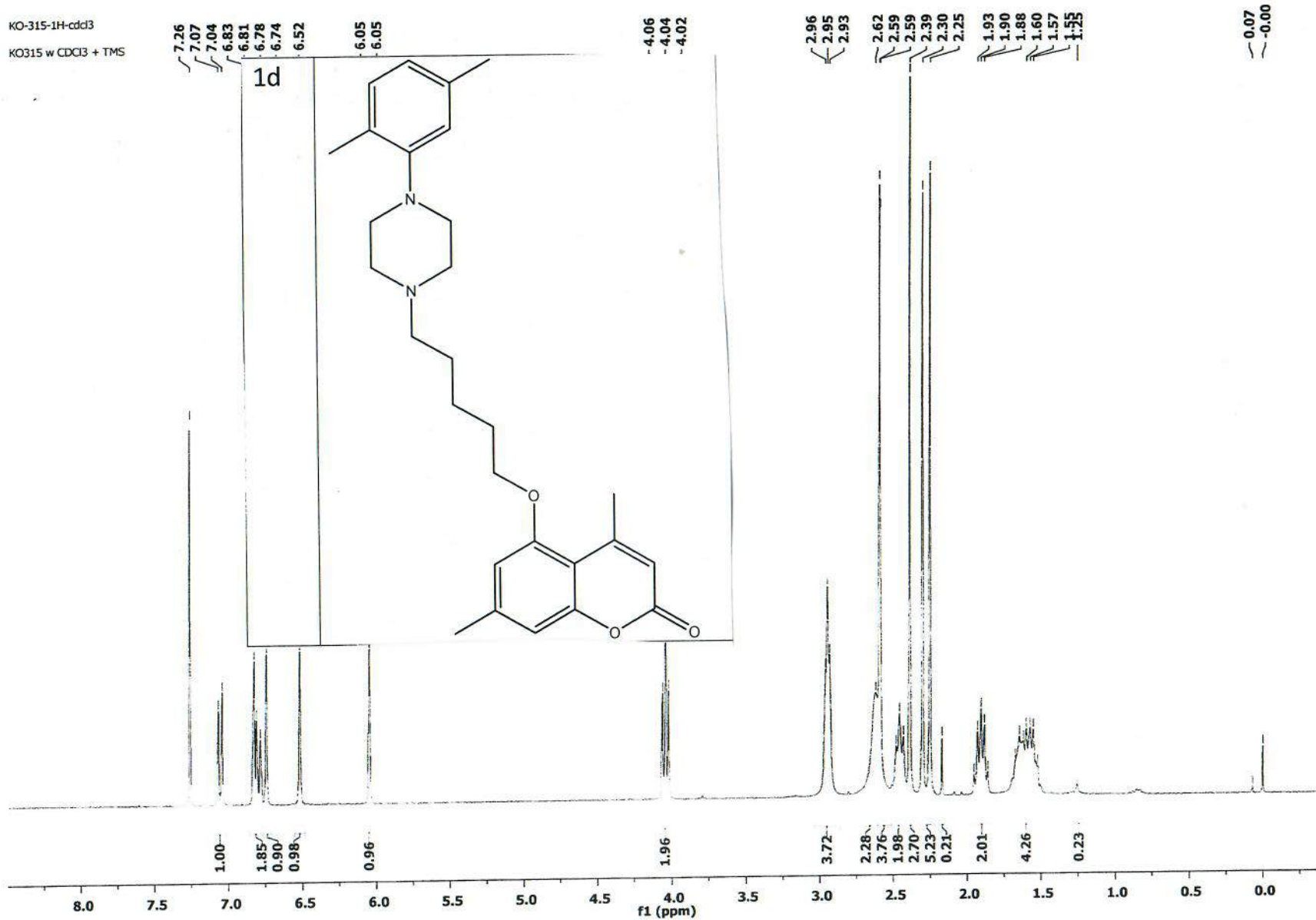


Ac

1c



KO-315-1H-cdd3
KO315 w CDCl3 + TMS



1d

1d

KO-315-13C
KO 315 13C

161.16
157.41
155.54
154.23

143.25

136.59

131.11
129.38

124.66
120.29

113.67
110.38
108.39
108.08

77.65
77.23
76.81

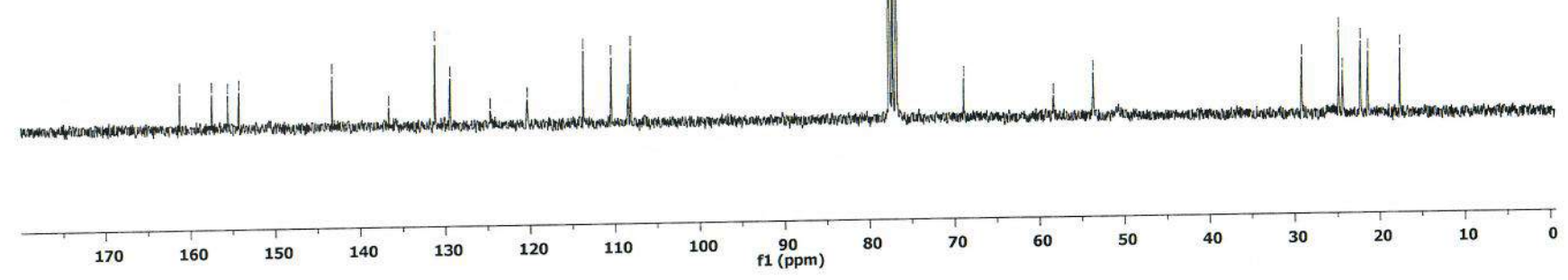
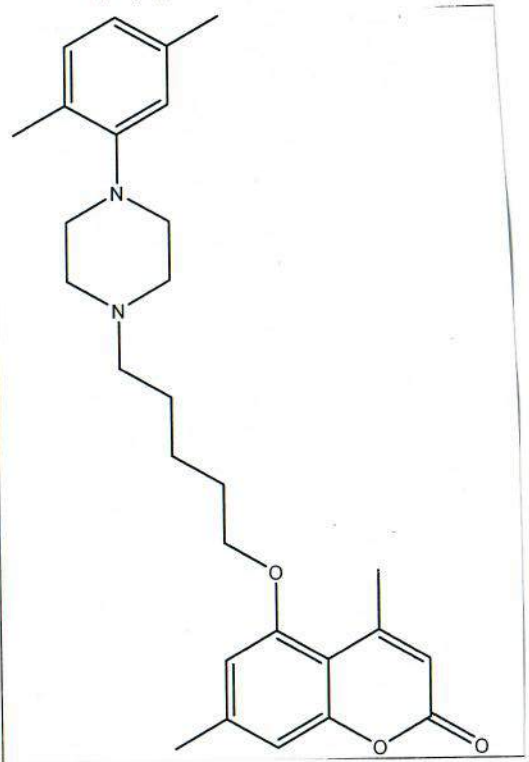
68.84

58.30

53.64

29.14
24.79
24.30
22.20
21.36
17.56

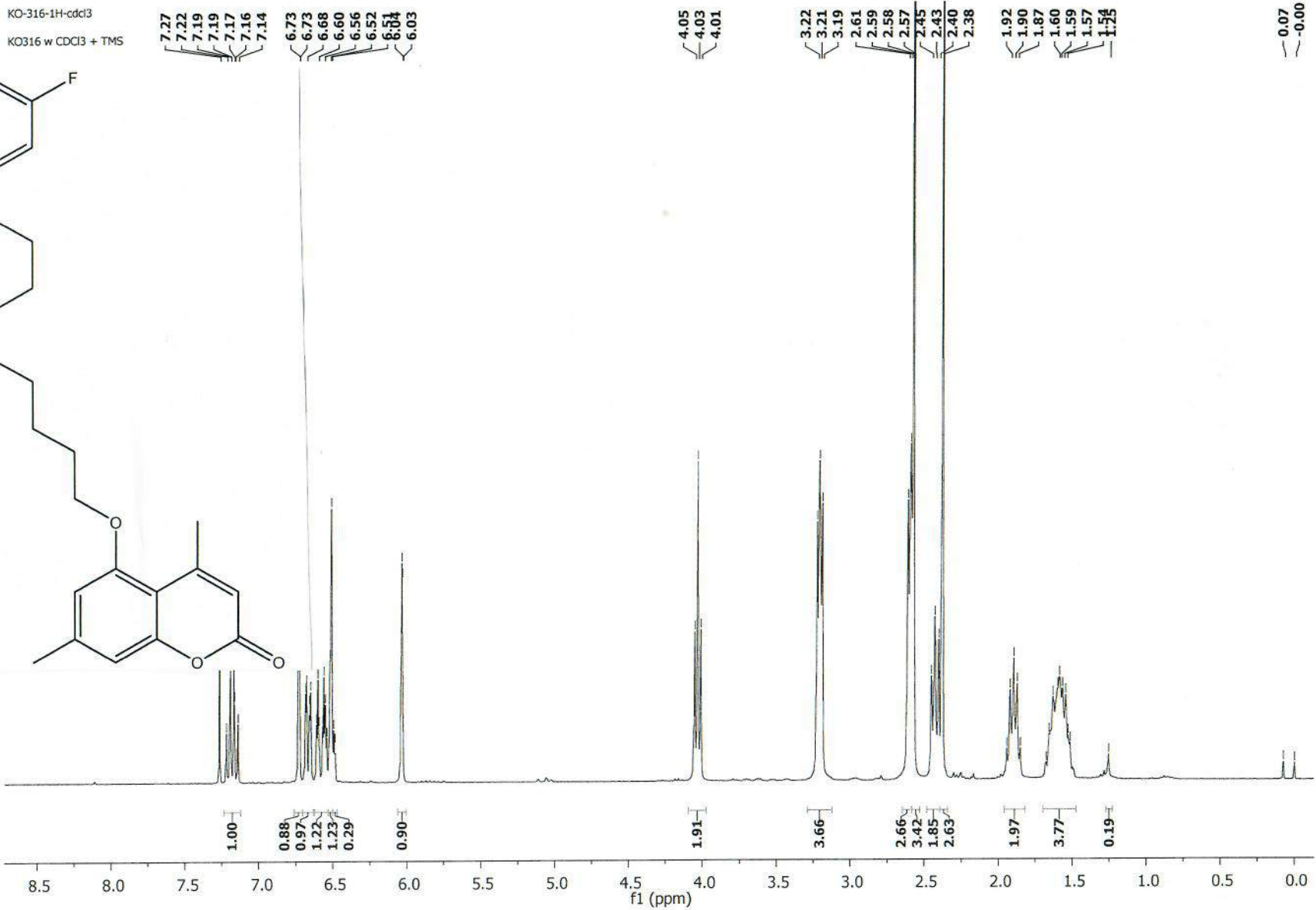
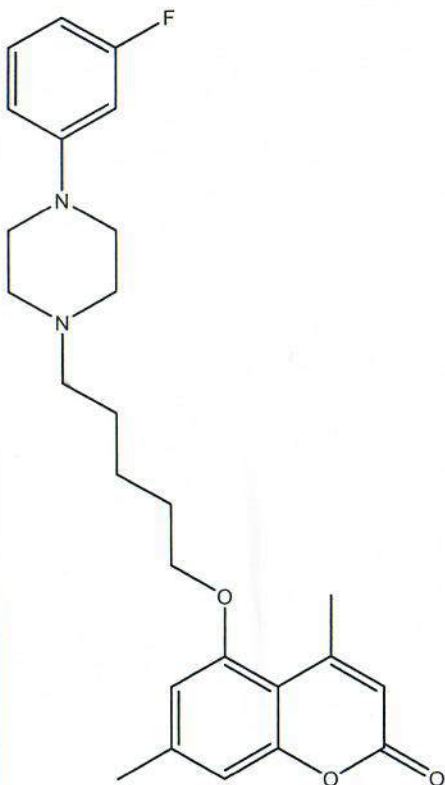
1d



1e

KO-316-1H-cdcl3

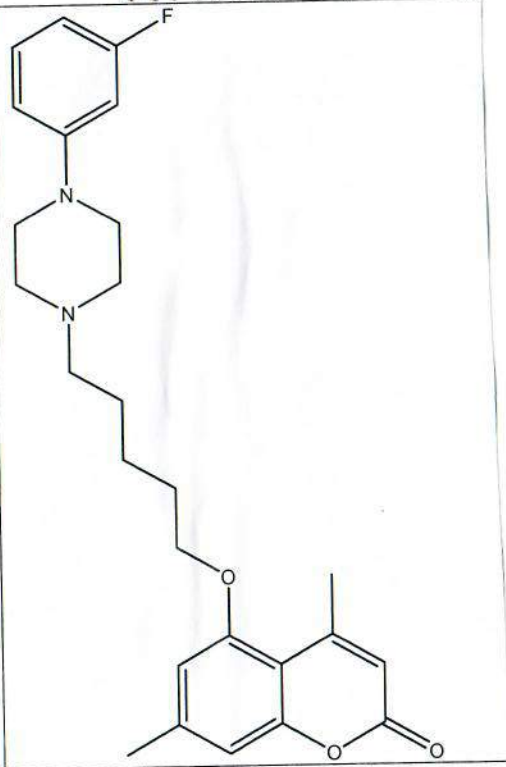
KO316 w CDCl3 + TMS



1e

KO-316-13C-cdd3
KO 316 13C w CDCl3

1e



165.66
162.44
161.17
157.49
155.54
154.29
153.15
153.02
143.19
130.37
130.24

113.63
111.28
111.25
110.30
108.39
108.01
106.18
105.90
102.98
102.65

77.65
77.23
76.81

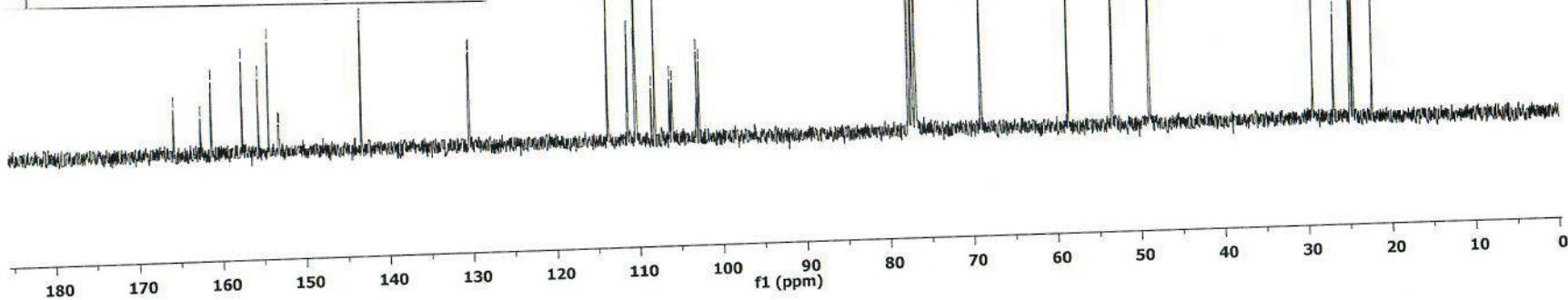
69.03

58.58

53.29

48.79

29.30
26.78
24.76
24.48
22.20

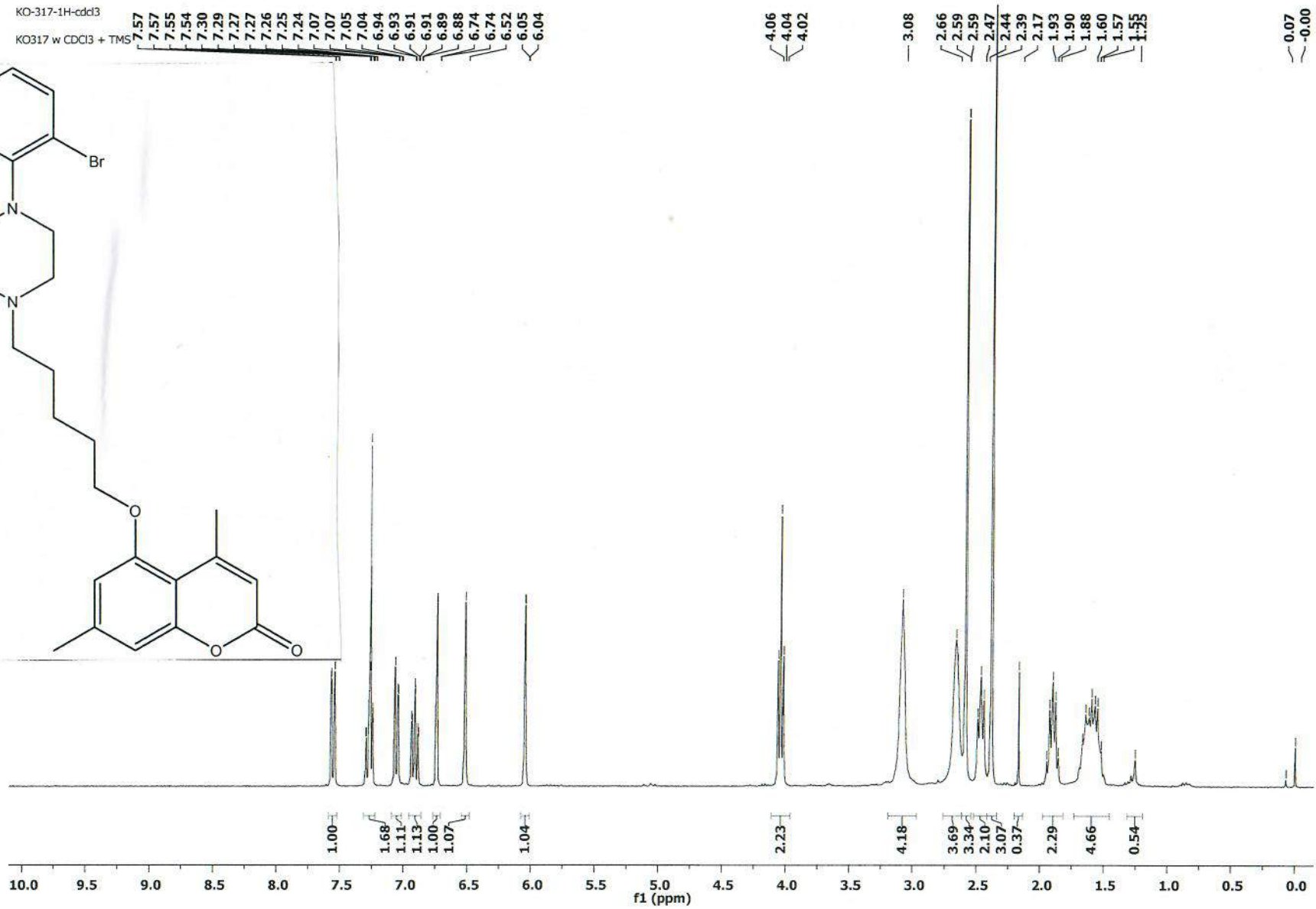
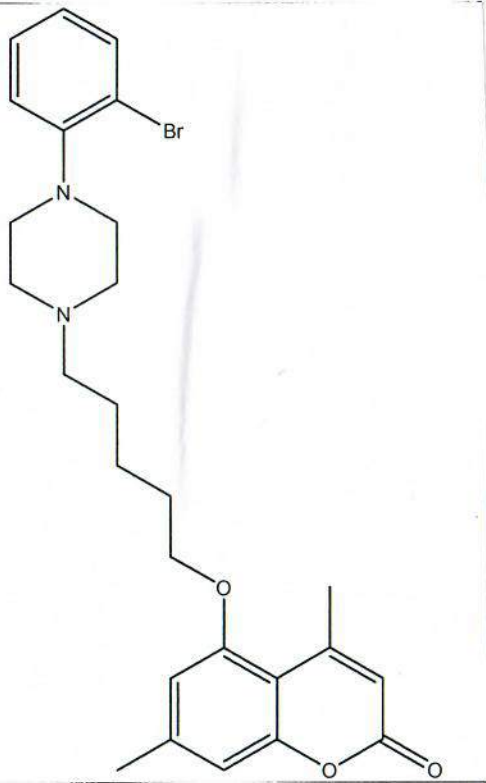


1f

KO-317-1H-cdd3

KO317 w CDCl3 + TMS

1f



1f

KO-317-13C-cdcl3
KO 317 13C w CDCl3

161.20
157.52
155.55
154.33

143.20

134.04

128.51
124.63
121.12
120.07

113.64
110.31
108.03

77.65
77.23
76.81

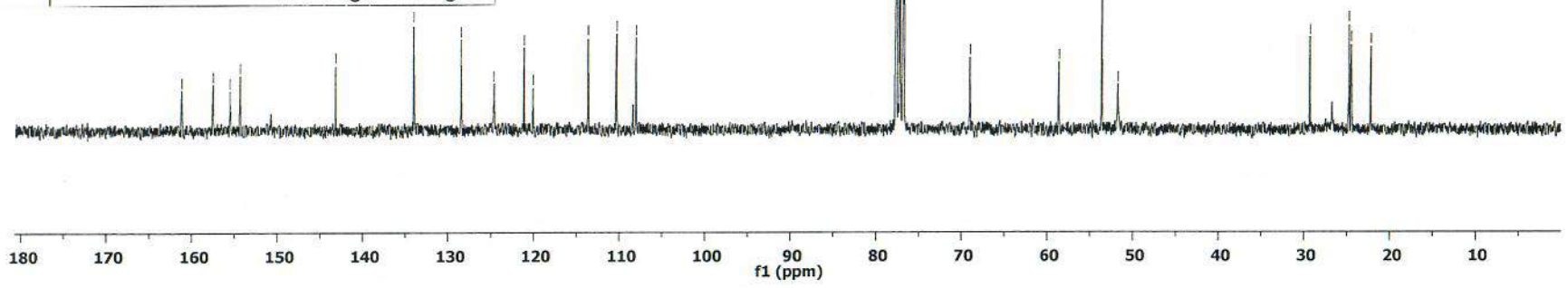
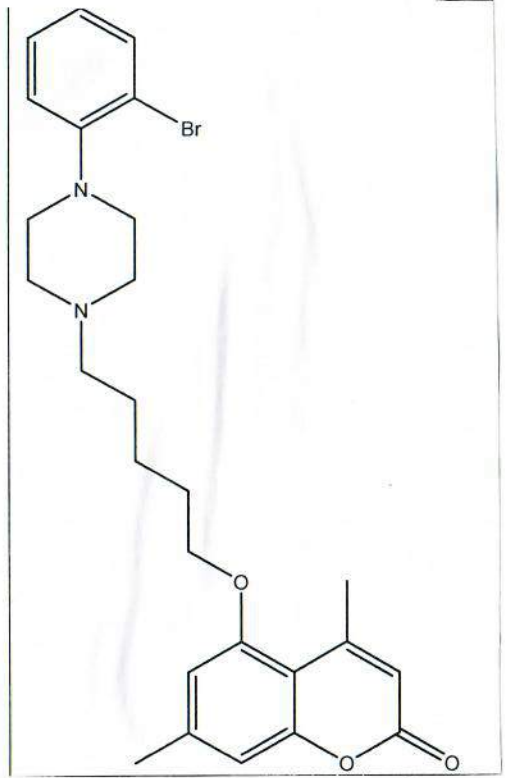
69.03

58.64

53.64
51.76

29.31
24.79
24.52
22.21

1f

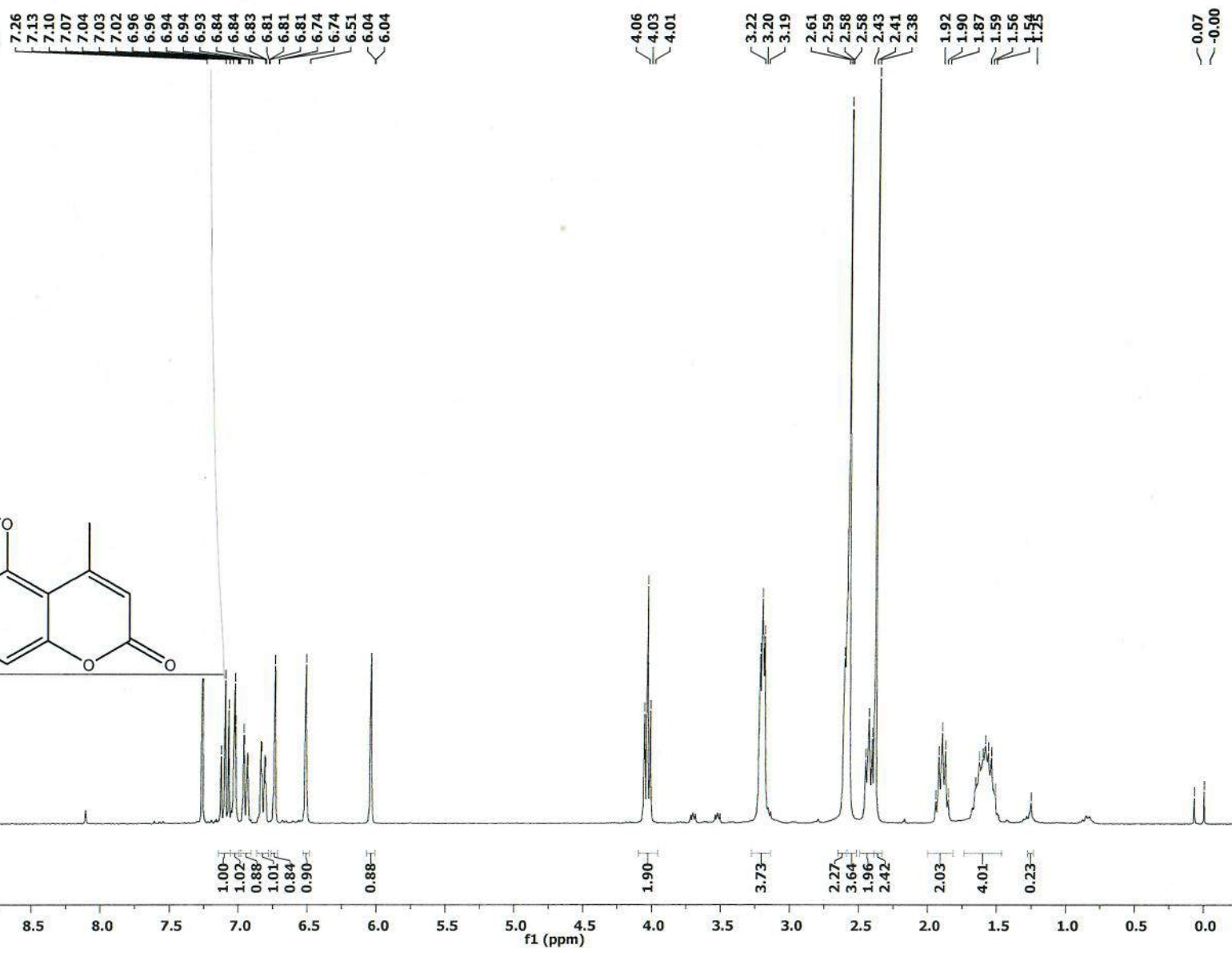
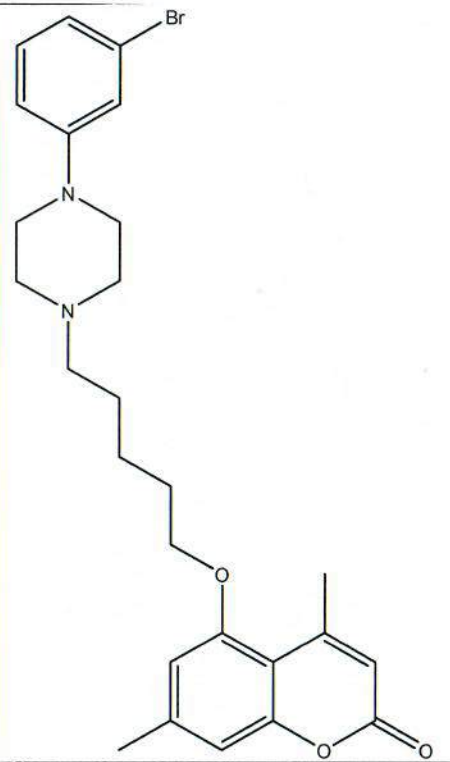


18

1g

KO-318-1H-cdcl3

KO318 w CDCl3 + TMS



1g

KO-318-13C-cdcl3
KO 318 13C w CDCl3

161.17
157.49
155.54
154.29
152.61

143.19

130.52

123.45
122.44
118.86
114.50
113.64
110.31
108.40
108.01

77.65
77.23
76.81

69.02

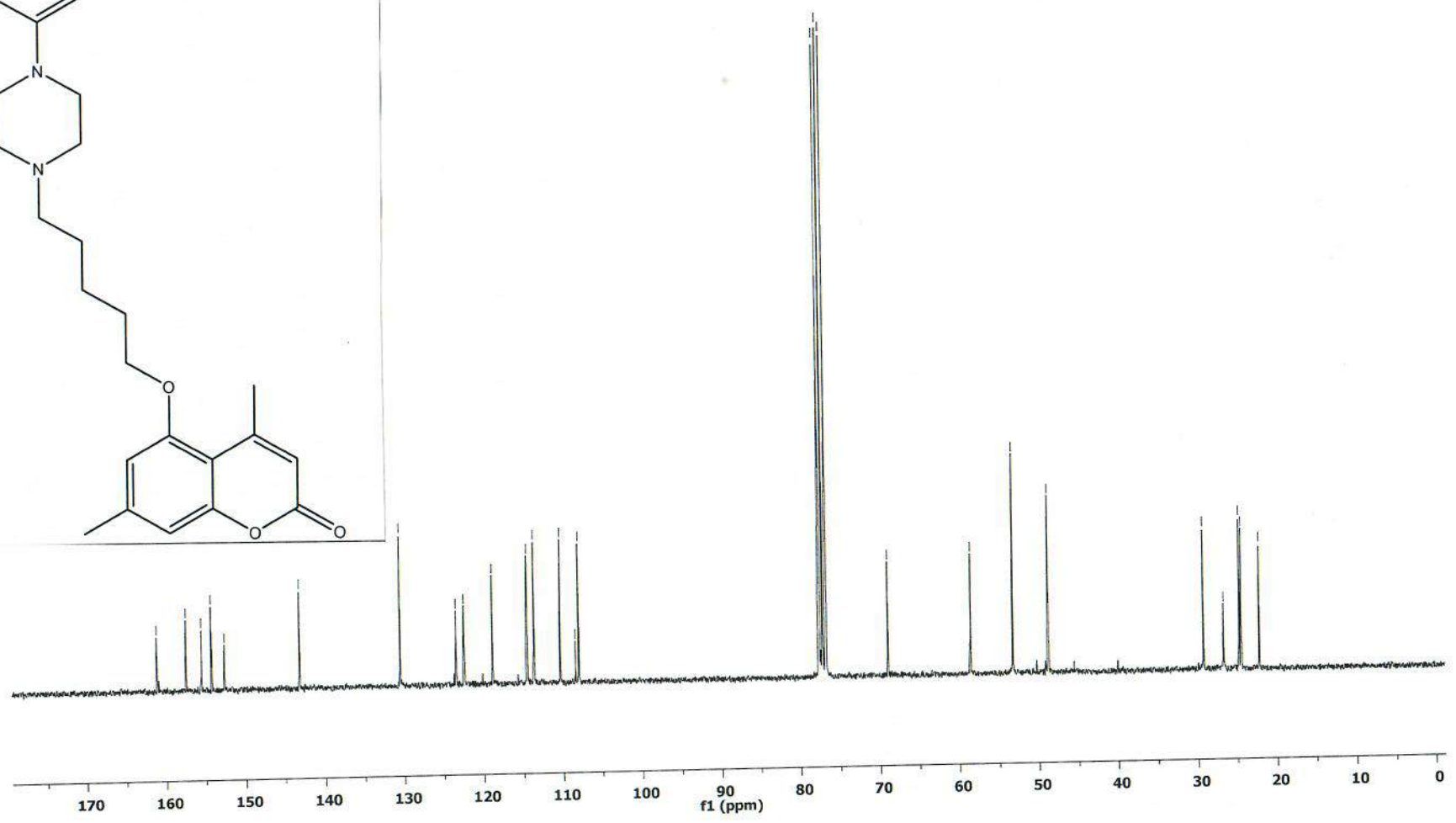
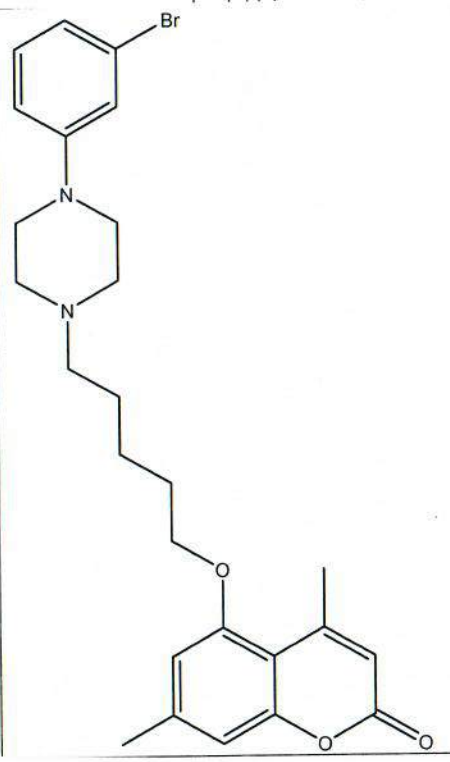
58.56

53.27

48.81

29.29
26.74
24.77
24.48
22.20

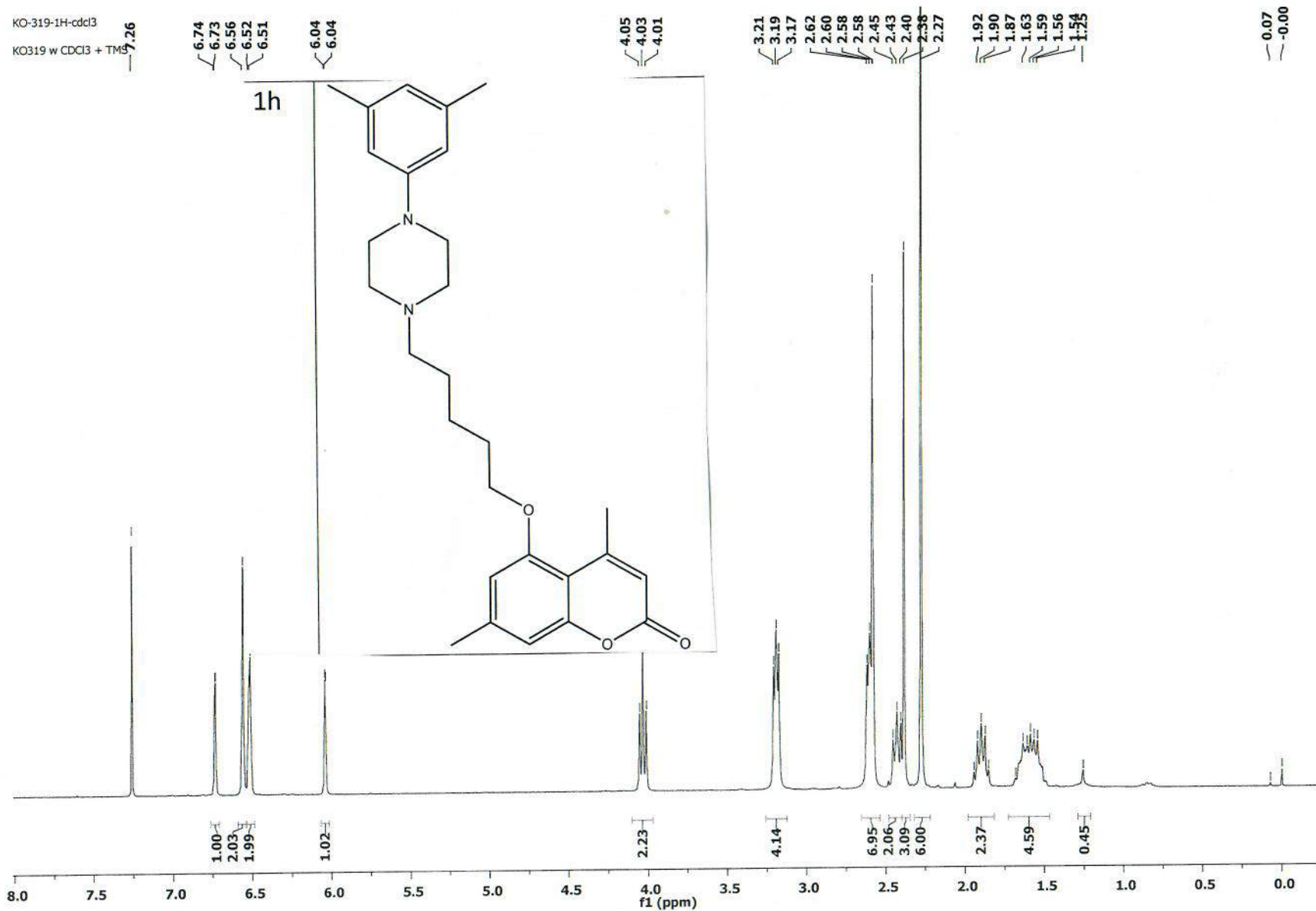
1g



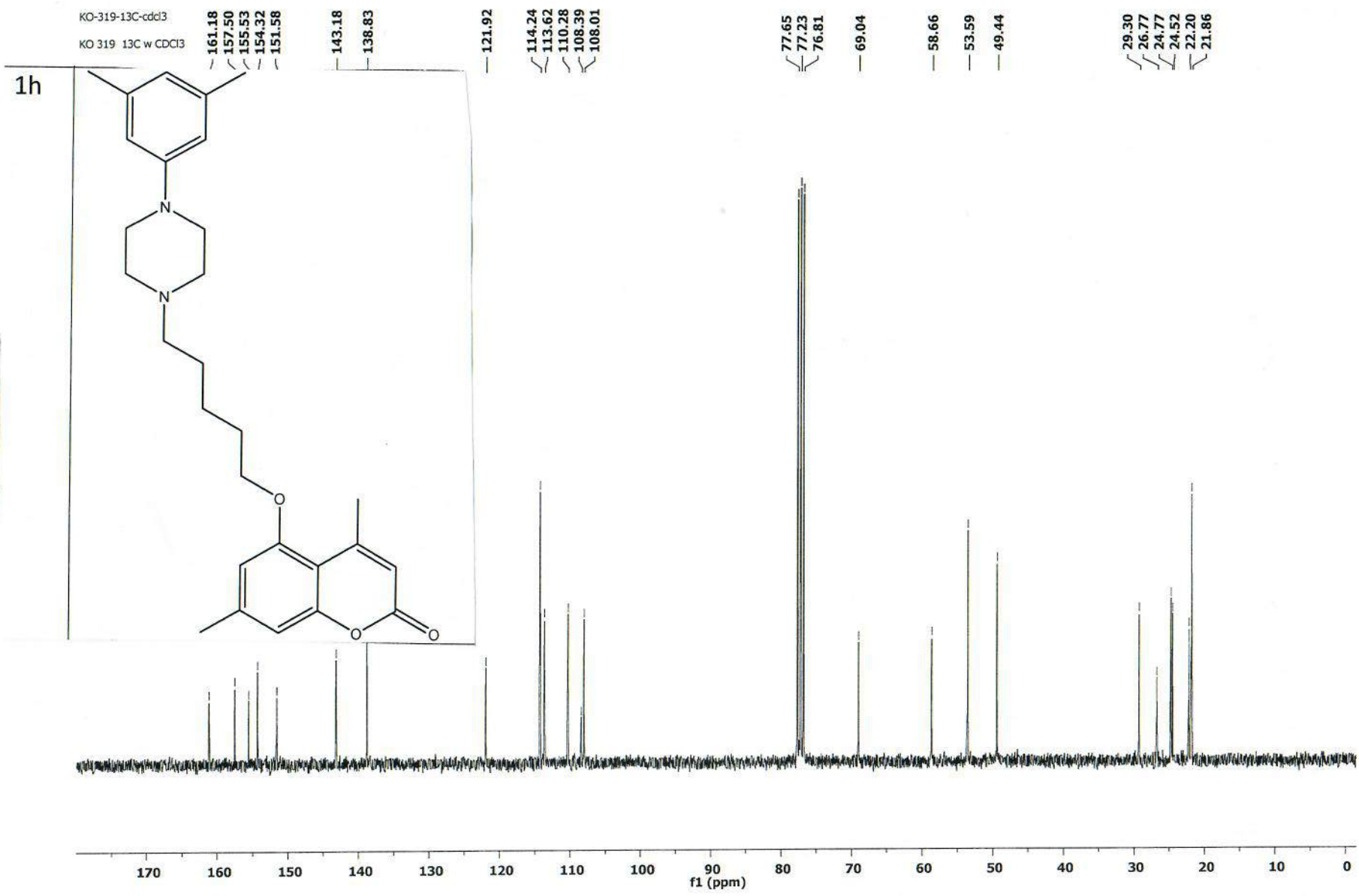
1h

KO-319-1H-cdcl3

KO319 w CDCl3 + TMS

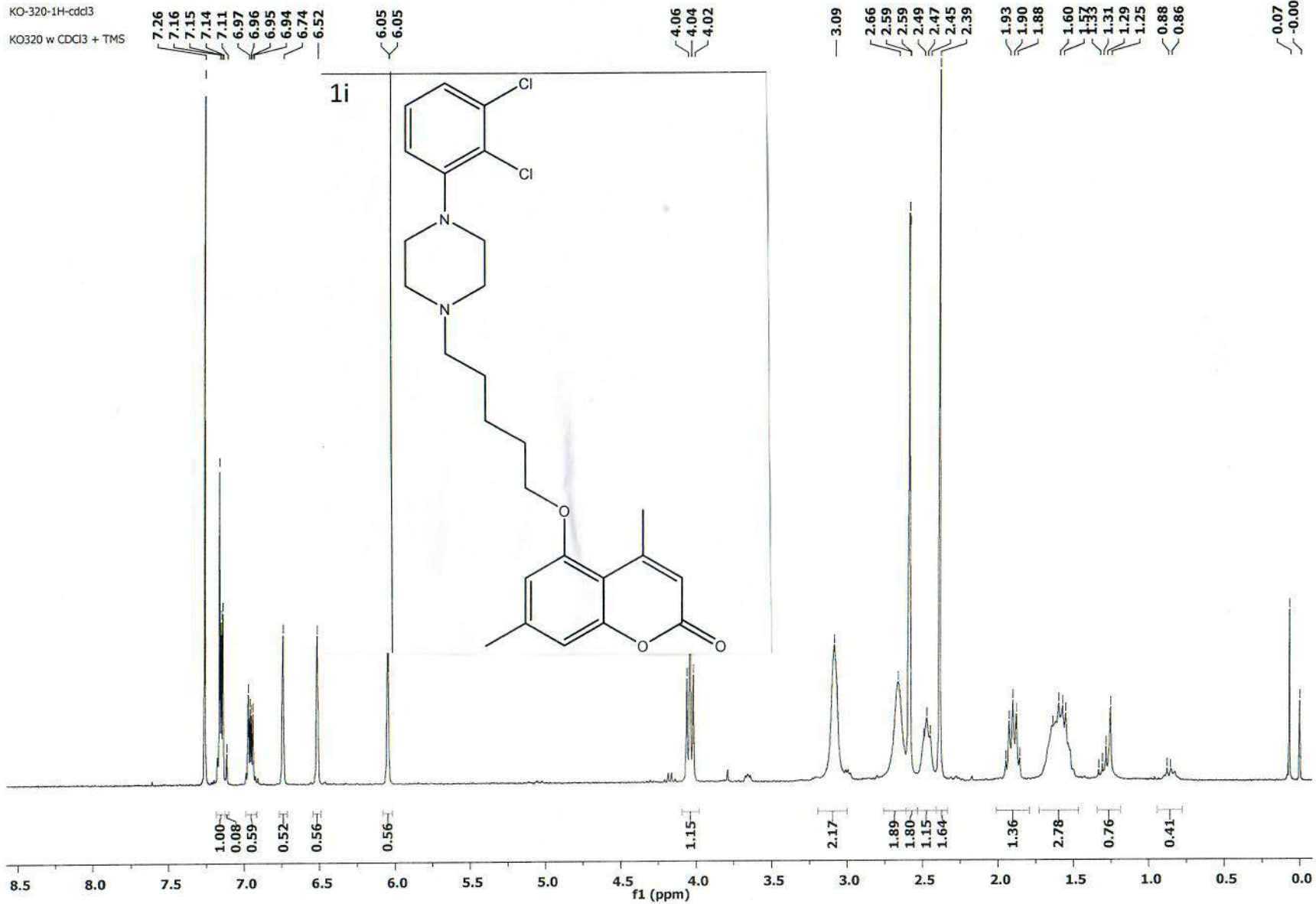


1h



10

KO-320-1H-cdd3
KO320 w CDCl3 + TMS



10

KO-320-13C-cdcl3
KO 320 13C w CDCl3

161.20
157.50
155.55
154.31

143.21

134.28

127.72

124.96

118.84

113.66

110.34

108.42

108.04

77.65

77.23

76.81

69.00

58.55

53.51

51.27

29.29

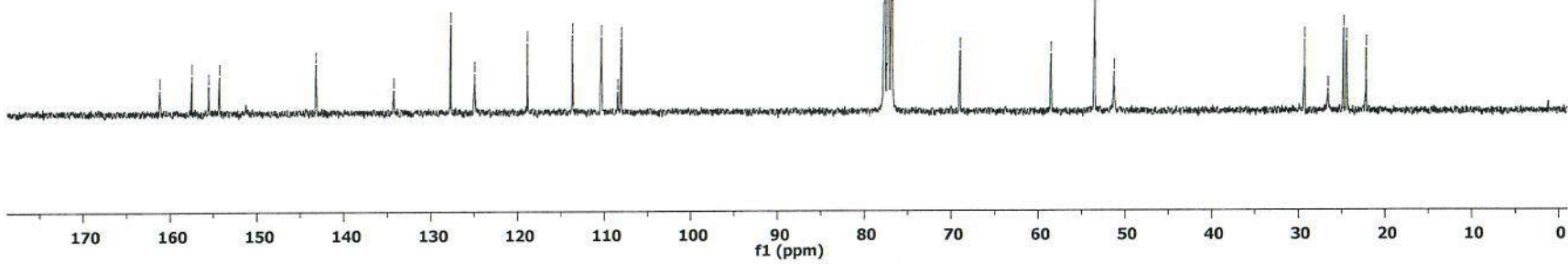
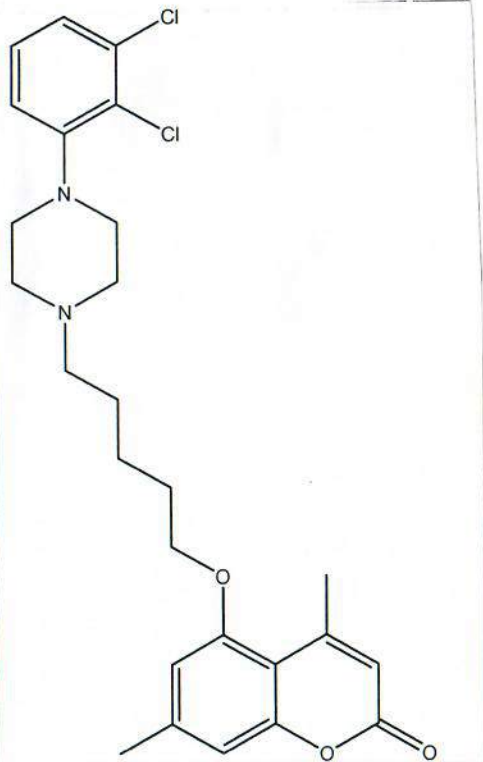
26.59

24.79

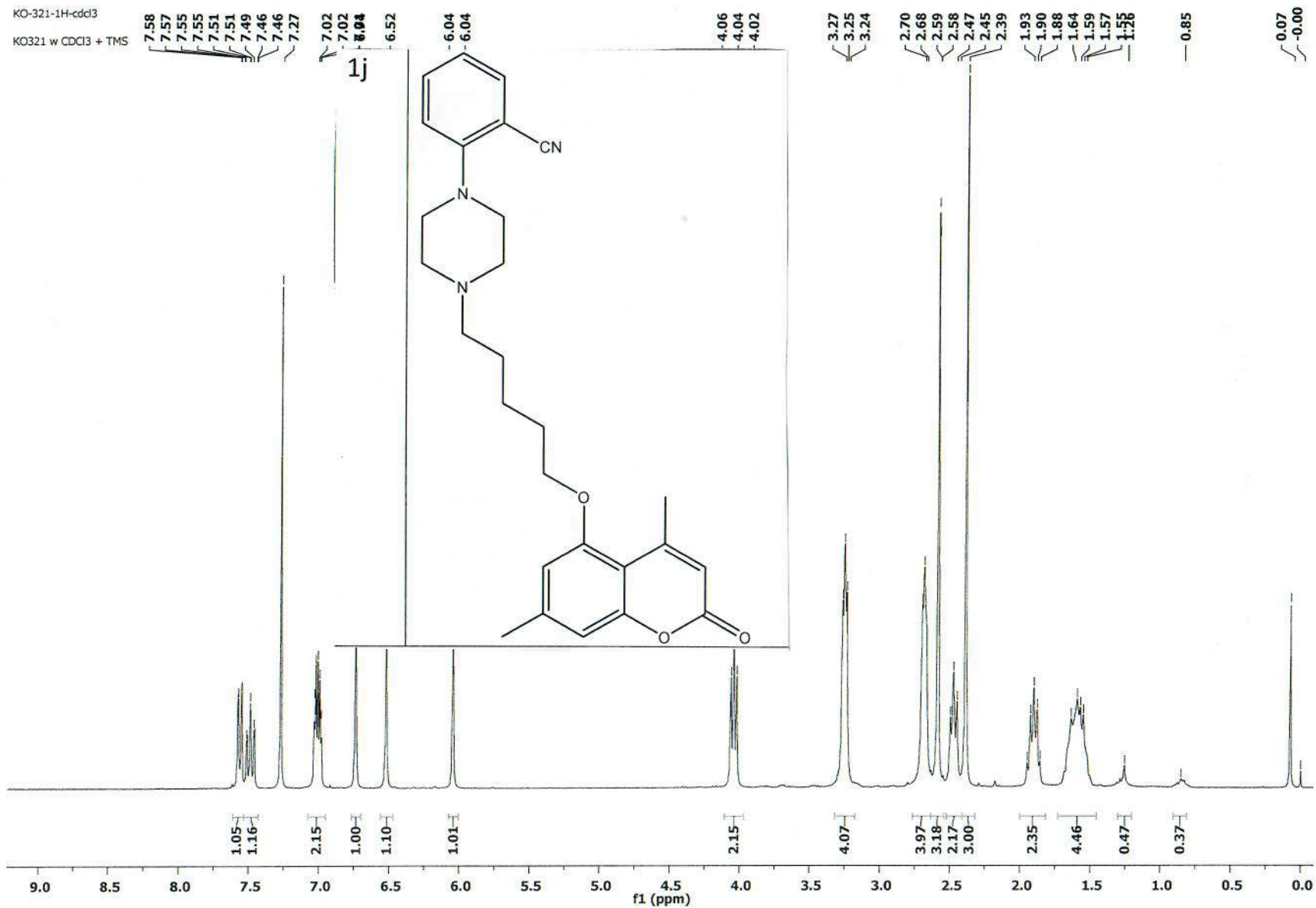
24.47

22.21

1i



KO-321-1H-cdd3
KO321 w CDCl3 + TMS



1j

KO-321-13C-cdd3
KO 321 13C w CDCl3

161.21
157.51
155.79
155.55
154.33

143.21

134.56
134.05

122.08
118.87
118.65

113.65
110.33
108.42
108.04
106.26

77.65
77.23
76.81

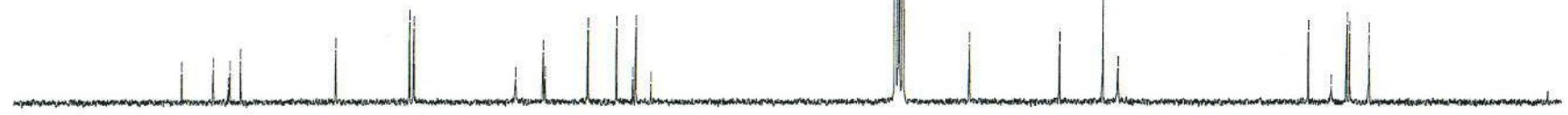
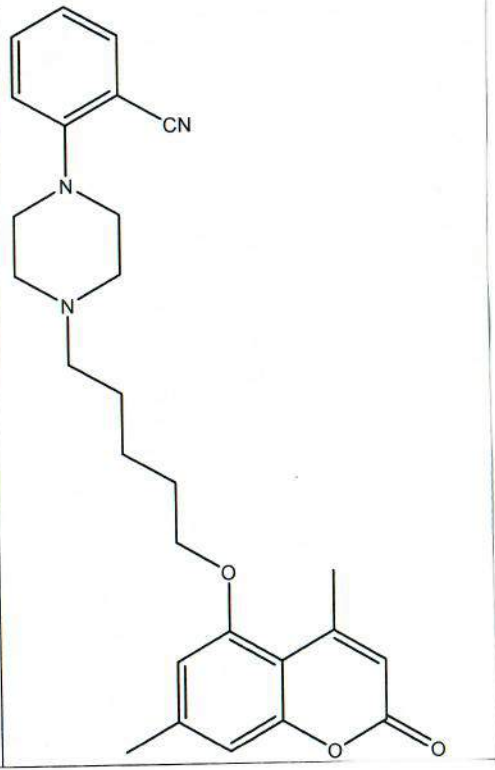
69.00

58.47

53.39
51.60

29.29
26.61
24.79
24.46
22.21

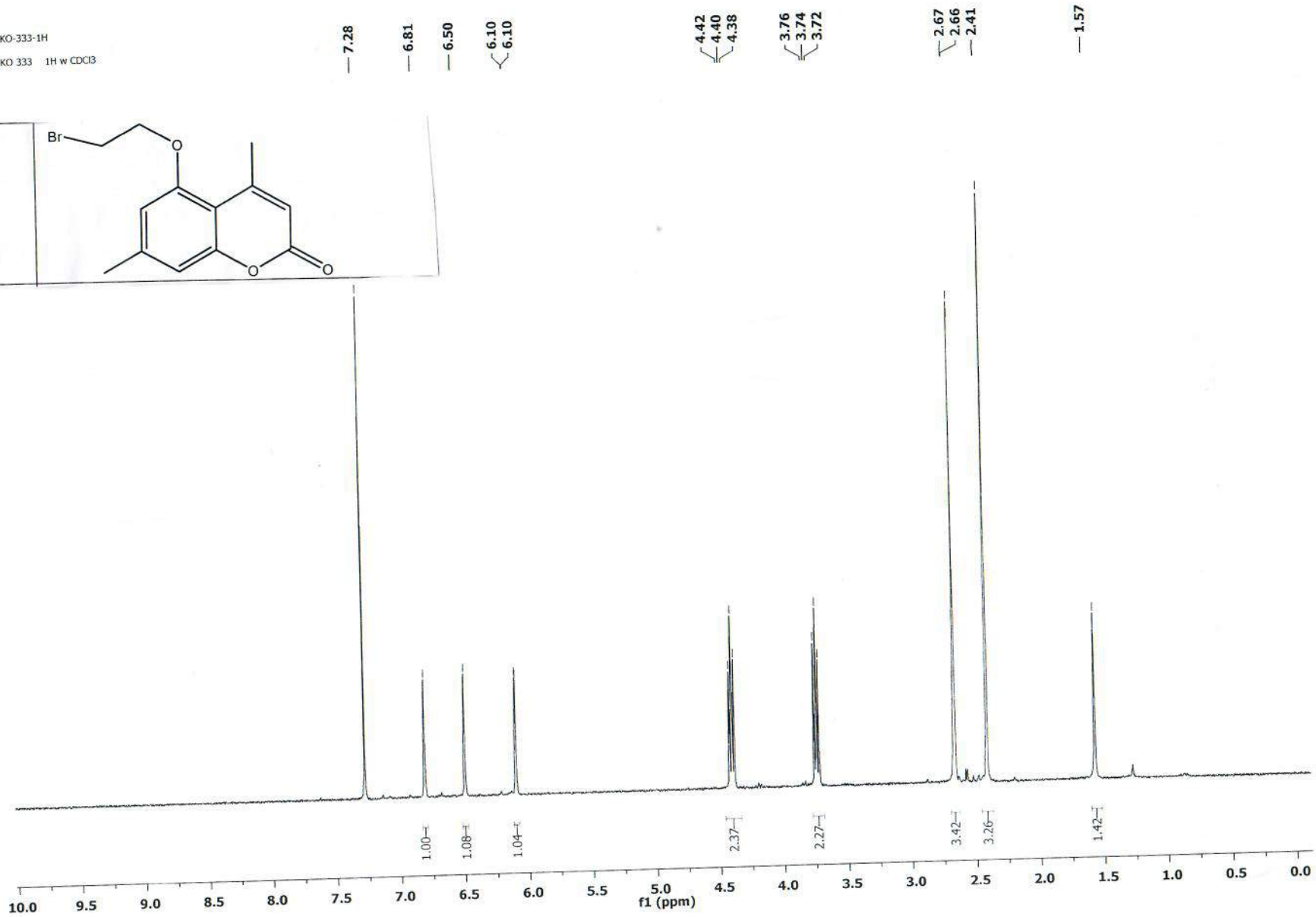
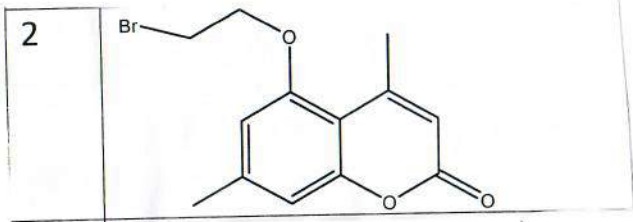
1j



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

264

KO-333-1H
KO 333 1H w CDCl3



2.47

KO-333-13C
KO 333 13C w CDCl3

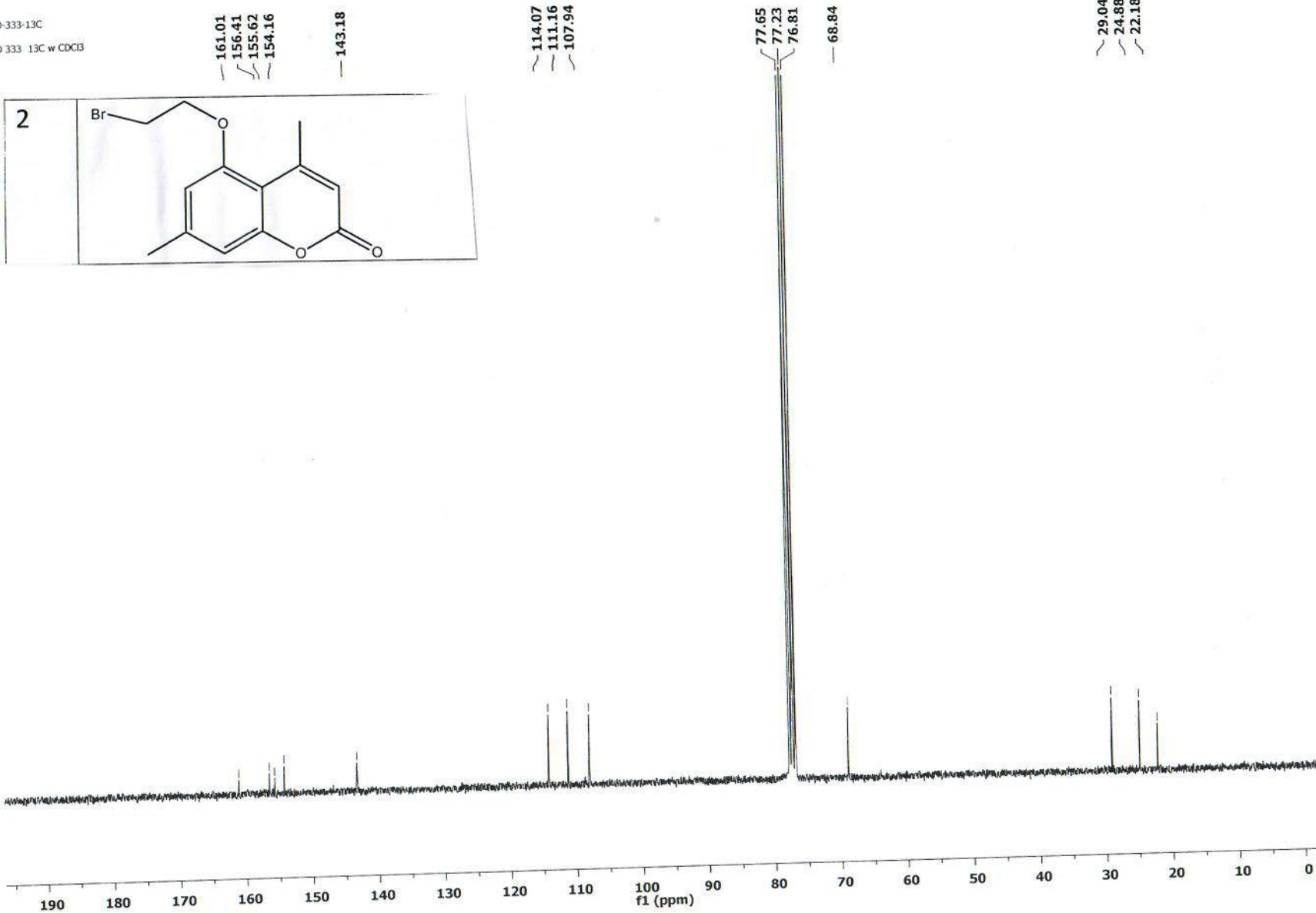
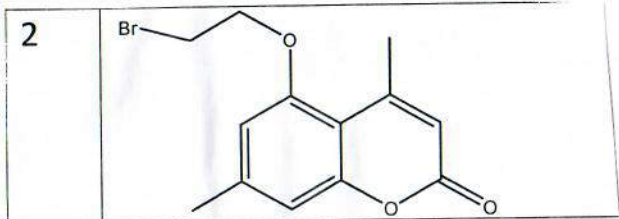
161.01
156.41
155.62
154.16
143.18

114.07
111.16
107.94

77.65
77.23
76.81

68.84

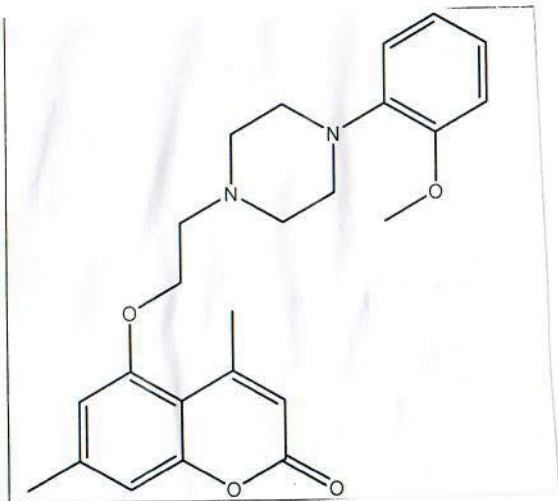
29.04
24.88
22.18



KO-334-1H-cdd3
KO 334 1H w CDC13

7.26
7.04
7.03
7.02
7.01
7.01
7.00
6.99
6.96
6.94
6.94
6.92
6.88
6.86
6.86
6.76
6.76
6.56
6.56
6.06
6.05

2a



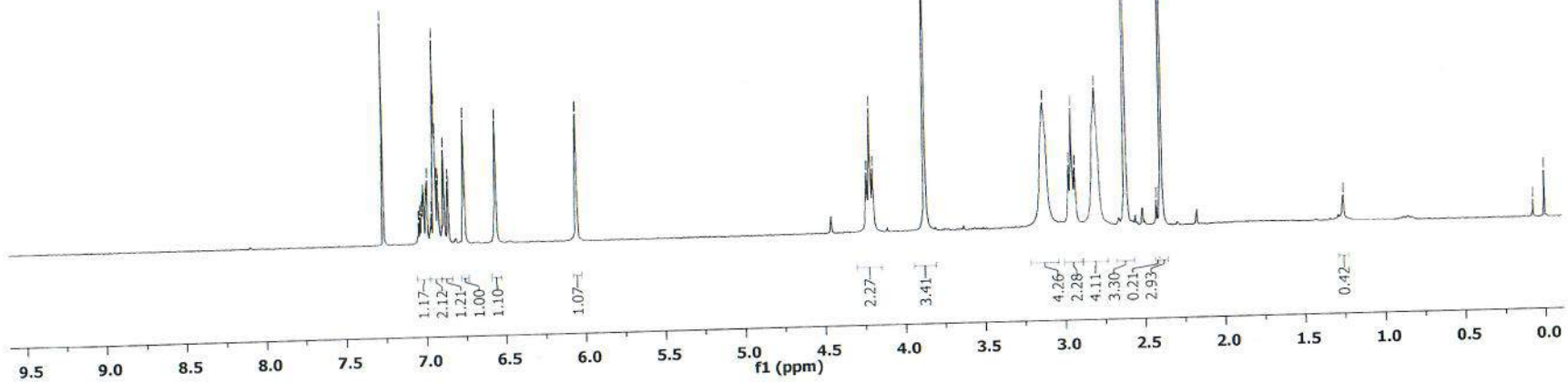
4.23
4.22
4.20

3.87

3.13
2.97
2.95
2.93
2.80
2.62
2.62
2.42
2.39

— 1.26

0.07
0.00



2e

KO-334-13C-cdCl3
KO 334 13C w CDCl3

161.14
157.18
155.52
154.36
152.45

143.22
141.25

123.34
121.21
118.44
113.74
111.41
110.60
108.33

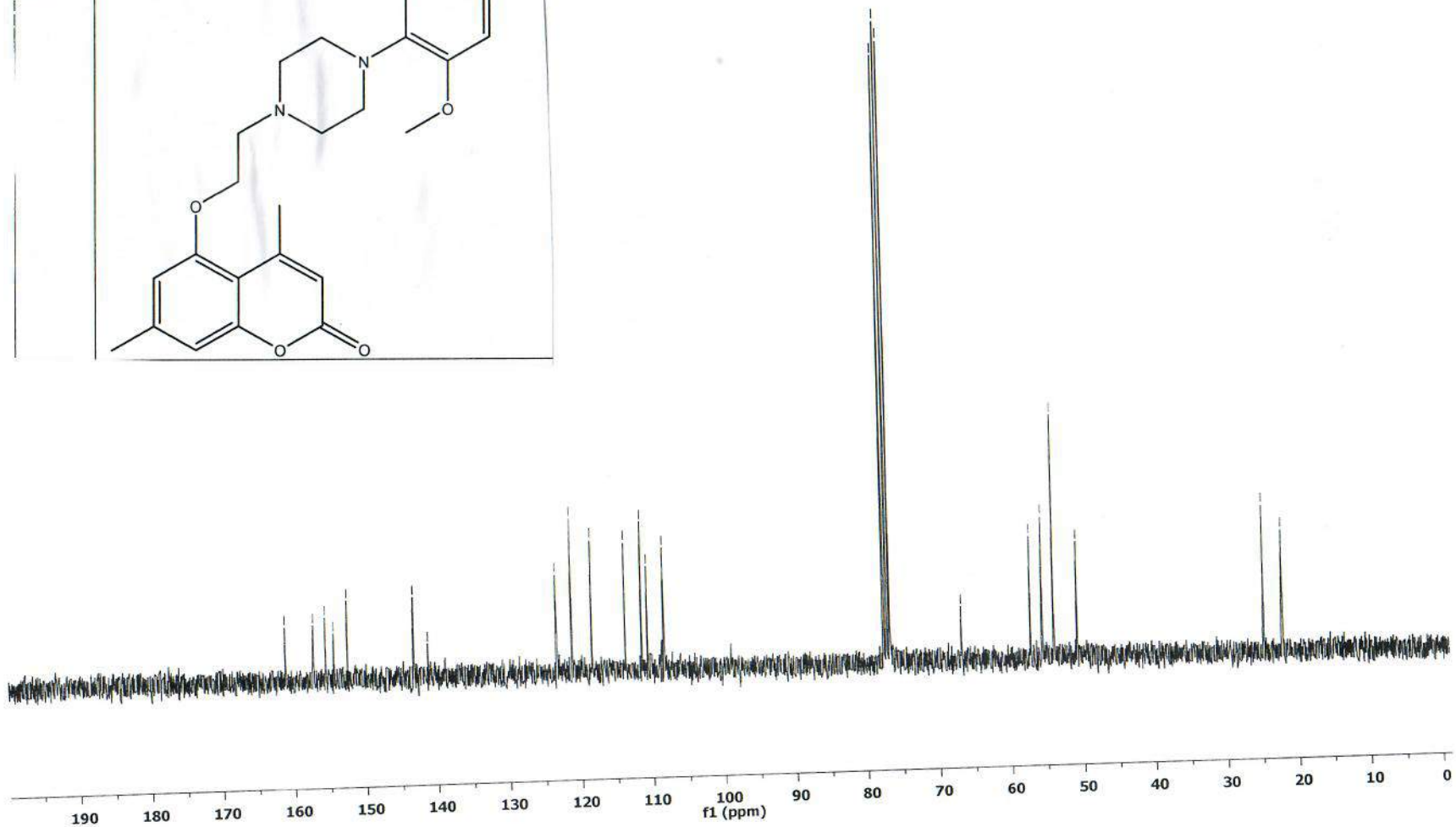
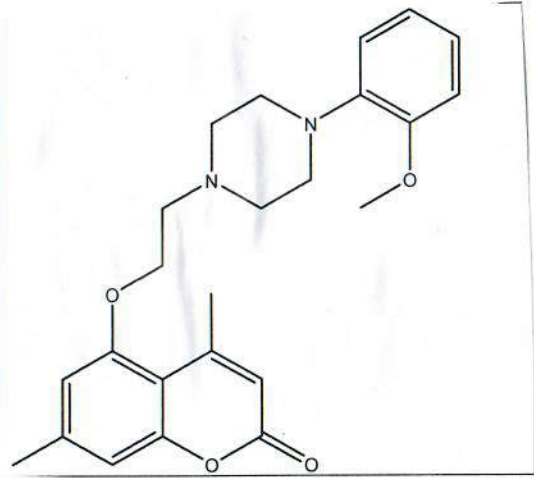
77.65
77.23
76.81

66.85

57.23
55.59
53.98
50.78

24.81
22.19

2a



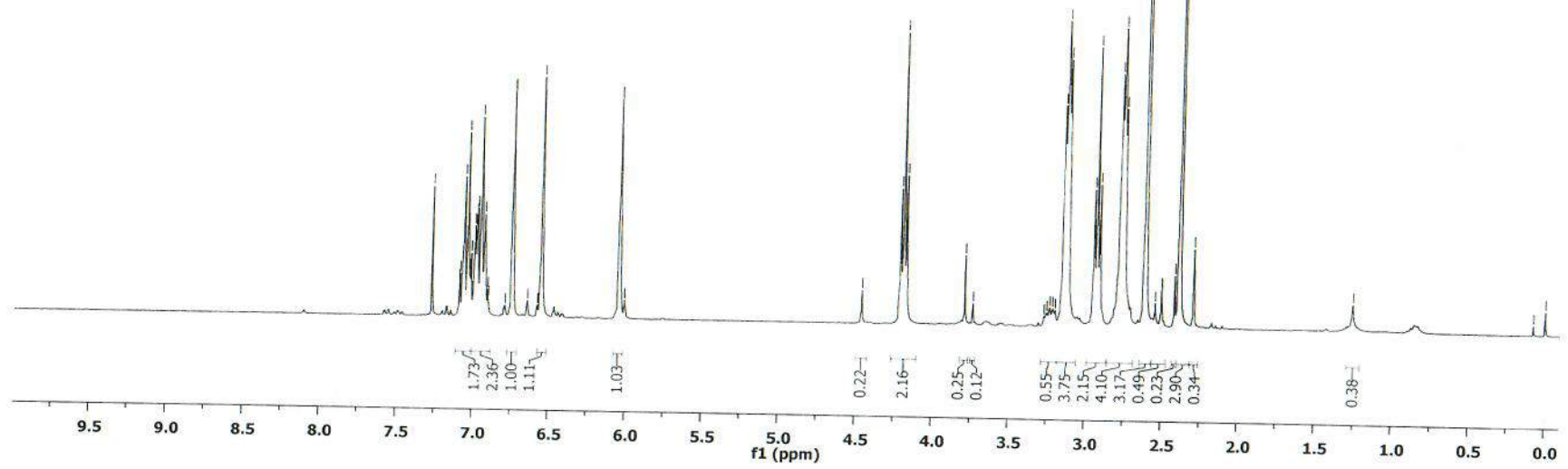
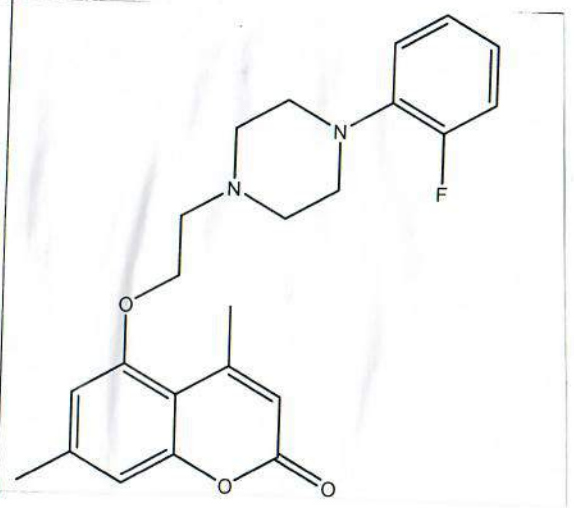
KO-338-1H-cdd13
KO 338 1H w CDCl3

7.27
7.09
7.07
7.06
7.04
7.02
7.01
6.99
6.99
6.98
6.97
6.95
6.94
6.93
6.91
6.90
6.79
6.74
6.74
6.64
6.58
6.55
6.04
6.04
6.01

4.46
4.21
4.19
4.17
3.79
3.74
3.23
3.15
3.14
3.12
2.95
2.93
2.91
2.78
2.77
2.75
2.62
2.61
2.54
2.51
2.50
2.42
2.39
2.28

0.08
0.00

2b



KO-338-13C
KO 338 13C w CDCl3

161.15
157.51
157.16
155.44
154.43
154.25

143.20
140.17
140.05

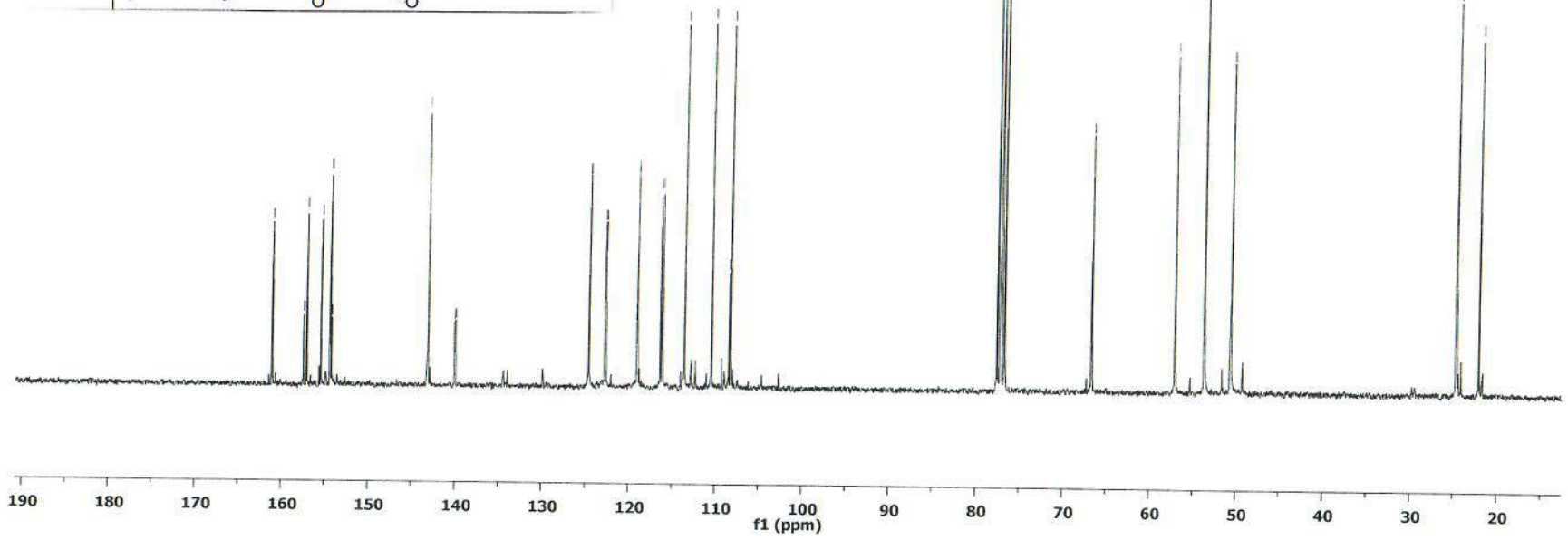
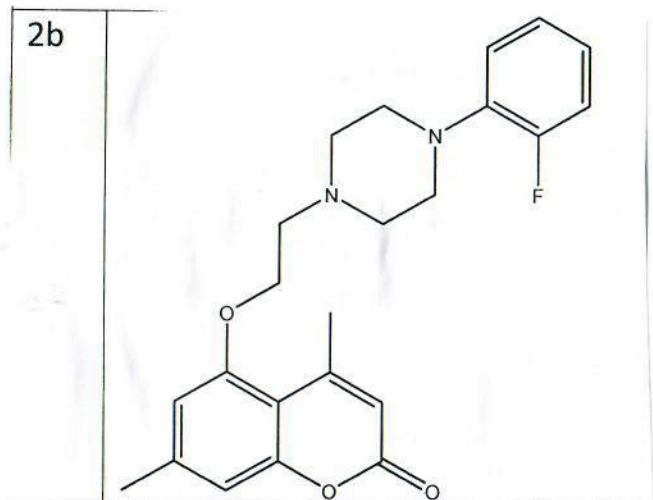
124.67
124.62
122.81
122.71
119.12
119.08
116.43
116.15
113.63
110.51
108.54
108.28

77.65
77.23
76.81

66.76

57.16
53.78
50.72
50.68

24.75
22.15



KO-337-1H
KO 337 1H w CDCl3

7.26
7.20
7.17
7.15
6.75
6.55
6.53
6.47
6.46
6.44
6.04

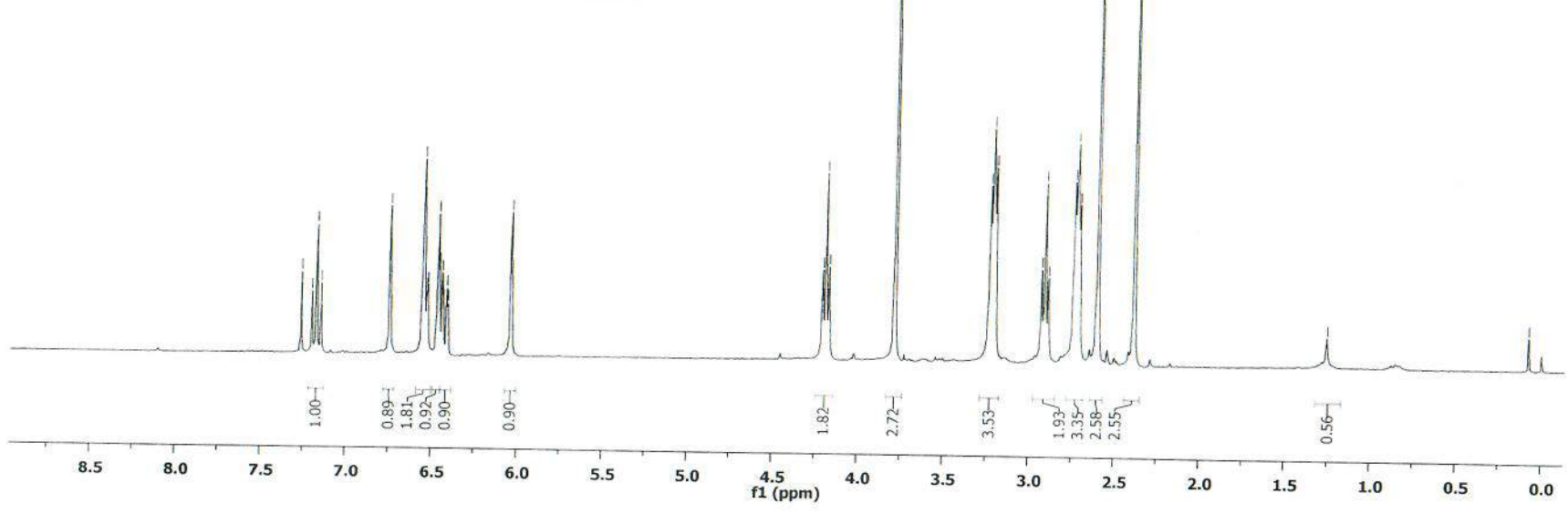
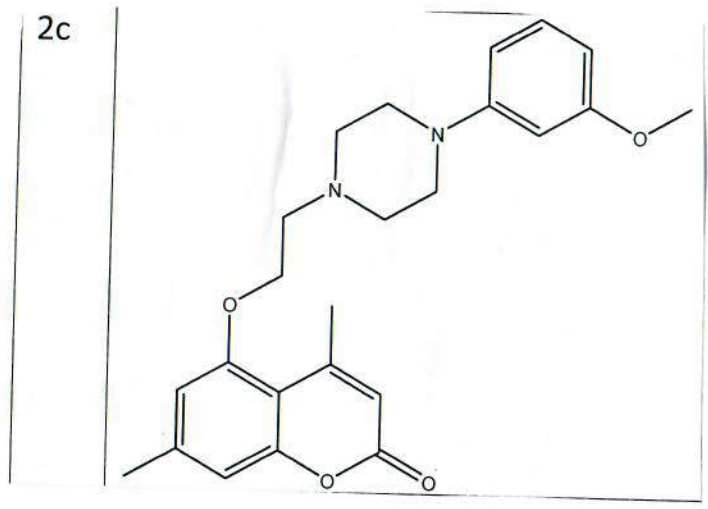
4.21
4.19
4.17

3.79

3.23
3.22
3.20
2.93
2.91
2.89
2.74
2.73
2.71
2.60
2.39

1.26

0.07



KO-337-13C
KO 337 13C

161.09
160.77
157.14
155.48
154.32
152.72

143.19

129.99

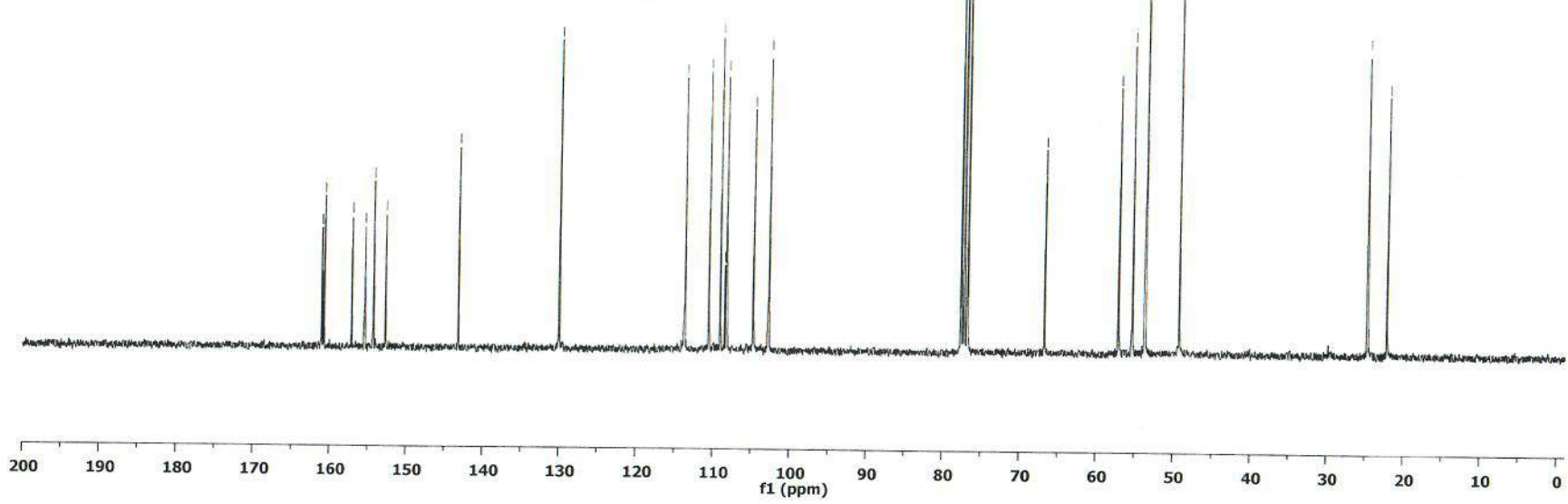
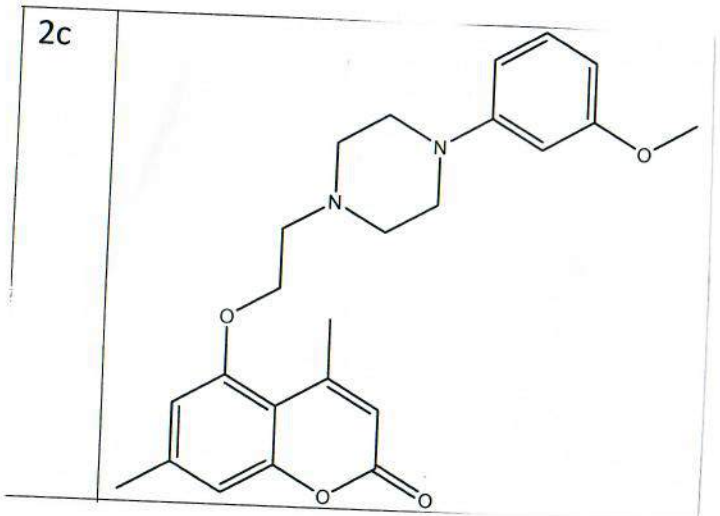
113.70
110.56
109.08
108.55
108.28
104.74
102.79

77.65
77.23
76.81

66.79

57.15
55.37
53.70
49.28

24.75
22.16



2d

KO-340-1H-cdd3

KO 340 1H w CDCl3

7.26
7.07
7.04
6.83
6.81
6.79
6.74
6.56

6.04

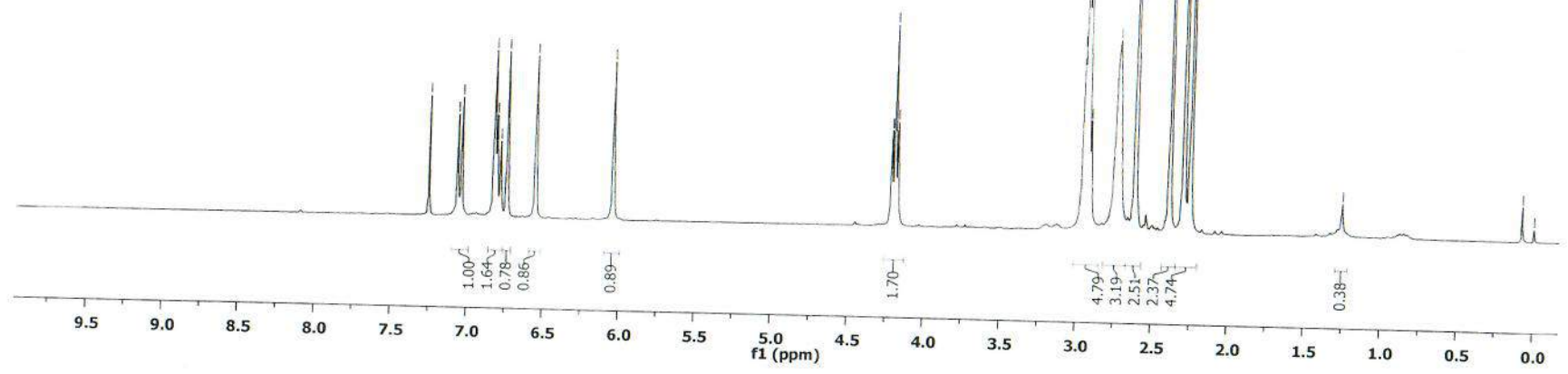
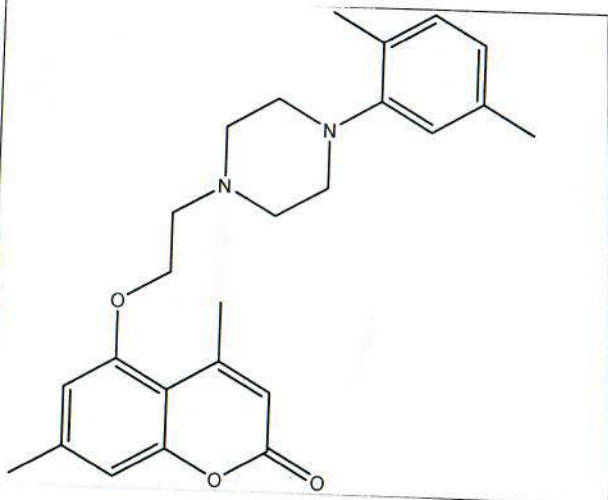
4.22
4.20
4.18

2.96
2.95
2.93
2.91
2.73
2.62
2.39
2.30
2.26

1.25

0.08
-0.00

2d



2d

KO-340-13C
KO 340 13C w CDCl3

161.10
157.19
155.46
154.40
151.28

143.18

136.29

131.06
129.41

124.04

119.89

113.65

110.49

108.55
108.28

77.65
77.43
77.23
76.81

66.83

57.23

54.28

53.79

51.85
48.92

29.88

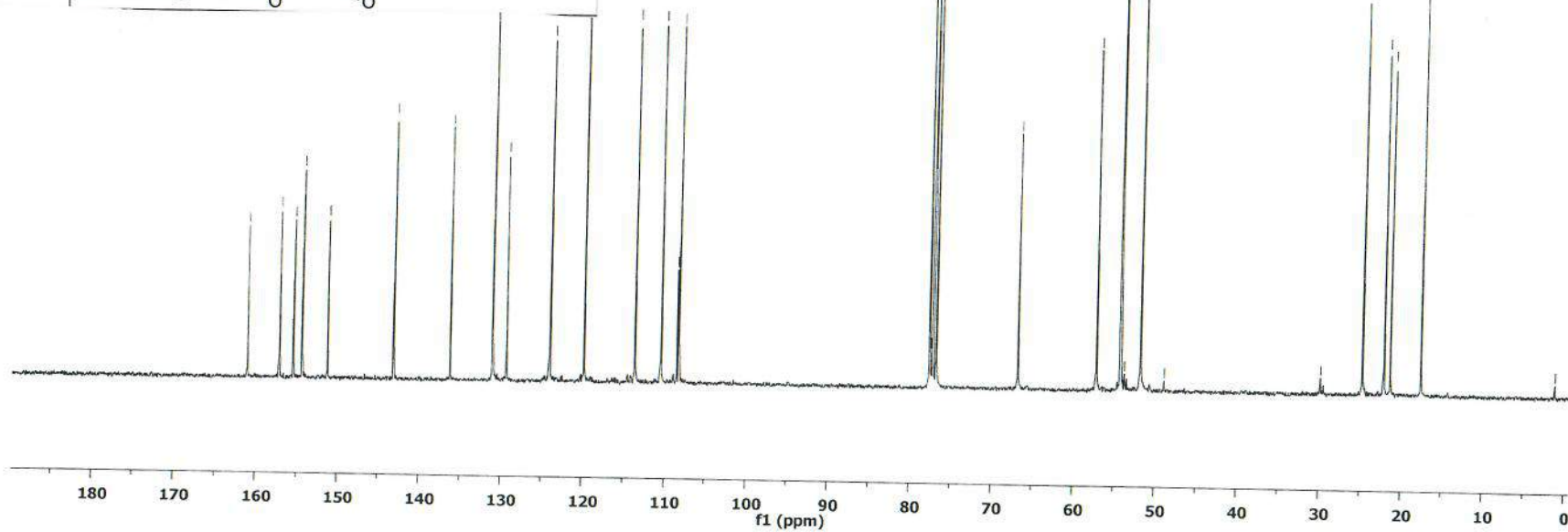
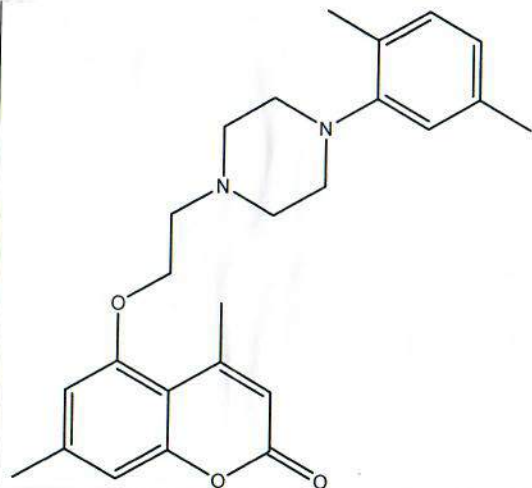
24.77

22.16

21.37
17.63

1.20

2d



2e

KO-341-1H-cdd3

KO 341 1H w CDCl3

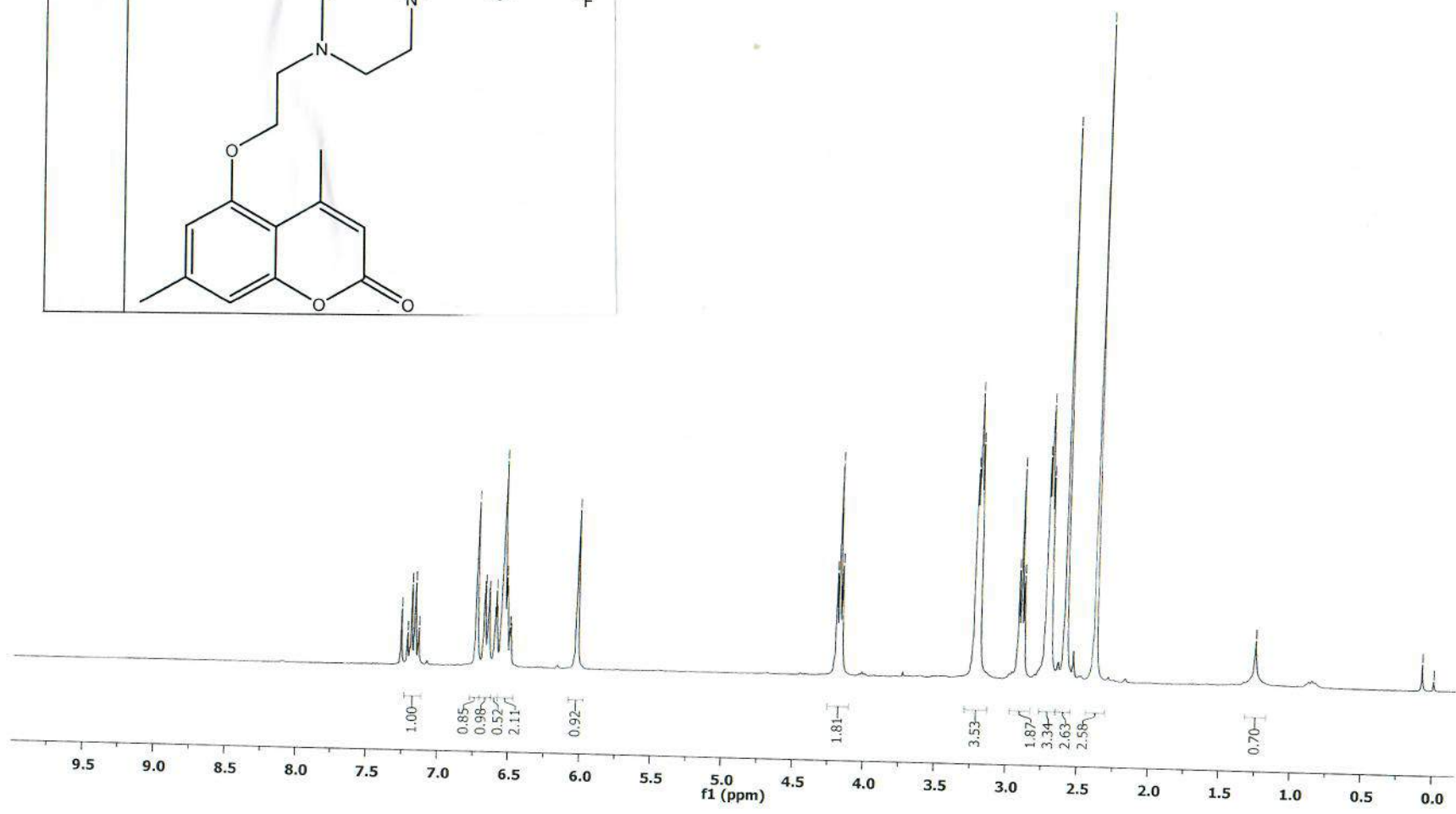
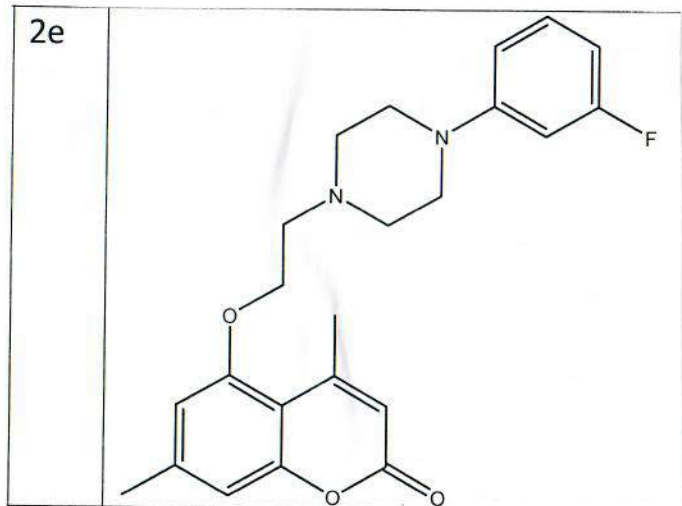
7.27
7.22
7.20
7.17
7.14
6.74
6.68
6.65
6.60
6.55
6.53

4.20
4.18
4.17

3.23
3.22
3.20
2.93
2.91
2.89
2.73
2.72
2.70
2.60
2.39

— 1.26

0.08
-0.00



2e

KO-341-13C-cdd3
KO 341 13C w CDCl3

165.60
162.37
161.06
157.11
155.45
154.30
153.03
152.90

143.18

130.37
130.23

113.66
111.32
111.29
110.52
108.51
108.25
106.26
105.98
103.02
102.68

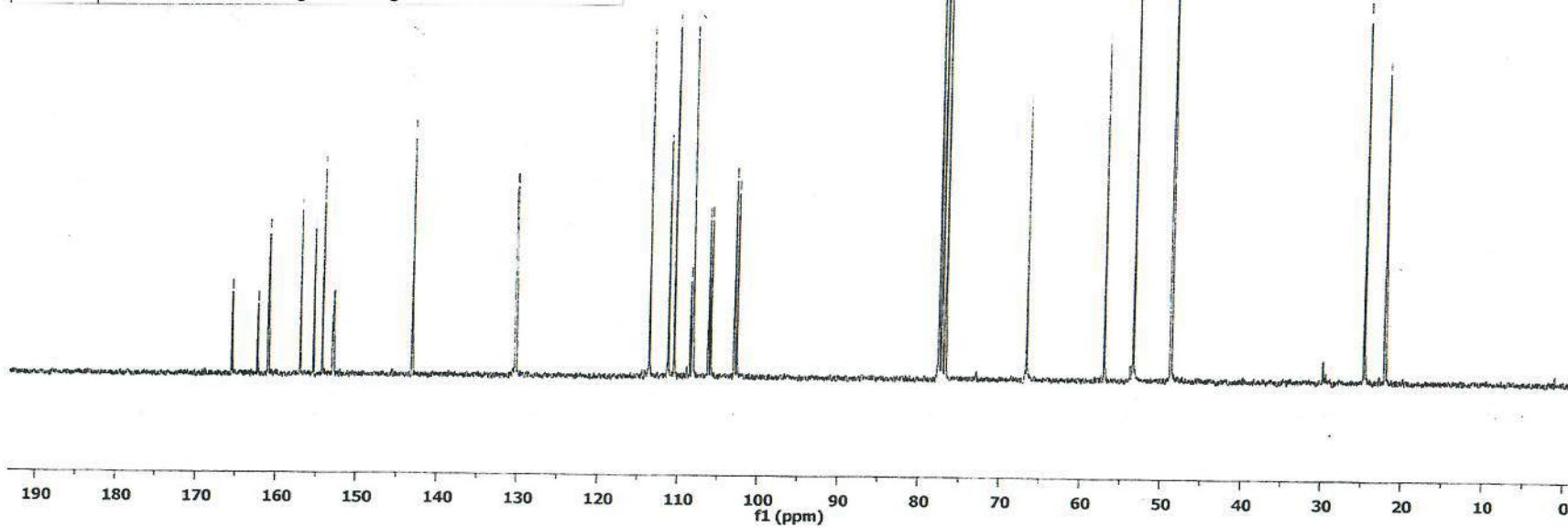
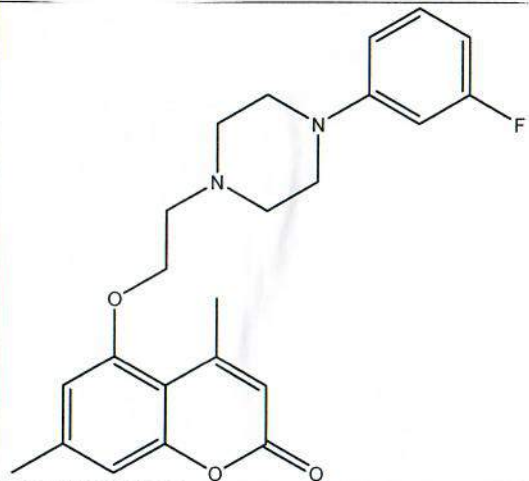
77.65
77.23
76.81

66.72

57.10
53.50
48.84

24.72
22.14

2e



2f

KO342-1H-cdcl3
KO342 1H w CDCL3

7.58
7.57
7.55
7.55
7.28
7.26
7.25
7.25
7.08
7.07
7.05
7.04
6.92
6.76
6.66

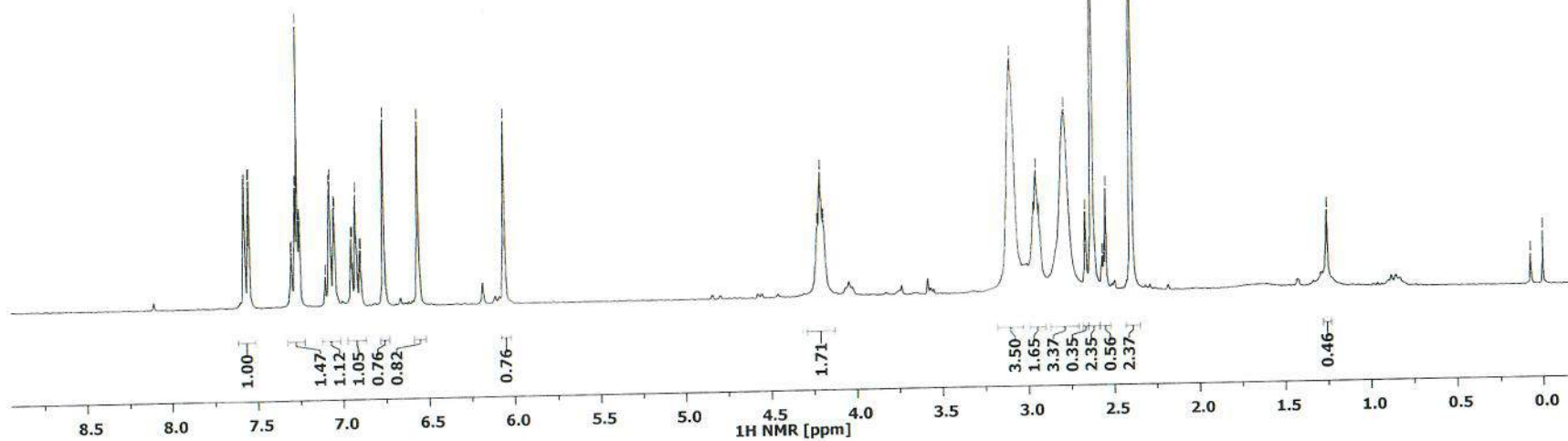
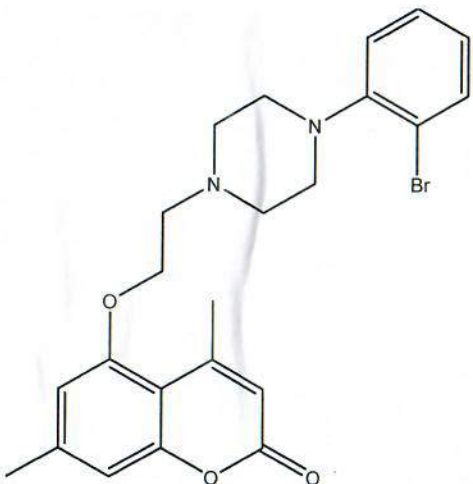
4.23
4.21
4.19

3.10
2.97
2.95
2.94
2.79
2.67
2.62
2.57
2.56
2.55
2.40

1.26

0.07
-0.00

2f



KO342-13C-cdcl3

KO 342 13C w CDCl3

161.07
157.01
155.52
154.17
150.37
146.81
143.28

134.06

128.56
124.87
121.19
120.06

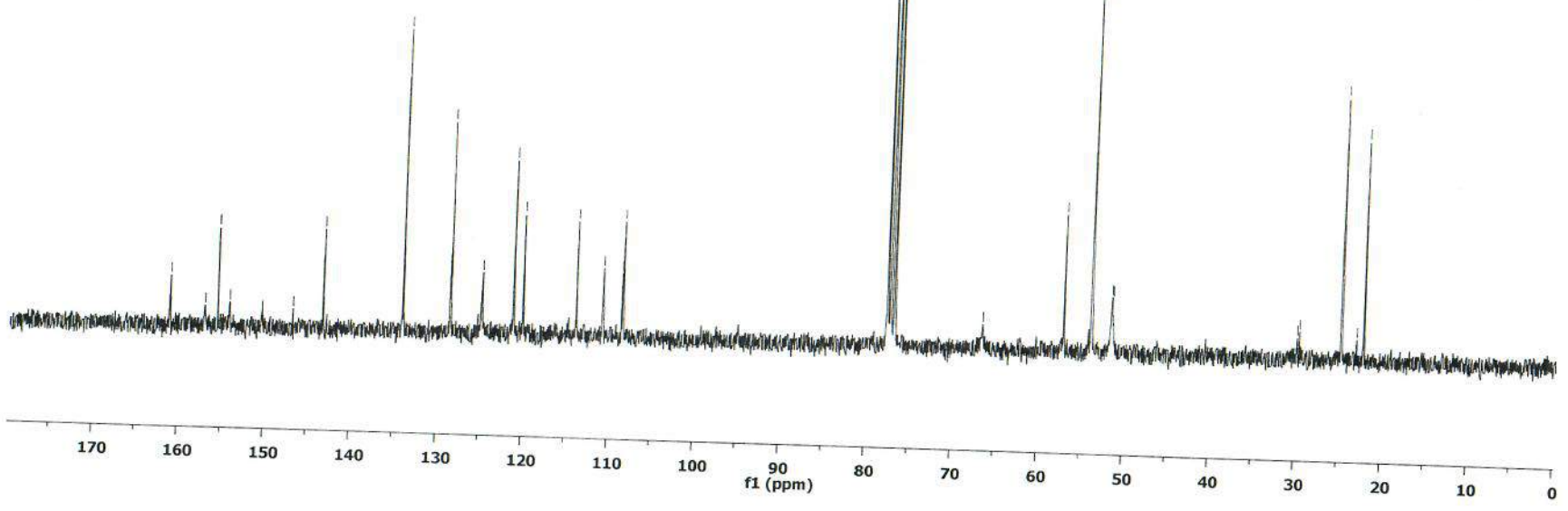
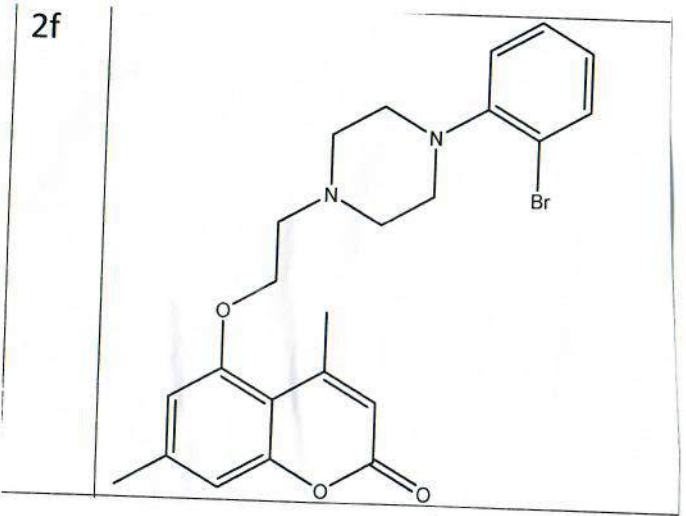
113.85
110.76
108.57
108.42

77.65
77.23
76.81

66.55

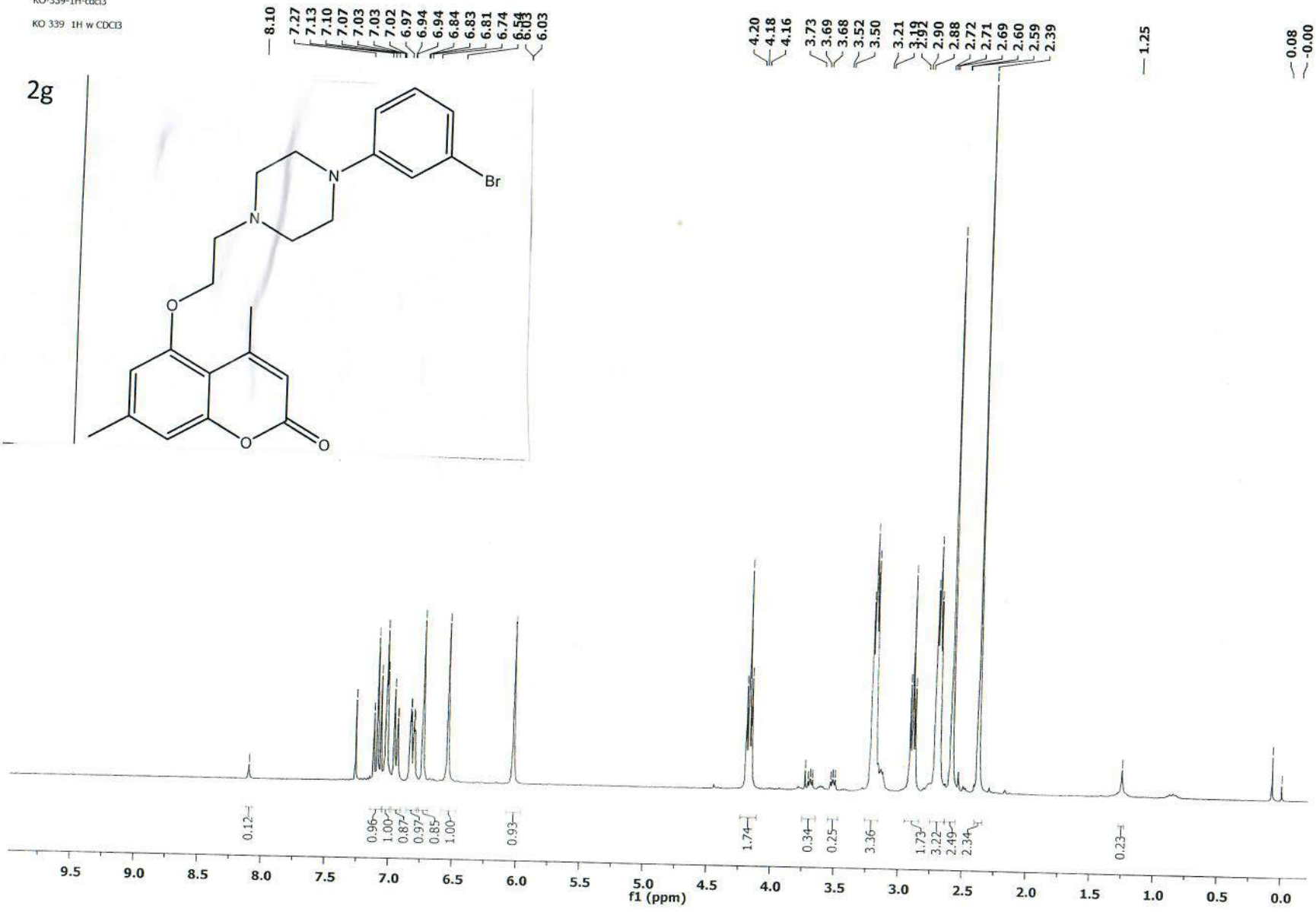
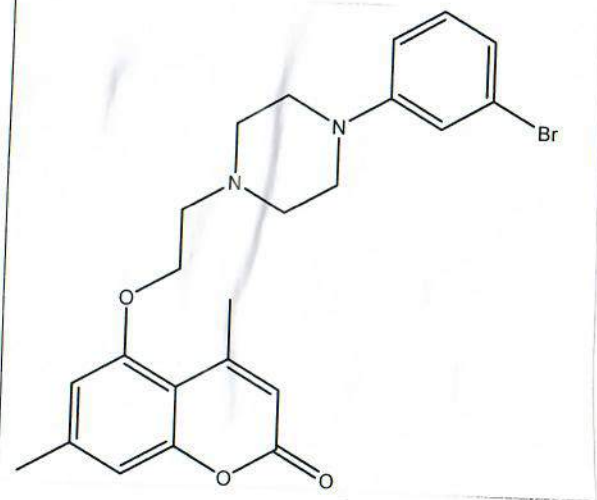
57.11
53.88
51.51
51.40

29.90
29.63
24.81
23.00
22.19



KO-339-1H-cdcl3
KO 339 1H w CDCl3

2g



2g

KO-339-13C
KO 339 13C w CDCl3

161.05
160.88
157.11
155.45
154.29
152.52

143.17

130.66
130.50
123.61
123.40
122.51
119.96
118.88
115.57
114.55
113.67
110.53
108.51
108.25

77.65
77.23
76.81

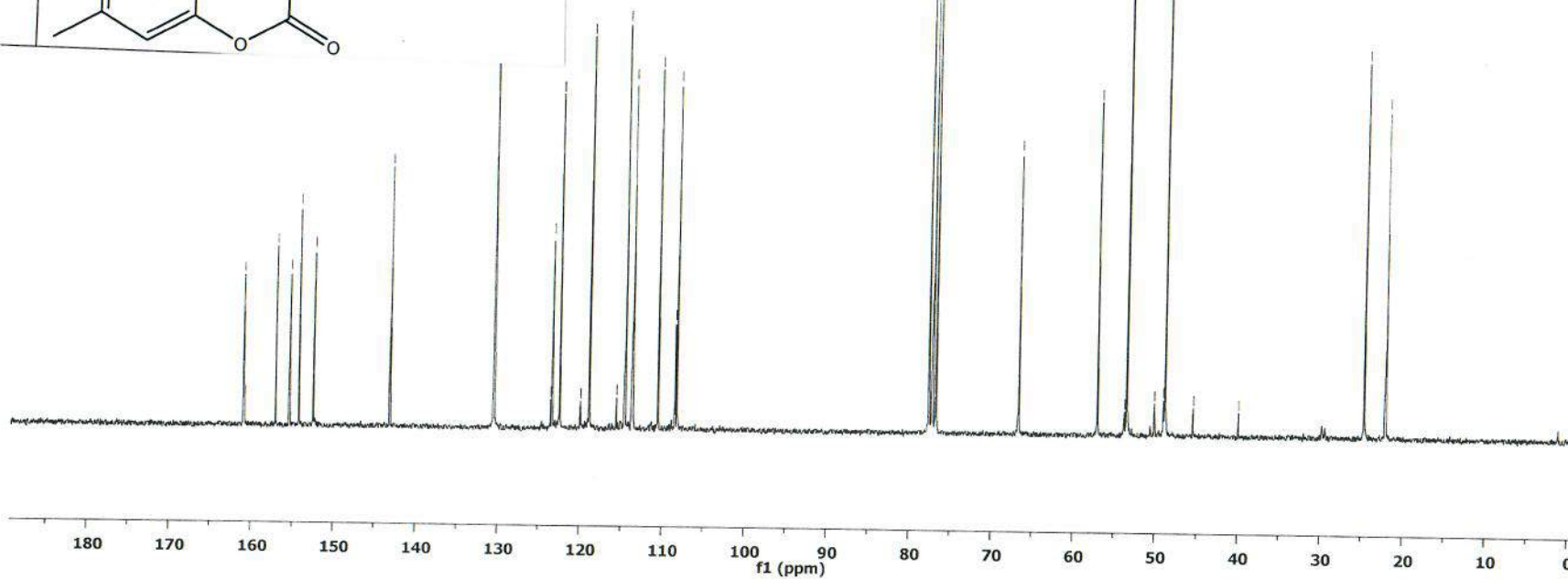
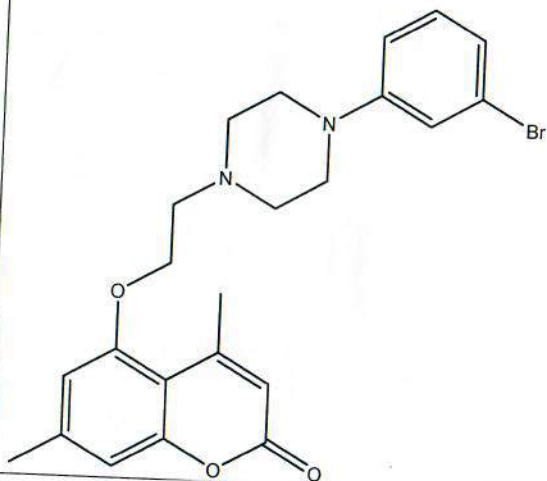
66.72

57.10
53.76
53.50
50.17
49.08
48.89
45.48

39.95

24.72
22.15

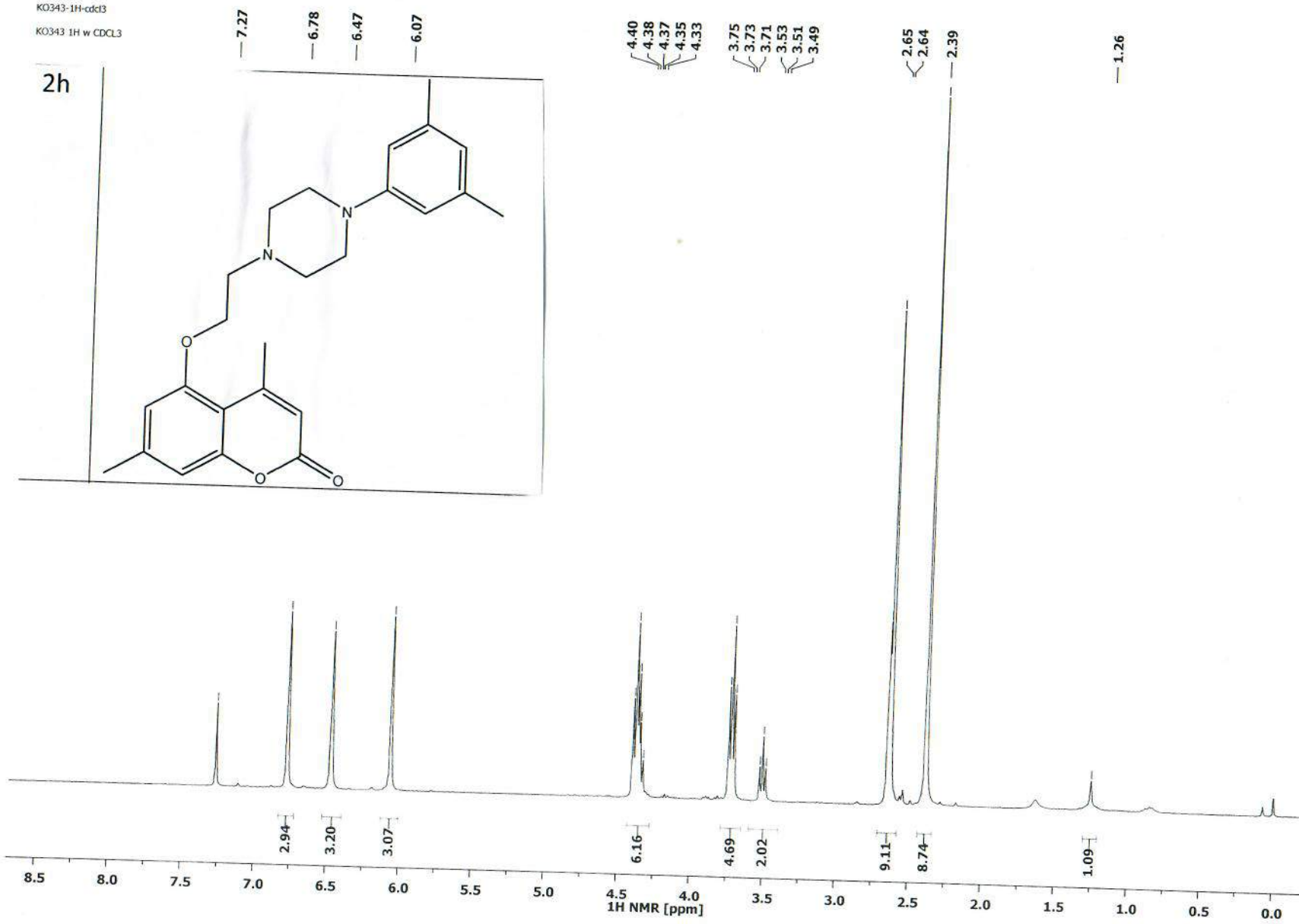
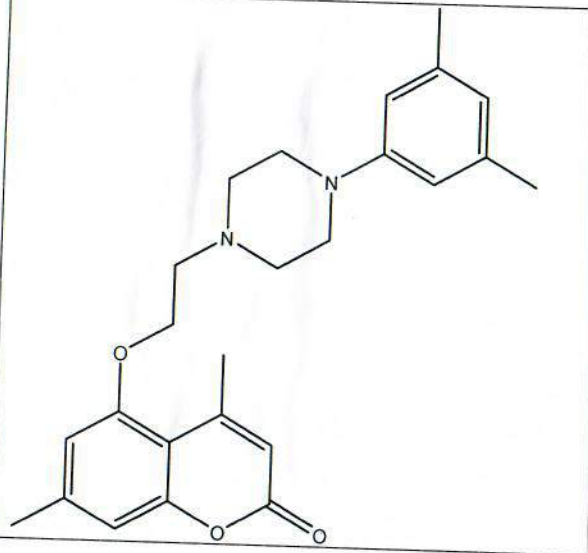
2g



2b

KO343-1H-cdcl3
KO343 1H w CDCL3

2h



2h

KO343-13C-cdCl3

KO 343 13C w CDCl3 13C

160.97
156.38
155.55
154.16
143.18

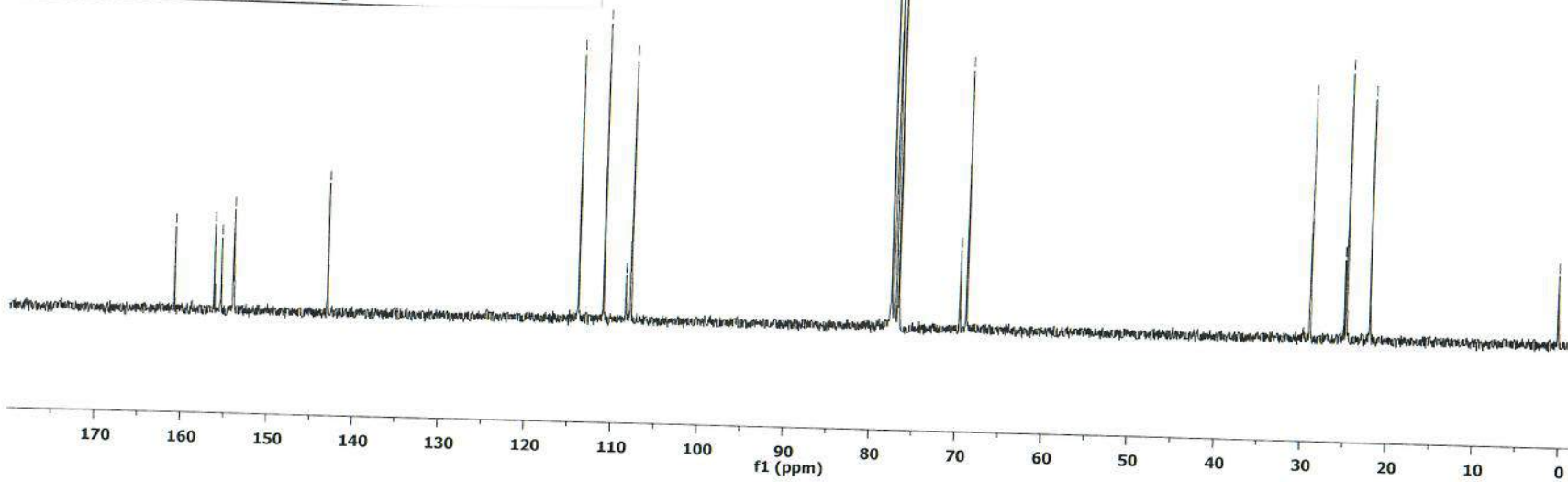
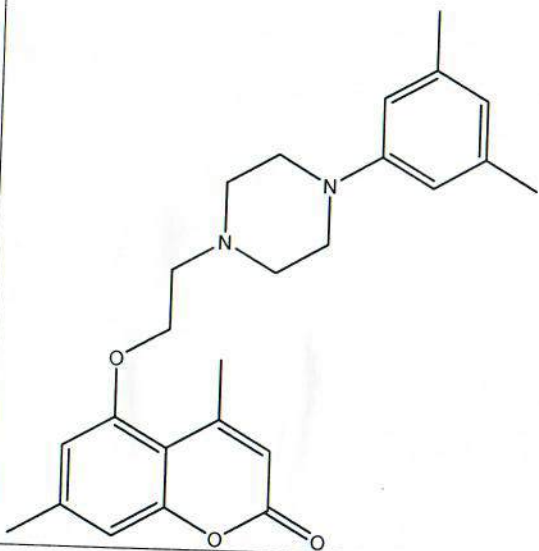
113.97
111.07
108.52
107.98
107.92

77.65
77.23
76.81
69.66
68.83

29.07
25.16
24.85
22.15

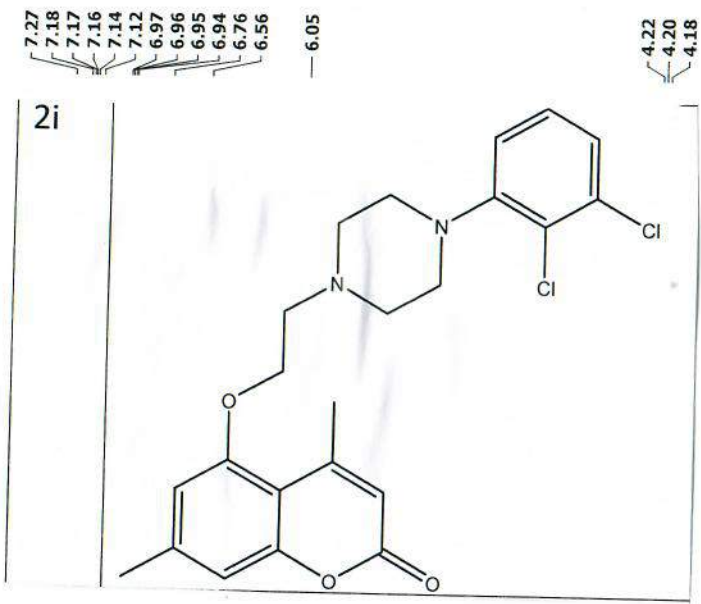
0.35

2h



2i

KO-335-1H-cdcl3
KO-335 1H w CDCl3



7.27
7.18
7.17
7.16
7.14
7.12
6.97
6.96
6.95
6.94
6.76
6.56

6.05

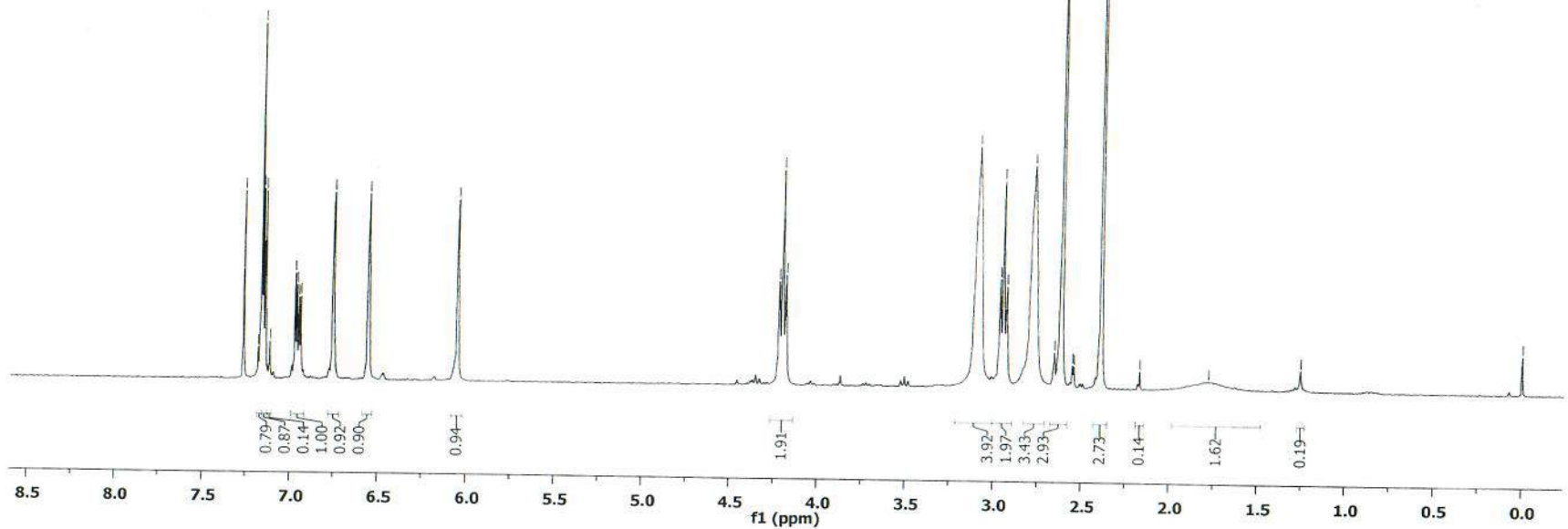
4.22
4.20
4.18

3.09
2.97
2.95
2.93
2.78
2.66
2.62
2.55
2.54
2.39
2.17

1.78

1.25

0.00



KO-335-13C-cde3
KO 335 13C w CDCl3

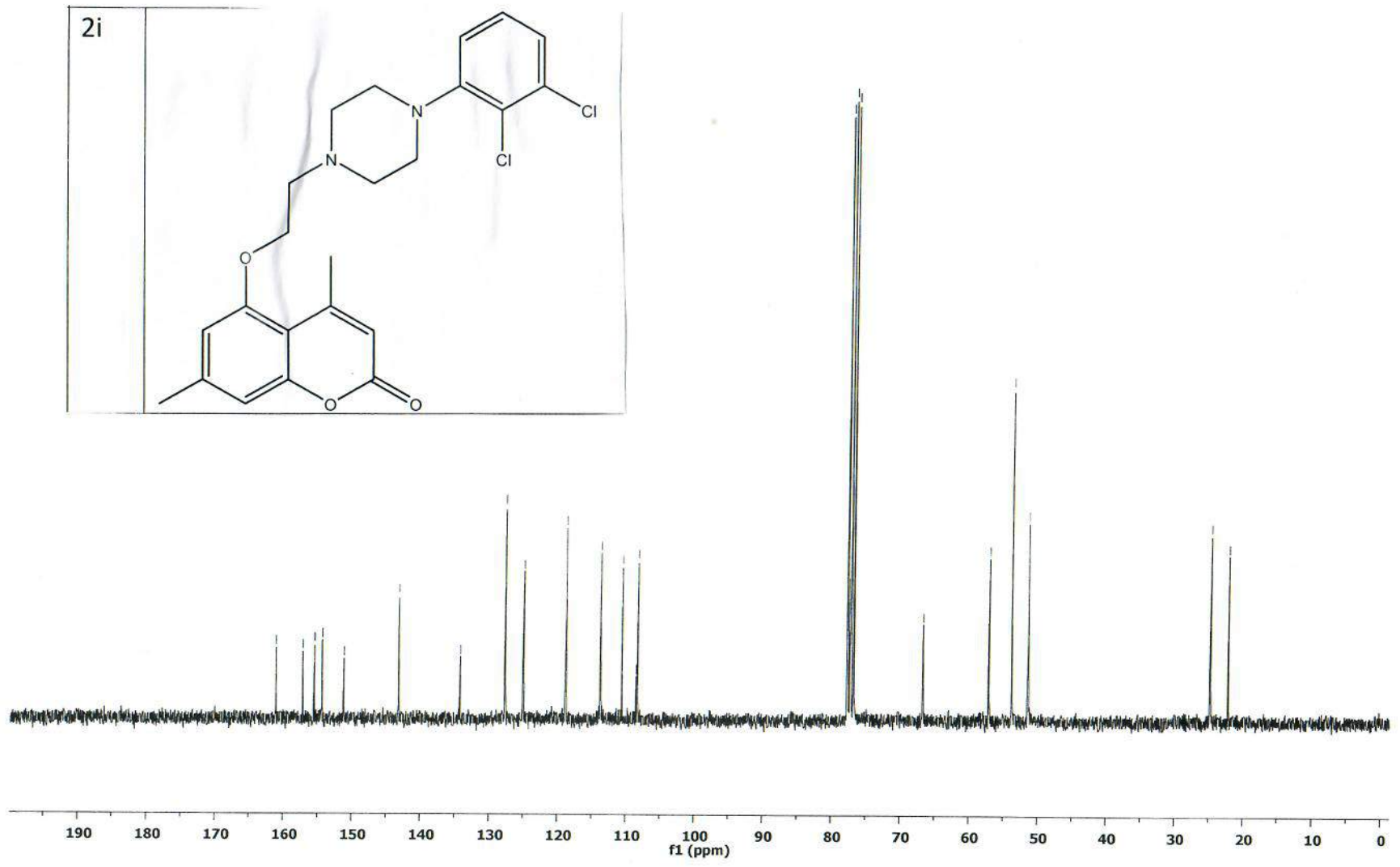
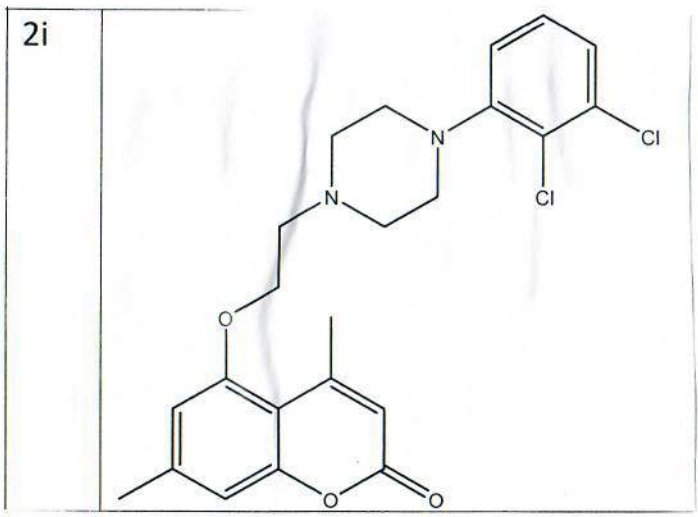
- 161.13
- 157.17
- 155.51
- 154.34
- 151.22
- 143.22
- 134.27
- 127.69
- 124.96
- 118.82
- 113.75
- 110.61
- 108.59
- 108.32

- 77.65
- 77.23
- 76.81

- 66.74

- 57.16
- 53.81
- 51.45

- 24.79
- 22.19



2j

KO-336-1H-cdcl3

KO 336 1H w CDCl3

7.58
7.56
7.53
7.52
7.50
7.47
7.28
7.03
7.02
6.95
6.56
6.05

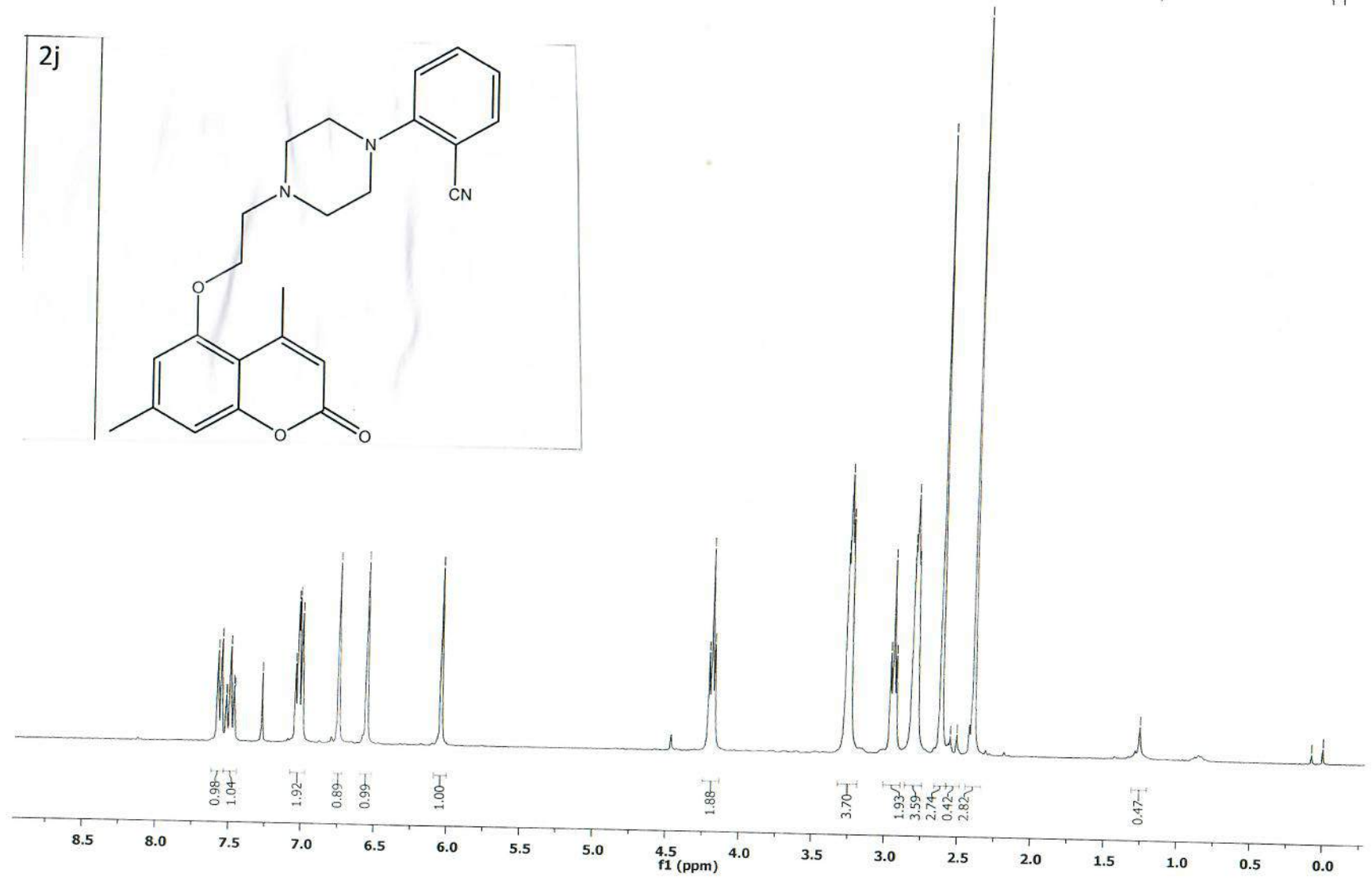
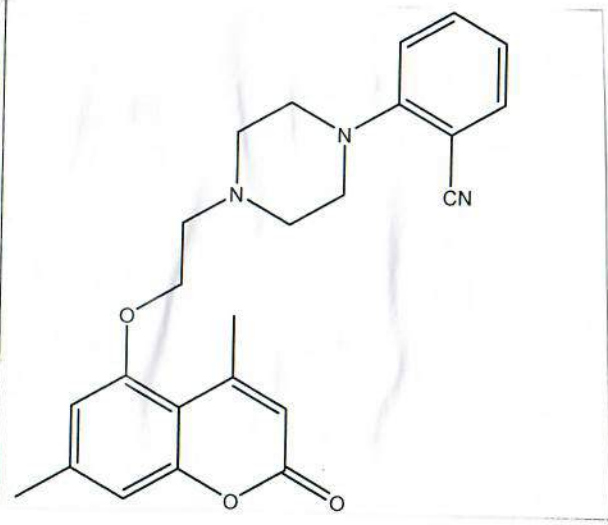
4.22
4.20
4.18

3.28
3.26
3.25
2.97
2.95
2.93
2.82
2.81
2.79
2.62
2.56
2.51
2.40

1.26

0.08
0.01

2j



2j

KO-336-13C-cdcl3
KO 336 13C w CDCl3

161.08
157.16
155.71
155.46
154.35

143.18
134.50
134.00

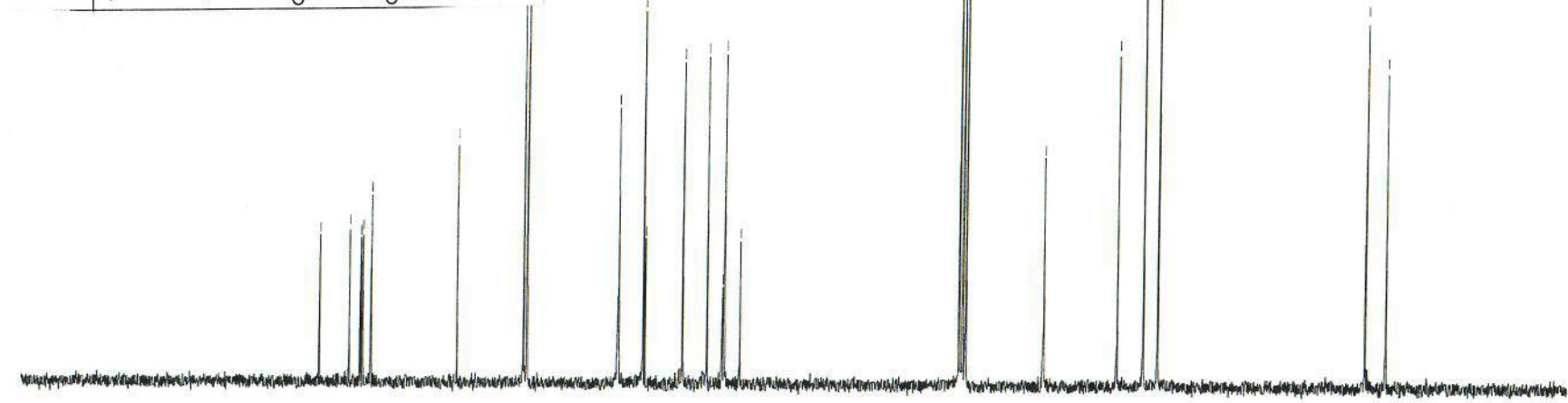
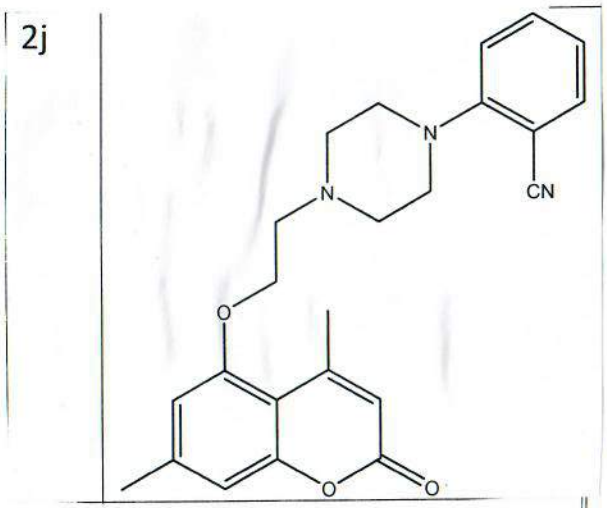
122.10
118.86
118.57
113.67
110.53
108.55
108.28
106.25

77.65
77.23
76.81

66.65

57.03
53.61
51.72

24.74
22.15

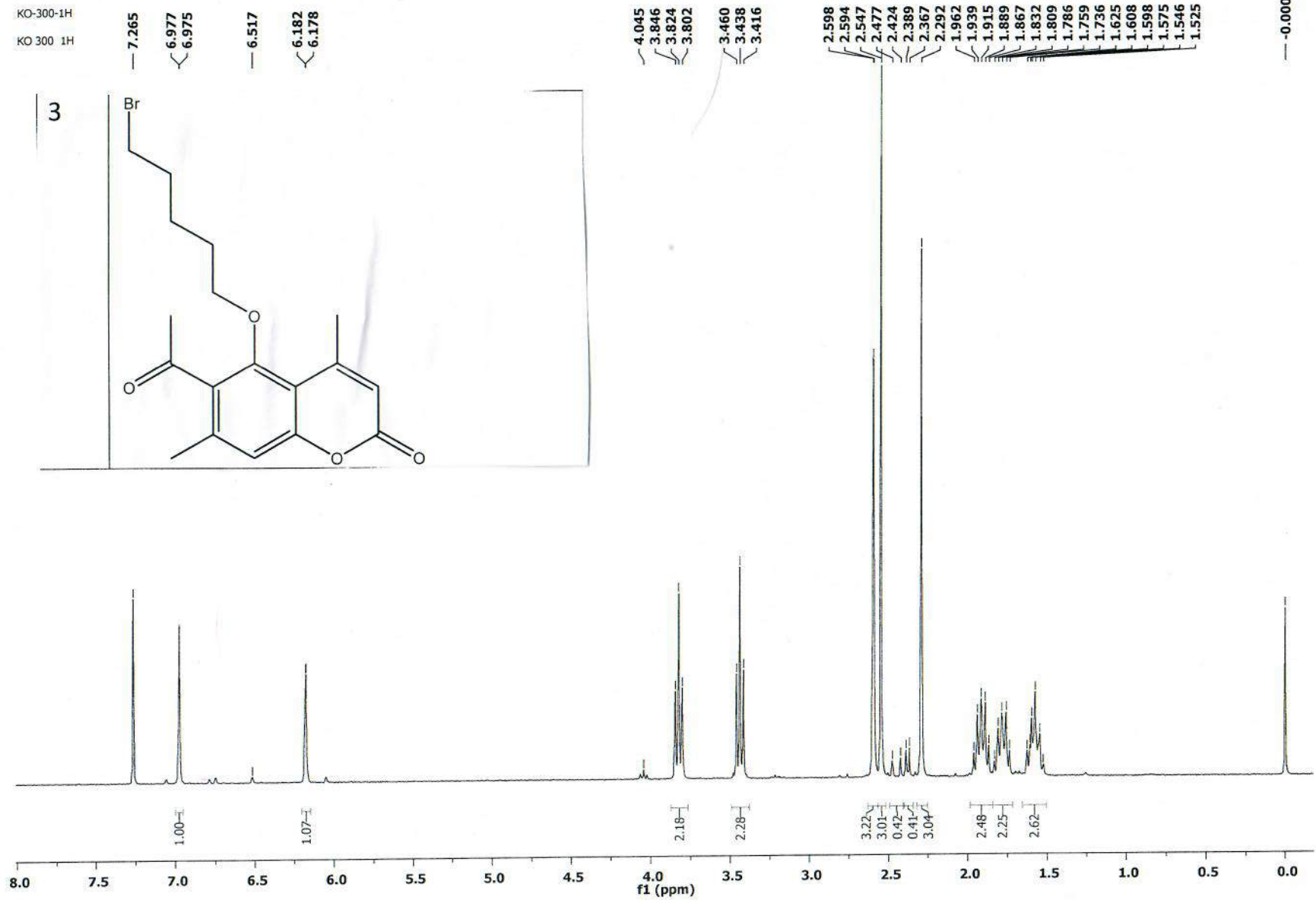
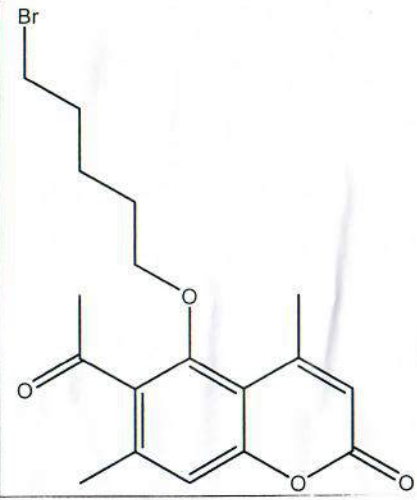


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

KO-300-1H
KO 300 1H

3



KO-300b-13C
KO 300b 13C

— 204.70

— 160.18
— 154.86
— 154.34
— 152.20

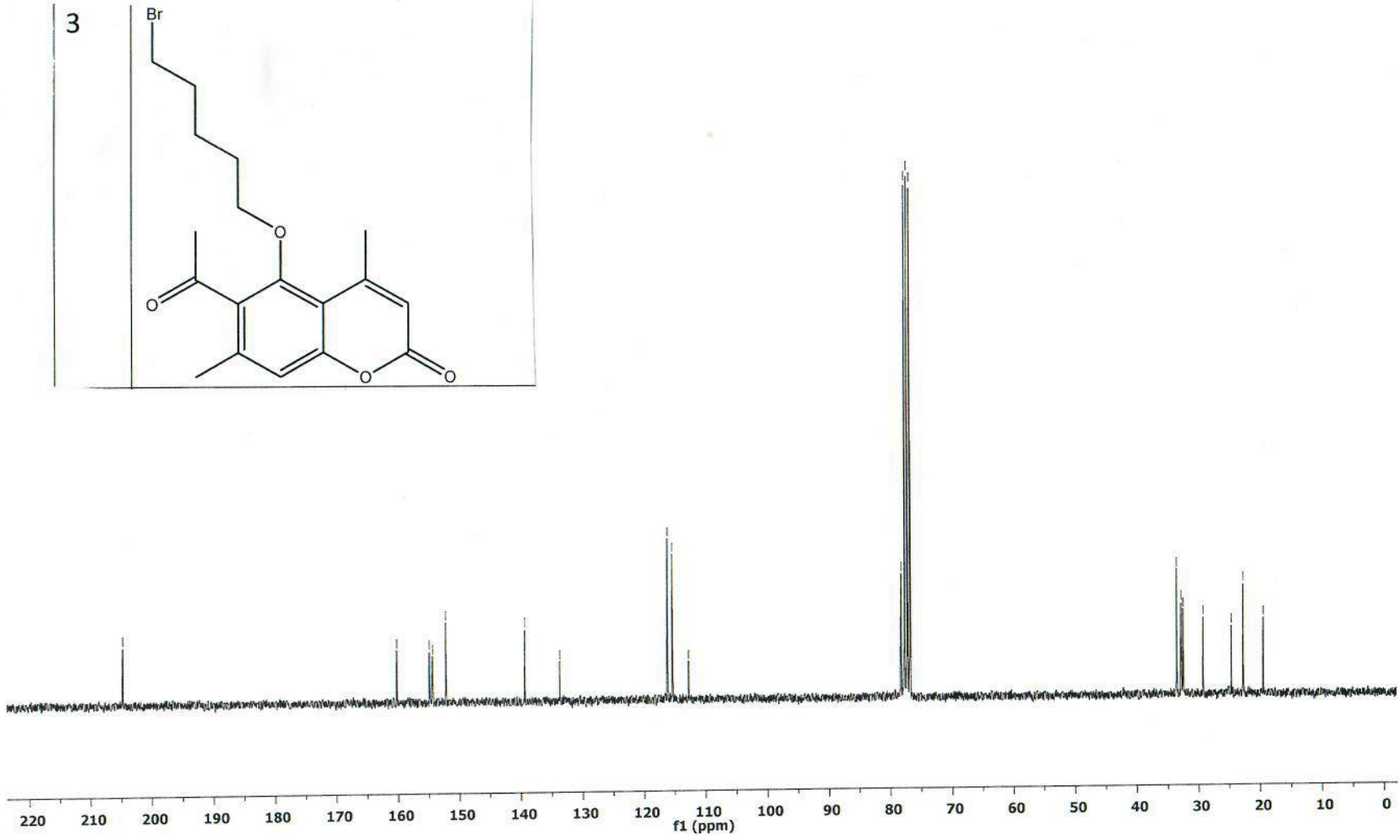
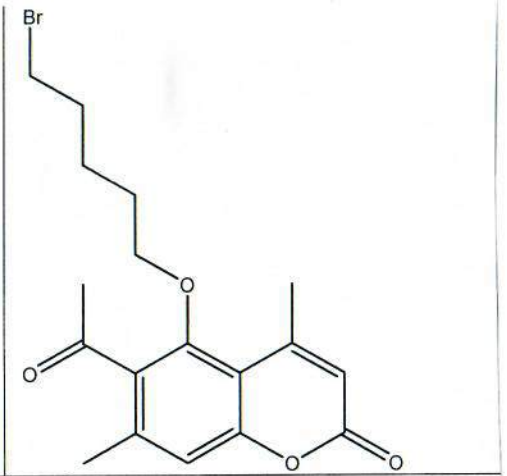
— 139.35
— 133.71

— 116.14
— 115.37
— 112.71

78.24
77.65
77.23
76.81

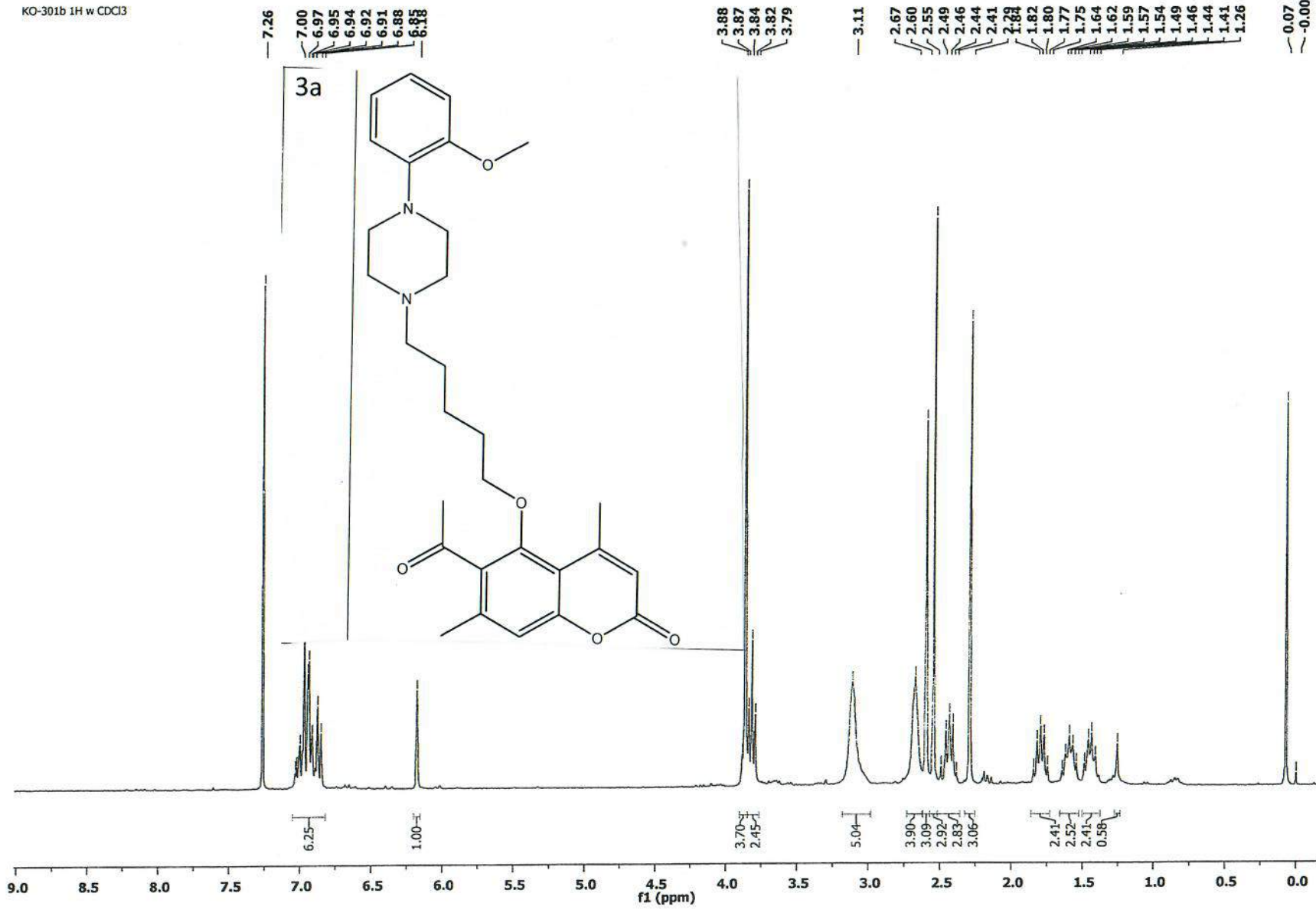
33.56
32.79
32.49
29.22
24.68
22.73
19.50

3



3a

KO-301b 1H w CDCl3



3a

301b
KO-301b-13C
204.69
KO 301b 13C w CDCl3

160.23
154.89
154.56
152.46
152.31

141.41
139.42
133.65

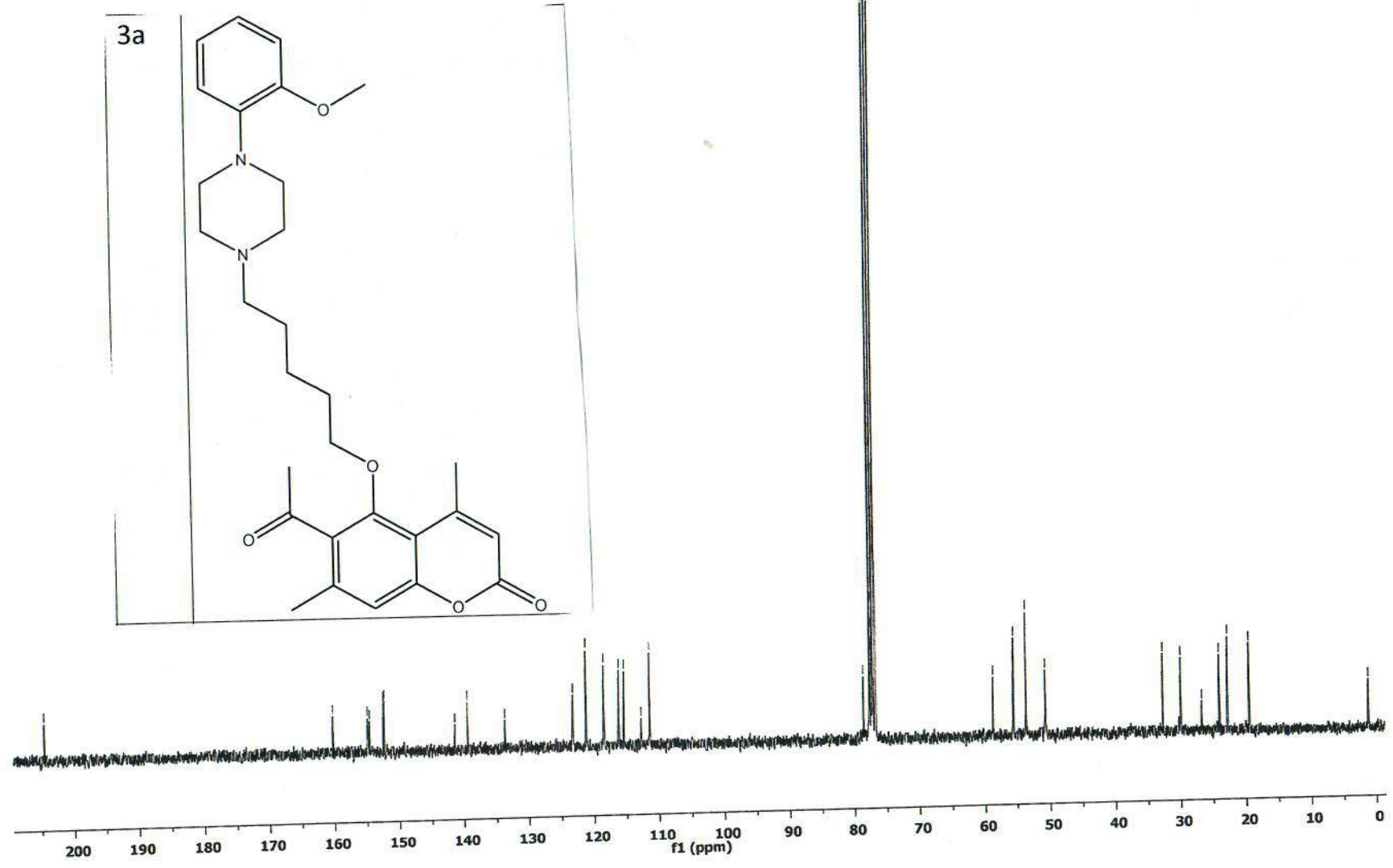
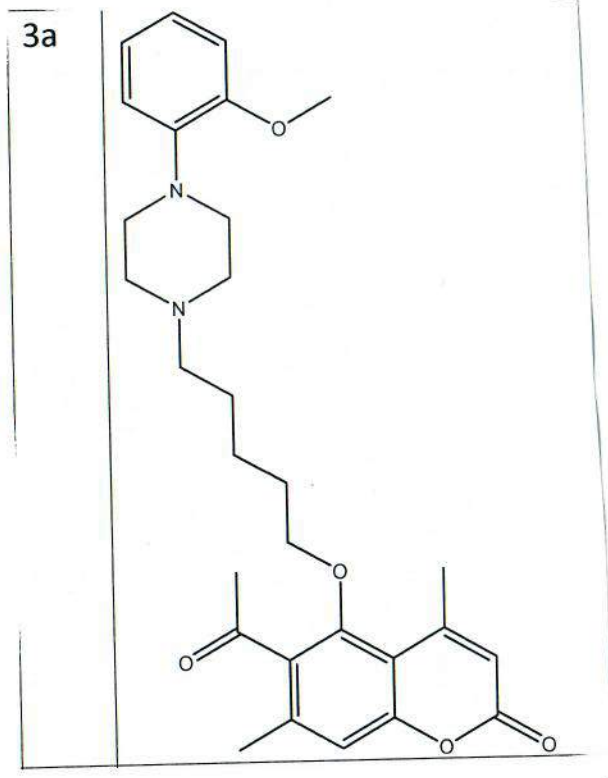
123.21
121.21
118.44
116.10
115.31
112.73
111.38

78.57
77.65
77.23
76.81

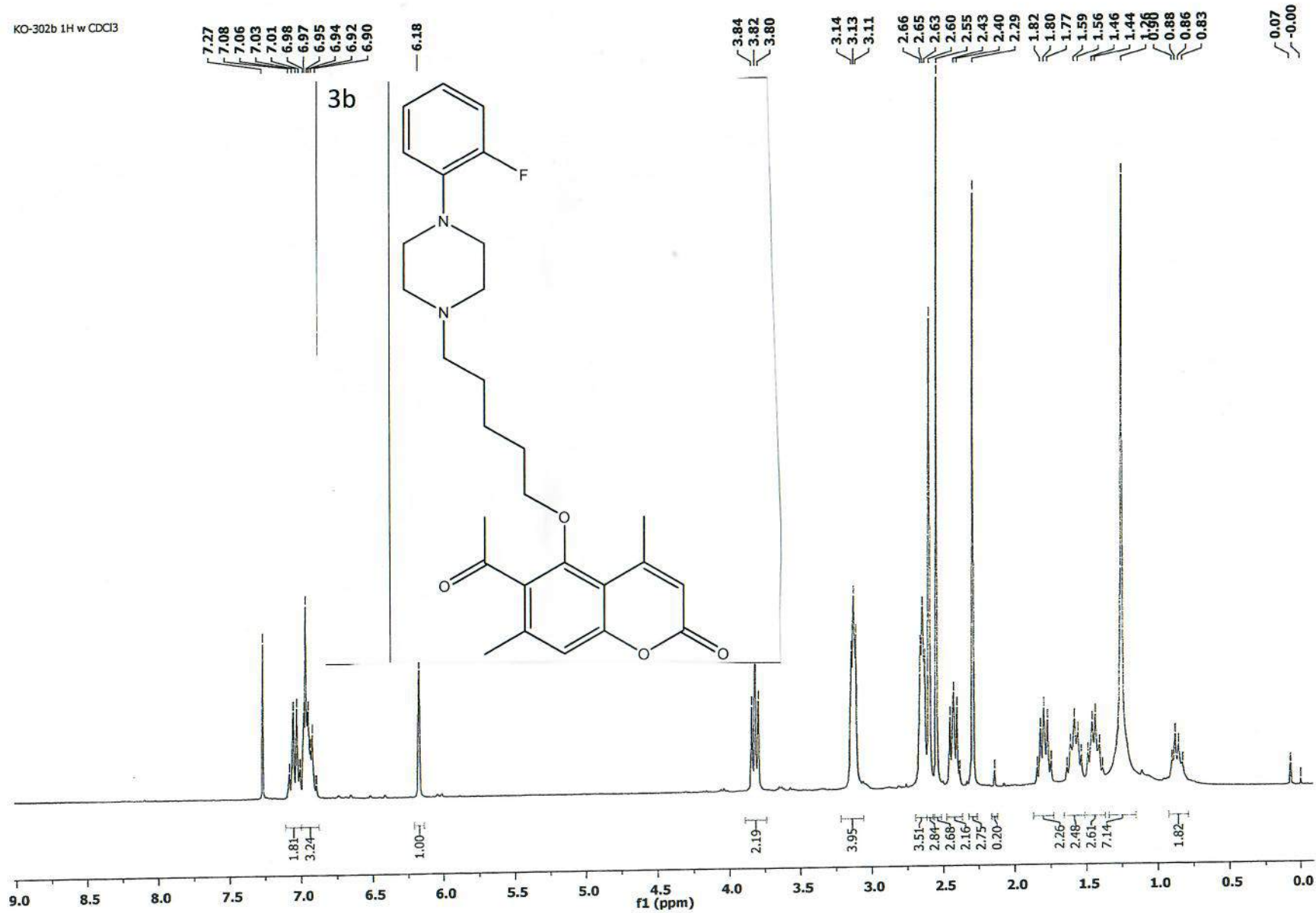
58.68
55.57
53.68
50.70

32.74
30.00
26.72
24.04
22.77
19.55

1.23



KO-302b 1H w CDCl3



3b

KO-302b-13C
KO 302b 13C w CDCl3

204.63

160.20
157.55
154.87
154.54
154.29
152.29

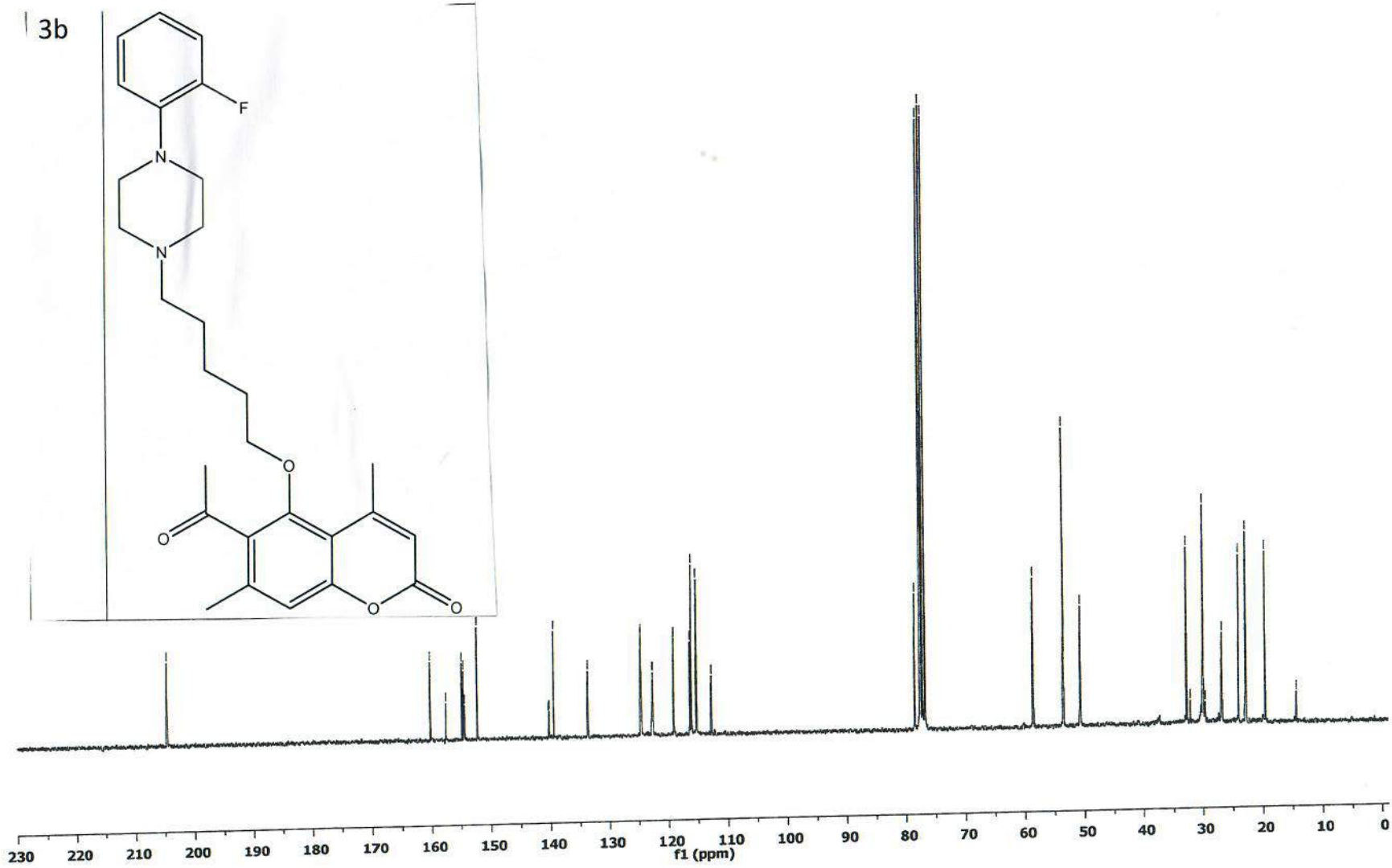
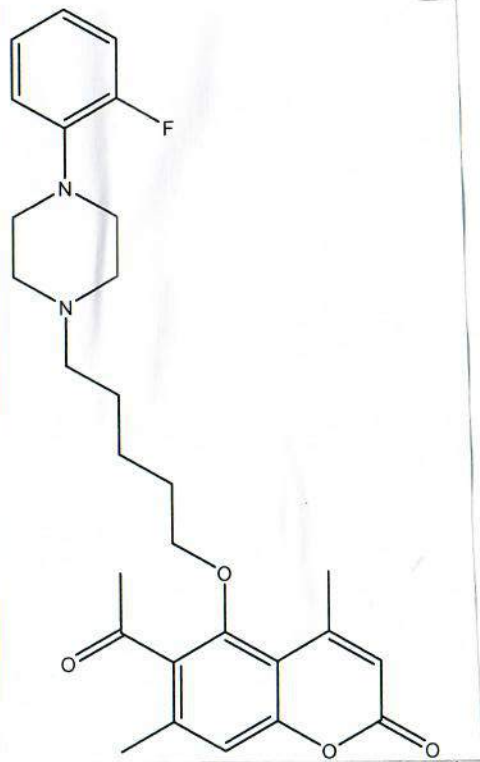
140.34
140.22
139.41
133.64
124.68
124.63
122.70
122.60
119.12
119.08
116.42
116.14
116.08
115.30
112.71

78.55
77.65
77.43
77.23
76.81

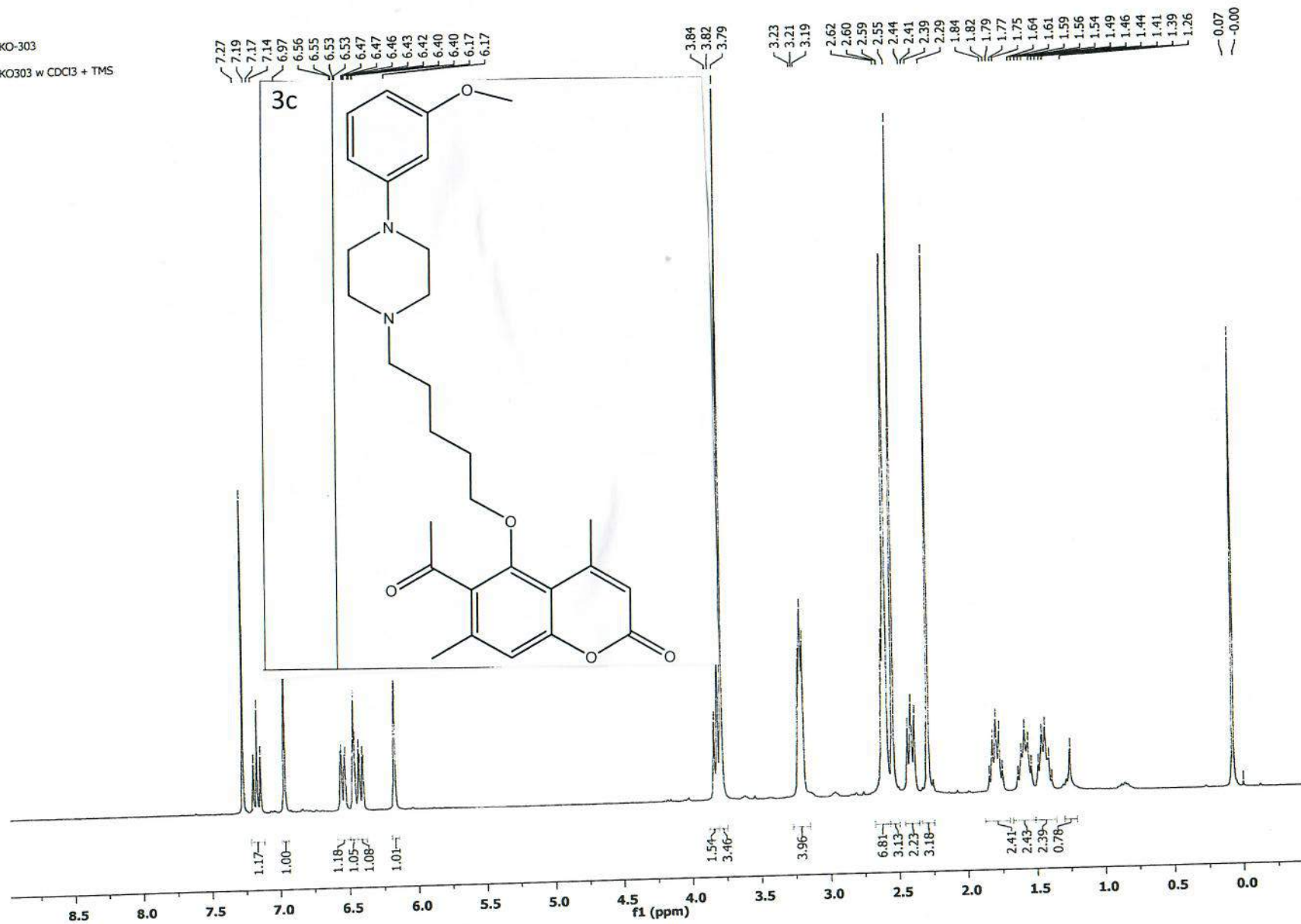
58.63
53.53
50.69
50.64

32.73
32.13
29.98
29.90
29.56
26.77
24.00
22.89
22.75
19.54
14.33

3b



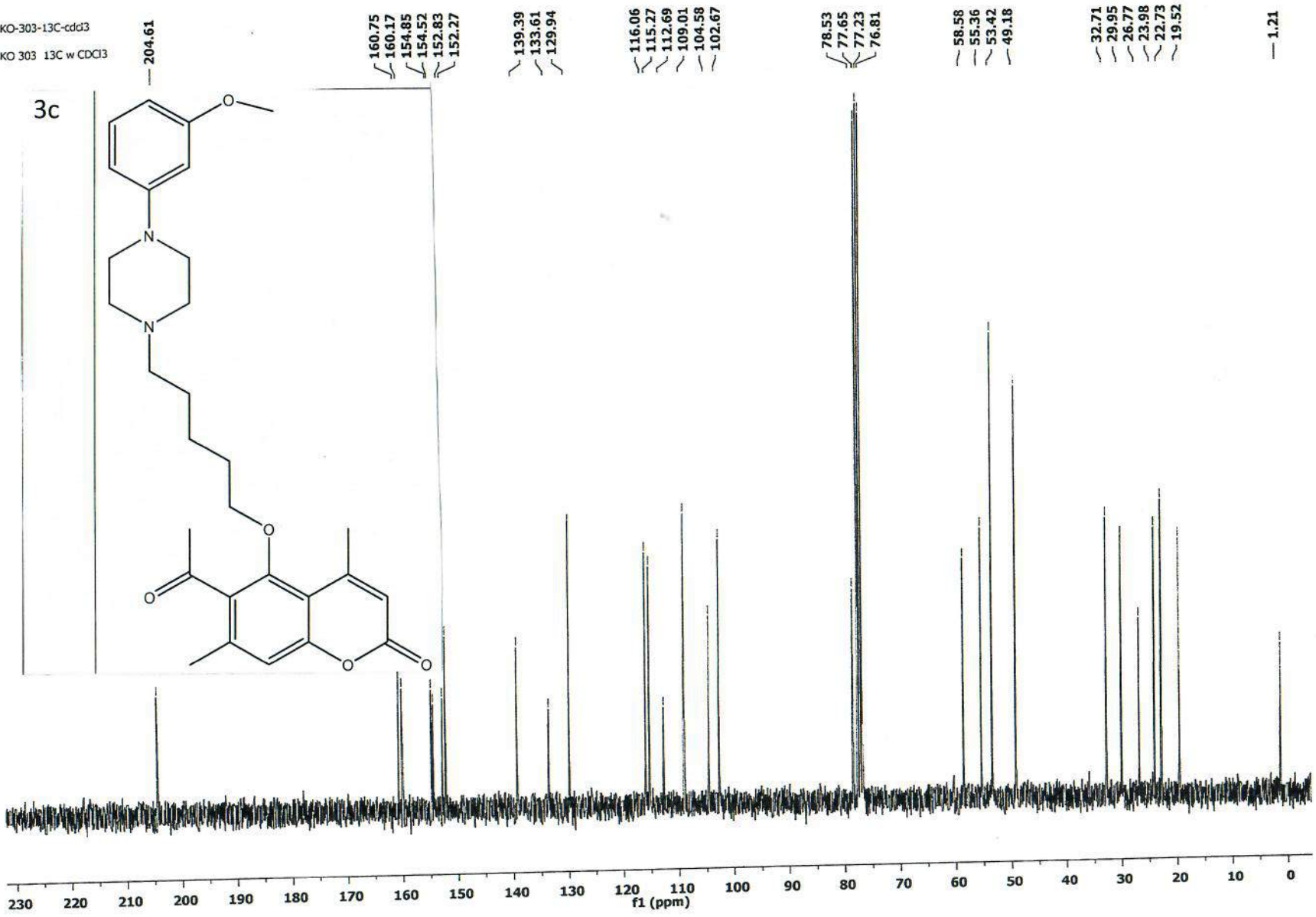
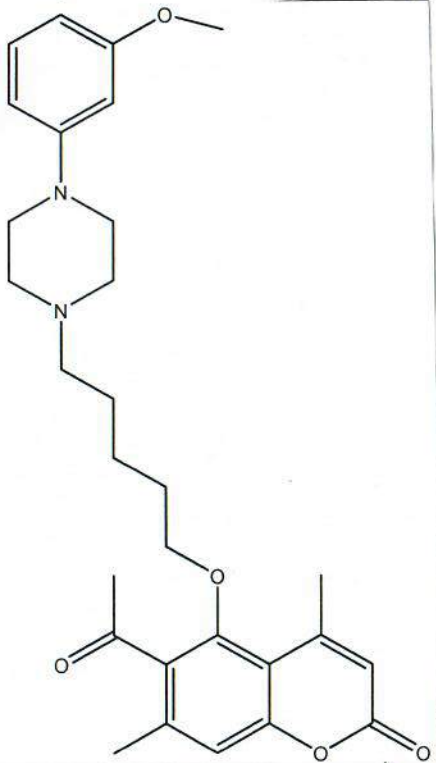
KO-303
KO303 w CDCl3 + TMS



3c

KO-303-13C-cdd3
KO 303 13C w CDCl3

3c





KO-304
KO304 w CDCl3 + TMS

7.26
7.06
7.04
6.97
6.83
6.80
6.78

6.18
6.17

3.85
3.82
3.80

2.96
2.94
2.93

2.60

2.55

2.43

2.40

2.29

2.15

1.83

1.80

1.78

1.75

1.64

1.62

1.59

1.57

1.54

1.49

1.47

1.44

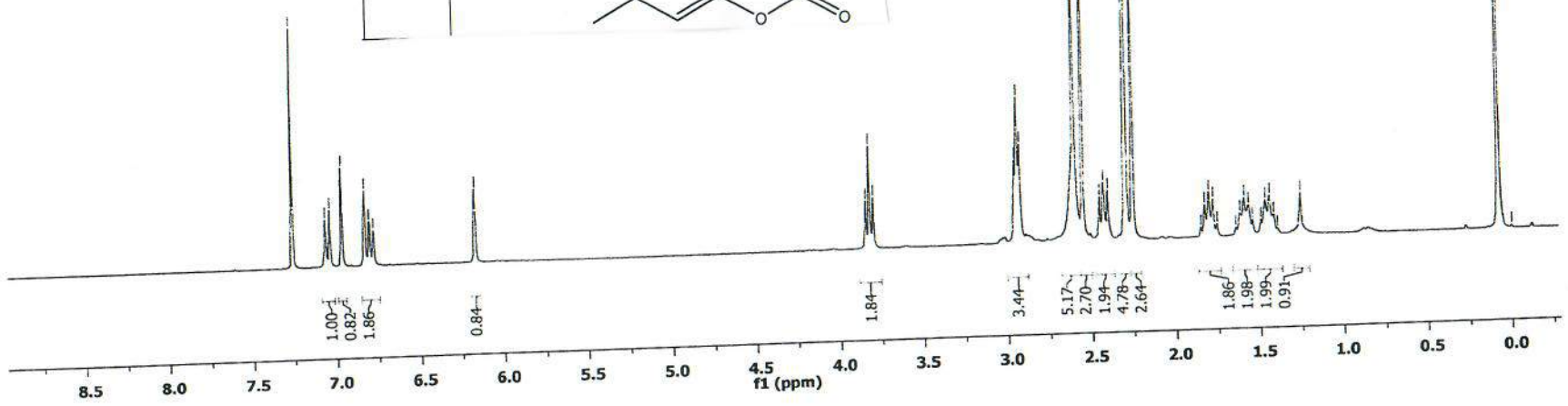
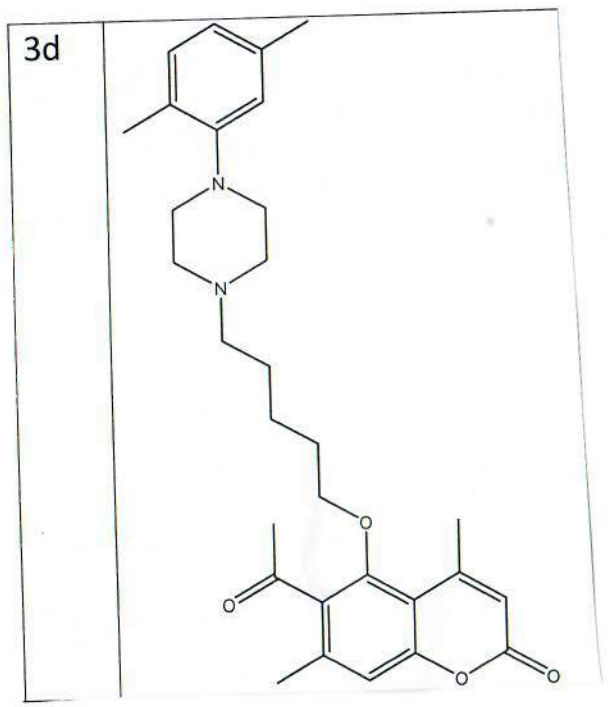
1.42

1.39

1.26

0.08
0.00

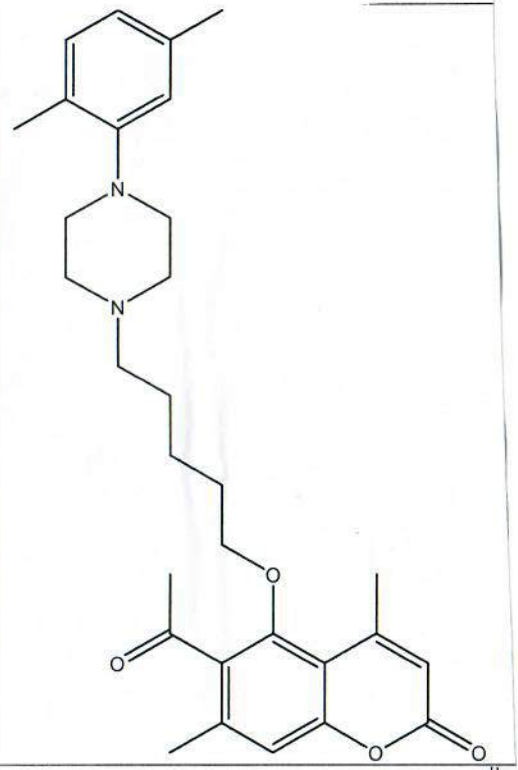
3d



3d

KO-304-13C-cdcl3
KO 304 13C w CDCl3

3d



204.60

160.17
154.85
154.56
152.29
151.47

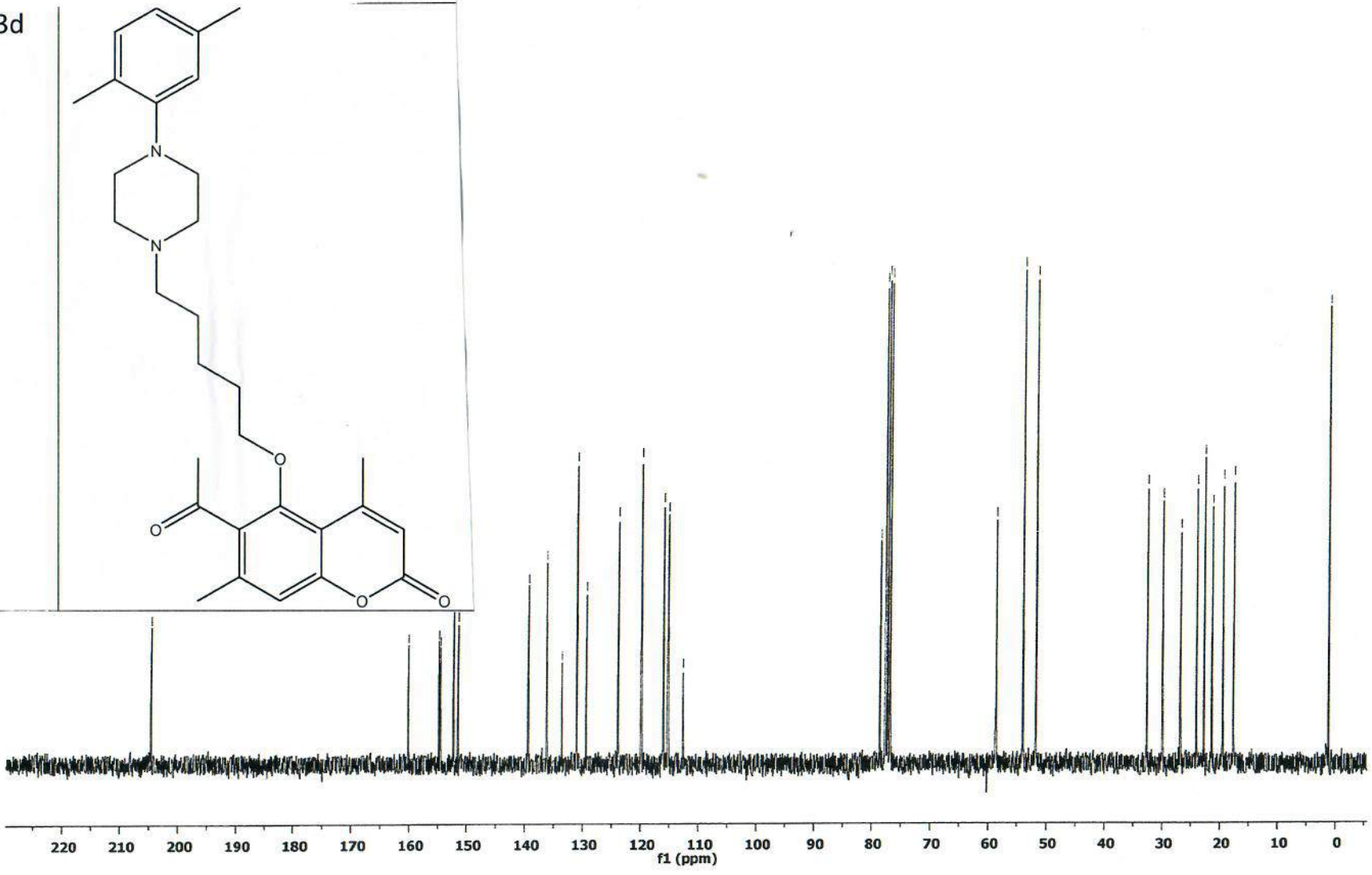
139.40
136.25
133.60
131.02
129.40
123.89
119.88
116.05
115.26
112.69

78.56
77.65
77.23
76.81

58.70
54.00
51.84

32.70
29.99
26.85
24.02
22.75
21.39
19.52
17.65

1.20



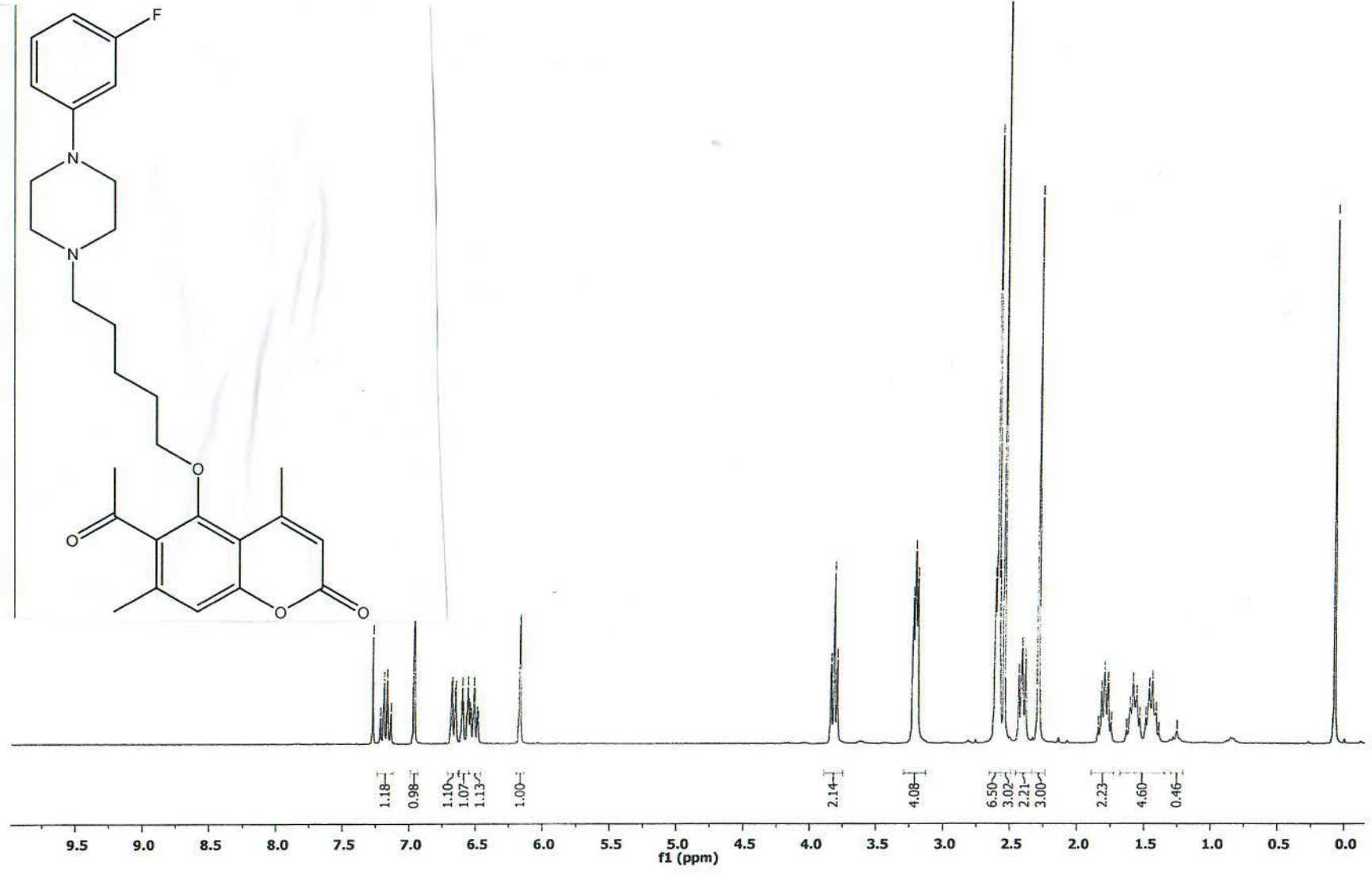
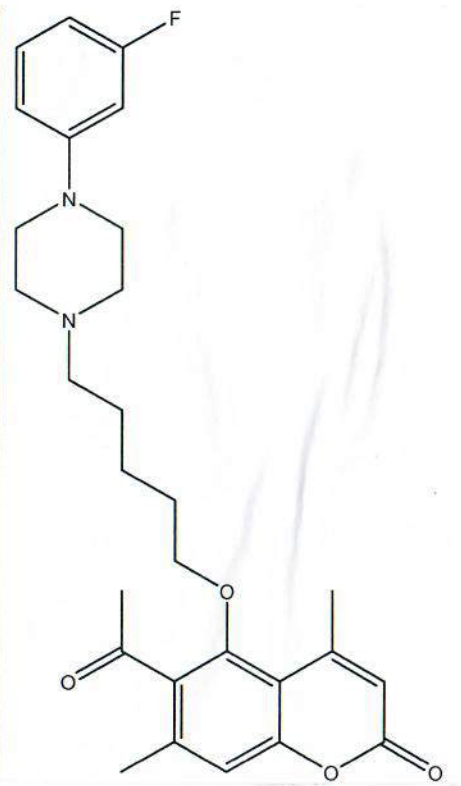


KO-305-1H-cdcl3
KO 305 1H w CDCl3

7.27
7.22
7.19
7.17
7.14
6.97
6.96
6.68
6.60
6.56
6.55
6.52
6.17

3.84
3.82
3.80
3.23
3.21
3.20
2.62
2.60
2.58
2.55
2.41
2.39
2.29
1.84
1.82
1.80
1.77
1.75
1.63
1.61
1.58
1.56
1.53
1.49
1.46
1.44
1.41
0.08

3e

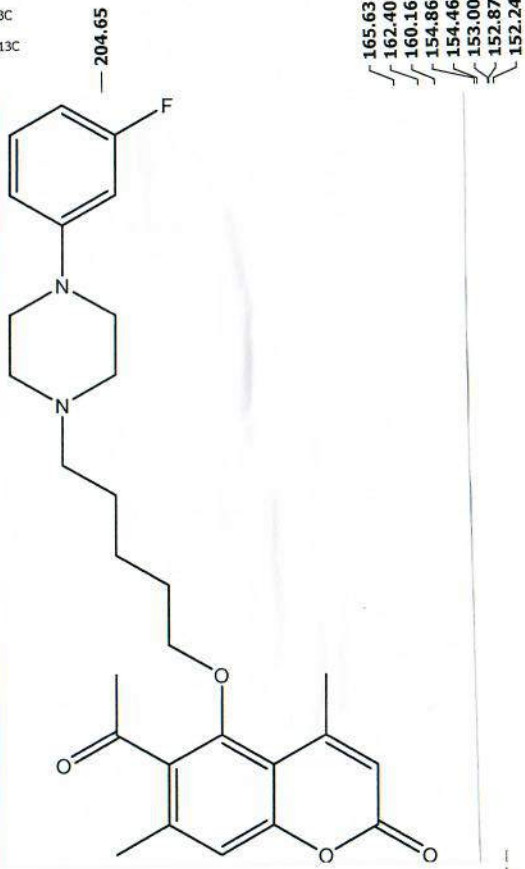


3e

3e

KO-305-13C
KO 305 13C

3e



- 165.63
- 162.40
- 160.16
- 154.86
- 154.46
- 153.00
- 152.87
- 152.24

- 139.36
- 133.64
- 130.38
- 130.25

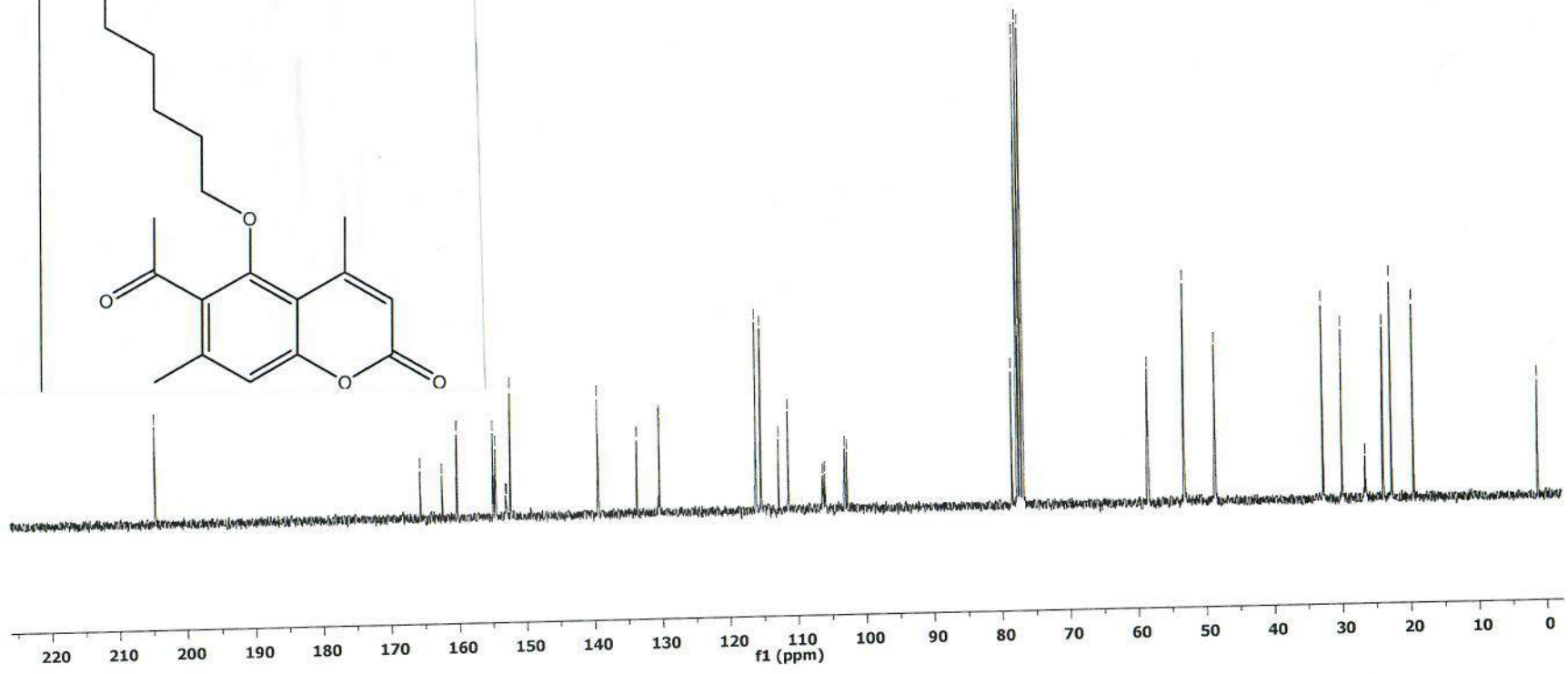
- 116.09
- 115.30
- 112.70
- 111.33
- 106.30
- 106.02
- 103.08
- 102.75

- 78.45
- 77.65
- 77.23
- 76.81

- 58.45
- 53.13
- 48.58

- 32.74
- 29.89
- 26.50
- 23.89
- 22.72
- 19.50

- 1.21



3f

KO-306-1H-cdcl3

KO 306 1H w CDCl3

7.57
7.57
7.54
7.54
7.30
7.29
7.27
7.25
7.24
7.08
7.08
7.05
7.05
6.97
6.94
6.93
6.91
6.89
6.88
6.18

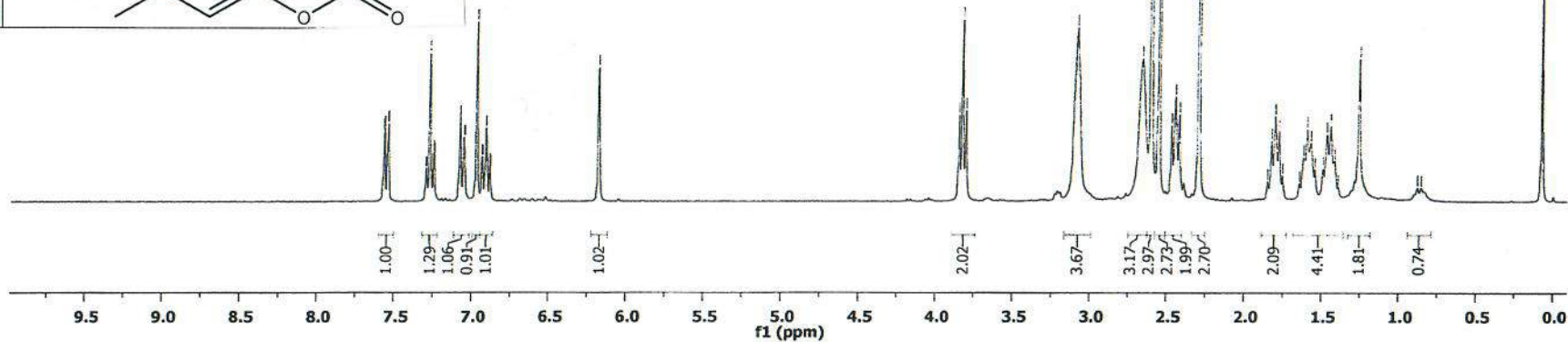
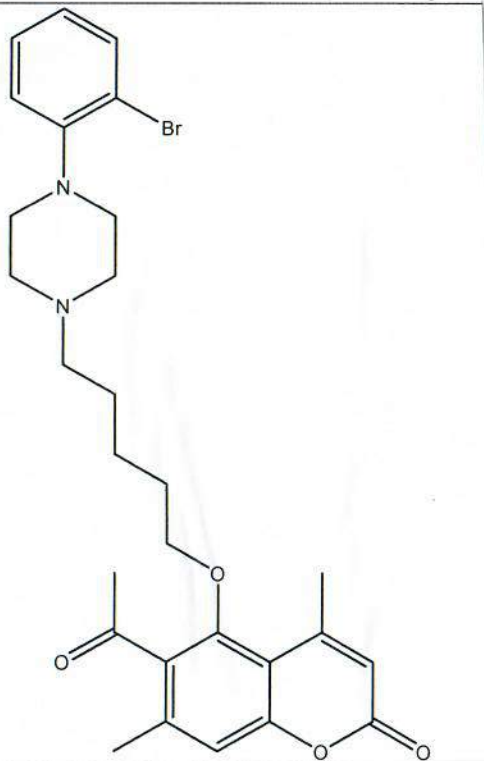
3.85
3.82
3.80

3.09
2.66
2.60
2.55
2.47
2.44
2.42
2.29

1.83
1.80
1.78
1.60
1.57
1.47
1.44
0.88
0.86

0.08

3f



3f

KO-306-13C-cdcl3
KO 306 13C

204.63

160.17
154.85
154.49
152.26
150.56

139.37
133.99
133.62
128.50
124.68
121.15
120.03
116.07
115.28
112.70

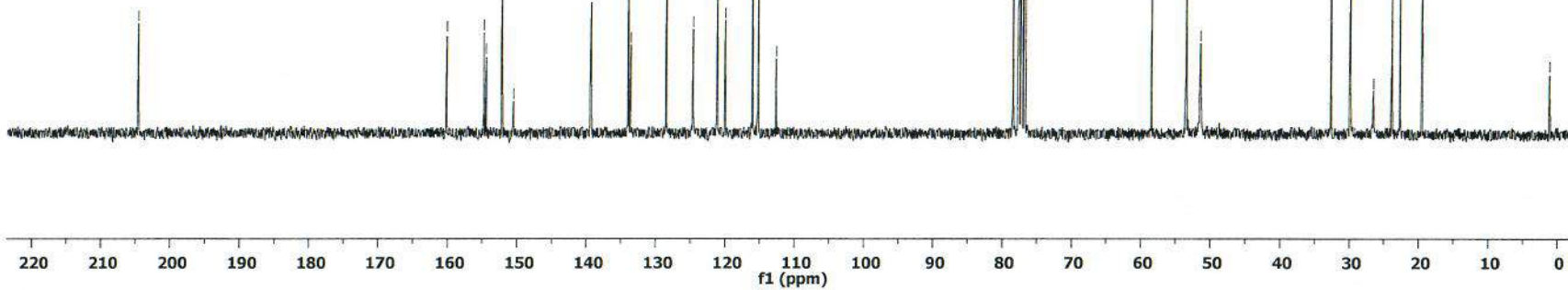
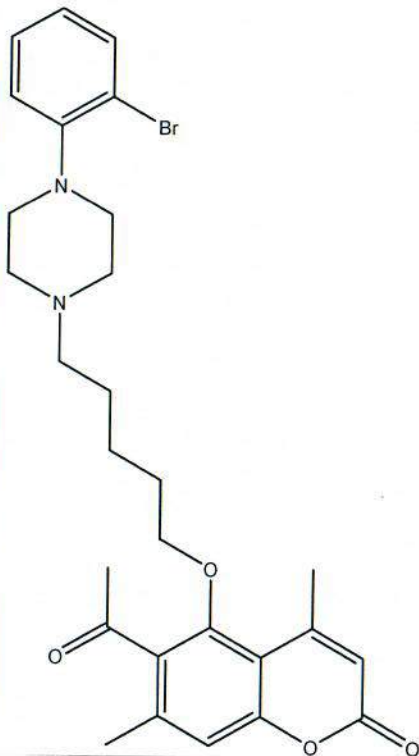
78.48
77.65
77.23
76.81

58.51
53.53
51.48

32.73
29.92
26.54
23.94
22.74
19.52

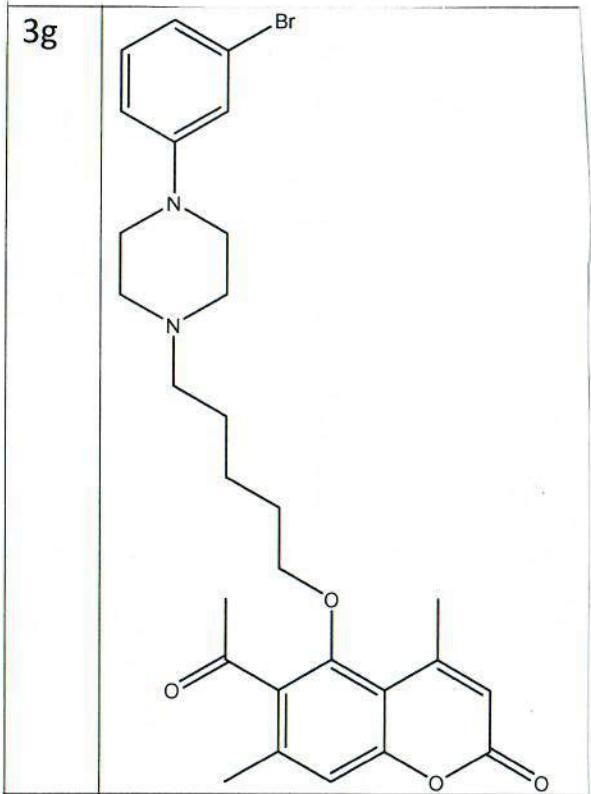
1.20

3f



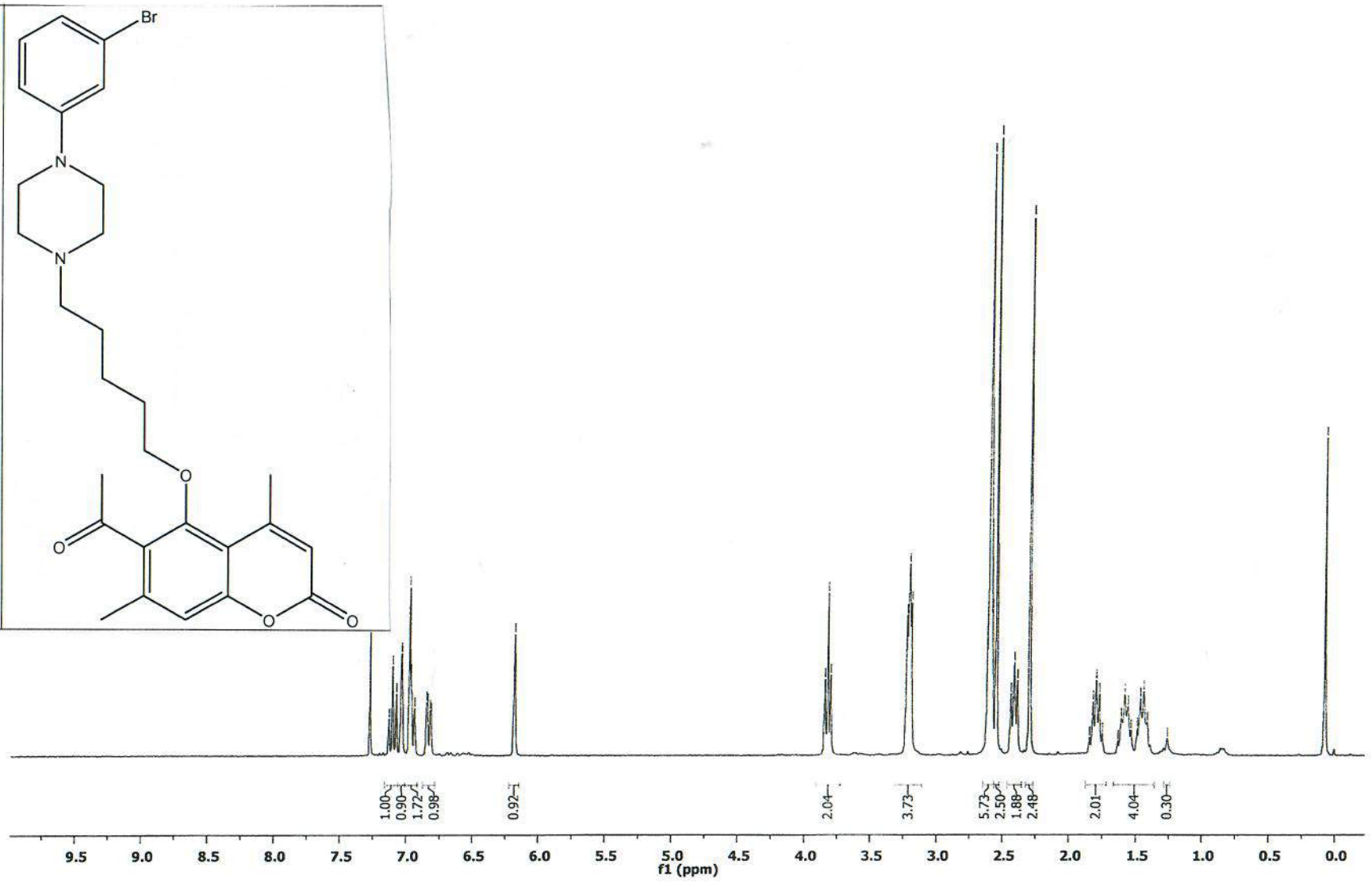
3g

KO-307-1H-cdcl3
KO 307 1H w CDCl3



7.27
7.13
7.10
7.08
7.04
6.98
6.97
6.94
6.85
6.84
6.82
6.81
6.18

3.85
3.82
3.80
3.23
3.21
3.20
2.60
2.58
2.55
2.44
2.41
2.39
2.30
1.85
1.82
1.80
1.78
1.75
1.64
1.61
1.59
1.56
1.54
1.49
1.47
1.44
1.42
1.26
0.08

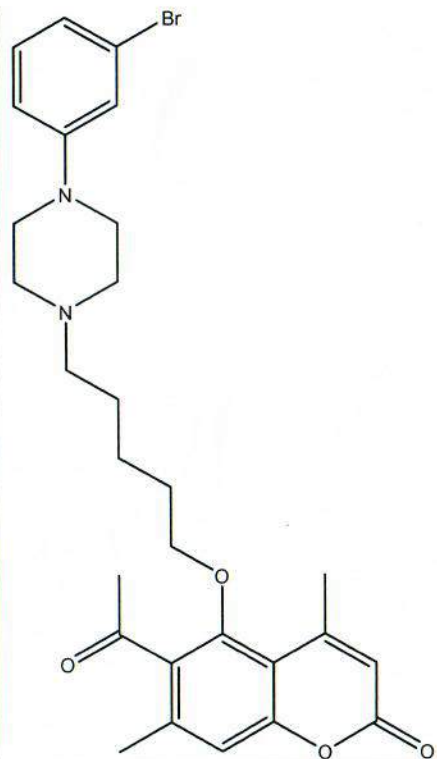


3g

KO-307-13C
KO 307 13C

— 204.65

3g



— 160.17
— 154.85
— 154.45
— 152.24

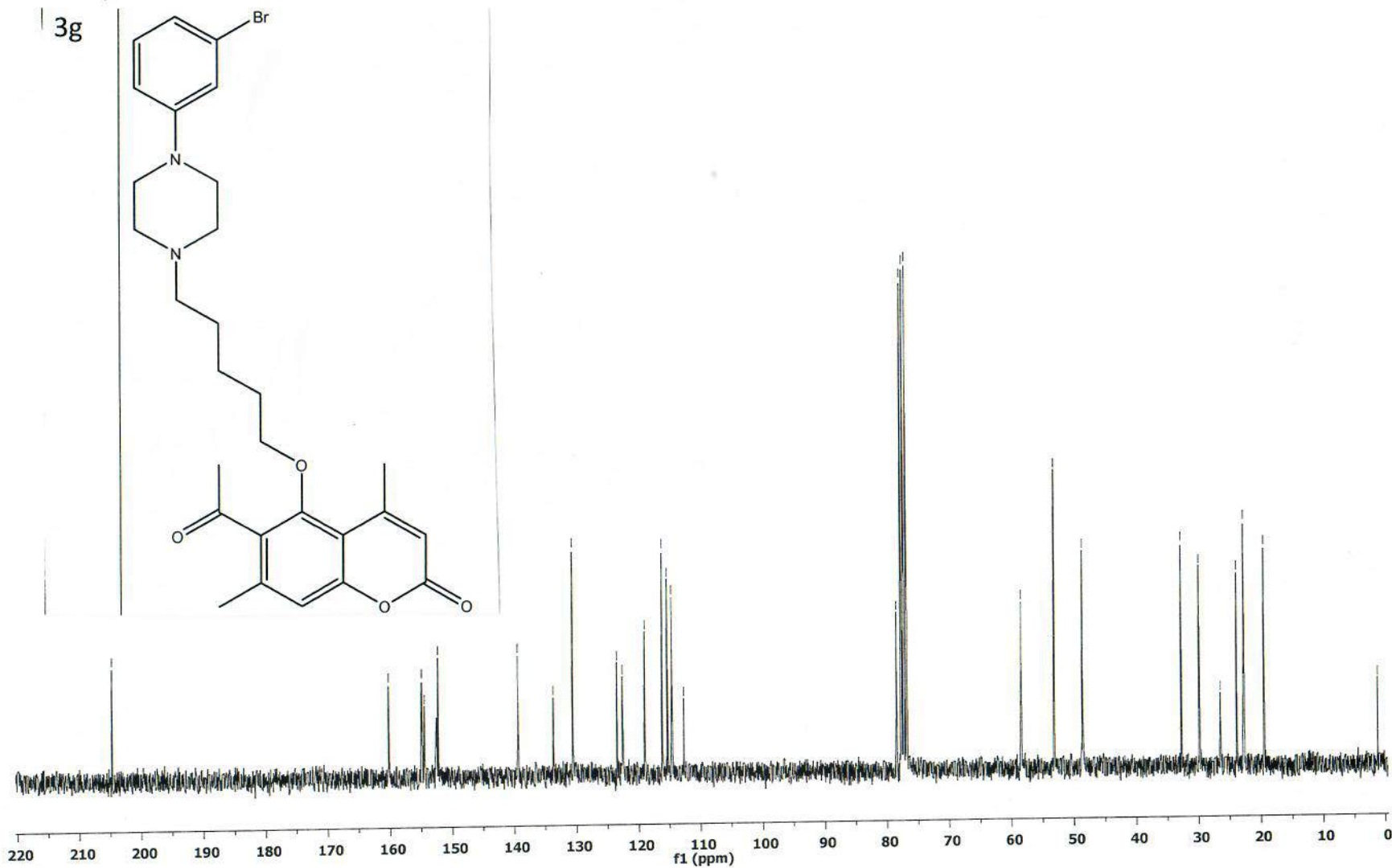
— 139.36
— 133.64
— 130.53
— 123.43
— 122.57
— 118.96
— 116.09
— 115.30
— 114.58
— 112.70

78.44
77.65
77.23
76.81

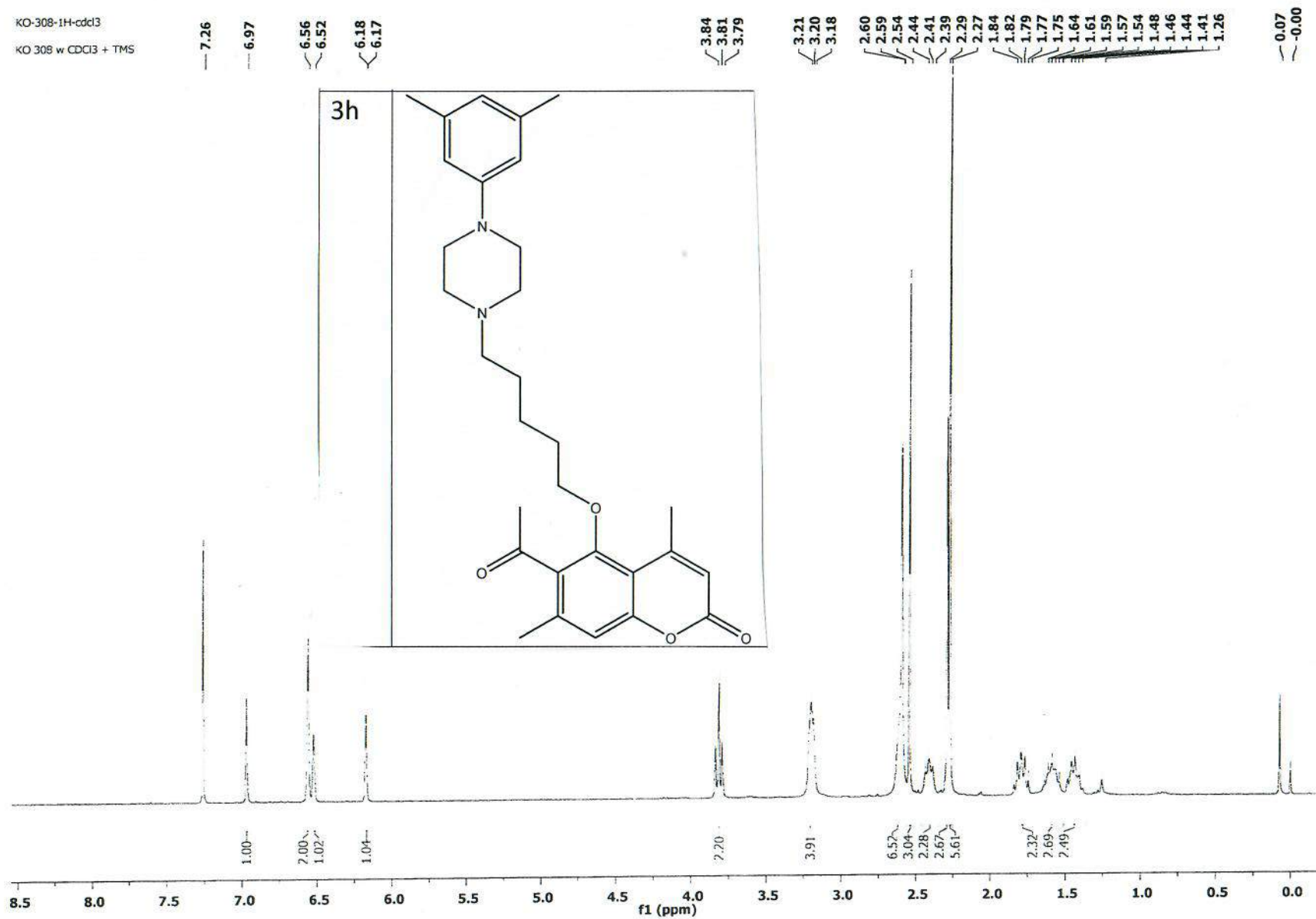
58.43
53.12
48.60

32.75
29.88
26.46
23.88
22.72
19.51

— 1.21

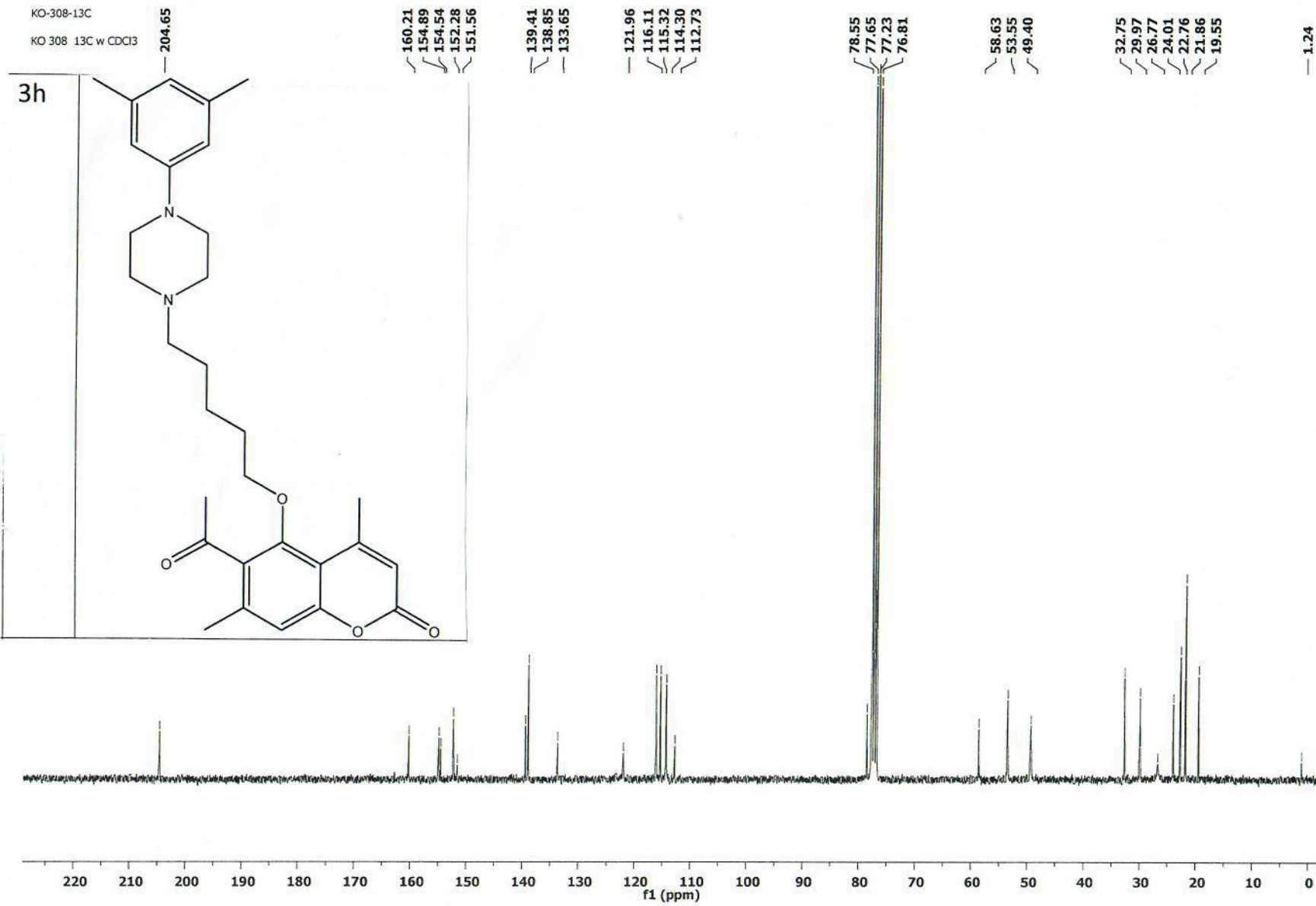


KO-308-1H-cdcl3
KO 308 w CDCl3 + TMS

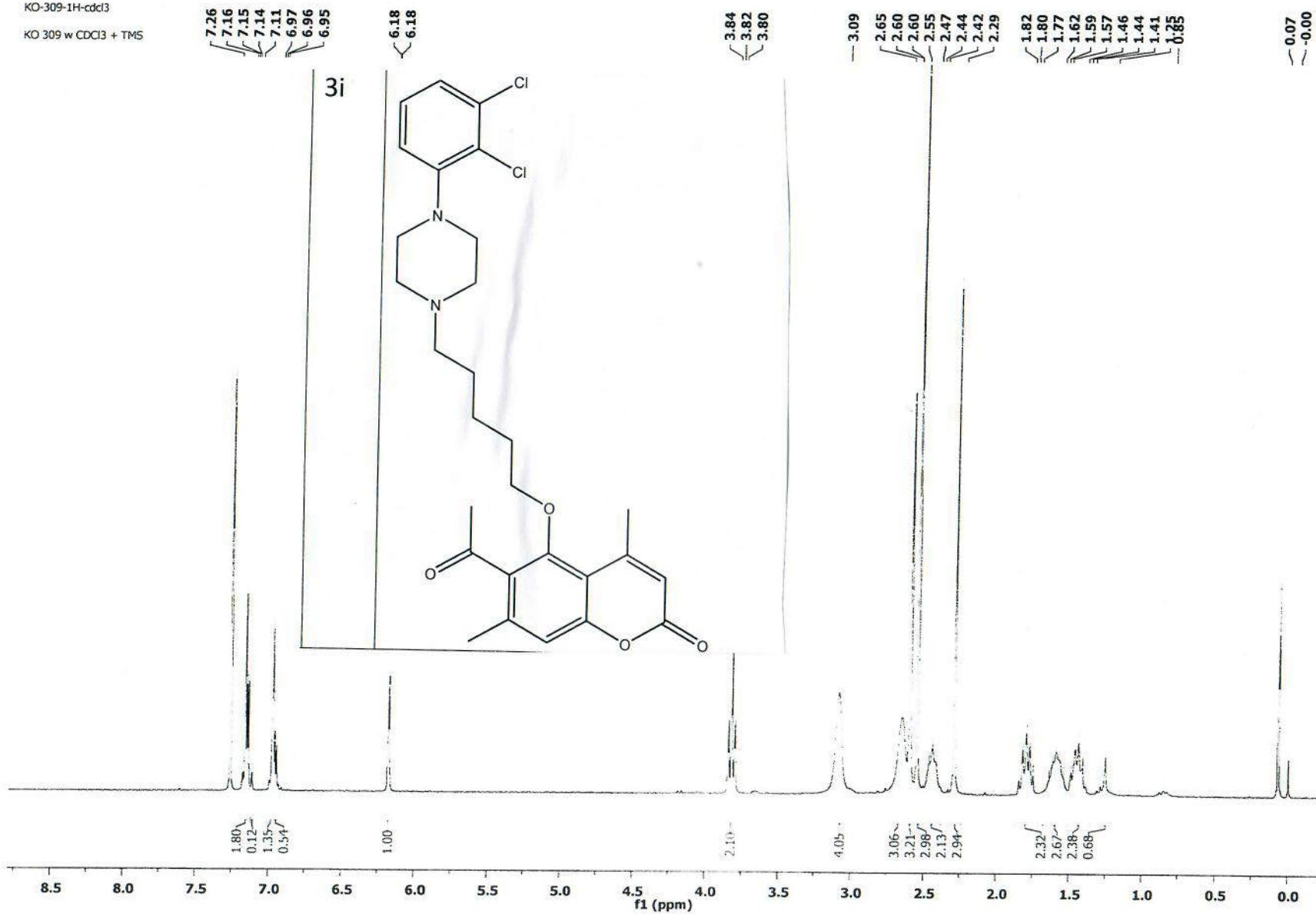


3h

3h



KO-309-1H-cdcl3
KO 309 w CDCl3 + TMS



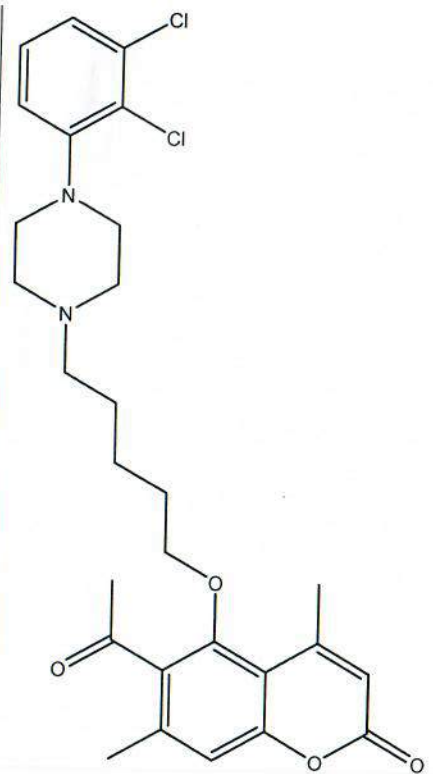
31

3i

KO-309-13C-cdd3

KO 309 13C in CDCl3

3i



204.67

160.21
154.90
154.53
152.28

139.42
134.26
133.65

127.69
124.88

118.84
116.12
115.33
112.73

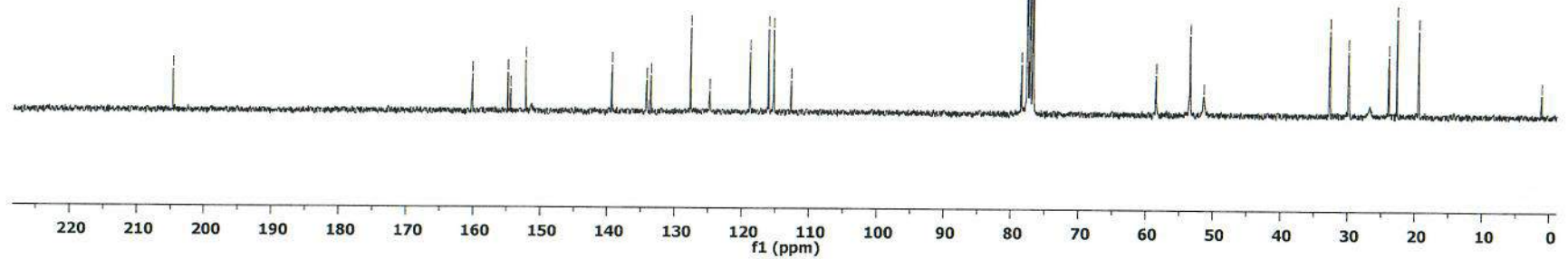
78.53
77.65
77.43
77.23
76.81

58.56
53.53
51.42

32.76
29.97

23.97
22.77
19.55

1.24



KO-310-1H-cdcl3

KO 310 w CDCl3 + TMS

7.58
7.57
7.55
7.55
7.51
7.51
7.49
7.48
7.48
7.46
7.46
7.27
7.03
7.00
6.98
6.97
6.97

6.18
6.18

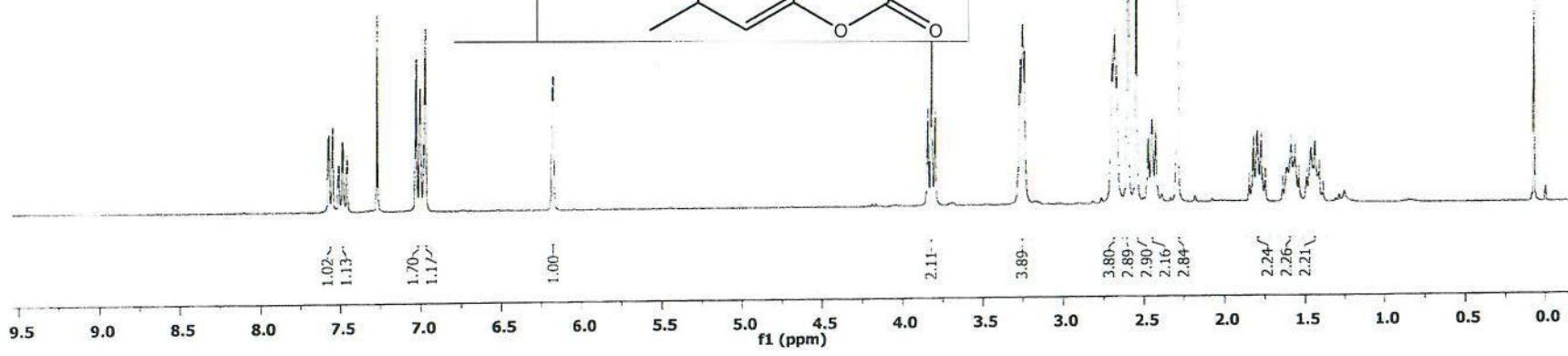
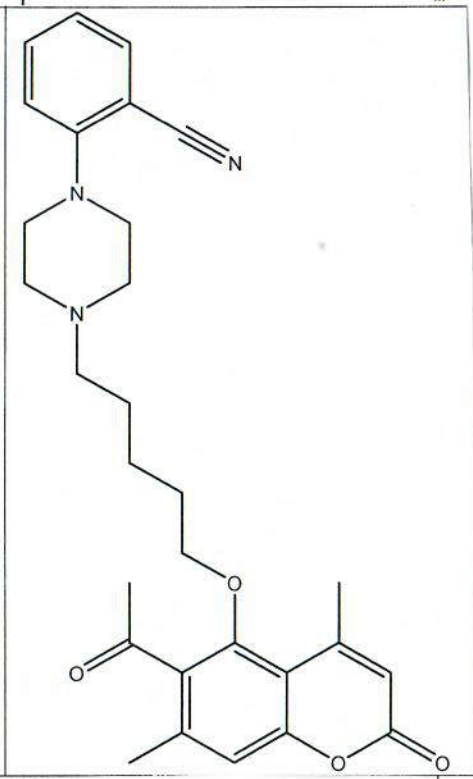
3.84
3.82
3.80

3.27
3.26
3.24

2.70
2.69
2.67
2.61
2.60
2.55
2.45
2.85
1.82
1.80
1.77
1.75
1.64
1.62
1.59
1.56
1.54
1.49
1.46
1.44
1.41
1.39

0.07
-0.00

3j



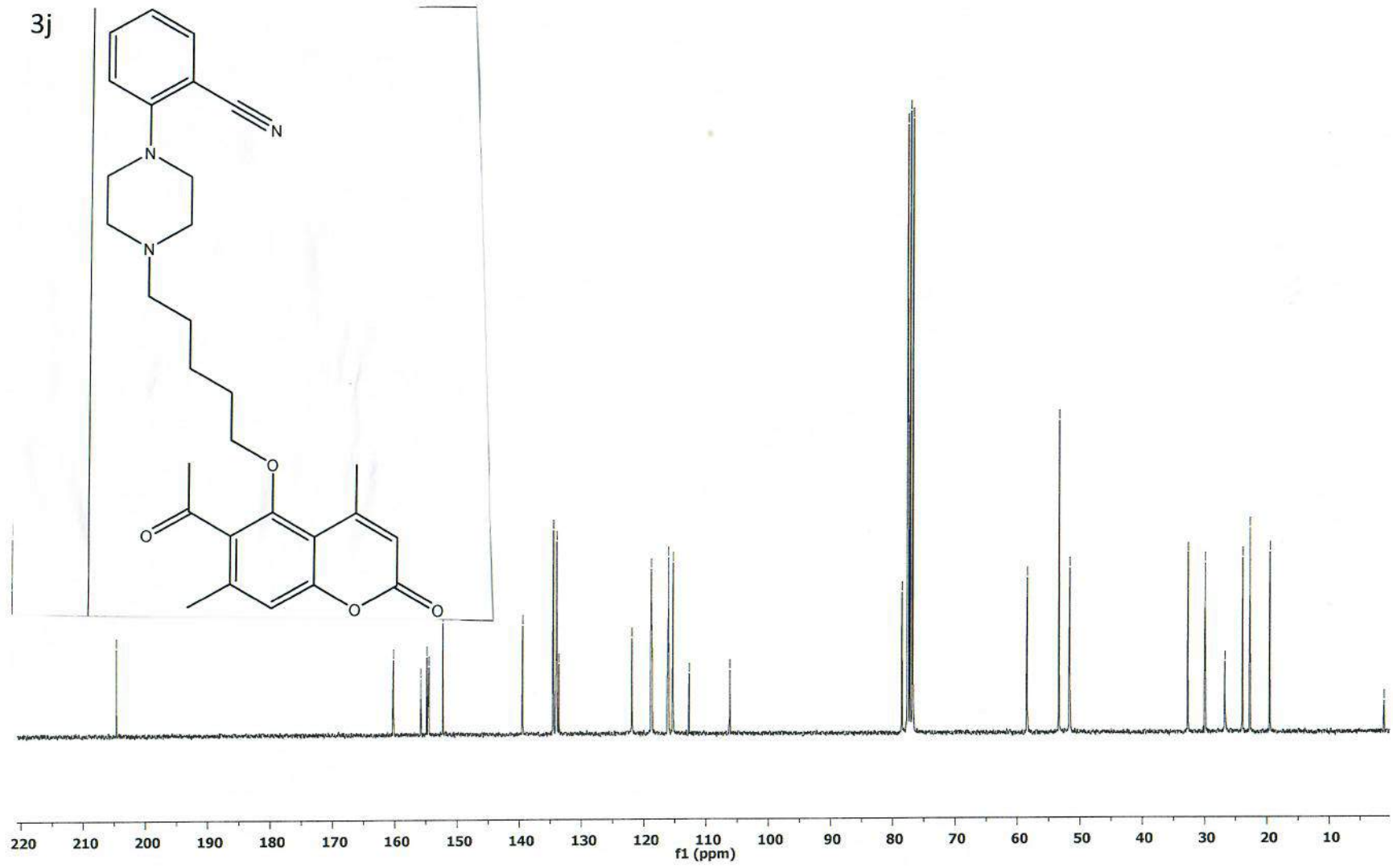
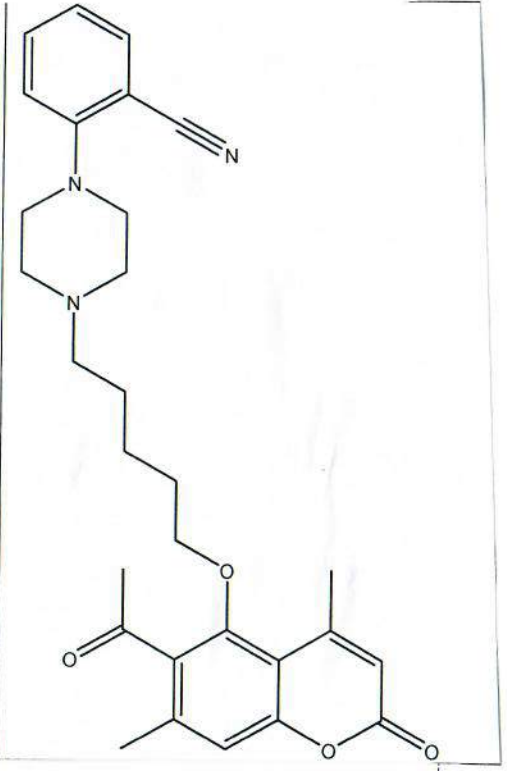
3j

3j

KO-310-13C-cdd
KO-310 13C in C₁₃

- 160.19
- 155.83
- 154.86
- 154.53
- 152.29
- 139.41
- 134.54
- 134.00
- 133.63
- 121.95
- 118.83
- 118.65
- 116.08
- 115.29
- 112.71
- 106.18
- 78.53
- 77.65
- 77.43
- 77.23
- 76.81
- 58.44
- 53.39
- 51.65
- 32.73
- 29.97
- 26.74
- 23.96
- 22.76
- 19.53
- 1.21

3j



KO-322-1H-cdcl3
KO 322 1H w CDCl3

— 7.26

— 7.01

6.20
6.20

4.17
4.15
4.13

3.59
3.57
3.55

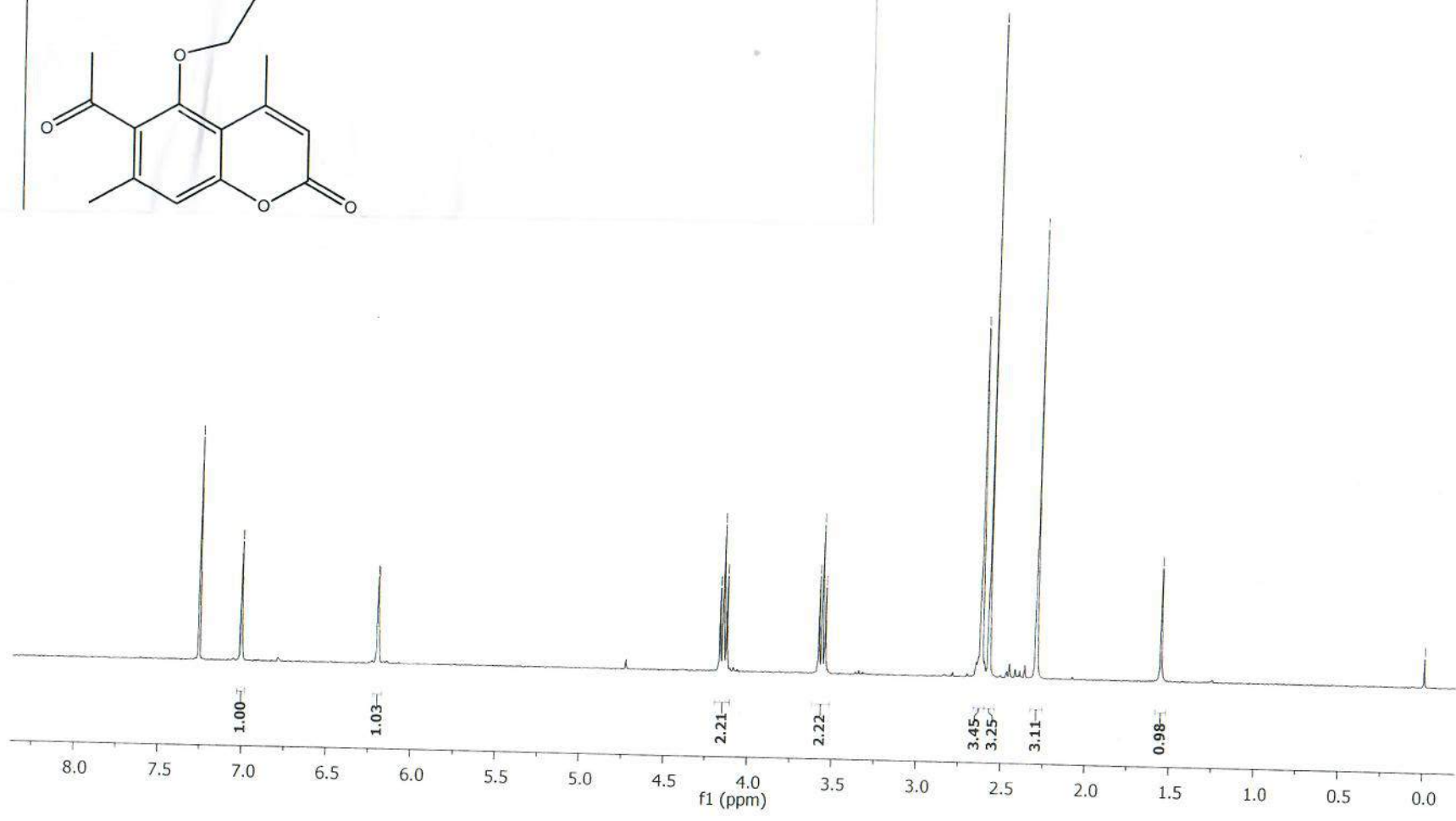
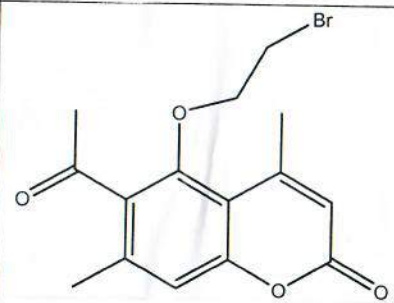
2.63
2.62
2.58

— 2.30

— 1.56

— 0.00

4



KO-322-13C

KO-322-13C w CDCl3

— 204.65

— 160.00
— 154.84
— 153.04
— 151.81

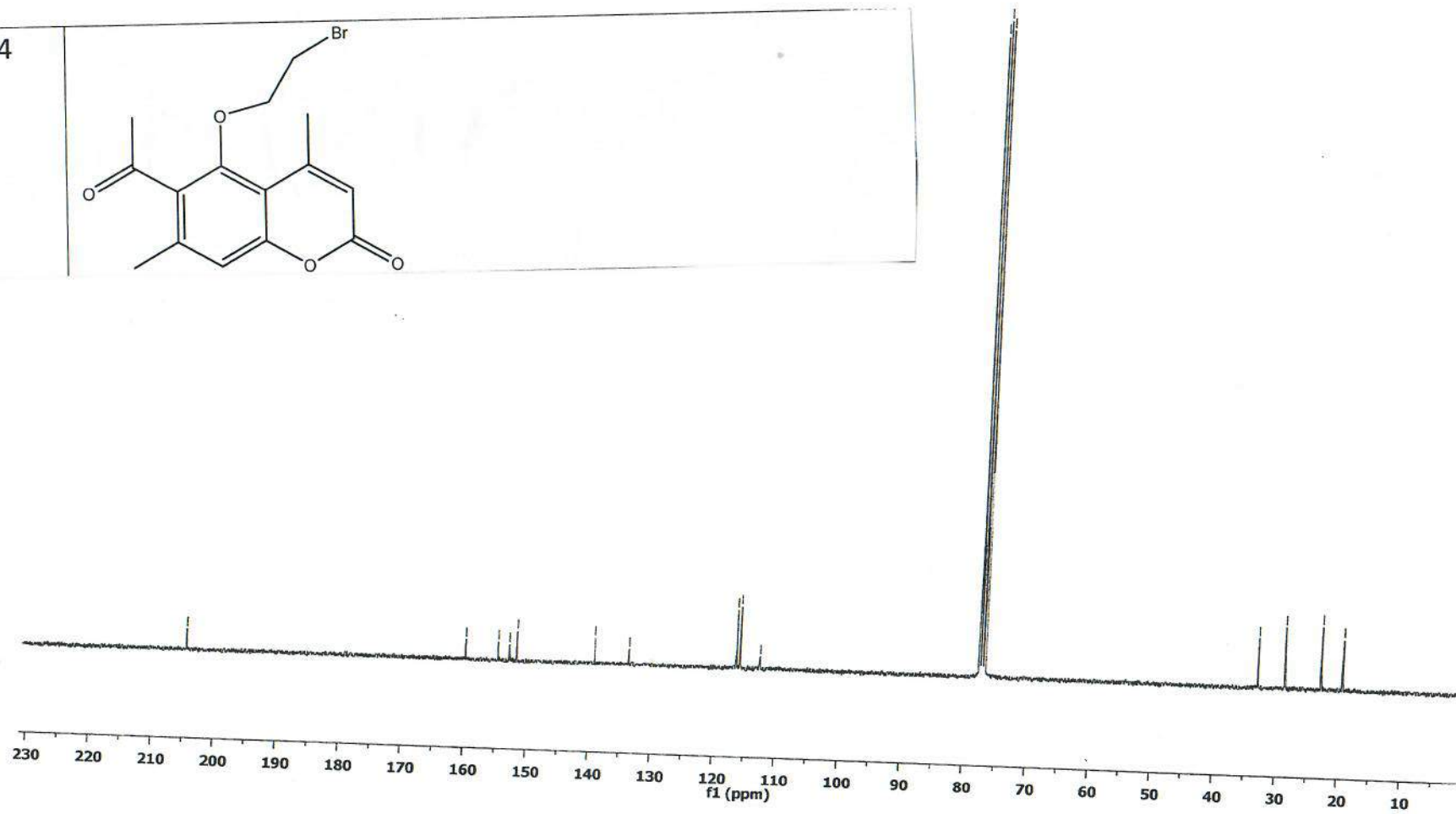
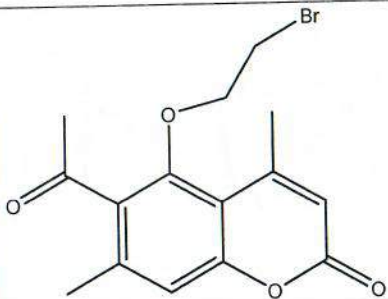
— 139.35
— 133.77

— 116.49
— 115.93
— 112.72

— 77.65
— 77.43
— 77.23
— 76.96
— 76.81

— 33.09
— 28.86
— 22.94
— 19.49

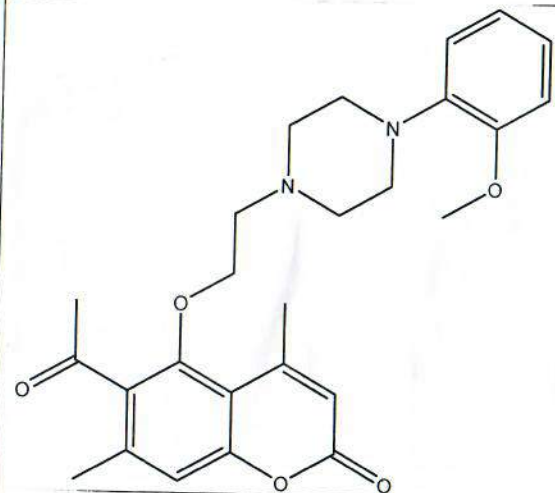
4



4a

KO-323-1h
KO 323 1H

4a

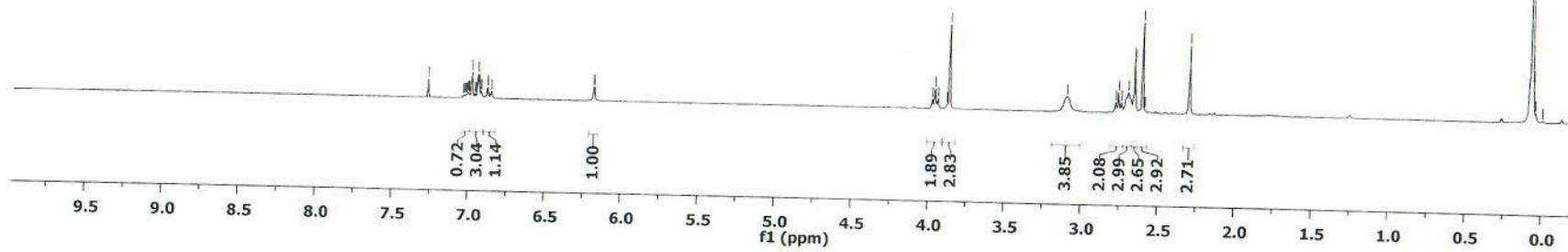


7.27
7.04
7.02
7.02
7.01
7.00
6.98
6.96
6.94
6.93
6.92
6.92
6.88
6.85
6.18
6.18

3.98
3.96
3.94
3.88
3.87

3.10
2.76
2.70
2.66
2.66
2.50

0.08
0.07
0.06
0.05
-0.00



4a

KO-323-13C
KO 323 13C in CDCl₃

— 203.93

— 160.11
— 154.86
— 152.41

— 139.40
— 133.56

— 123.39
— 121.74
— 118.48
— 116.23
— 115.59
— 112.78
— 111.45

— 77.65
— 77.23
— 76.81

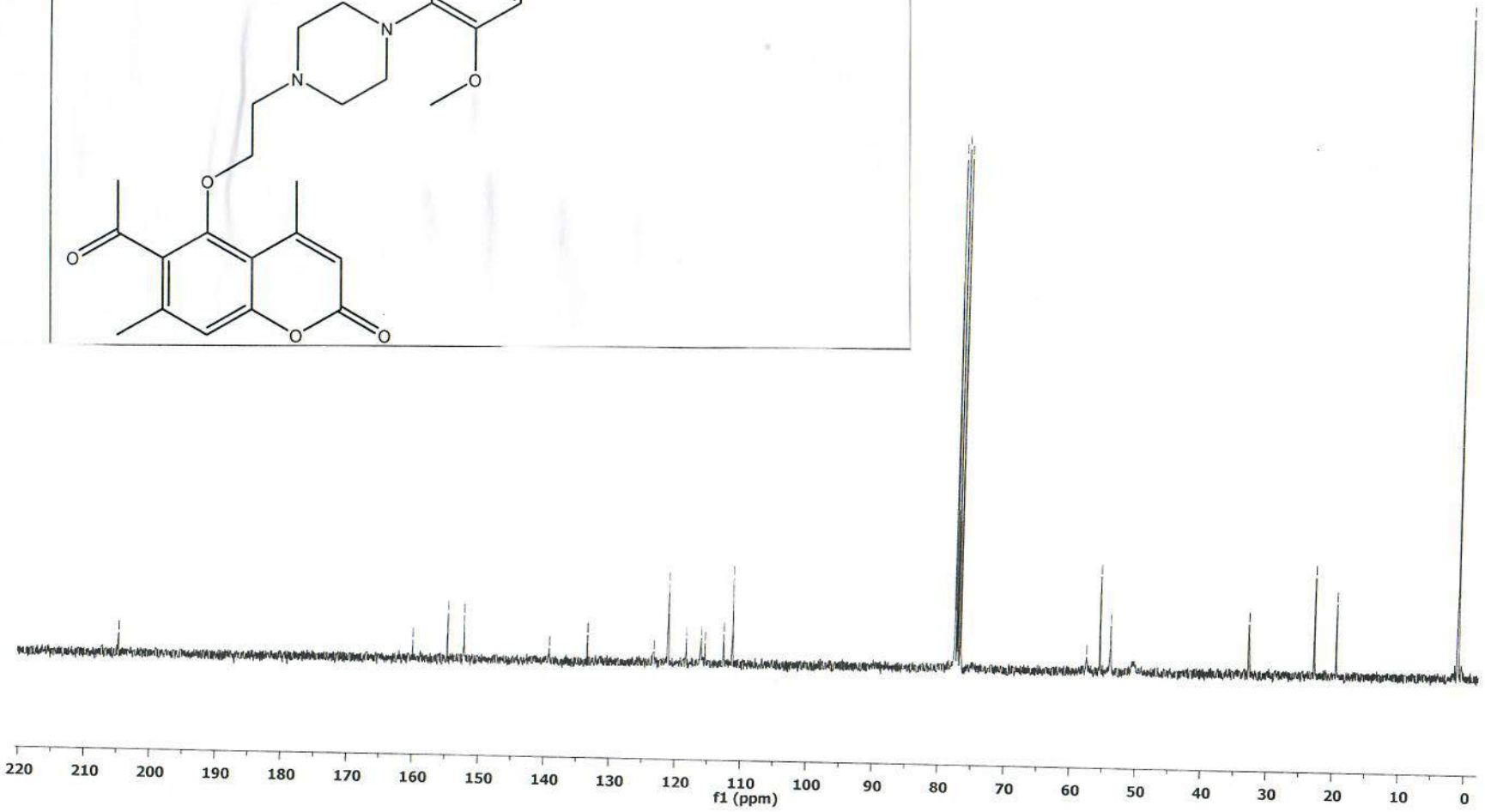
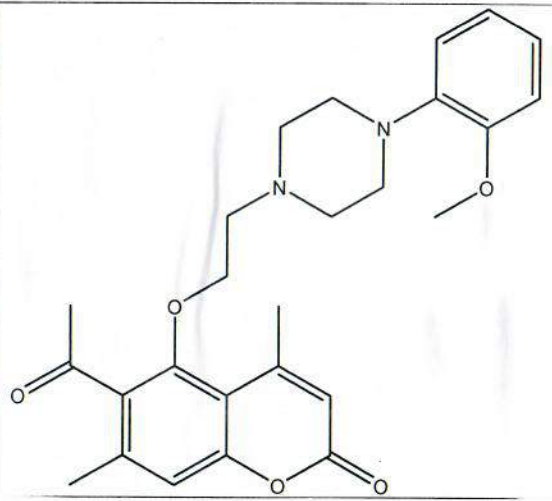
— 57.65
— 55.59
— 54.02

— 32.95

— 22.91
— 19.59

— 1.22

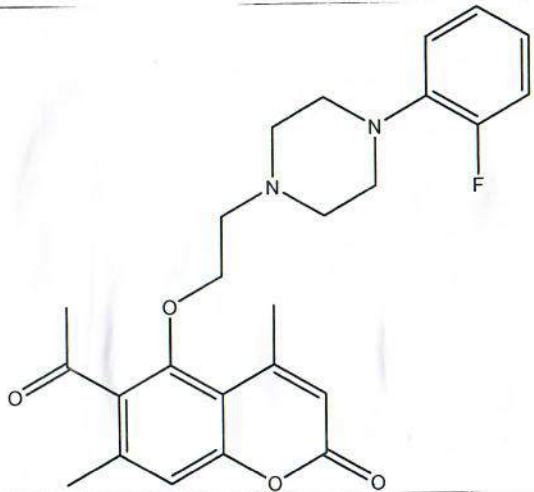
4a



4b

KO-327A-1h
KO 327A 1H

4b



8.10
7.32
7.26
7.10
7.09
7.07
7.06
7.04
7.04
7.02
6.99
6.95
6.93
6.91
6.19

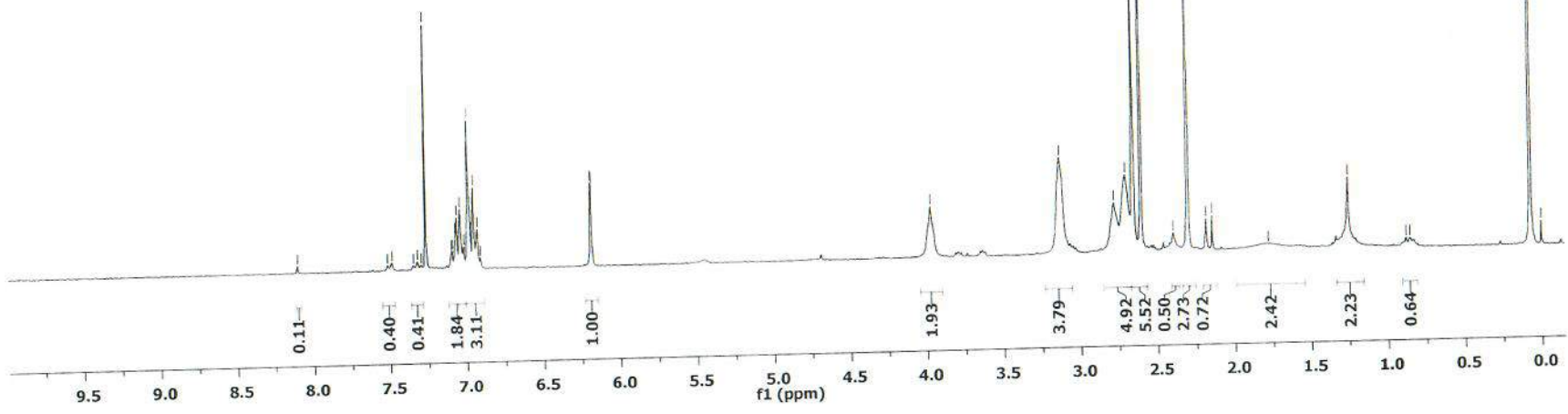
3.97

3.13
2.78
2.71
2.66
2.65
2.61
2.40
2.30
2.18
2.14
1.78

1.26

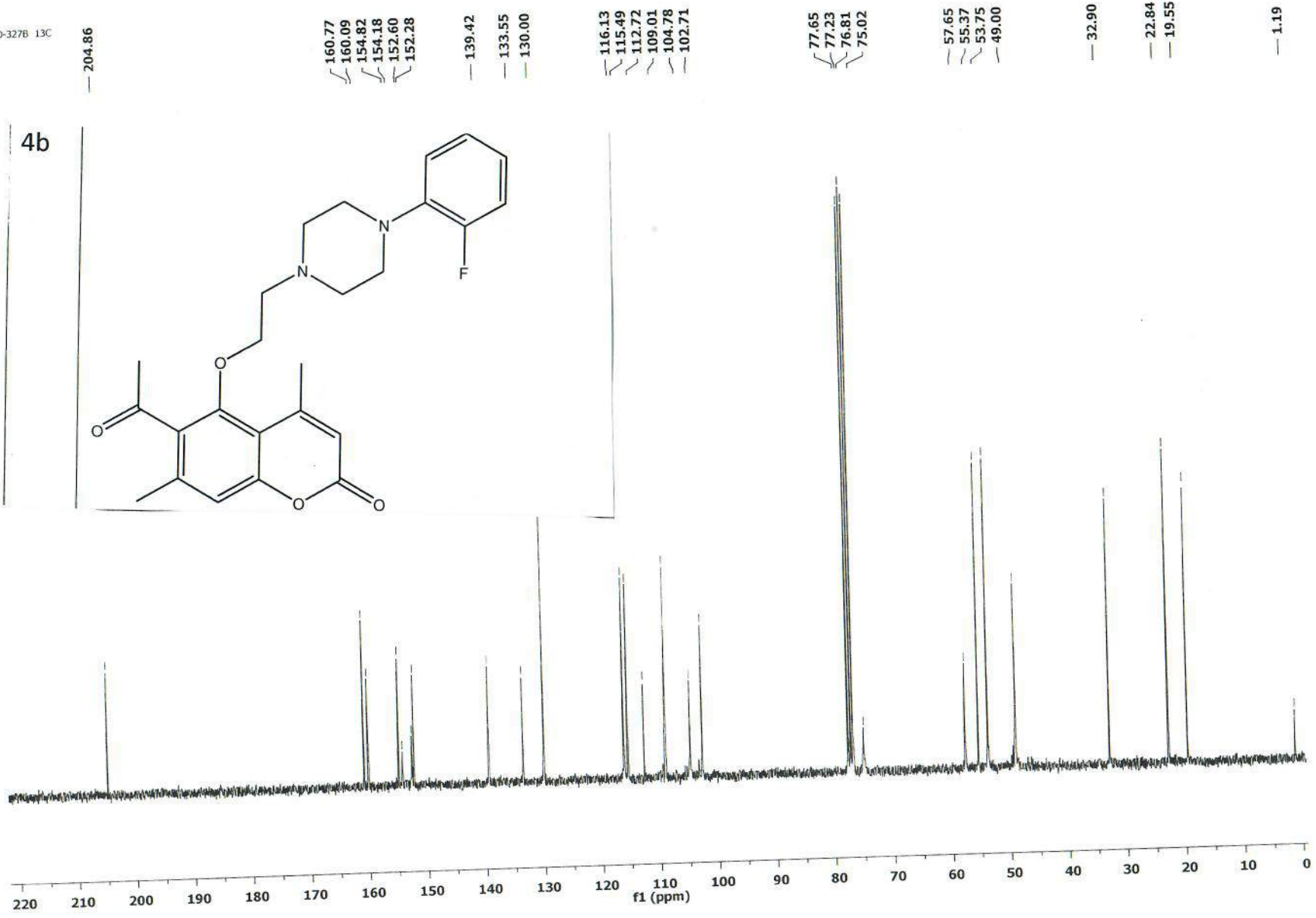
0.88
0.85

0.07
0.00



4b

KO-327B 13C



4c

KO-326-1h
KO 326 1H

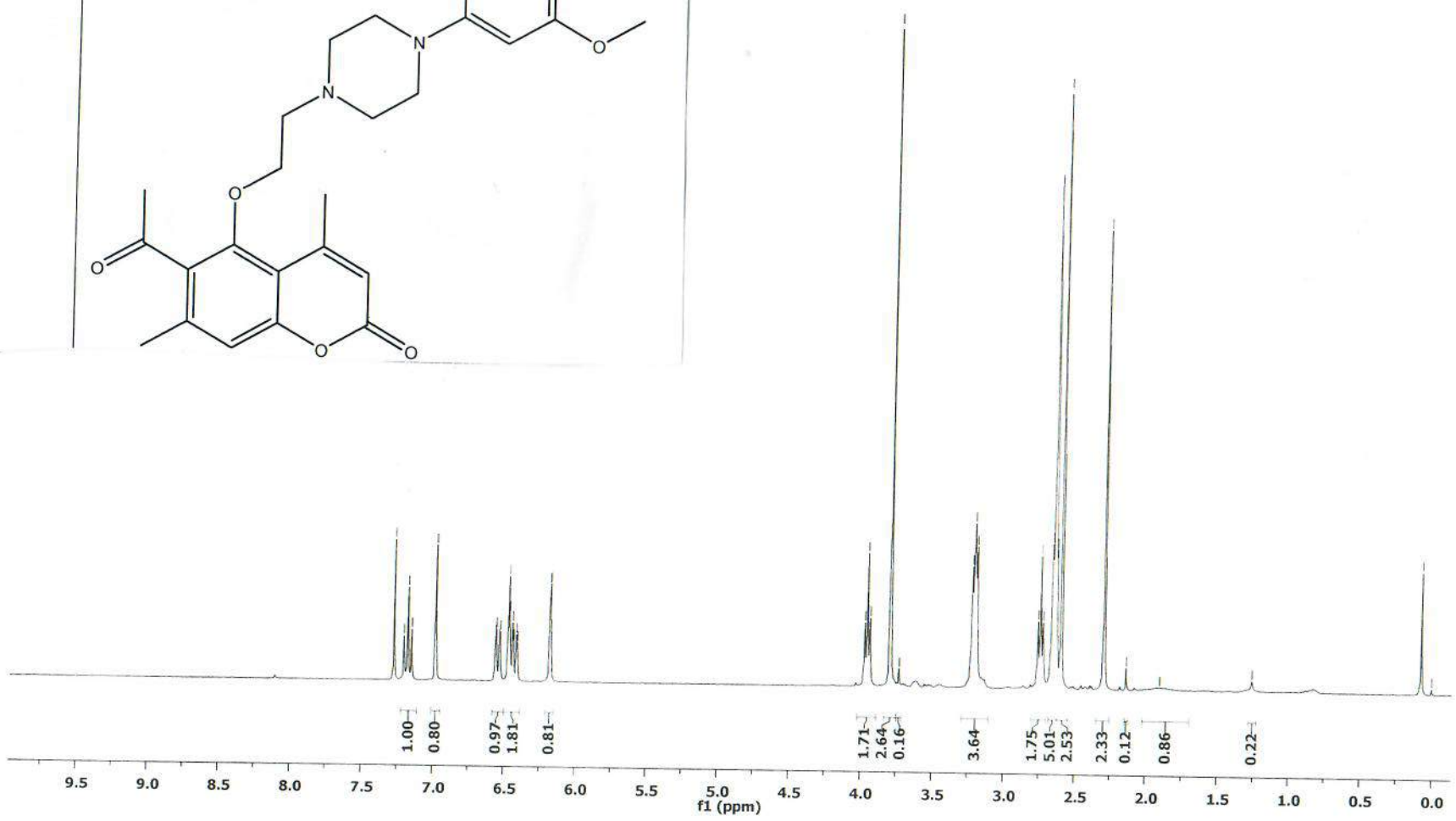
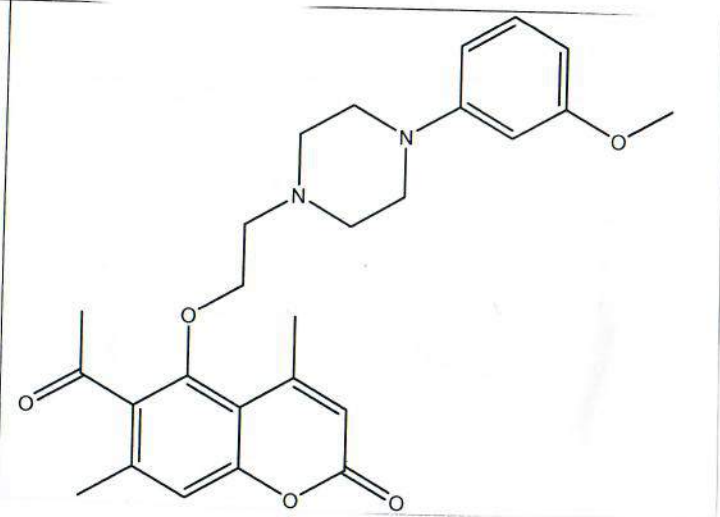
7.27
7.20
7.18
7.15
6.98
6.56
6.56
6.54
6.53
6.48
6.47
6.46
6.44
6.44
6.42
6.41
6.18
6.18

3.97
3.96
3.94
3.80
3.73
3.23
3.21
3.19
2.67
2.65
2.65
2.64
2.60
2.50
2.14
1.91

1.26

0.08
0.00

4c



4c

KO-326-13C
204.92
204.91

160.11
157.53
154.87
154.27
152.37
152.28
152.22
139.45
139.43
139.35
133.58
124.74
124.69
119.20
116.50
116.23
115.61
115.58
112.77

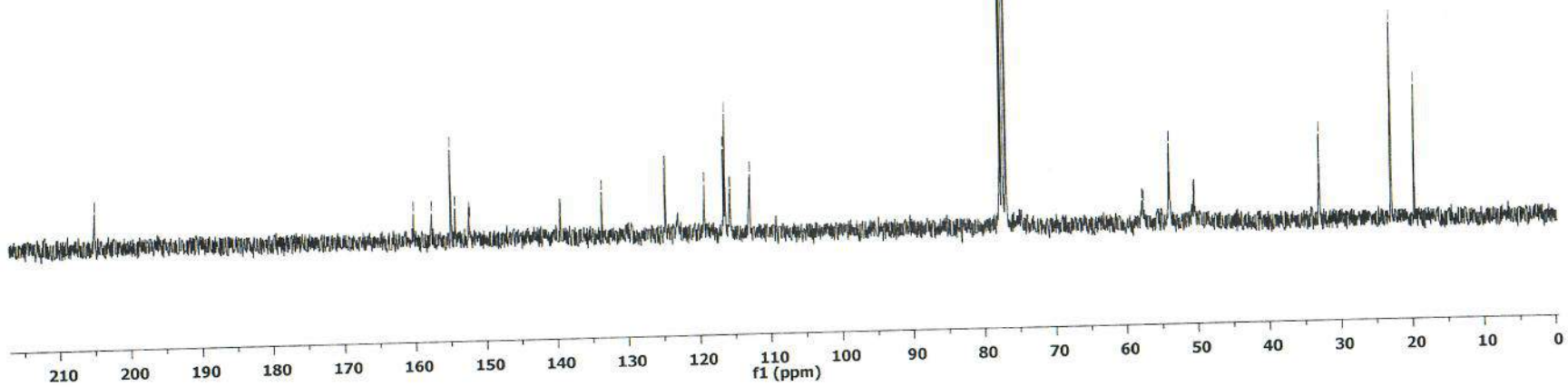
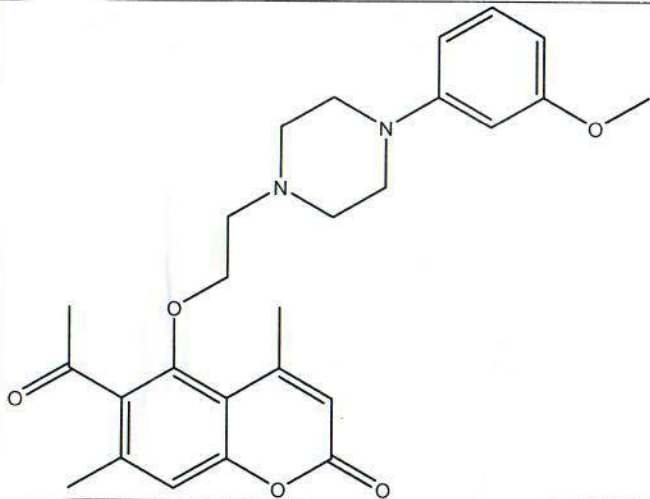
77.65
77.43
76.81

57.68
57.54
53.86
50.47
50.41
50.35

32.96

22.89
19.58

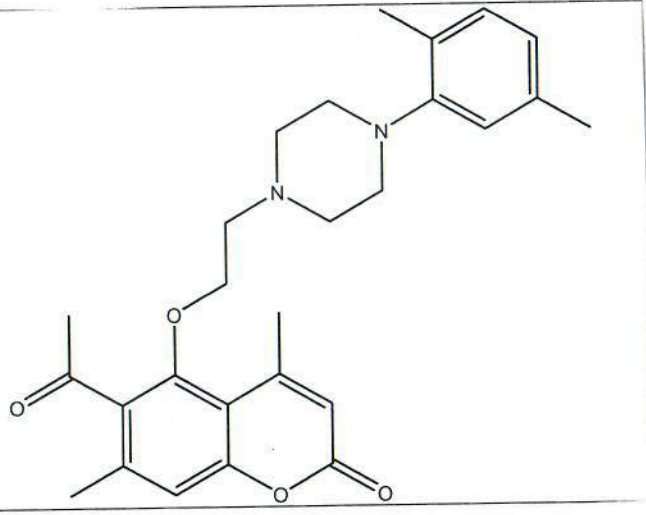
4c



4d

KO-329-1H-cdd3
KO 329 1H w CDCl3

4d



7.26
7.07
7.04
6.98
6.98
6.82
6.79

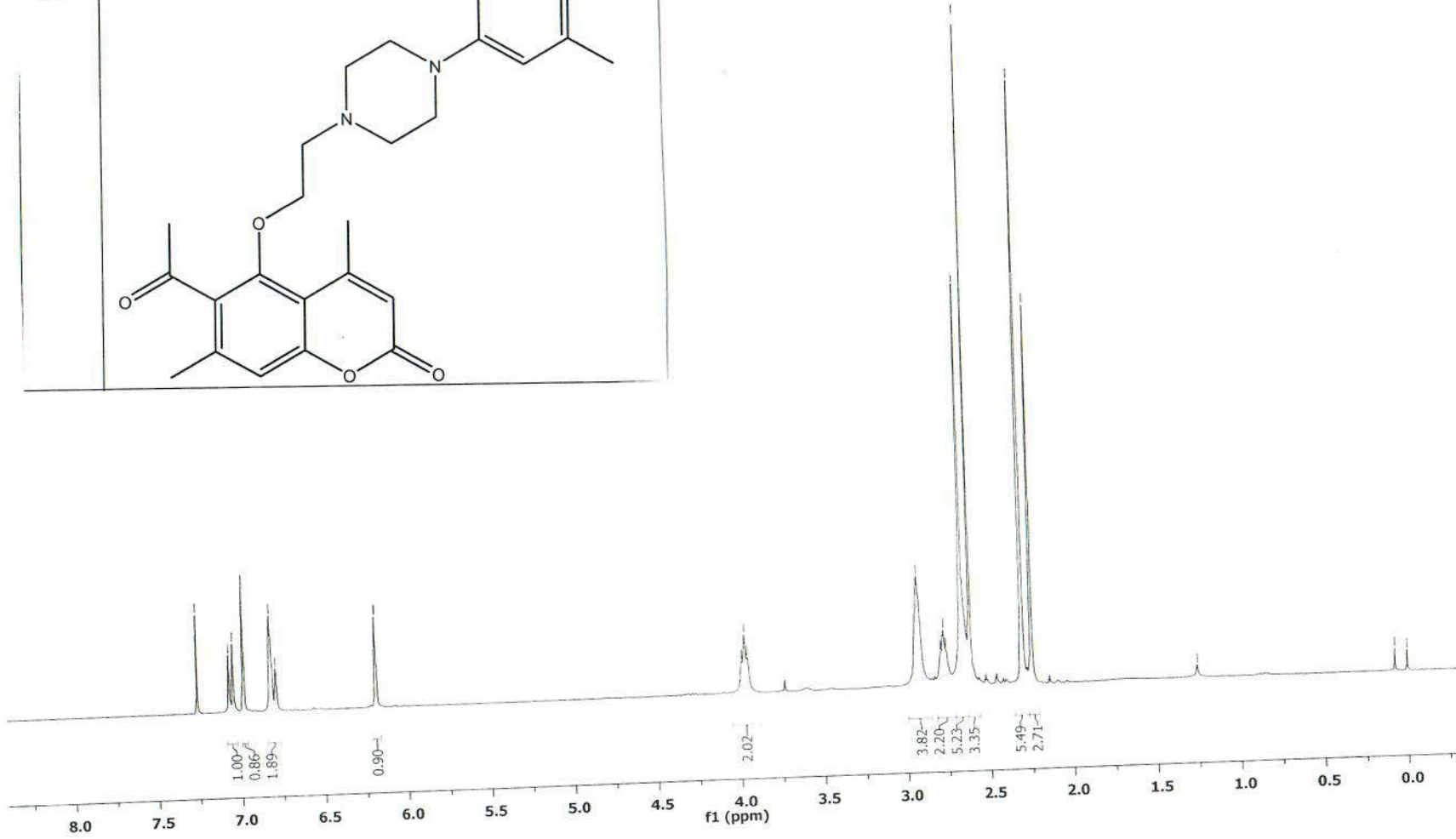
6.19
6.19

3.99
3.97
3.95

2.93
2.79
2.78
2.76
2.67
2.66
2.62
2.30
2.25

— 1.26

0.07
-0.00



4d

KO-329-13C-cdcl3
KO 329 13C w CDCl3

— 204.86

— 160.17
— 154.86
— 152.45
— 151.30

— 139.51
— 136.32
— 133.52
— 131.10
— 129.41
— 124.03
— 119.84
— 116.11
— 115.45
— 112.77

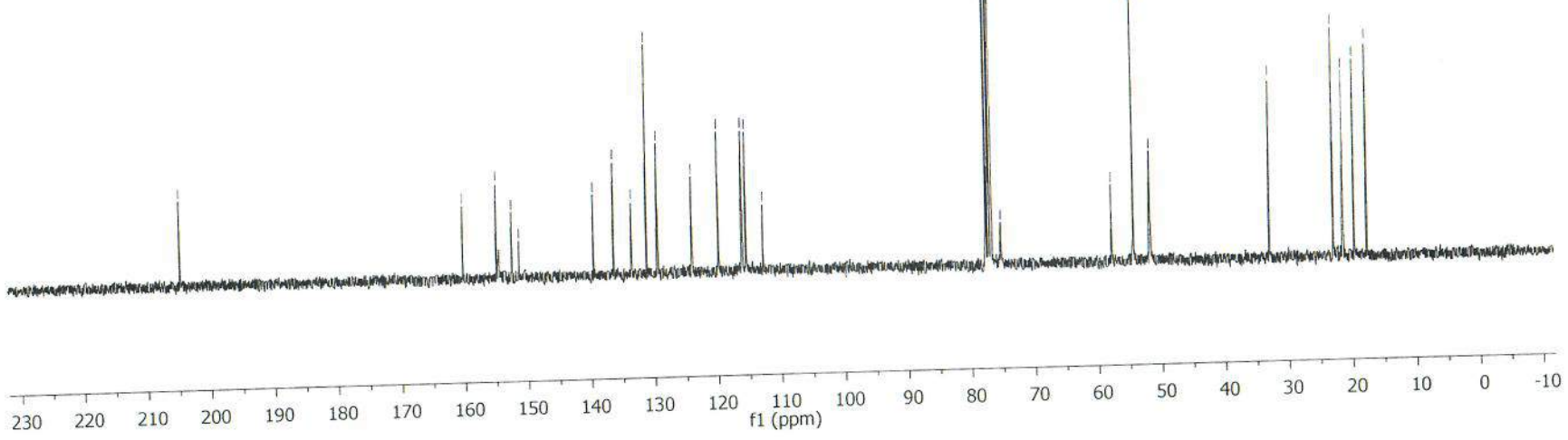
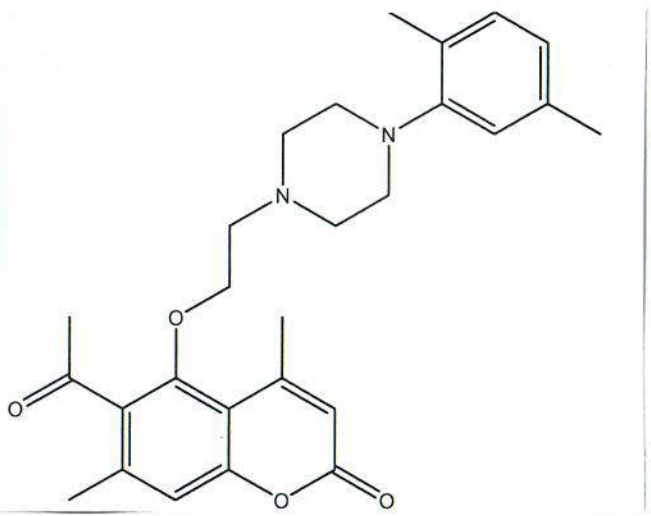
— 77.65
— 77.23
— 76.81
— 75.26

— 57.84
— 54.40
— 51.76

— 32.91

— 22.92
— 21.39
— 19.61
— 17.66

4d



4e

KO-330-1H-cdcl3
KO 330 1H w CDCl3

7.27
7.23
7.20
7.18
7.15
7.02
6.98
6.68
6.61
6.57
6.56
6.53
6.18
6.18

3.98
3.96
3.94

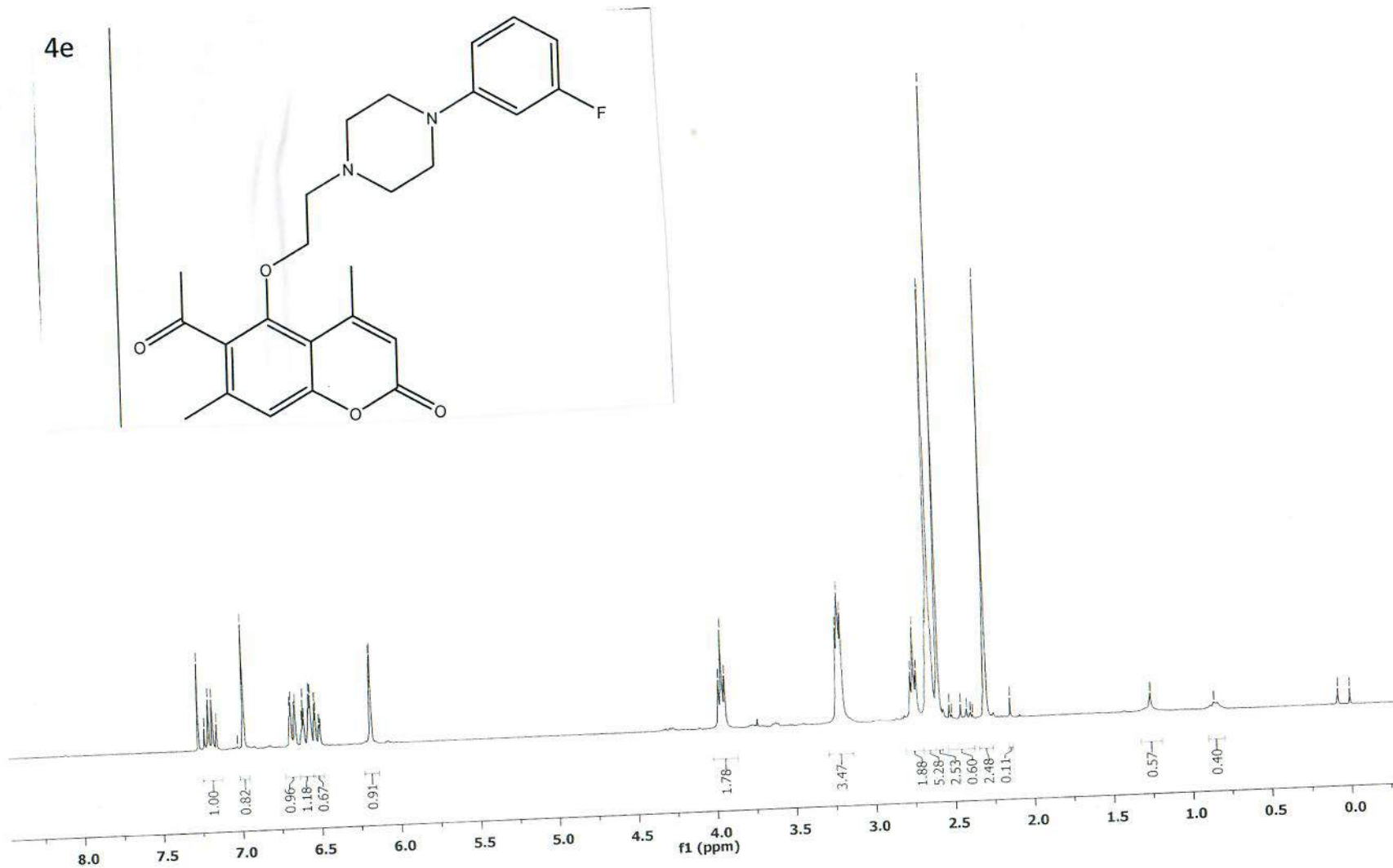
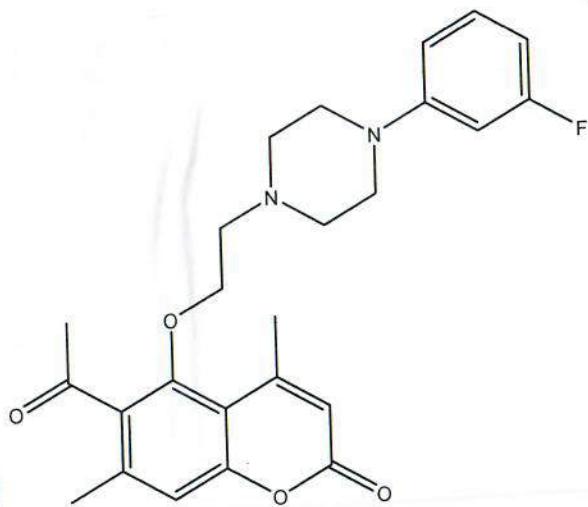
3.23
3.22
3.20
2.77
2.75
2.73
2.67
2.65
2.60
2.60
2.53
2.51
2.45
2.42
2.39
2.38
2.30
2.14

— 1.26

— 0.85

— 0.07
— -0.00

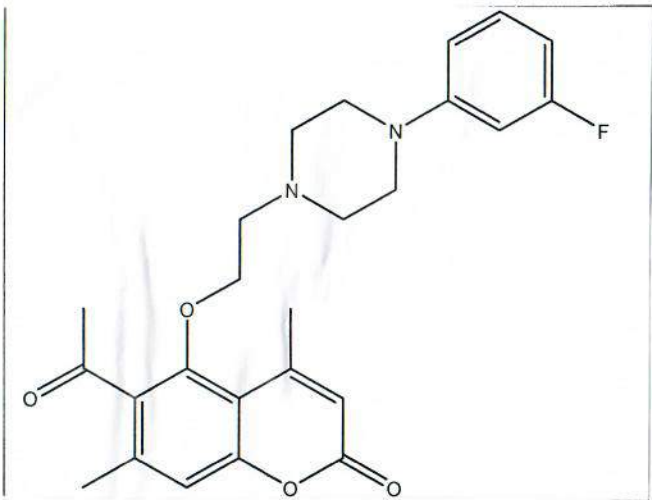
4e



4e

KO-330-13C-cdcl3
KO 330 13C w CDCl3

4e



— 204.86

165.64
162.42
160.12
154.84
154.24
153.02
152.89
152.28

139.47
133.57
130.39
130.26

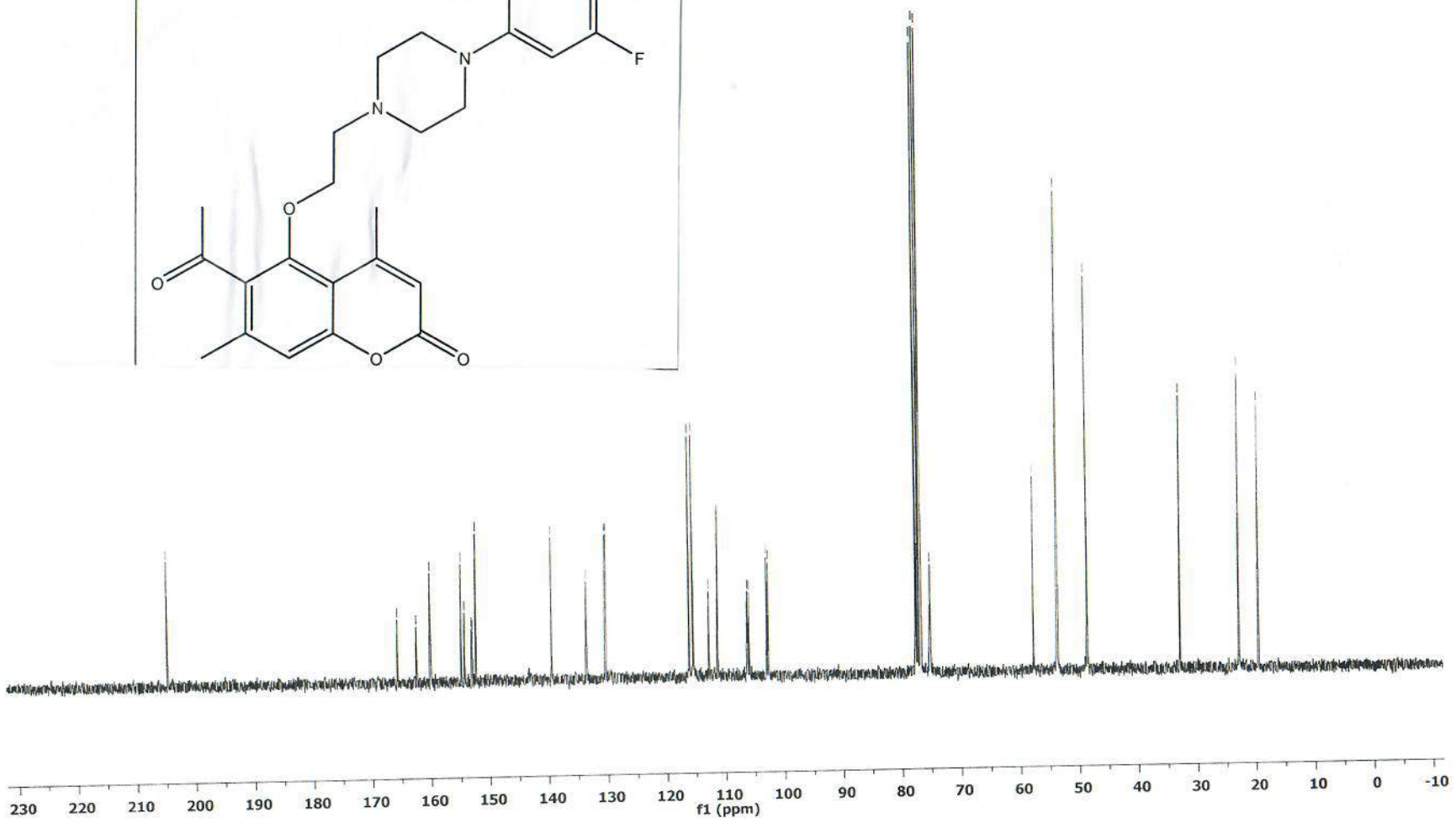
116.15
115.49
112.73
111.29
111.25
106.26
105.97
103.00
102.67

77.65
77.23
76.81
75.18

57.73
53.66
48.71

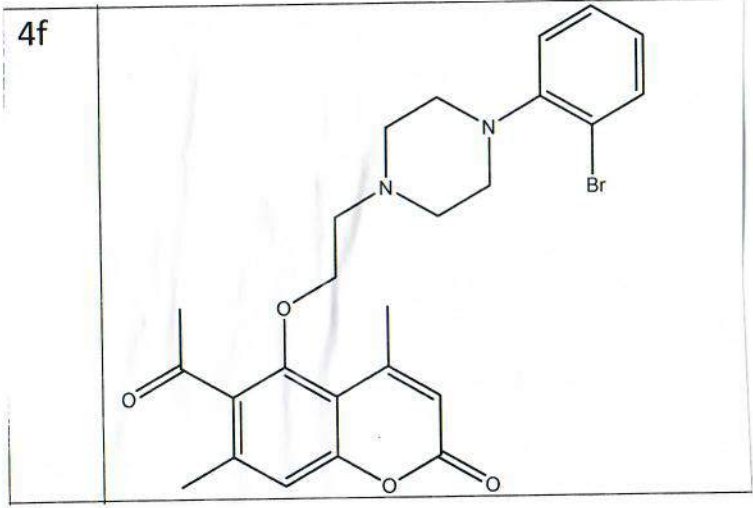
— 32.92

— 22.84
— 19.57



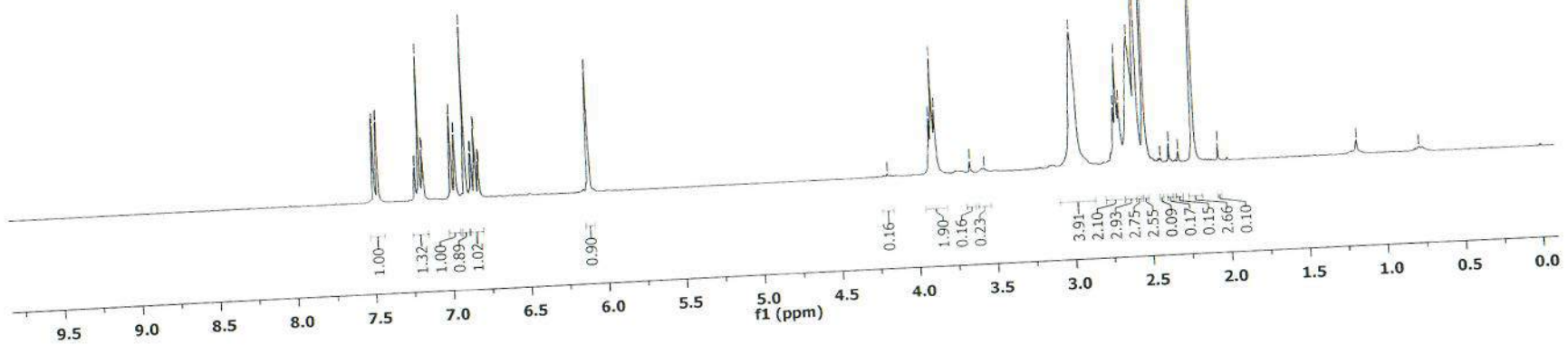
4f

KO-331-1H
KO 331 1H w CDCl3



7.50
7.49
7.47
7.47
7.23
7.22
7.20
7.19
7.18
7.17
7.00
6.99
6.97
6.97
6.91
6.87
6.86
6.84
6.84
6.82
6.81
6.11
6.11

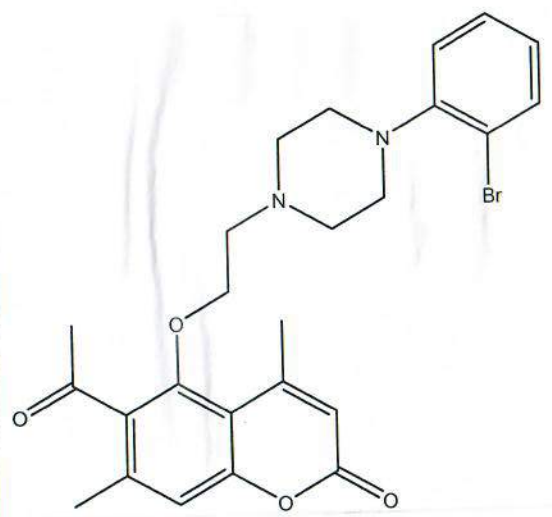
4.19
3.92
3.90
3.88
3.66
3.57
2.99
2.73
2.71
2.69
2.63
2.59
2.59
2.54
2.44
2.38
2.32
2.23
2.07
1.18
0.78



4f

KO-331-13C
KO 331 13C w CDCl3

4f



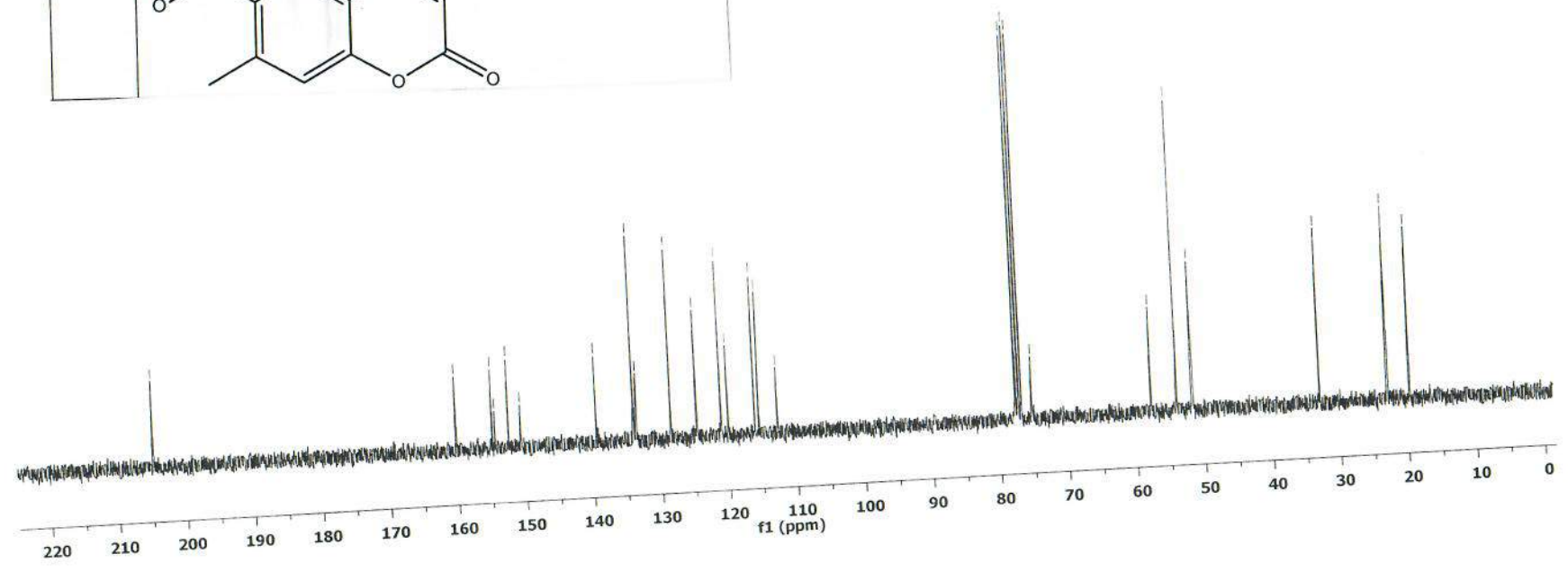
- 160.15
- 154.84
- 154.42
- 152.41
- 150.62
- 139.50
- 134.03
- 133.50
- 128.47
- 124.63
- 121.07
- 120.03
- 116.09
- 115.43
- 112.75

- 77.65
- 77.23
- 76.81
- 75.25

- 57.75
- 54.00
- 51.71

- 32.89

- 22.91
- 19.61



4g

KO-328-13C
KO 328 13C

— 204.87

160.07
154.81
154.11
152.40
152.21
— 139.40
— 133.57
— 130.53
123.43
122.58
118.89
116.16
115.51
114.57
112.71

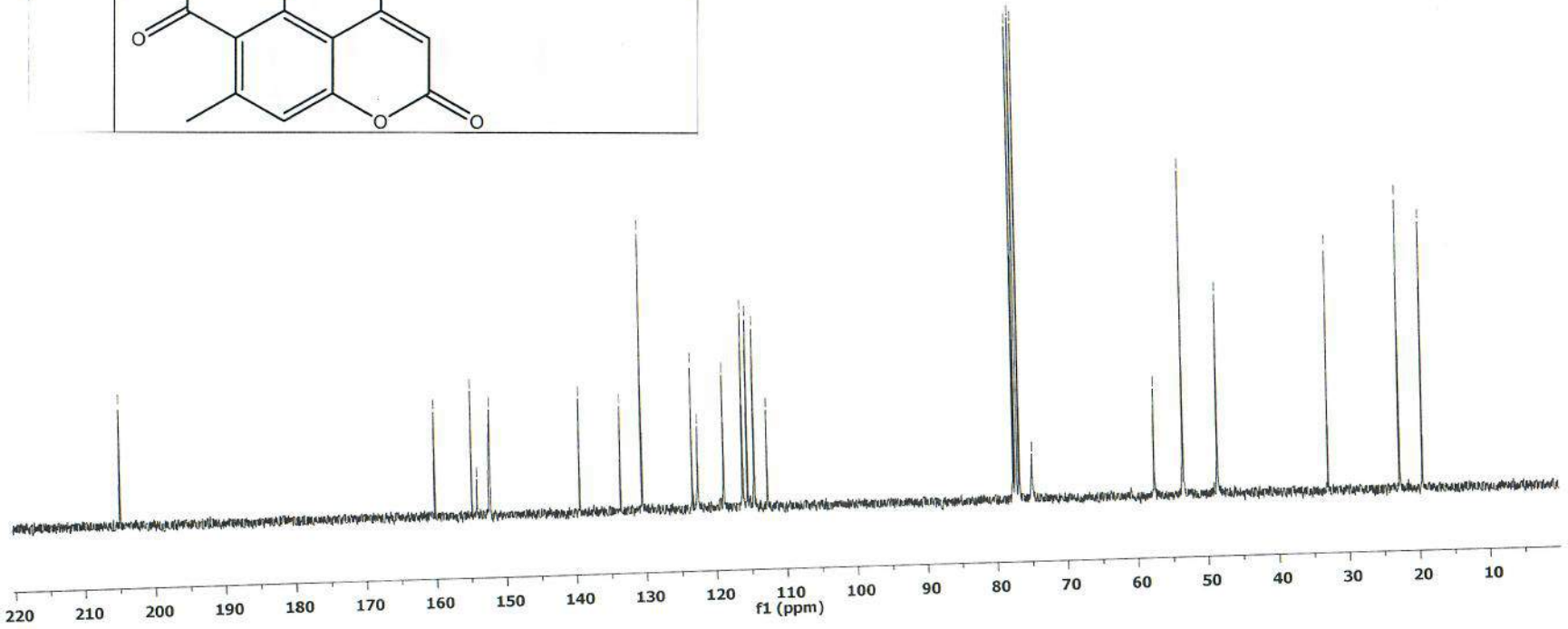
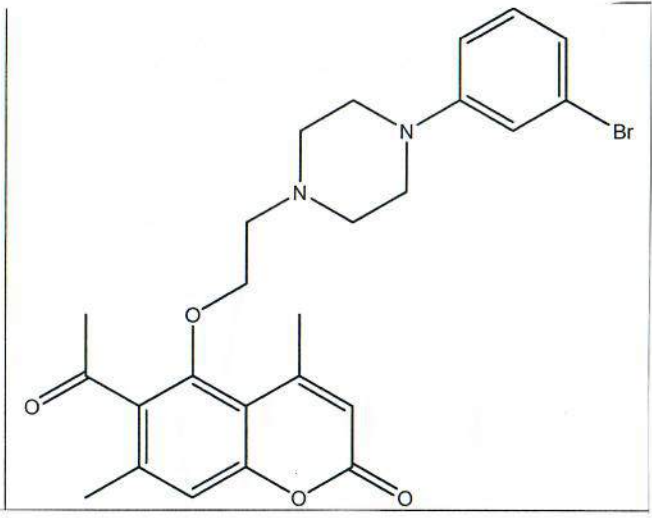
77.65
77.23
76.81
74.97

57.61
53.57
48.61

— 32.93

— 22.82
— 19.54

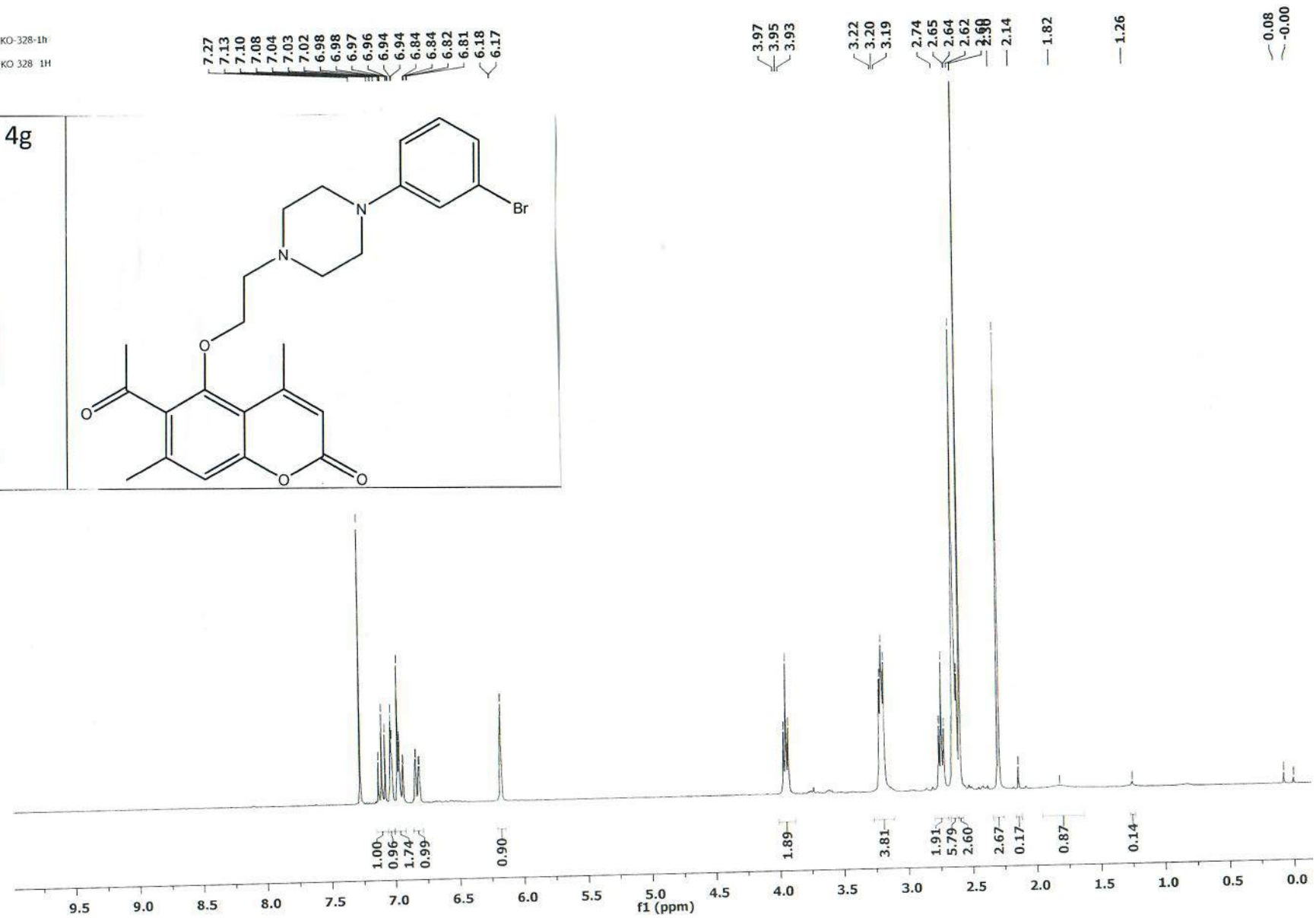
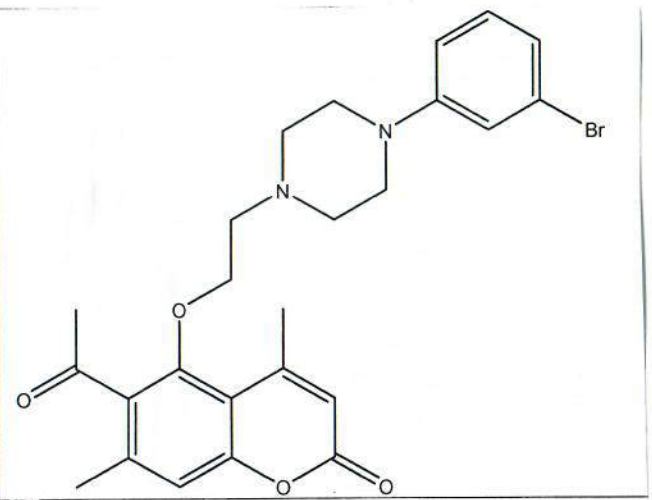
4g



4g

KO-328-1h
KO 328 1H

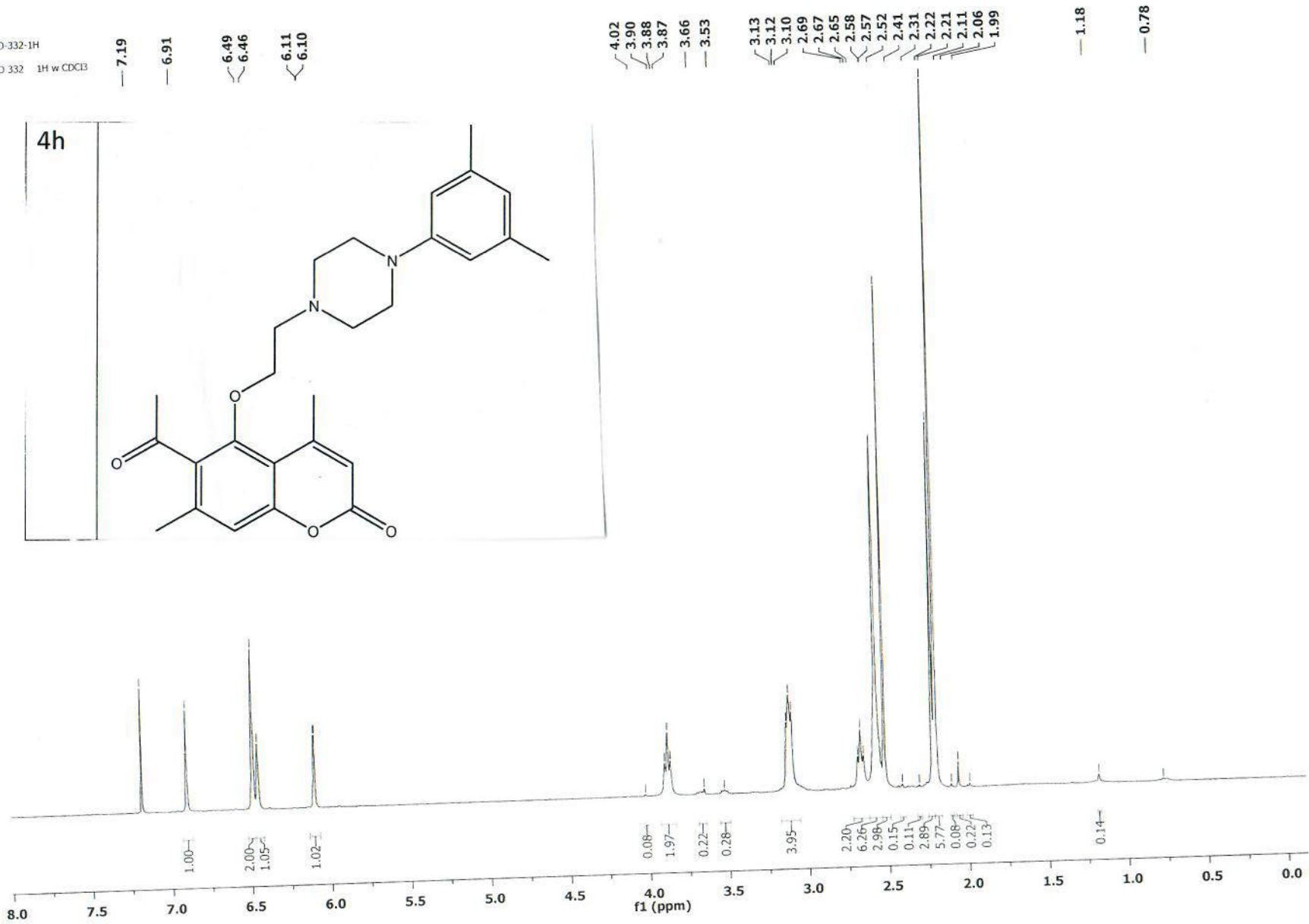
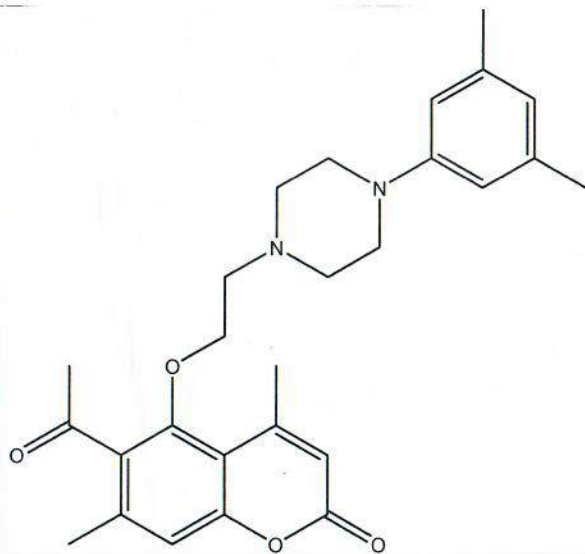
4g



4h

KO-332-1H
KO 332 1H w CDCl3

4h



4h

KO-332-13C-cdCl3
KO-332-13C w CDCl3

204.89

160.14
154.85
154.28
152.35
151.40

139.47
138.87
133.56

122.04
116.13
115.49
114.86
114.24
112.75

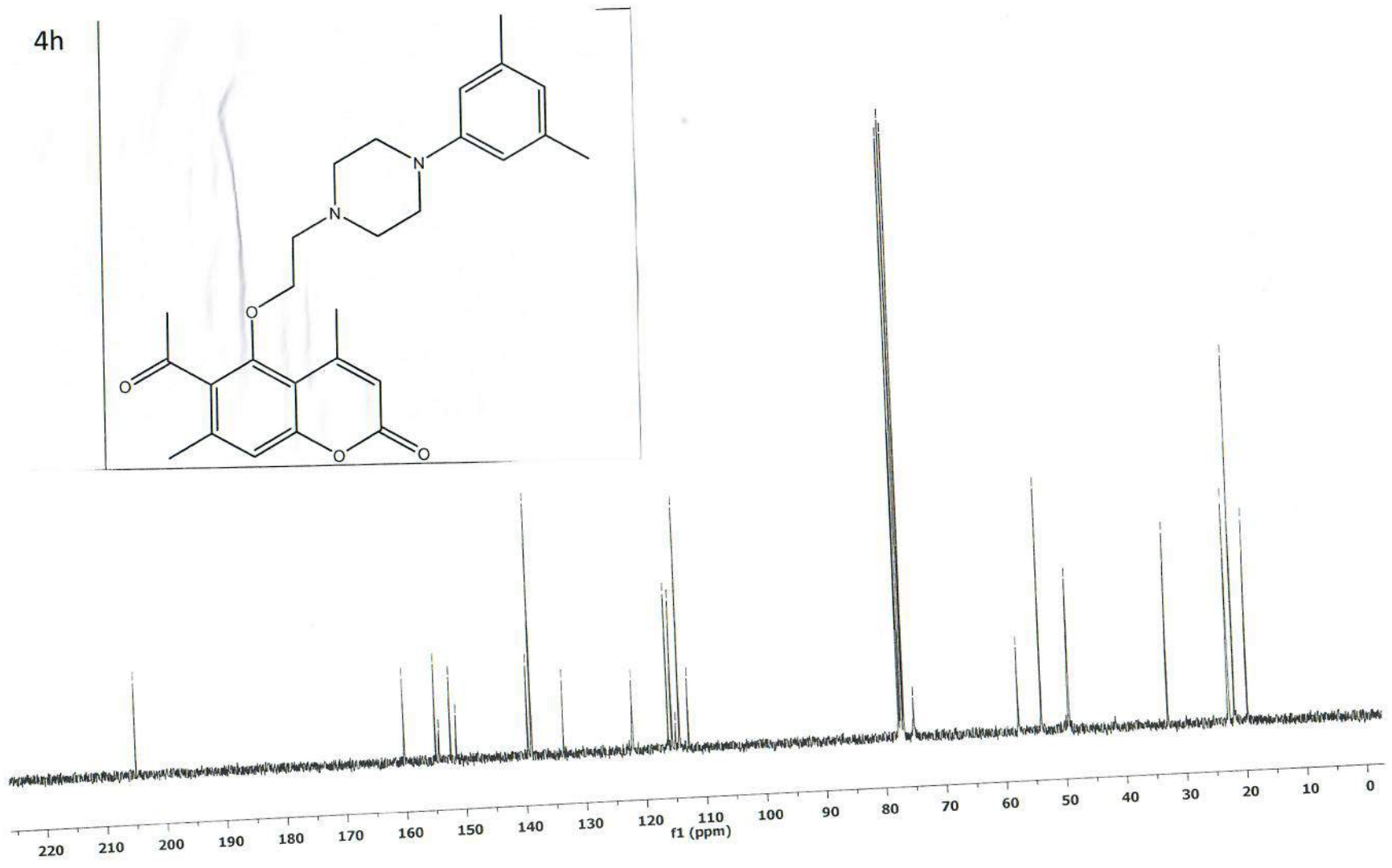
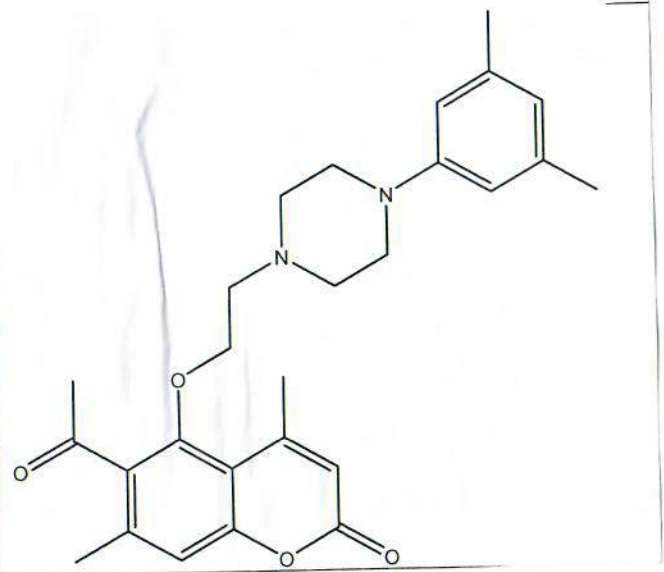
77.65
77.23
76.81
75.13

57.75
53.93
49.32

32.92

22.88
21.84
19.59

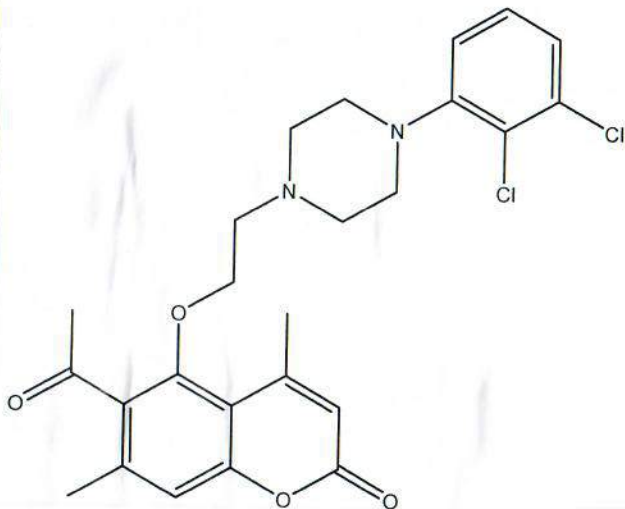
4h



90'

KO-324-1h
KO 324 1H

4i



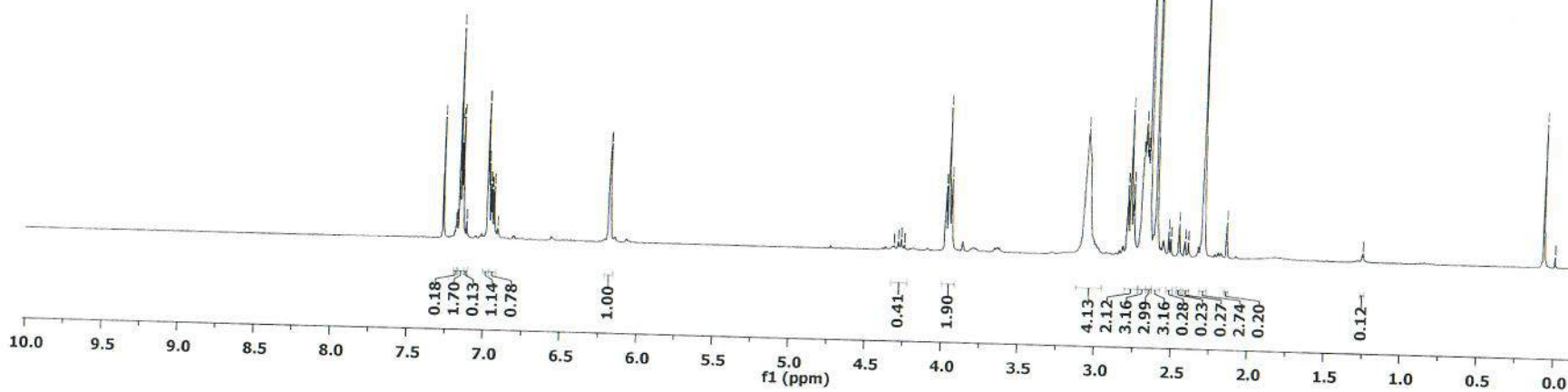
7.27
7.19
7.18
7.17
7.15
7.15
7.12
6.99
6.98
6.97
6.96
6.95
6.94
6.92
6.19
6.18

4.32
4.29
4.27
4.25
3.98
3.96
3.94

3.06

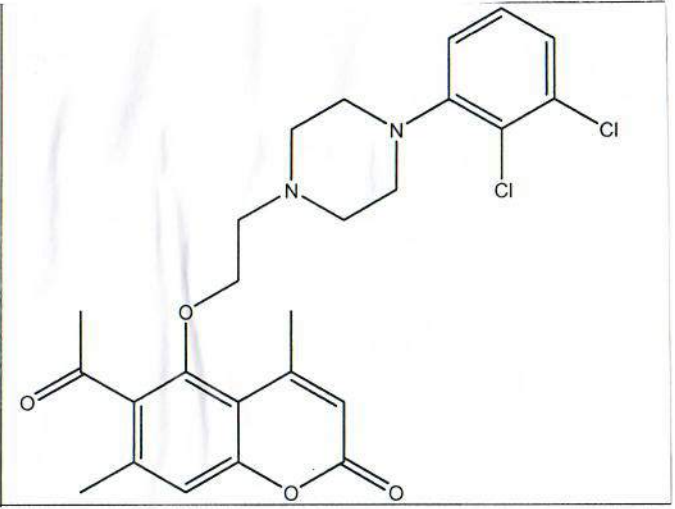
2.80
2.78
2.76
2.70
2.69
2.68
2.66
2.66
2.61
2.53
2.46
2.30
1.26

0.08
0.00



KO-324-13C
KO 324 13C in CDCl3

4i



— 204.84

~ 160.10
~ 154.84
~ 152.29

~ 139.43
~ 134.26
~ 133.53

~ 127.69
~ 124.98

~ 118.82
~ 116.17
~ 115.52
~ 112.74

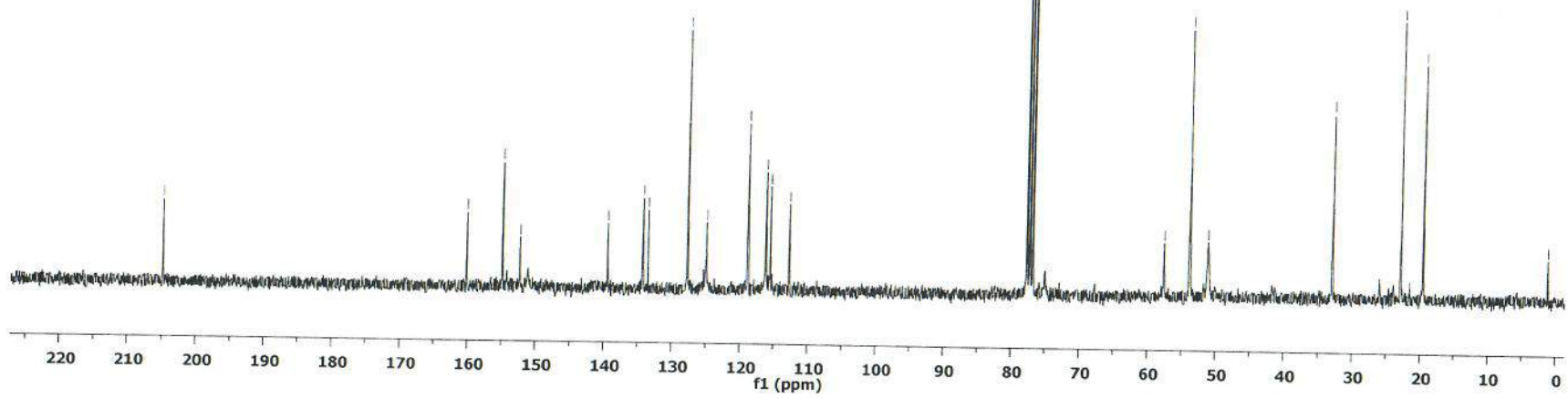
~ 77.65
~ 77.23
~ 76.81

~ 57.58
~ 53.86
~ 51.21

— 32.93

— 22.88
— 19.58

— 1.21

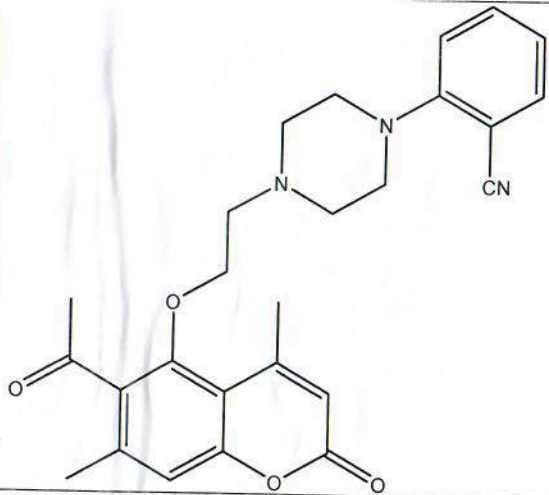


4j

KO-325-1h

KO 325 1H

4j



7.59
7.58
7.56
7.56
7.53
7.52
7.50
7.47
7.47
7.27
7.05
7.03
7.03
7.01
6.99
— 6.19

3.99
3.98
3.96
3.87

— 3.25

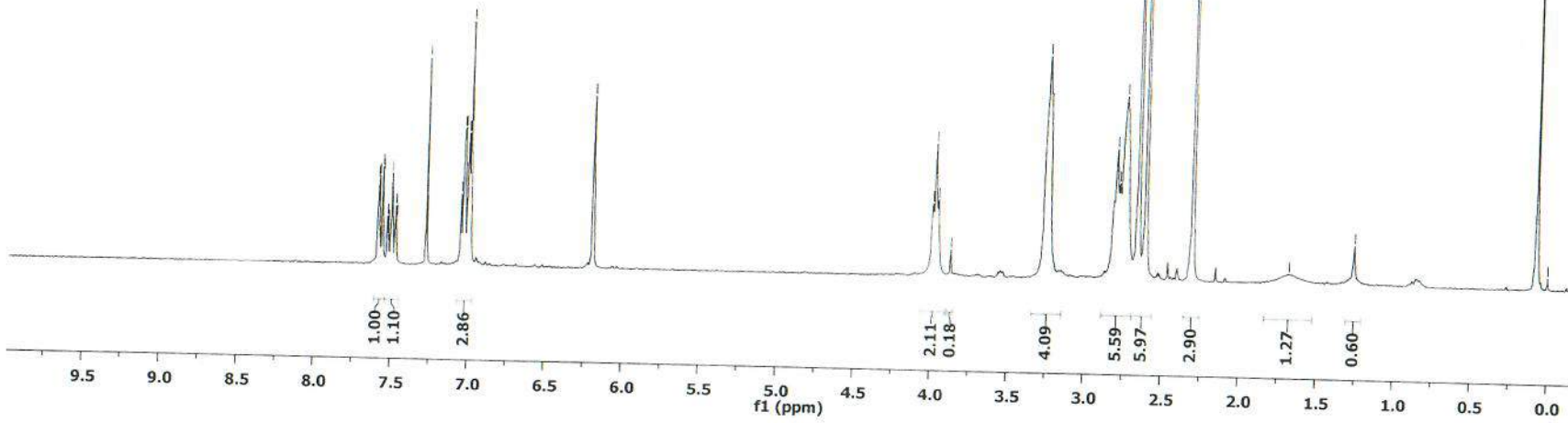
2.80
2.78
2.75

2.66
2.61
2.31

— 1.68

— 1.26

0.08
0.00



4j

KO-325-13C

KO-325-13C in CDCl₃

— 204.86

— 160.10
— 154.85
— 152.22

— 139.41
— 134.52
— 134.07
— 133.58

— 118.97
— 118.52
— 116.23
— 115.60
— 112.75

— 77.65
— 77.23
— 76.81

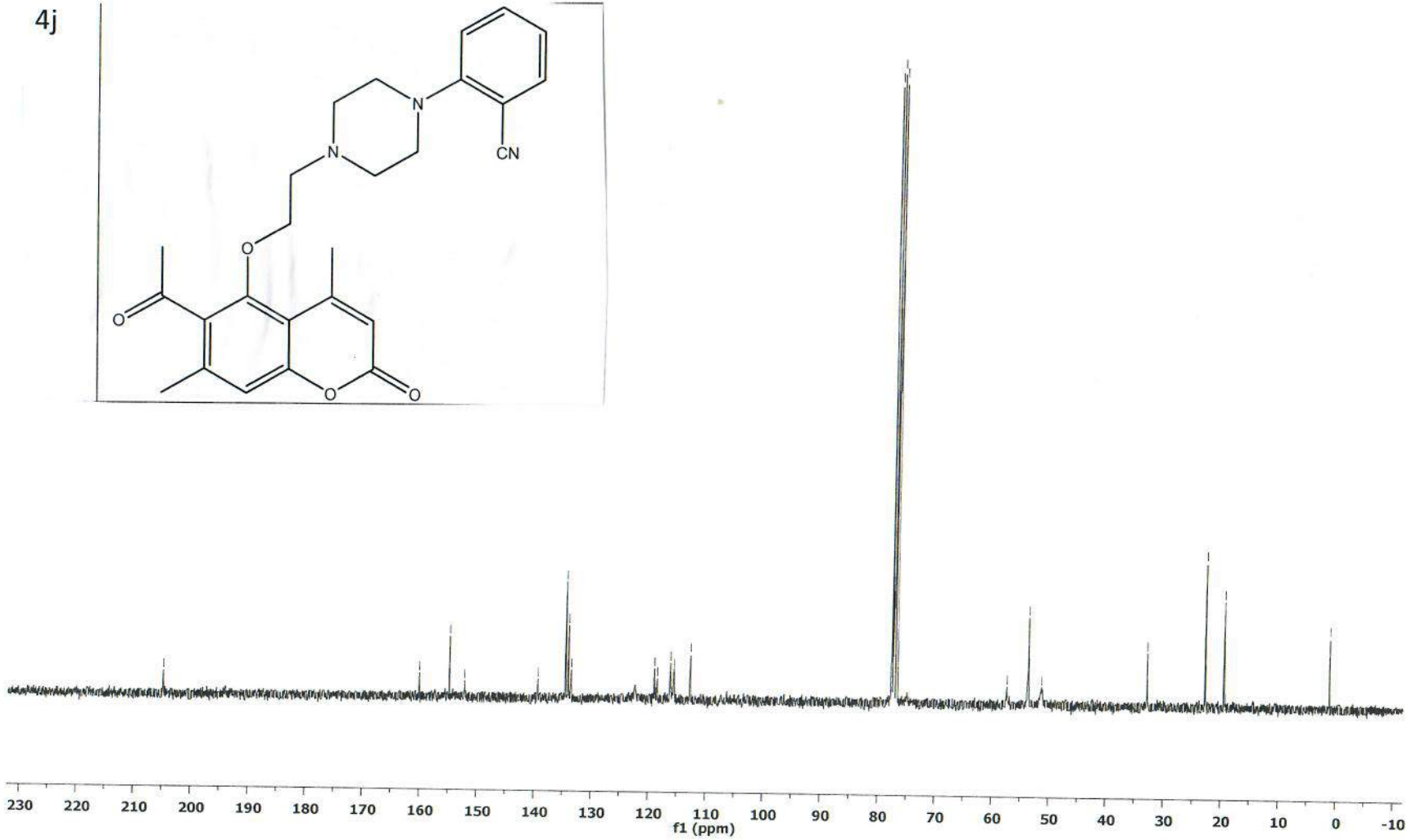
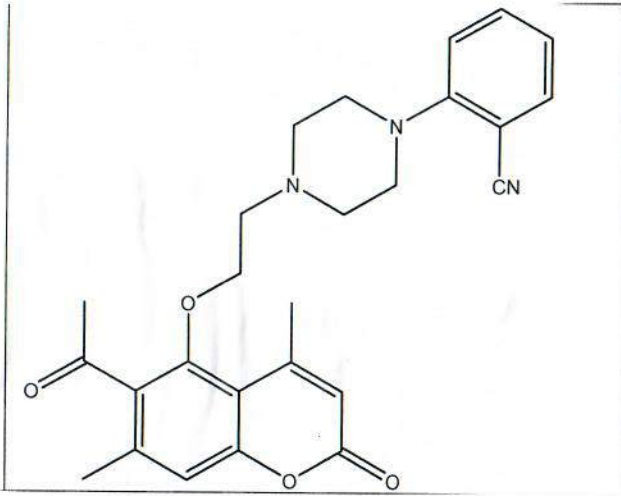
— 57.49
— 53.73
— 51.40

— 32.98

— 22.88
— 19.58

— 1.22

4j



5

KO-400-13C

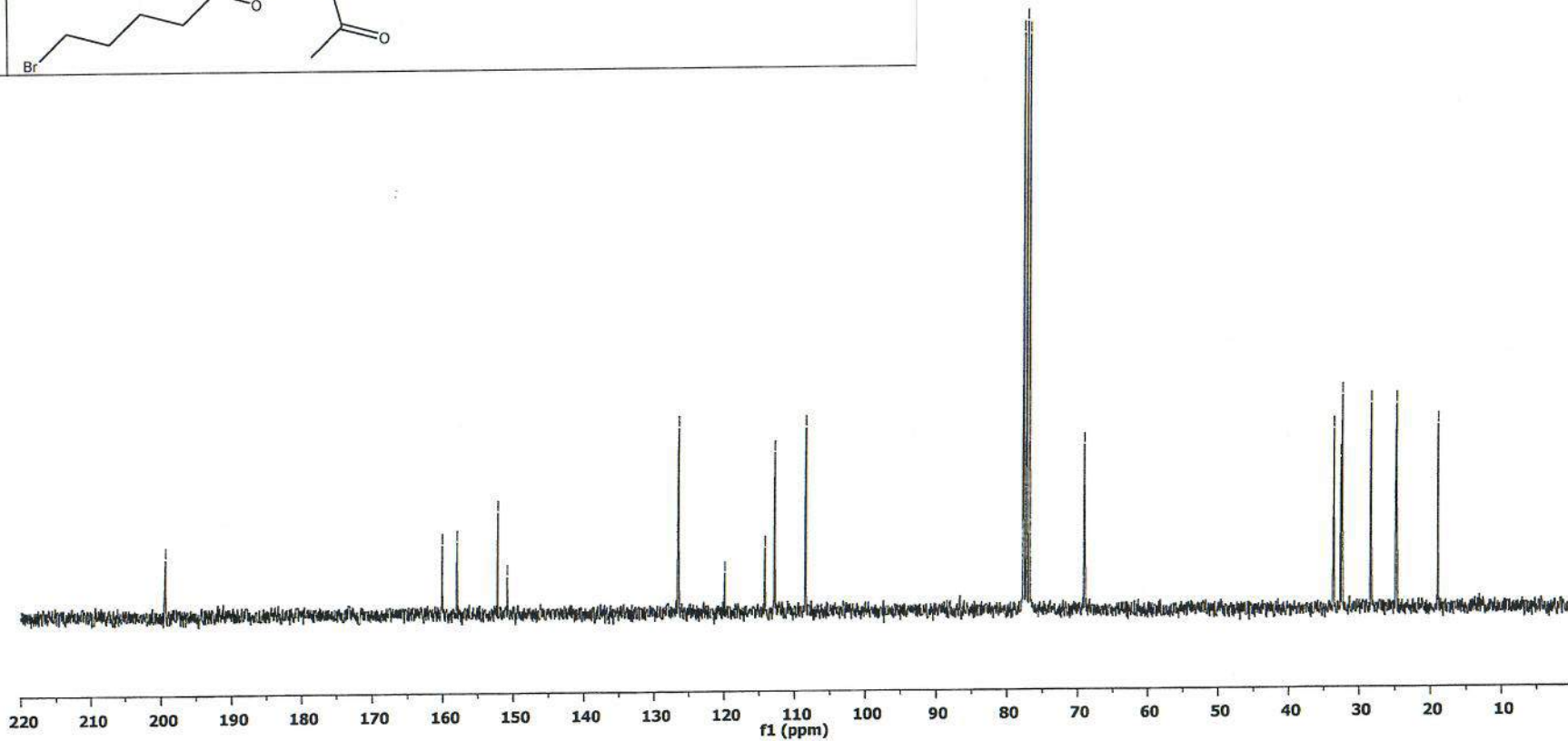
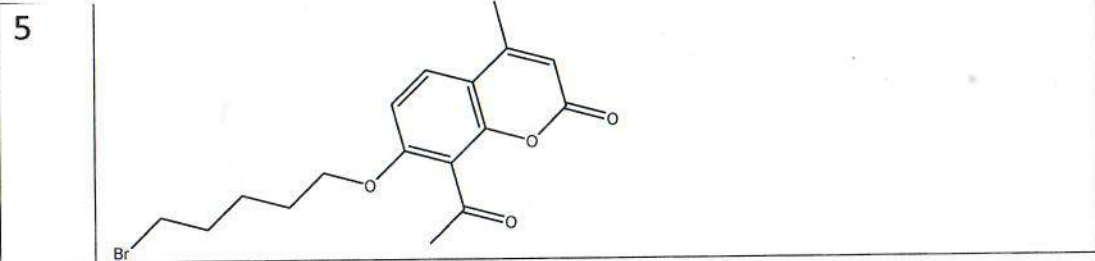
— 199.42

160.13
158.03
152.22
150.88

— 126.50
— 119.88
114.18
112.83
108.45

77.65
77.23
76.81
— 69.07

33.64
32.64
32.43
28.33
24.81
— 18.96



KO-100-1H

7.569
7.539

7.269

6.881
6.851

6.146
6.142

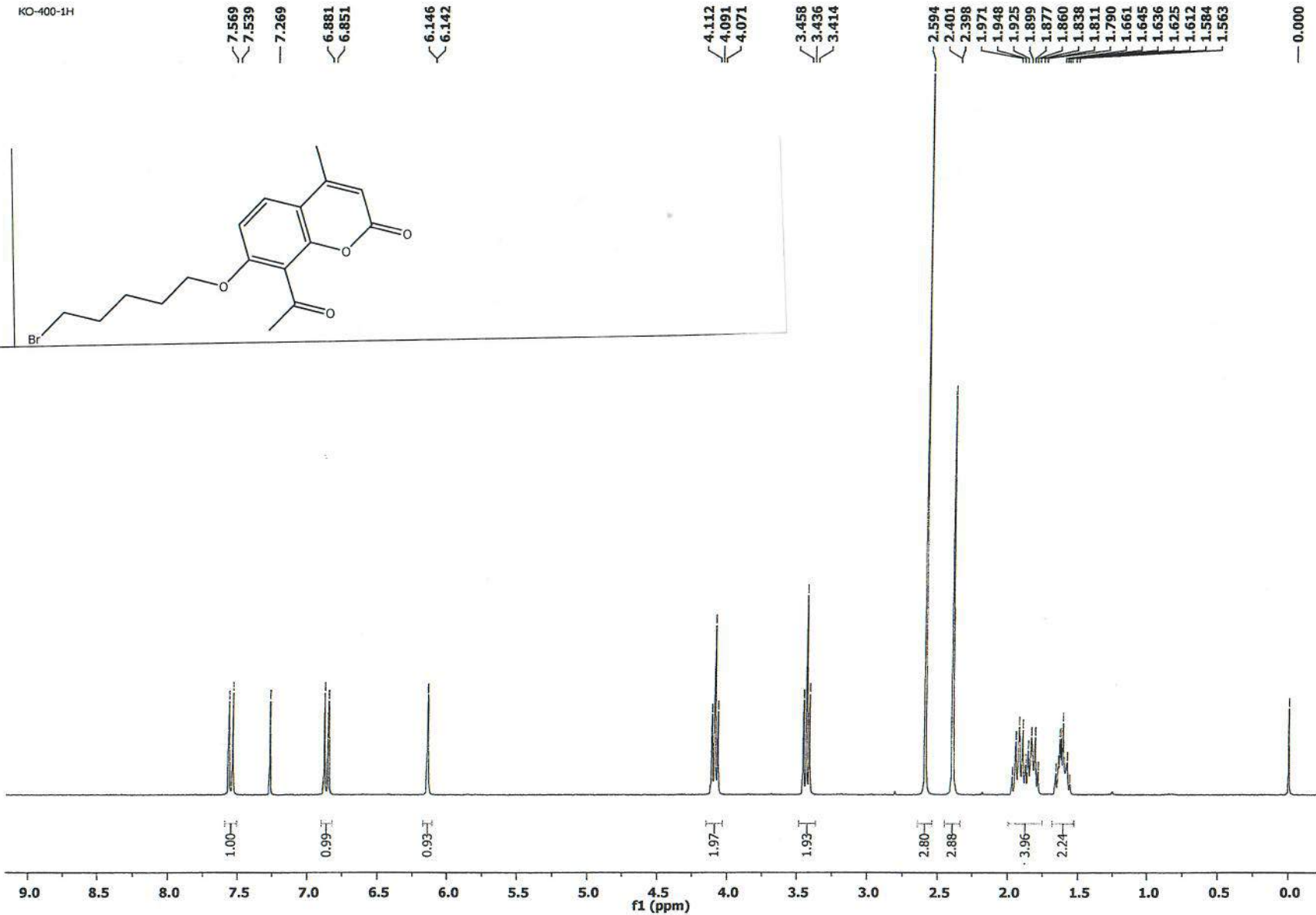
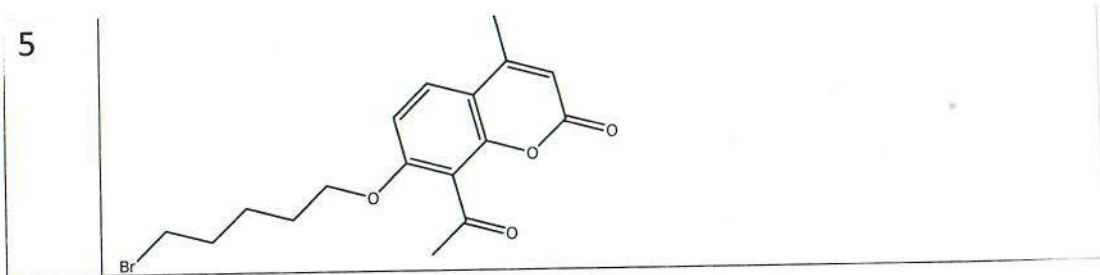
4.112
4.091
4.071

3.458
3.436
3.414

2.594
2.401
2.398
1.971
1.948
1.925
1.899
1.877
1.860
1.838
1.811
1.790
1.661
1.645
1.636
1.625
1.612
1.584
1.563

0.000

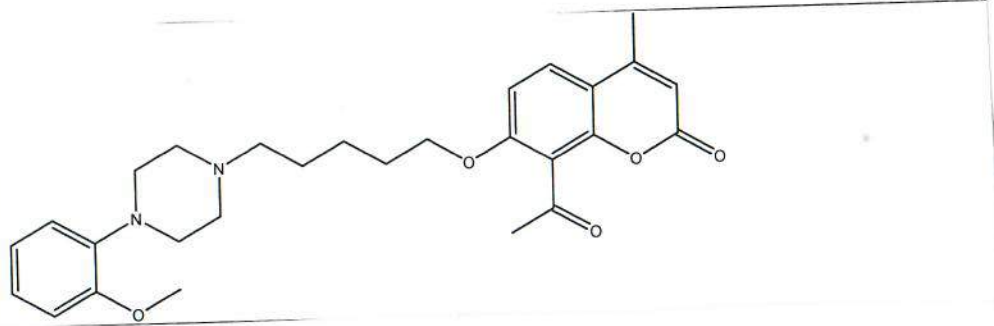
5



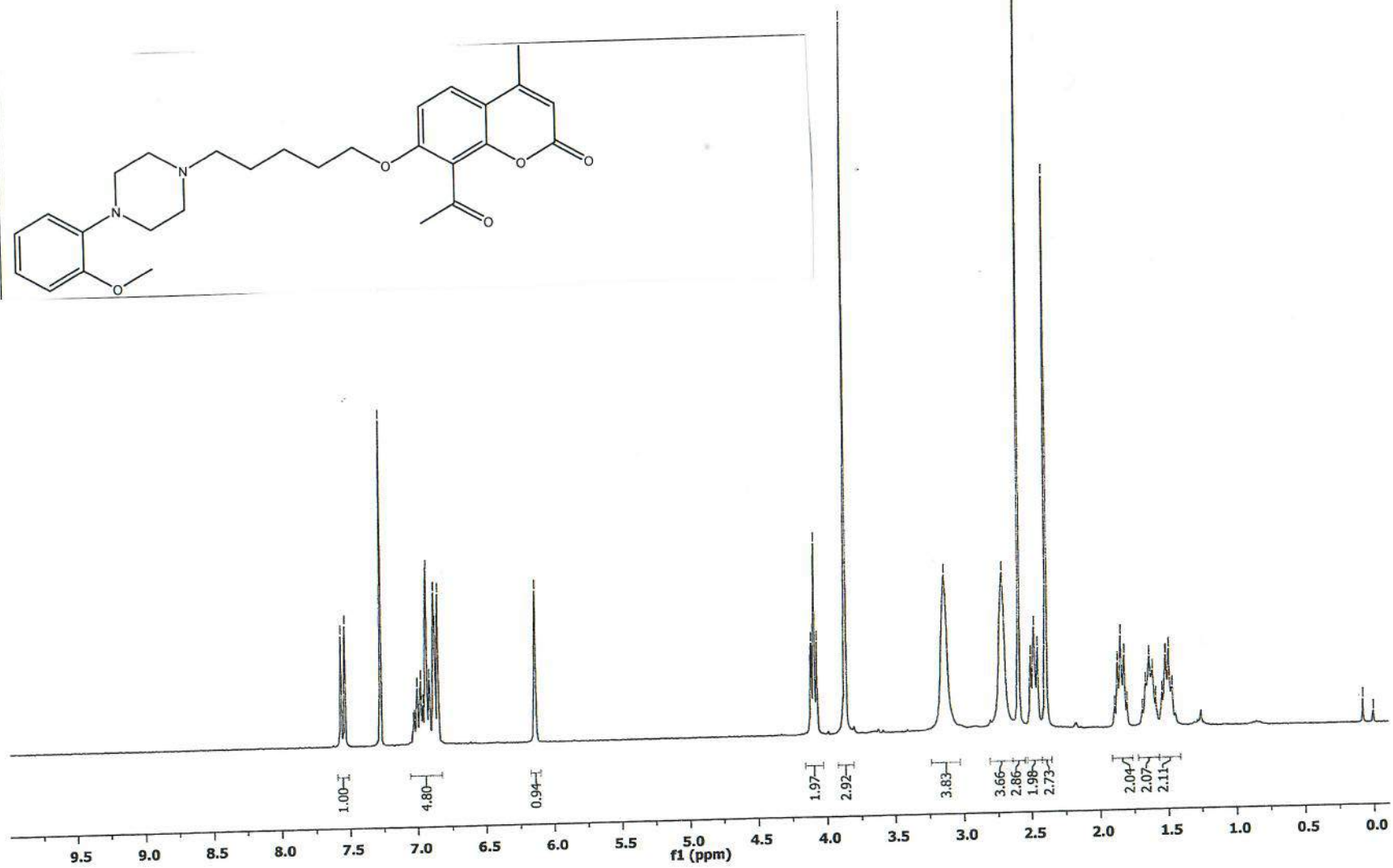
5a

KO-401-1H

5a



7.564
7.535
7.273
7.002
6.975
6.942
6.935
6.915
6.883
6.876
6.853
6.838
4.113
4.091
4.070
3.863
3.140
2.717
2.592
2.504
2.480
2.454
2.394
1.891
1.868
1.845
1.821
1.799
1.688
1.664
1.638
1.613
1.588
1.543
1.518
1.495
1.469
0.074
0.000



5a

KO-401-13C
KO 401 13C

— 199.46

— 160.14
— 158.09
— 152.37
— 152.26
— 150.81

— 141.03

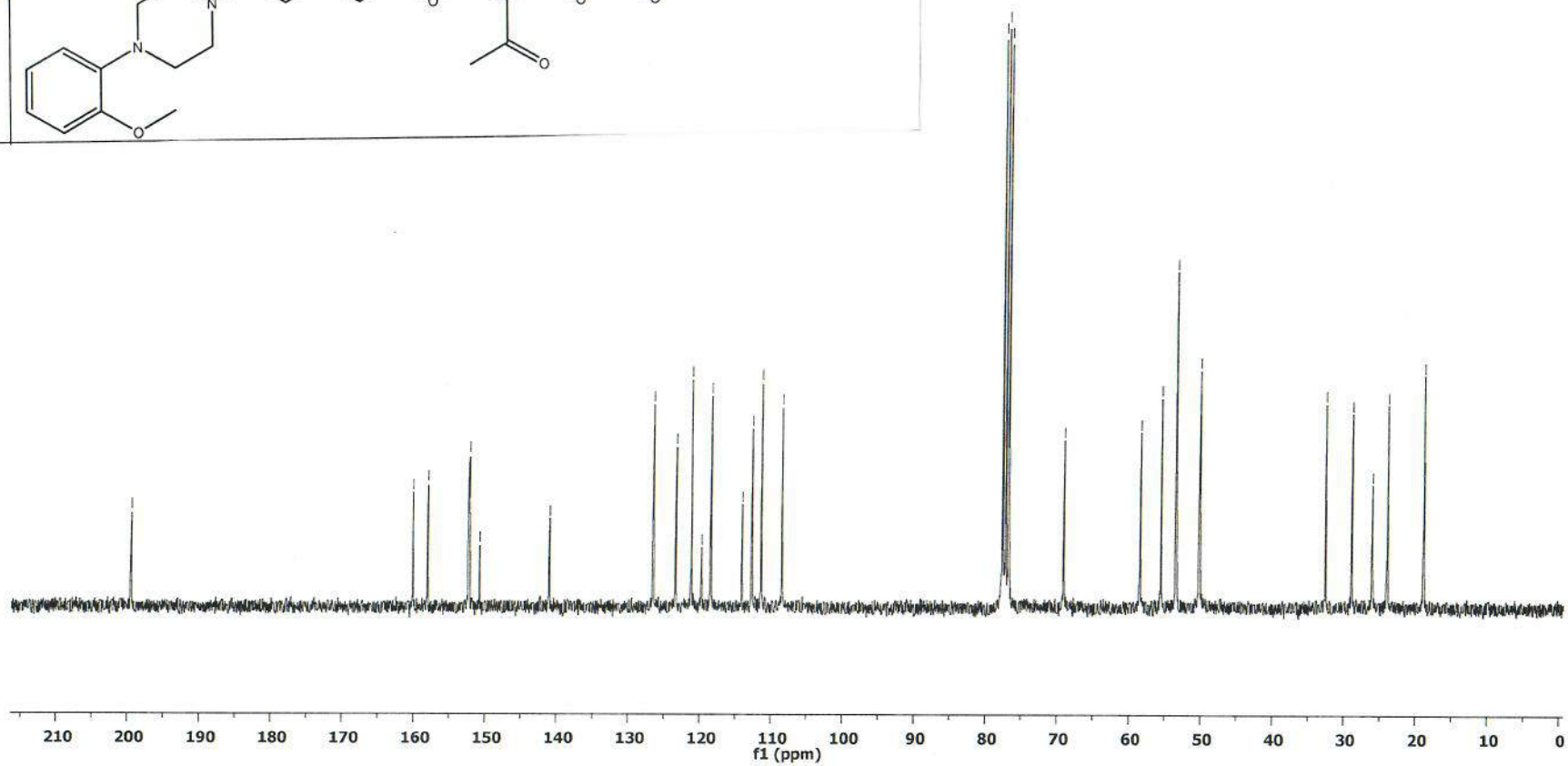
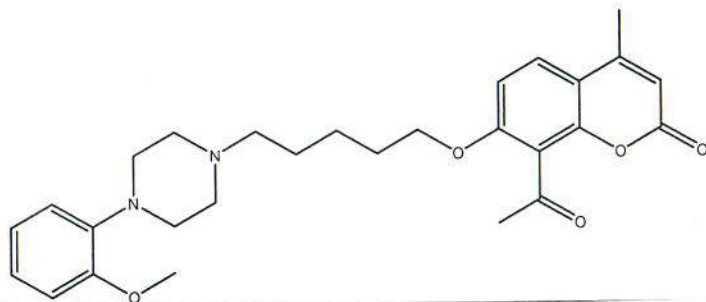
— 126.50
— 123.33
— 121.18
— 119.76
— 118.47
— 114.06
— 112.70
— 111.36
— 108.49

— 77.65
— 77.23
— 76.81
— 69.11

— 58.45
— 55.54
— 53.46
— 50.18

— 32.61
— 28.91
— 26.06
— 23.98
— 18.92

5a



KO-405-1H
KO-405 1H w CDCl3

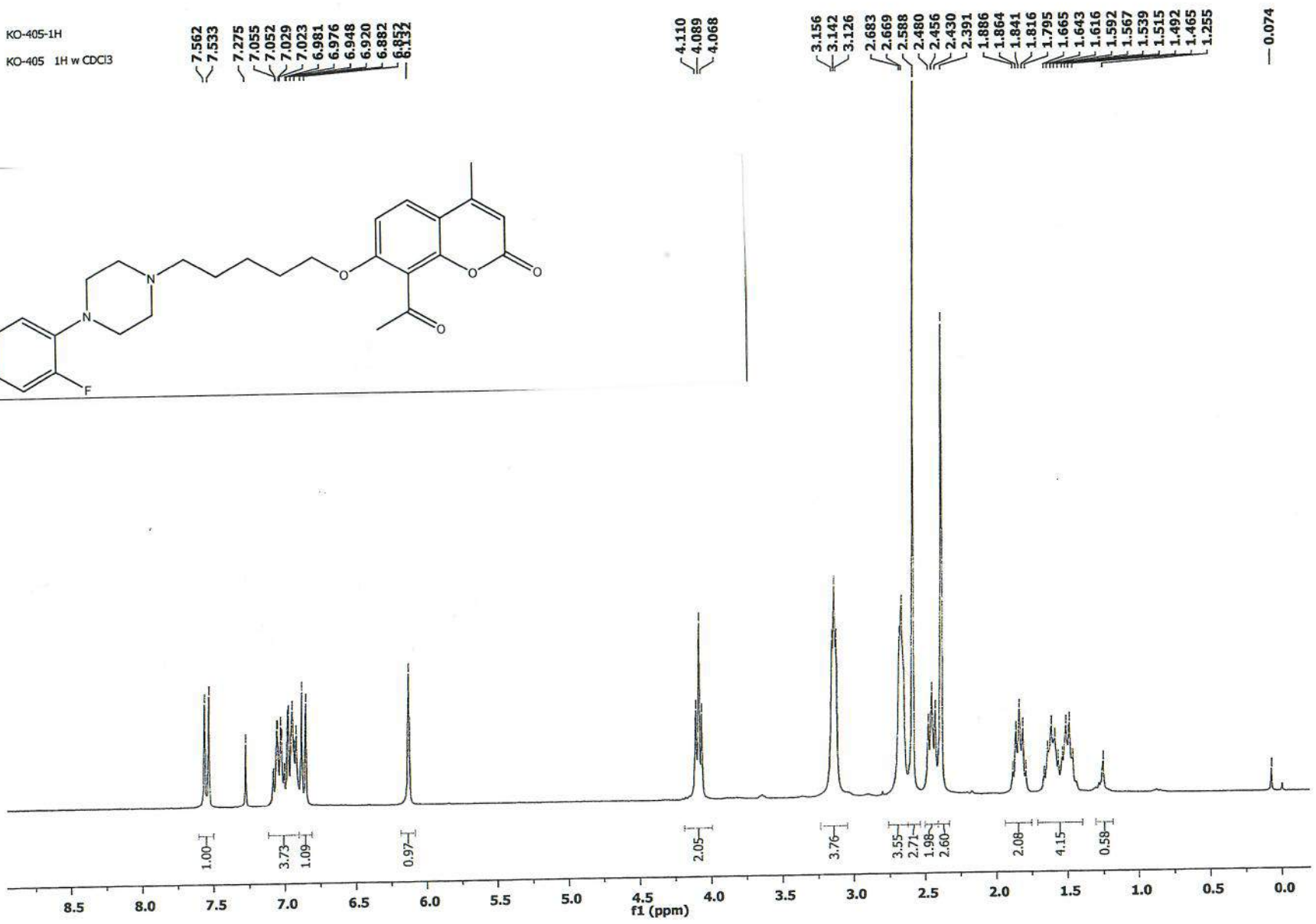
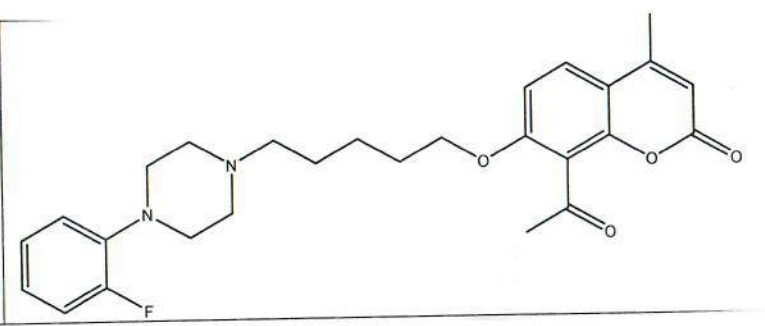
7.562
7.533
7.275
7.055
7.052
7.029
7.023
6.981
6.976
6.948
6.920
6.882
6.852

4.110
4.089
4.068

3.156
3.142
3.126
2.683
2.669
2.588
2.480
2.456
2.430
2.391
1.886
1.864
1.841
1.816
1.795
1.665
1.643
1.616
1.592
1.567
1.539
1.515
1.492
1.465
1.255

0.074

5b



KO-405-13C

KO 405 13C w CDCl3

— 199.45

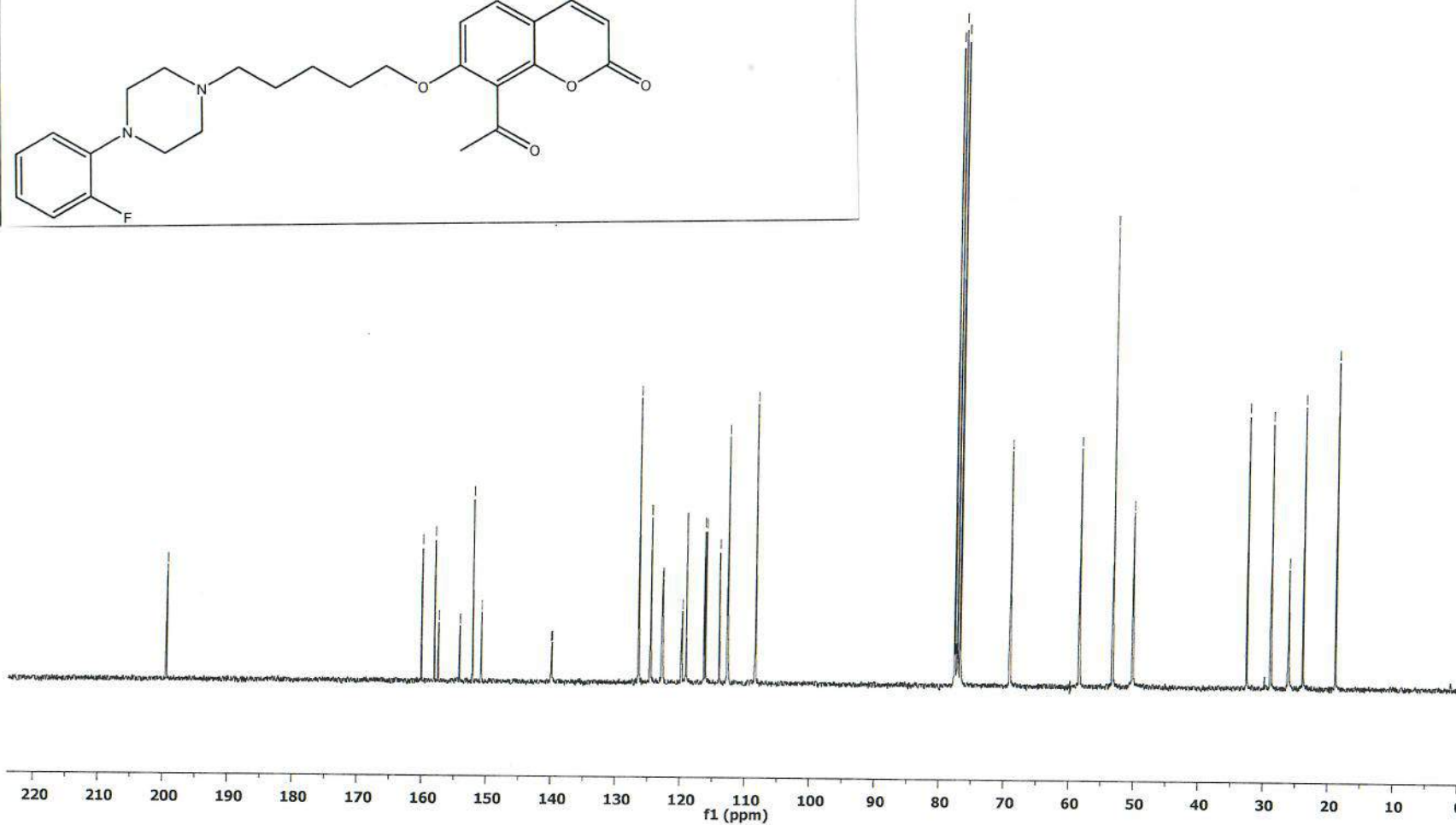
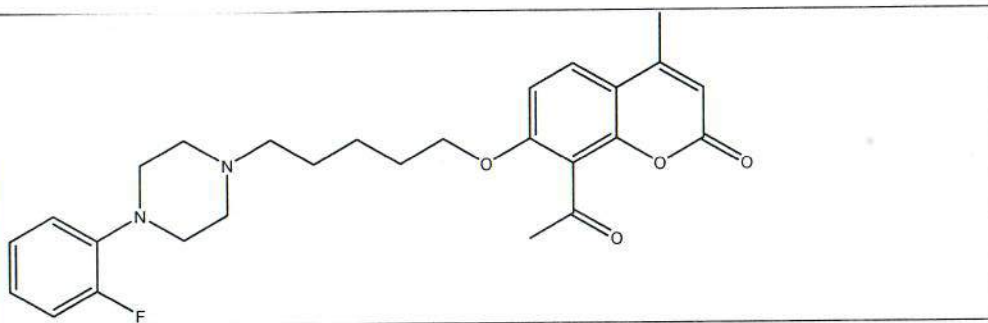
160.14
158.11
157.50
154.24
152.24
150.84
140.05
139.94
126.50
124.70
124.65
122.88
122.77
119.80
119.19
119.15
116.41
116.14
114.09
112.74
108.48

77.65
77.43
77.23
76.81
— 69.14

58.44
53.35
50.21

32.62
28.95
26.19
24.00
18.93

5b



5c

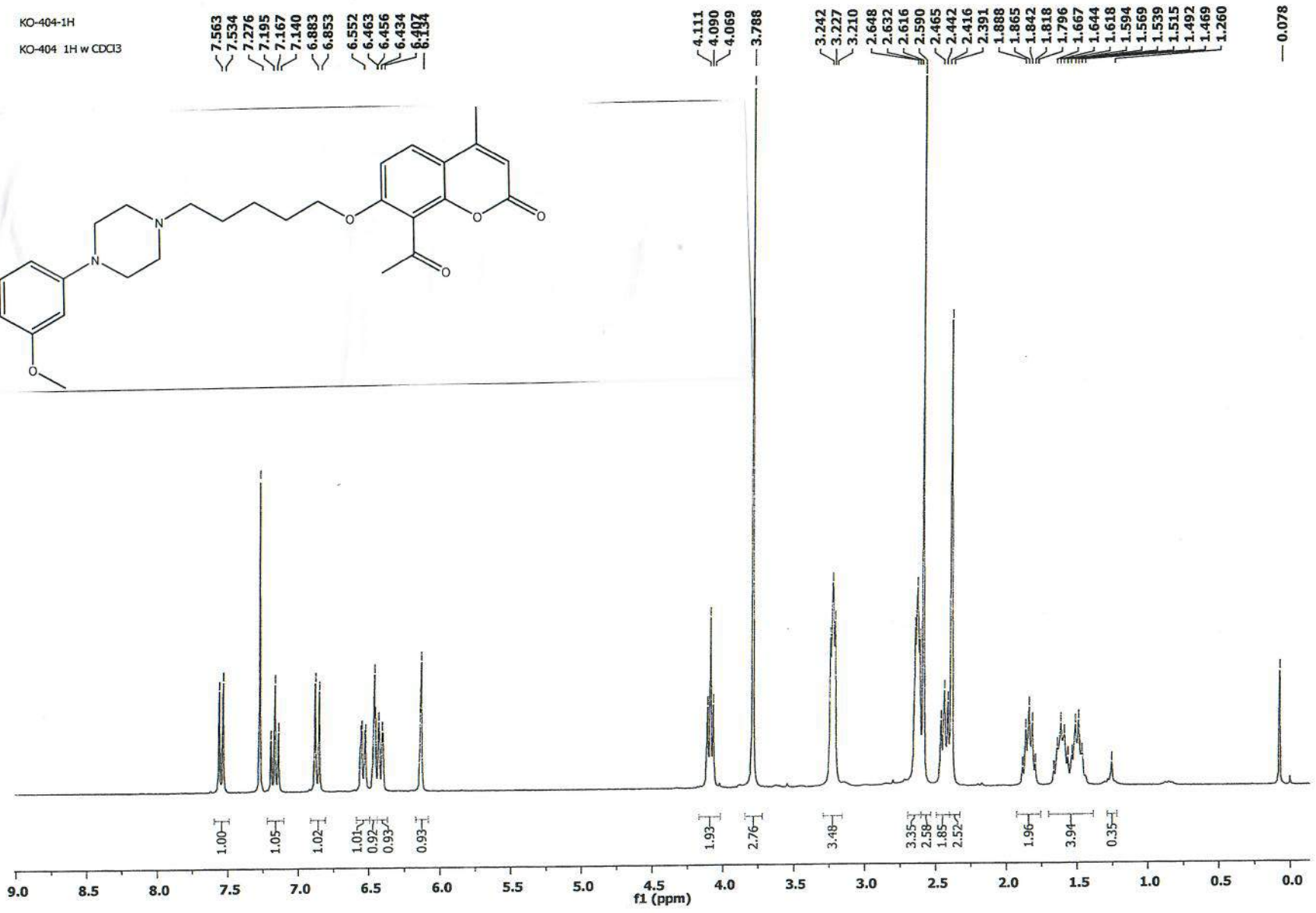
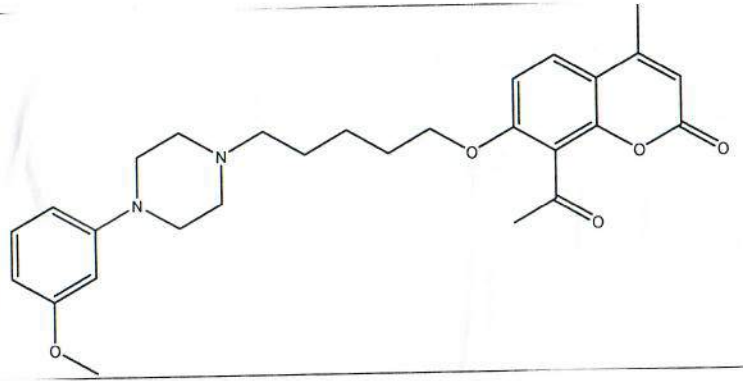
KO-404-1H
KO-404 1H w CDCl3

7.563
7.534
7.276
7.195
7.167
7.140
6.883
6.853
6.552
6.463
6.456
6.434
6.402
6.134

4.111
4.090
4.069
3.788

3.242
3.227
3.210
2.648
2.632
2.616
2.590
2.465
2.442
2.416
2.391
1.888
1.865
1.842
1.818
1.796
1.667
1.644
1.618
1.594
1.569
1.539
1.515
1.492
1.469
1.260
0.078

5c



5c

KO-404-13C
KO 404 13C w CDCl₃

199.47

160.74
160.14
158.10
152.59
152.25
150.82

129.97
126.51

119.77
114.07
112.72
109.09
108.47
104.82
102.76

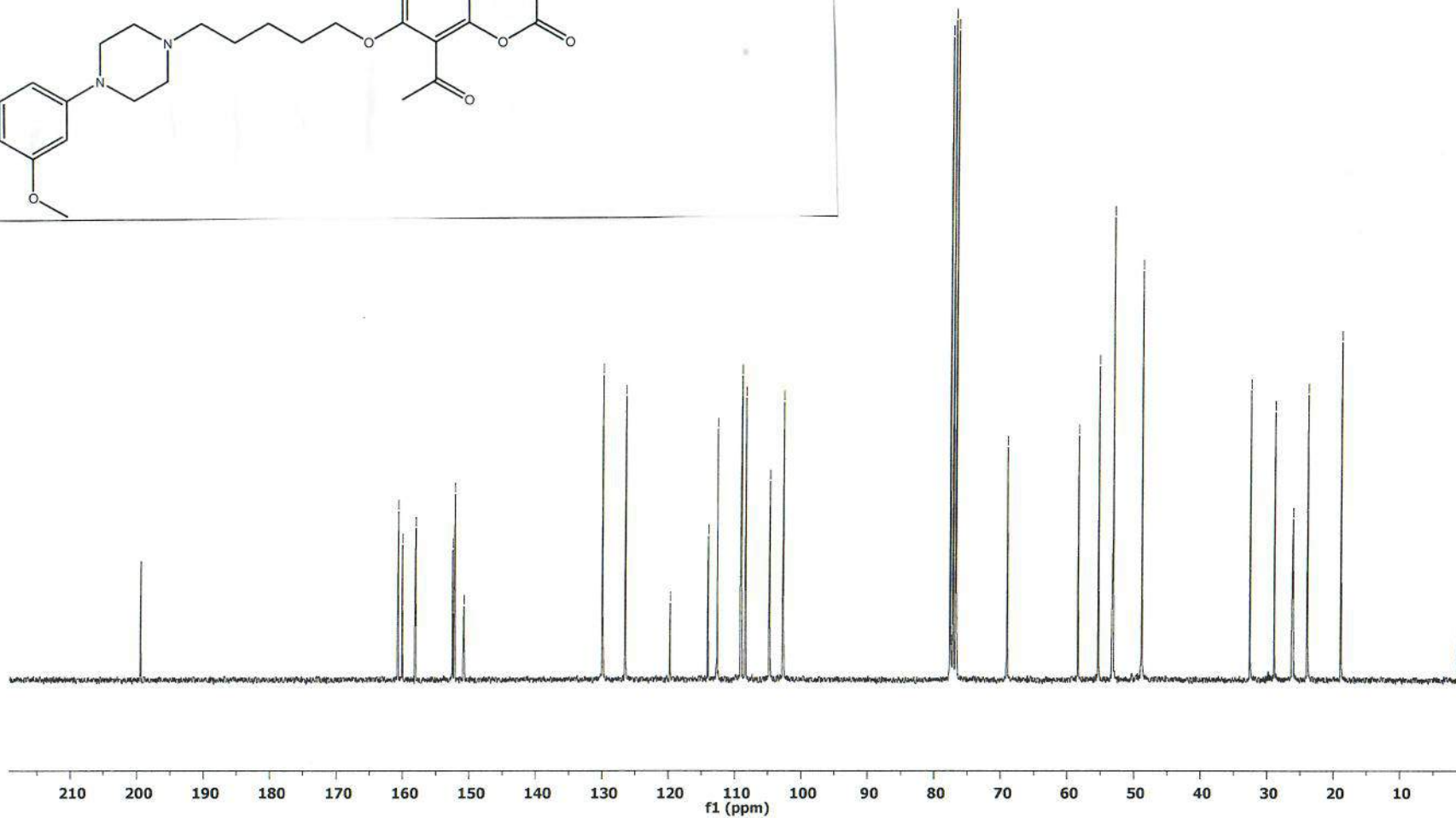
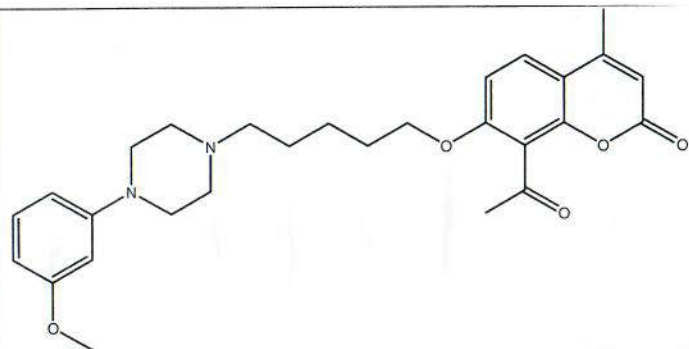
77.65
77.43
77.23
76.81
69.14

58.43
55.36
53.21
48.86

32.61
28.93
26.23
24.00
18.92

1.19

5c



5d

KO-407-1H-cdcl3

KO407 w CDCl3 + TMS

7.56
7.53
7.26
7.06
7.04
6.88
6.85
6.83
6.80
6.77

6.13
6.13

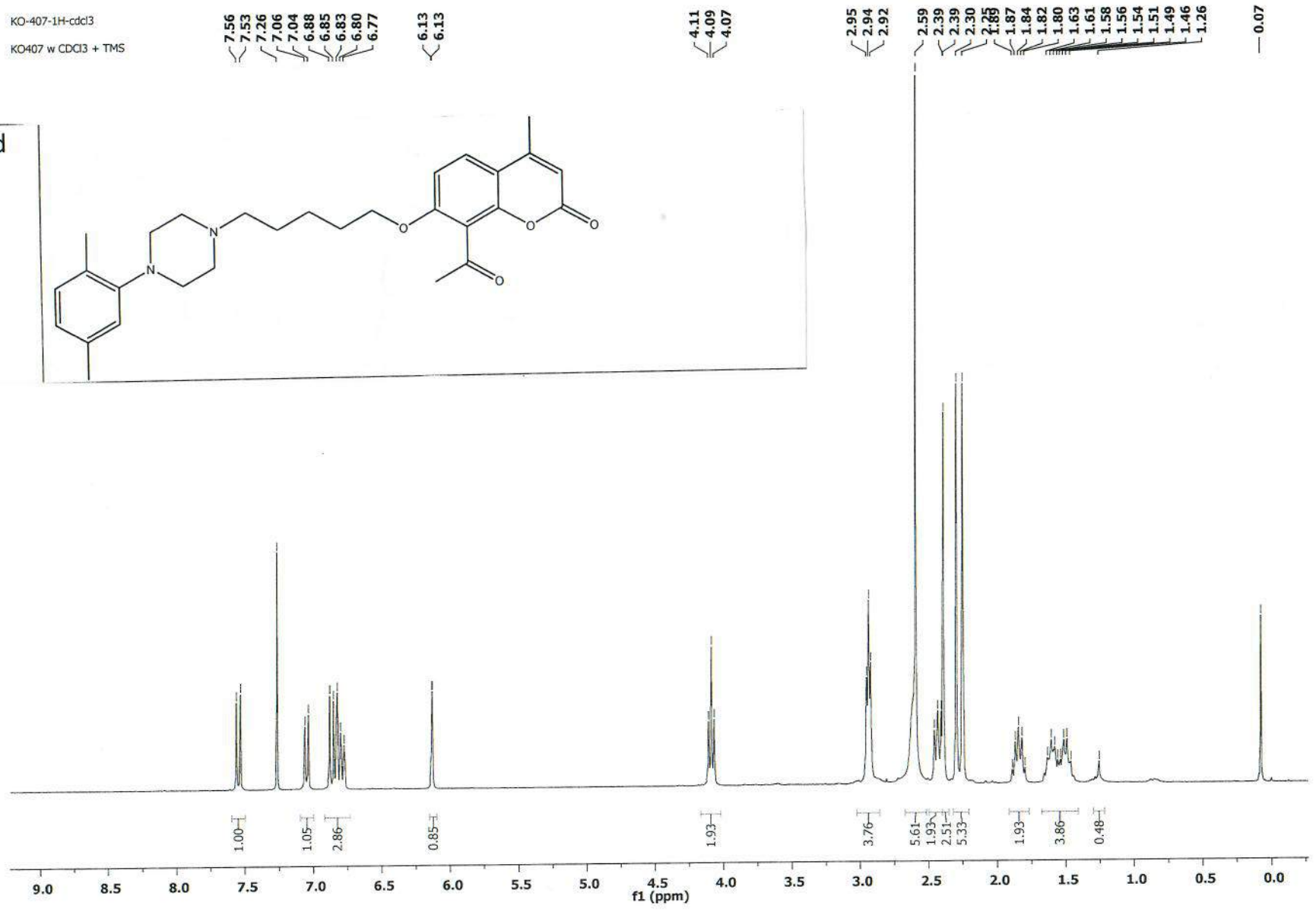
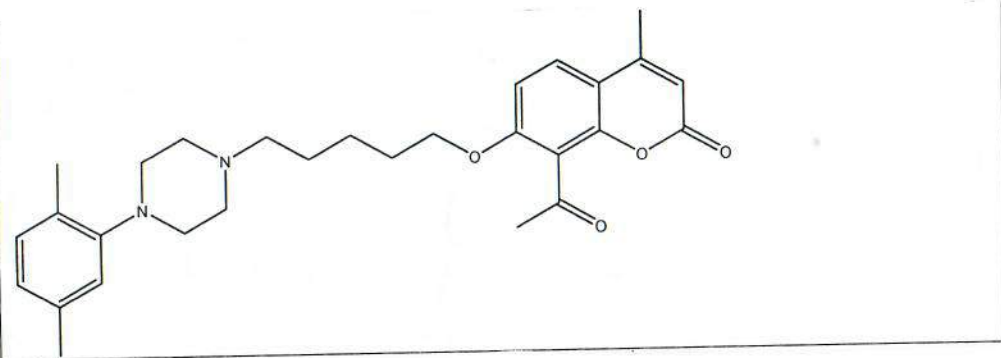
4.11
4.09
4.07

2.95
2.94
2.92

2.59
2.39
2.39
2.30
2.25
1.87
1.84
1.82
1.80
1.63
1.61
1.58
1.56
1.54
1.51
1.49
1.46
1.26

0.07

5d



5d

KO-407-13C-cdcl3

KO-407 w CDCl3 13C-NMR

— 199.40

160.14
158.16
152.23
151.44
150.83

136.23
131.01
129.40
126.47
123.88
119.86
119.79

114.05
112.71
108.44

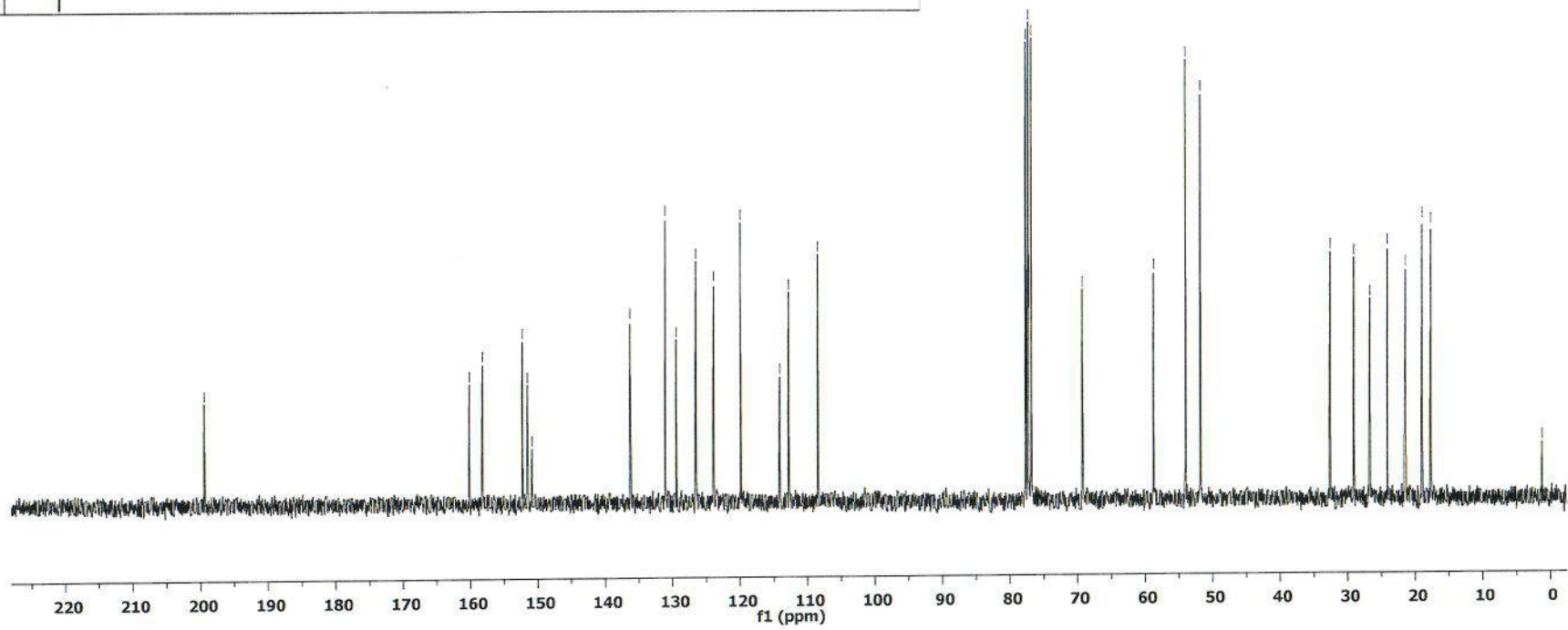
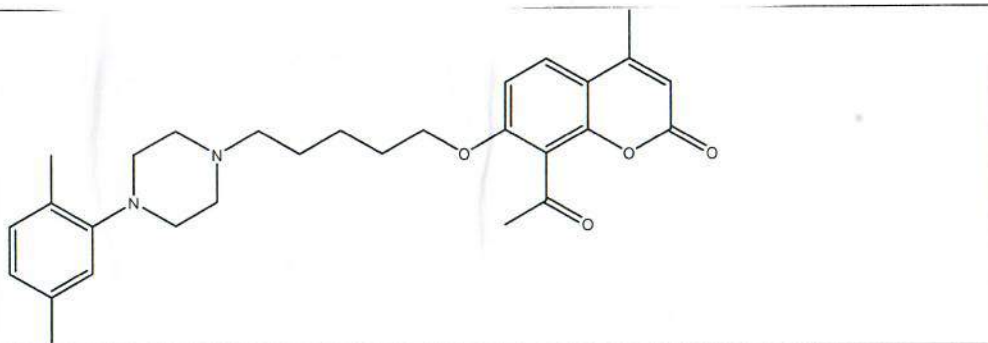
77.65
77.23
76.81
— 69.22

58.69
53.97
51.79

32.59
29.05
26.67
24.11
21.38
18.92
17.64

— 1.19

5d



5e

KO-408-1H-cdcl3

KO408 w CDCl3 + TMS

7.56
7.53
7.27
7.19
7.16
7.14
6.88
6.85
6.68
6.65
6.60
6.56
6.51
6.13
6.13

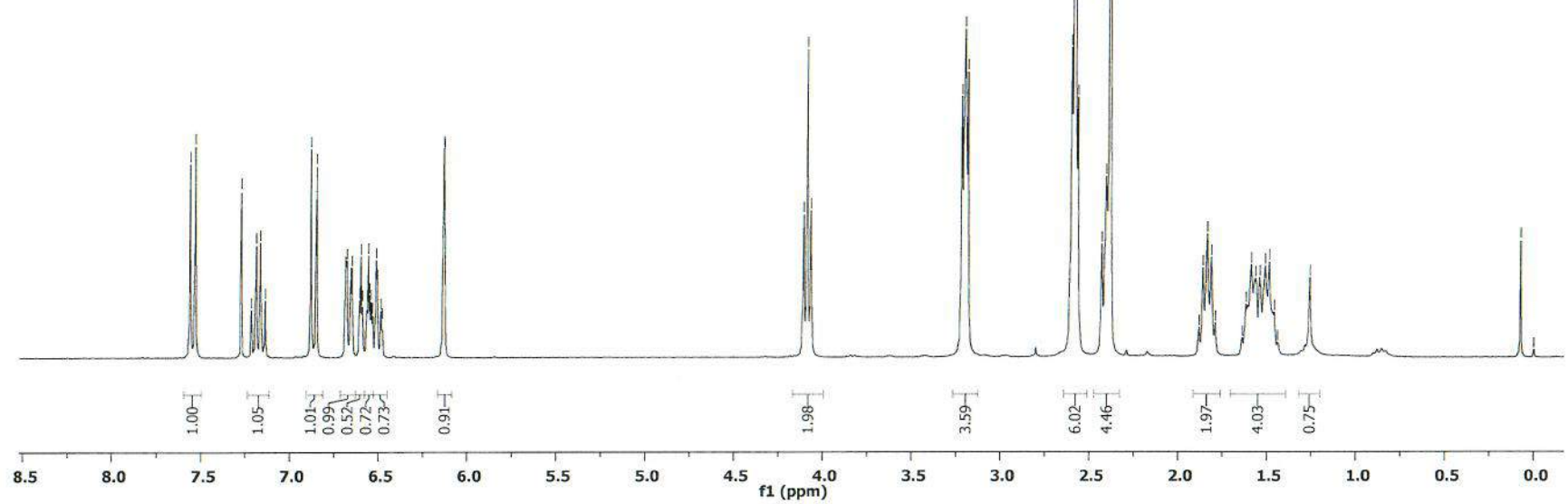
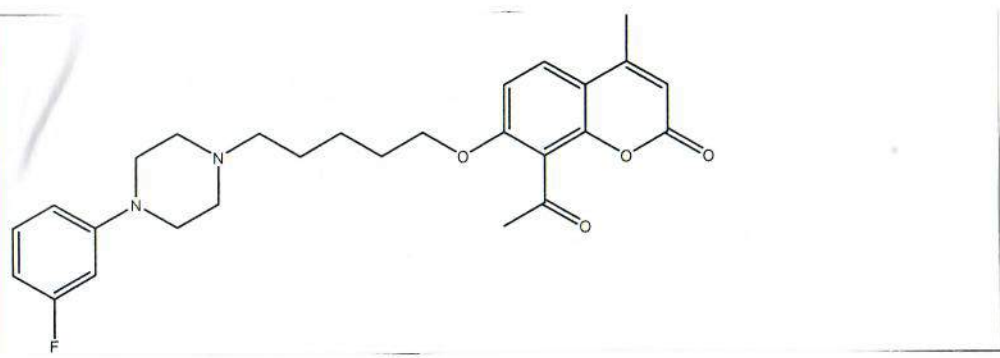
4.11
4.09
4.06

3.22
3.20
3.18

2.60
2.59
2.57
2.43
2.41
2.39
2.39
1.88
1.86
1.84
1.81
1.79
1.64
1.62
1.59
1.57
1.54
1.51
1.49
1.46
1.44
1.26

0.08
-0.00

5e



KO-408-13C-cdcl3

KO-408 w CDCl3 13C-NMR

199.40

165.62
162.40
160.13
158.14
153.17
153.04
152.22
150.84

130.32
130.19
126.48

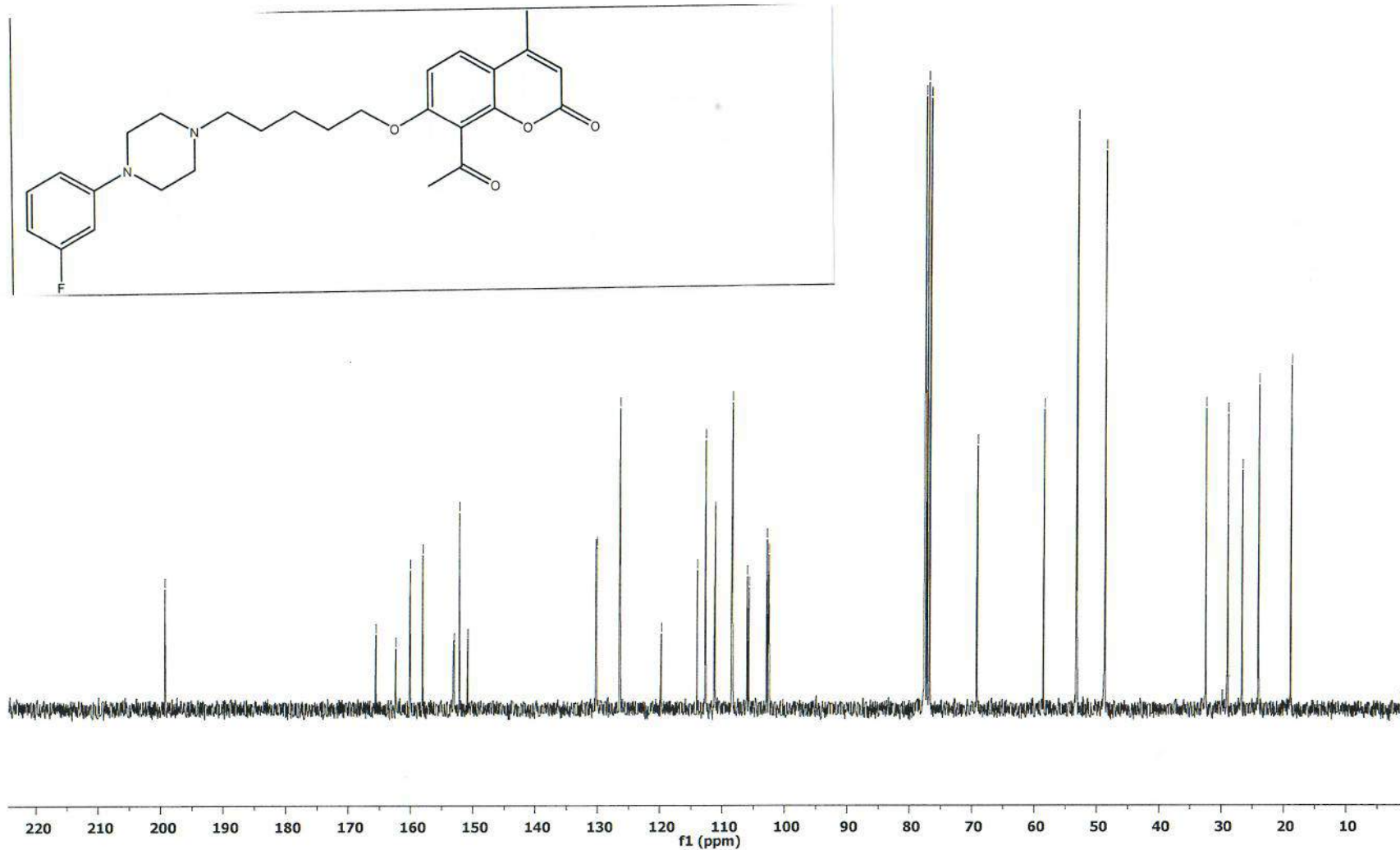
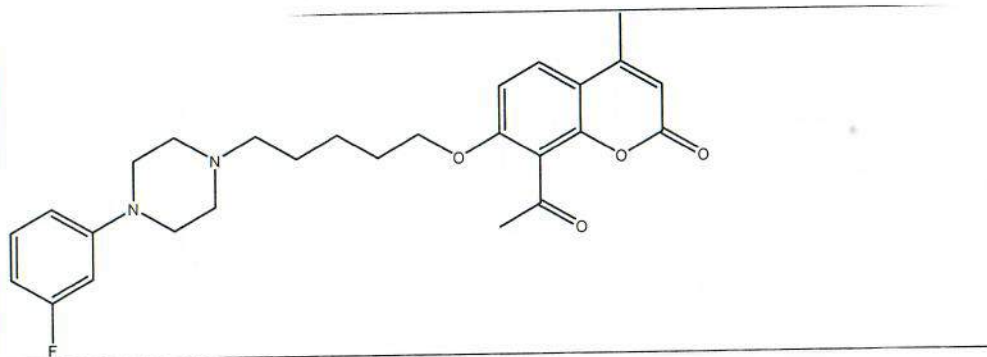
119.80
114.07
112.74
111.24
111.20
108.44
106.04
105.76
102.89
102.56

77.65
77.23
76.81
69.22

58.53
53.25
48.76

32.60
29.05
26.69
24.07
18.92

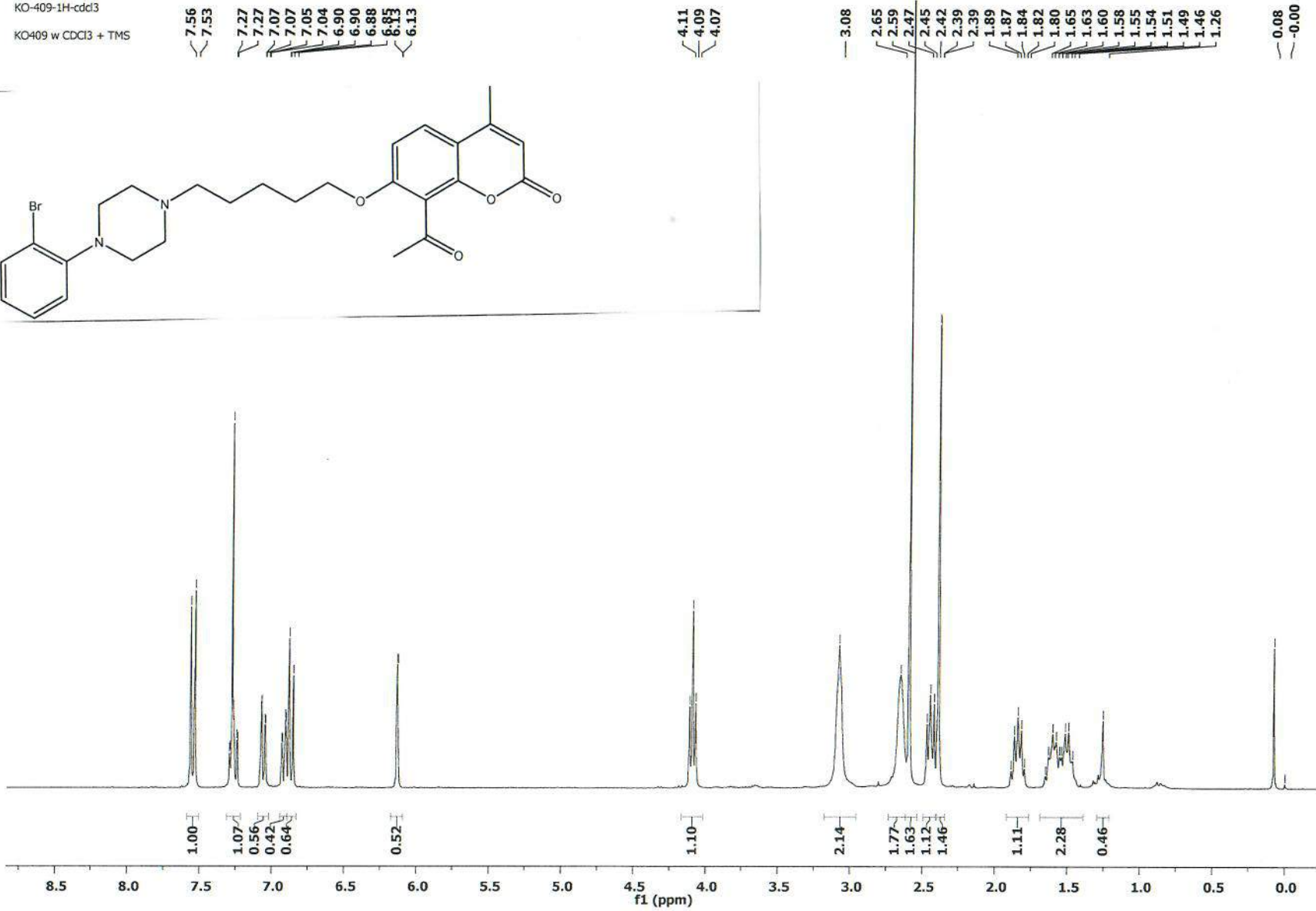
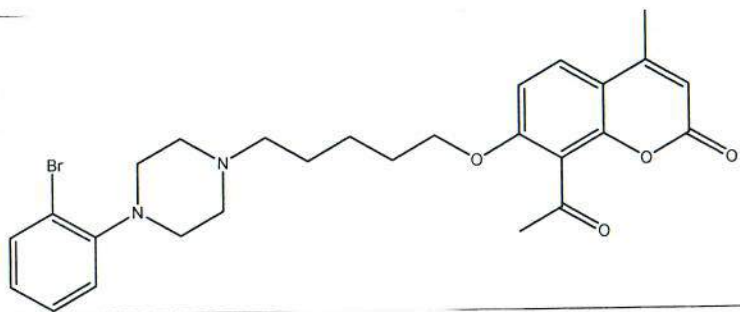
5e



5f

KO-409-1H-cdcl3
KO409 w CDCl3 + TMS

5f



5f

KO-409-13C-cdcl3
KO 409 13C w CDCl3

— 199.39

160.15
158.16
152.22
150.84
150.77

133.98
128.45
126.47
124.51
121.09
120.02
119.80
114.06
112.73
108.44

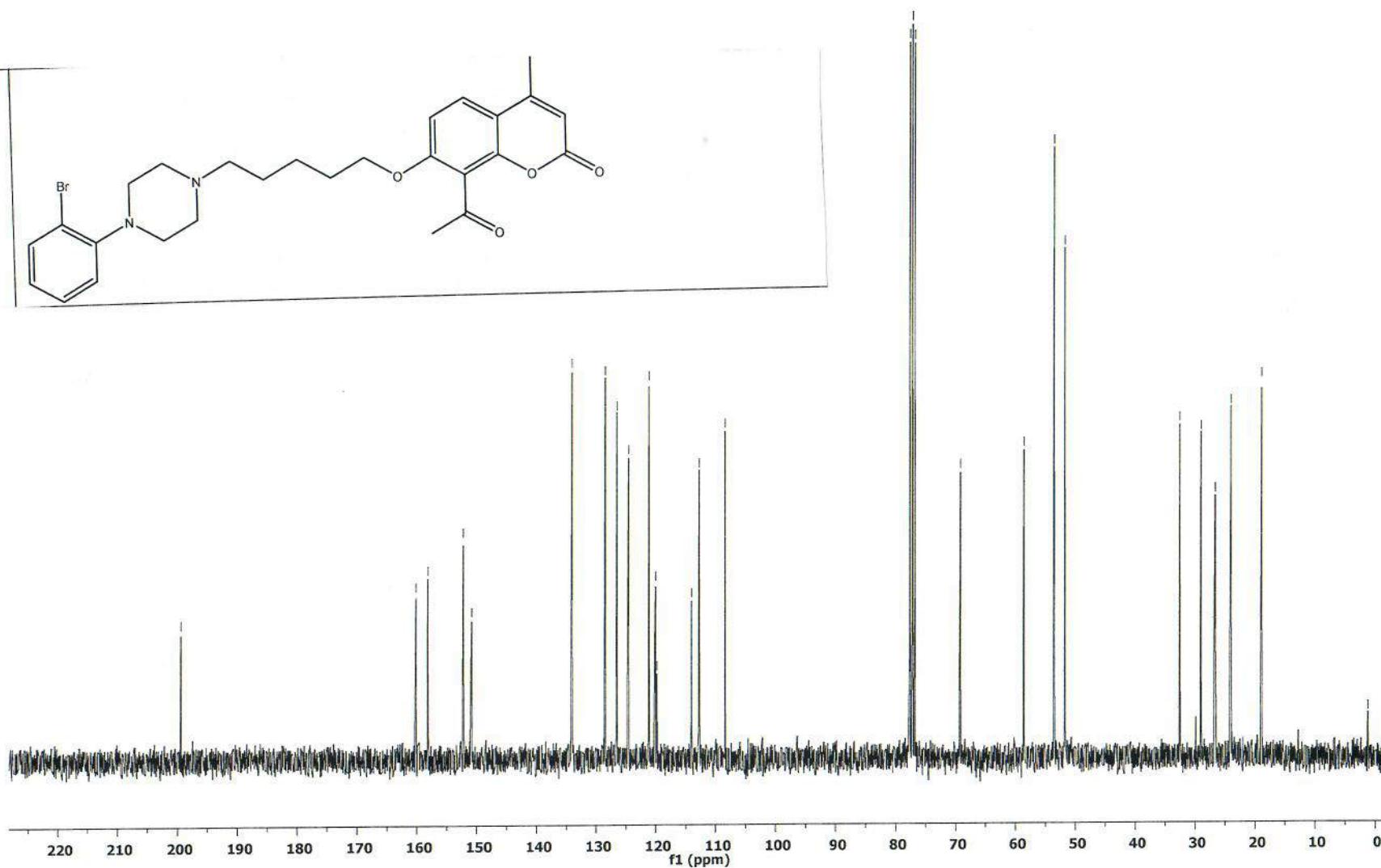
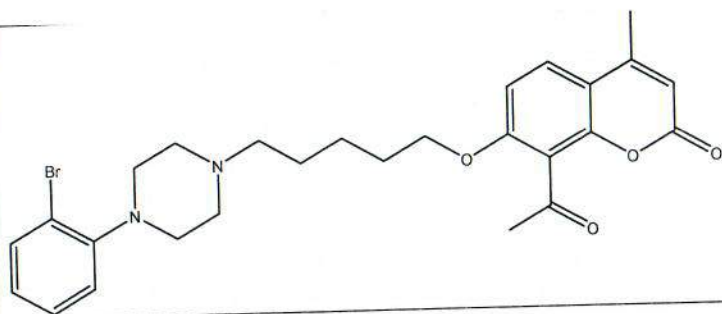
77.65
77.23
76.81
— 69.22

58.59
53.59
51.75

32.60
29.05
26.68
24.09
18.93

— 1.20

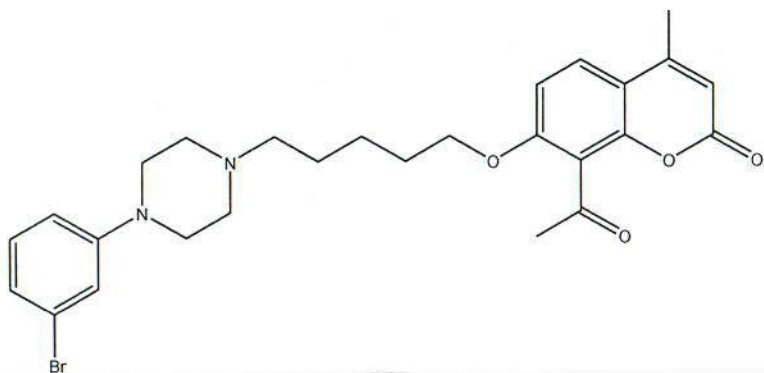
5f



5g

KO-406 1H w CDCl3

5g

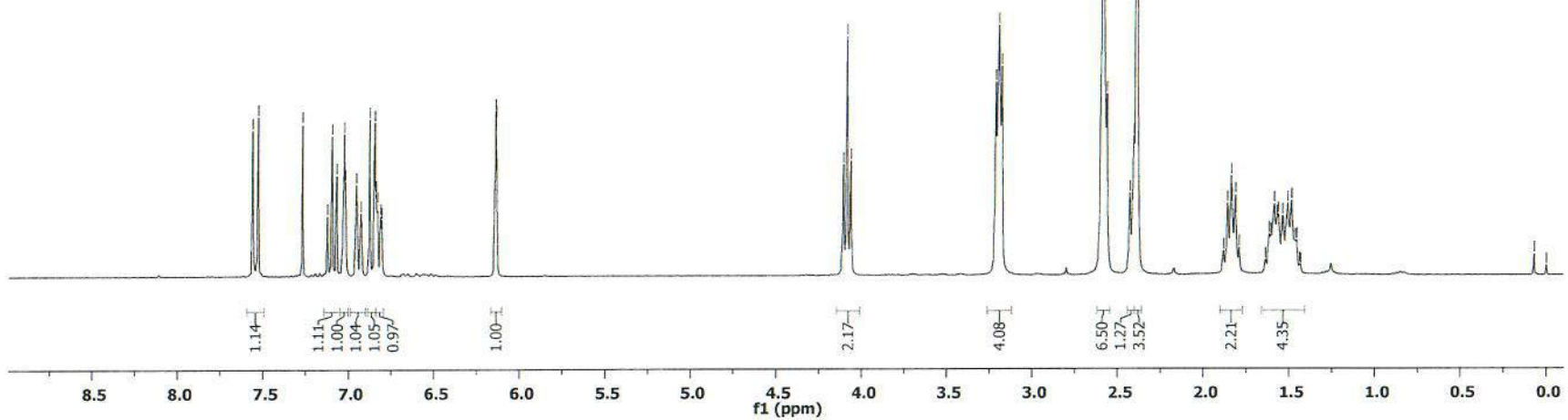


7.56
7.53
7.27
7.09
7.07
7.03
7.02
7.02
6.95
6.88
6.85
6.84
6.14

4.11
4.09
4.06

3.21
3.20
3.18
2.60
2.59
2.56
2.43
2.41
2.39
2.39

1.88
1.86
1.84
1.81
1.79
1.64
1.62
1.61
1.59
1.57
1.56
1.54
1.51
1.49
1.46
1.46
0.09
-0.00



5g

KO-406 13C

— 199.41

— 160.15
— 158.16
— 152.65
— 152.20
— 150.88

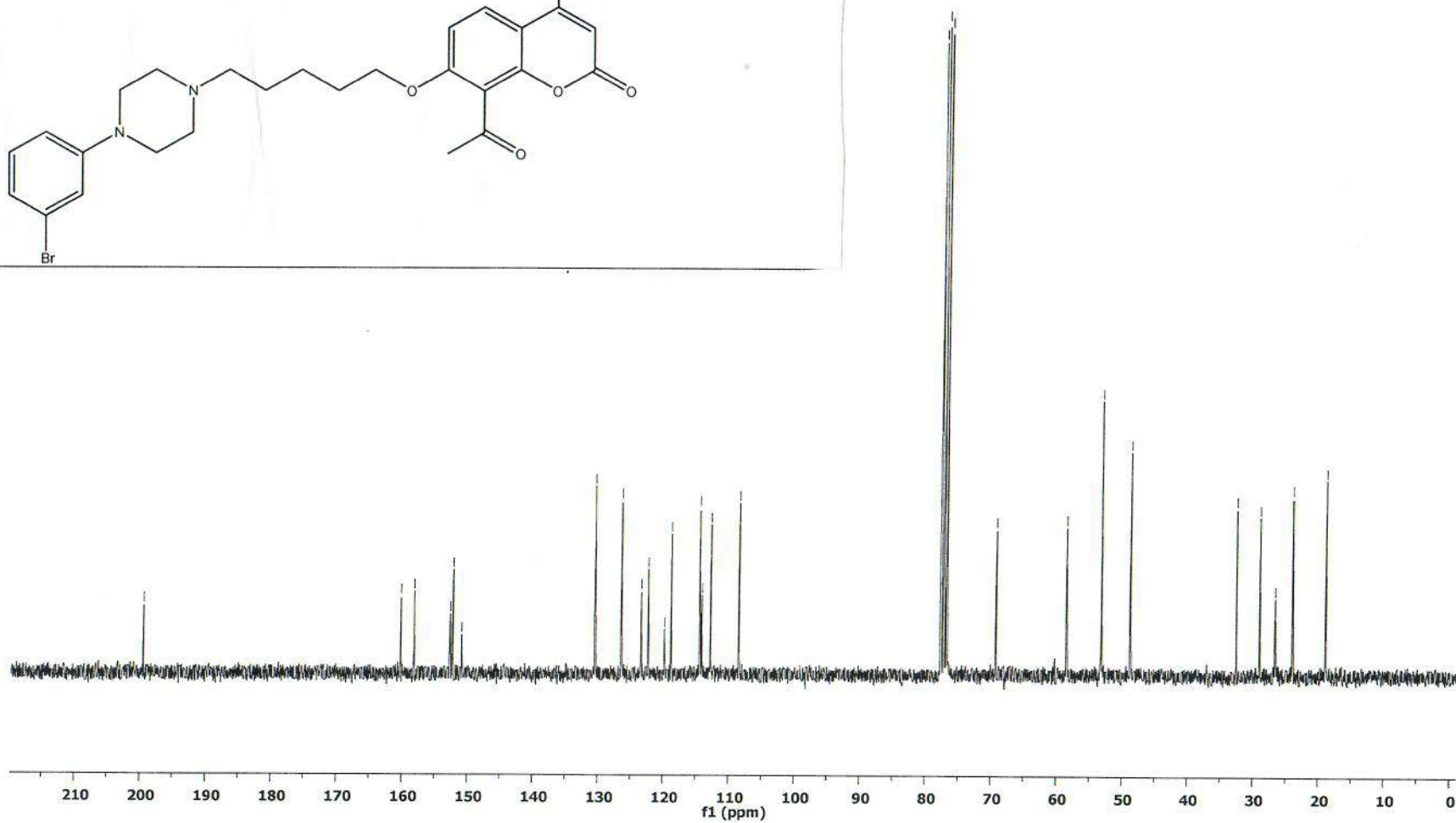
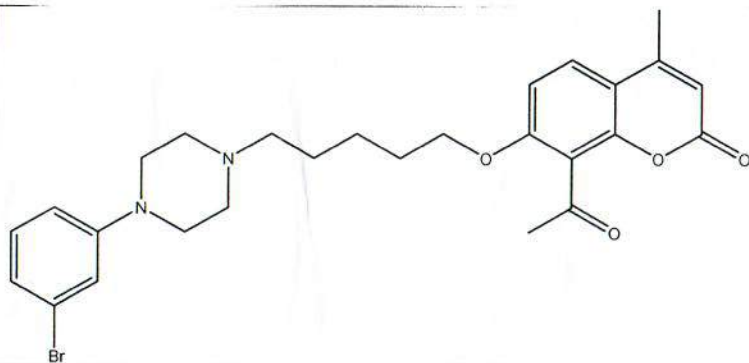
— 130.50
— 126.47
— 123.42
— 122.35
— 119.85
— 118.80
— 114.48
— 114.11
— 112.80
— 108.45

— 77.65
— 77.23
— 76.81
— 69.24

— 58.54
— 53.26
— 48.79

— 32.63
— 29.06
— 26.67
— 24.09
— 18.95

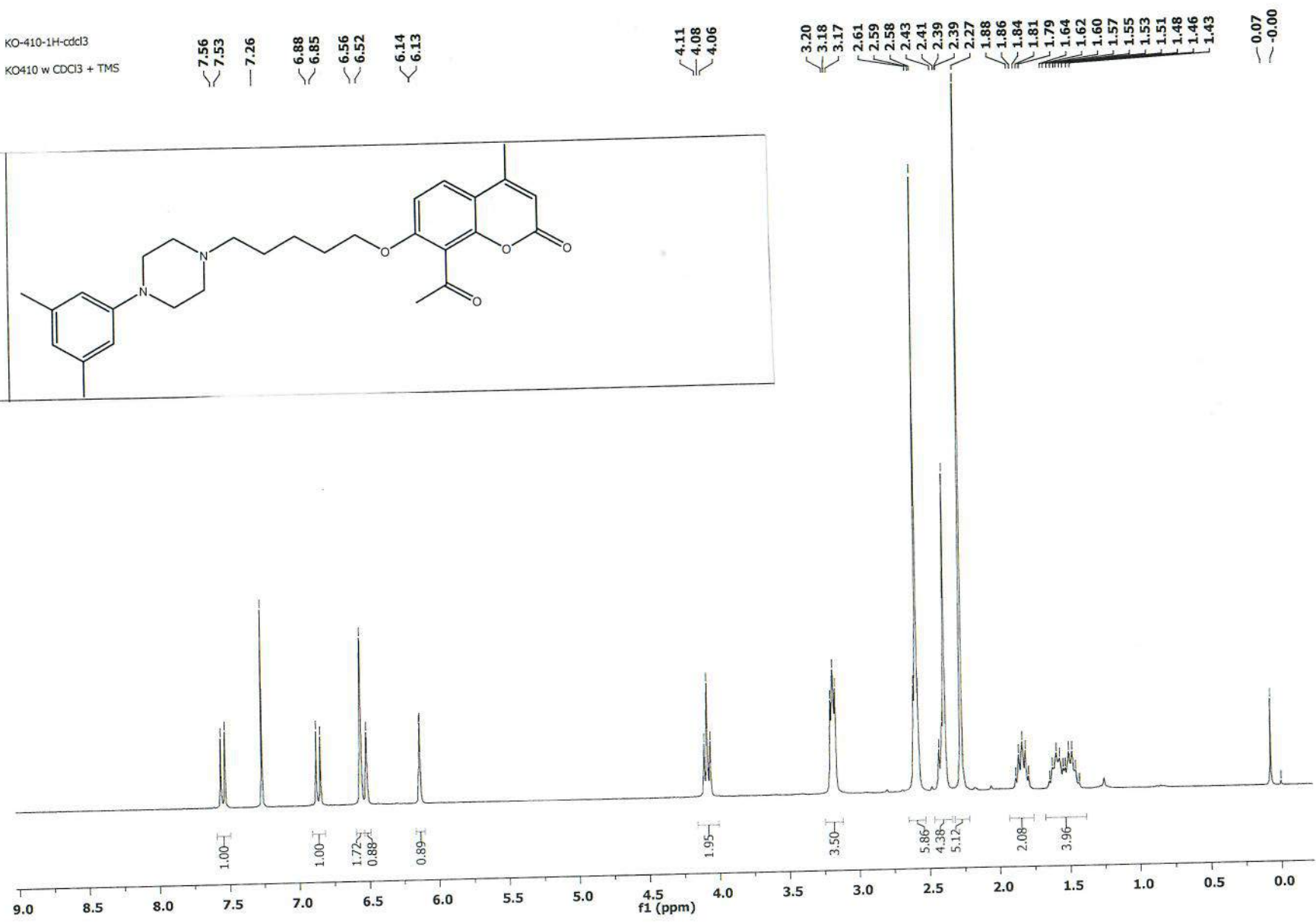
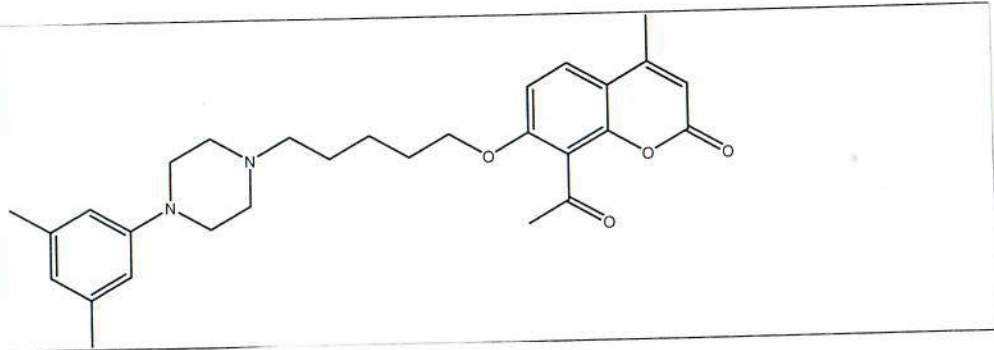
5g



5h

KO-410-1H-cdcl3
KO410 w CDCl3 + TMS

5h



5h

KO-410-13C-cdcl3

KO 410 13C w CDCl3

199.41

160.16
158.17
152.21
151.60
150.87

138.79

126.47
121.85
119.84

114.21
114.09
112.77
108.45

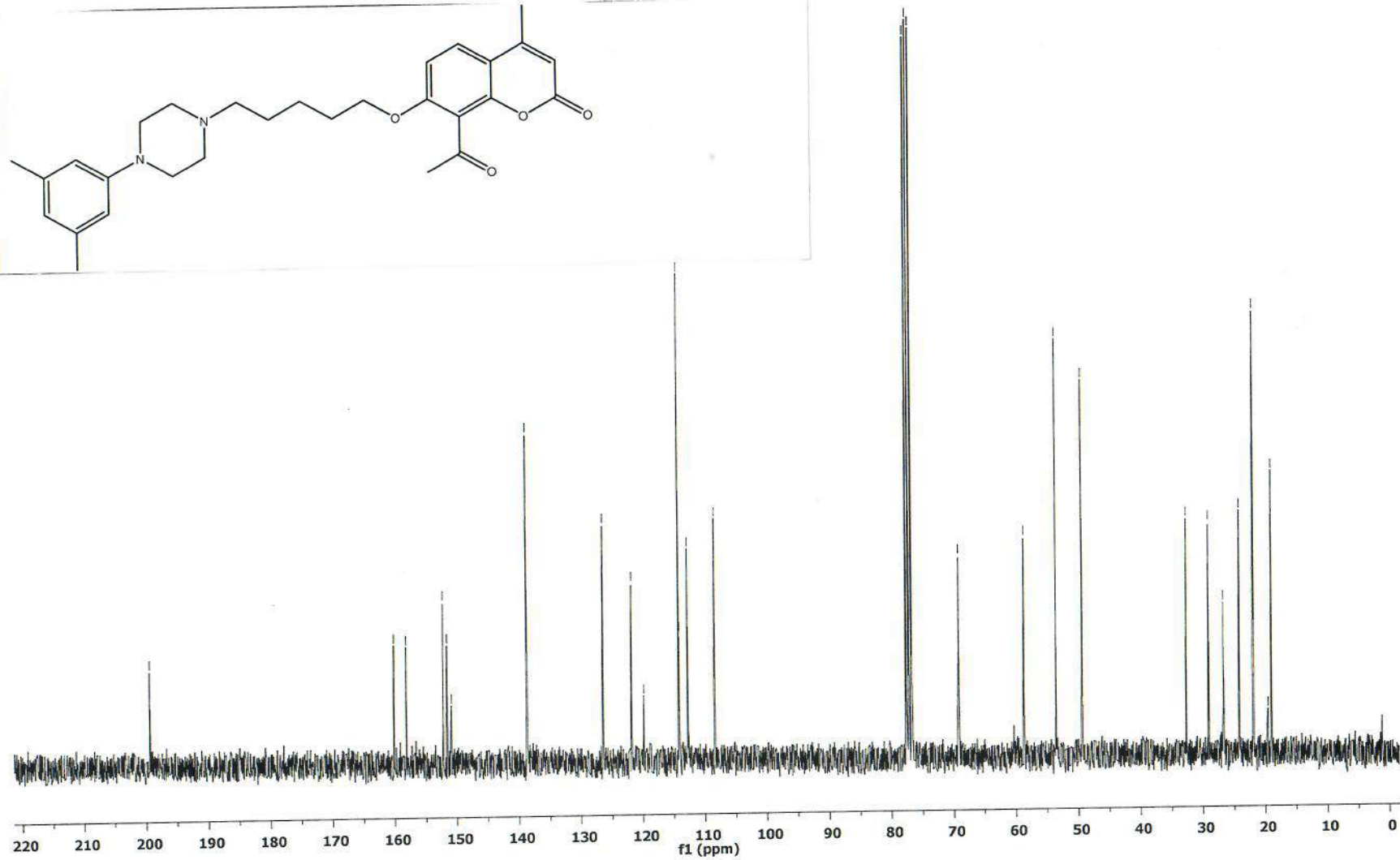
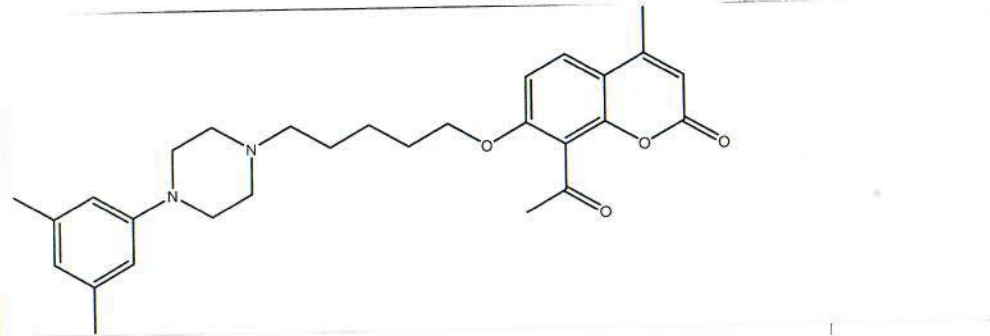
77.65
77.23
76.81

69.24

58.65
53.57
49.42

32.62
29.07
26.69
24.12
21.85
19.55
18.94

5h



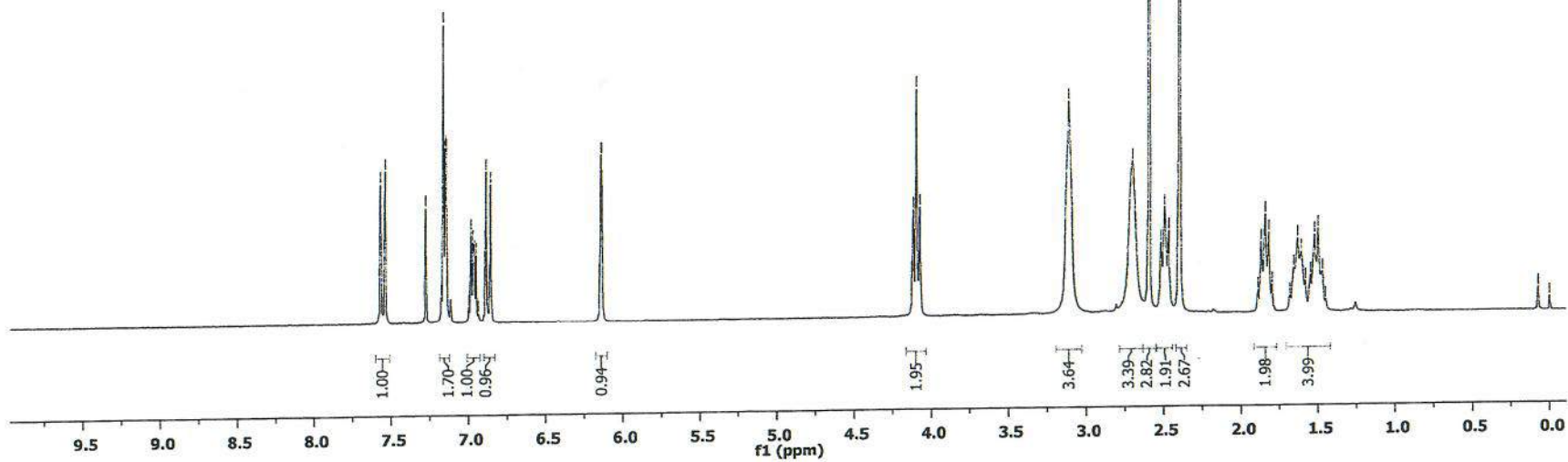
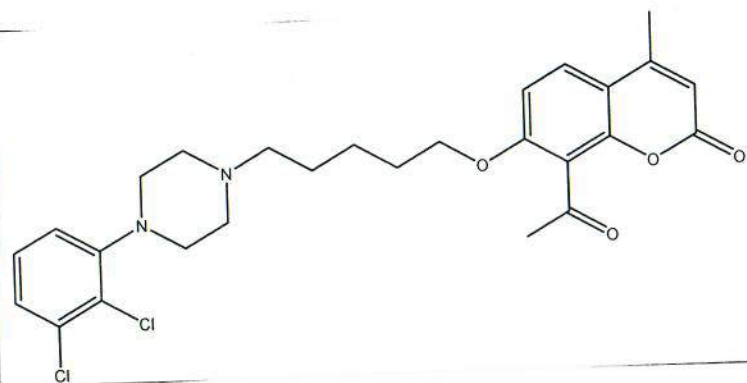
KO-402-1H
KO-402 1H w CDCl3

7.566
7.537
7.276
7.160
7.148
7.140
6.982
6.969
6.962
6.886
6.858
6.838
6.135

4.116
4.095
4.074

3.111
2.701
2.593
2.515
2.491
2.466
2.397
2.394
1.892
1.870
1.846
1.822
1.800
1.684
1.660
1.634
1.610
1.585
1.548
1.523
1.501
1.473
1.453
0.075
0.000

5i



5i

5i

KO-402-13C
KO 402 13C w CDC3

199.48

160.14
158.09
152.24
150.86

134.23

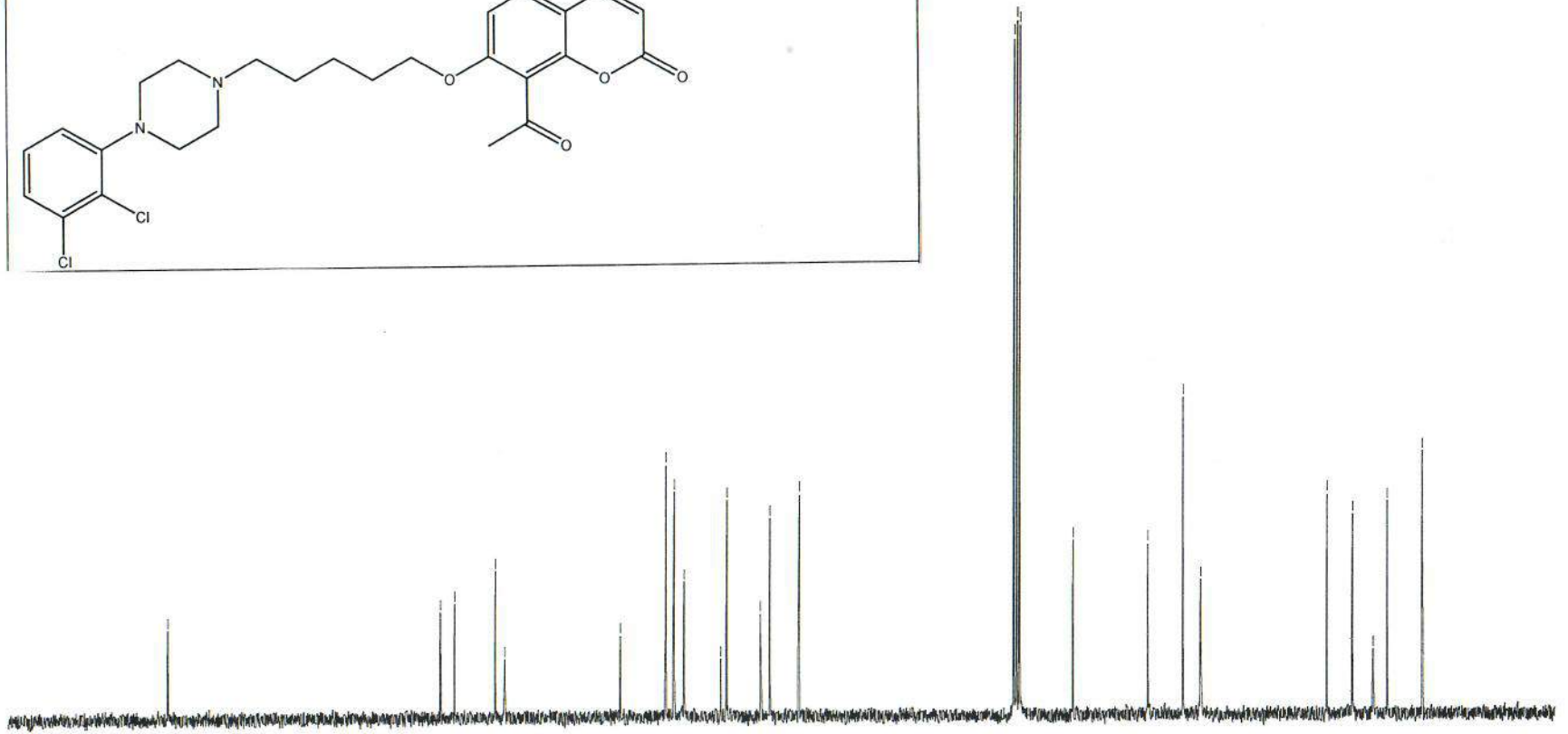
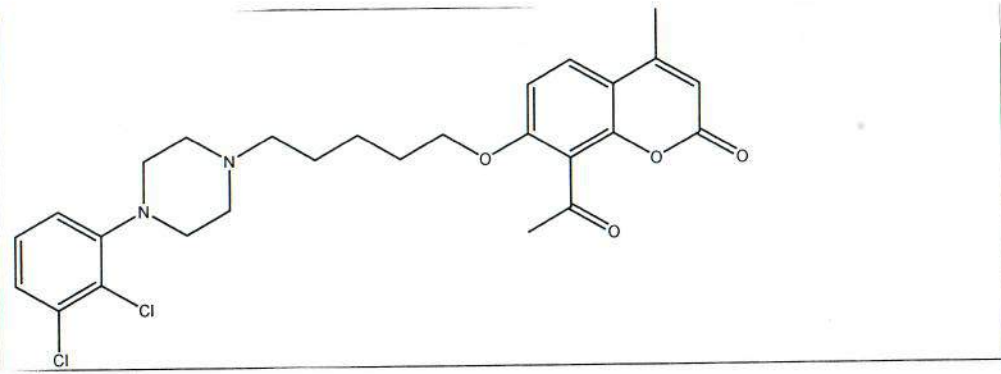
127.73
126.52
125.08
119.81
118.93
114.12
112.77
108.50

77.65
77.23
76.81
69.11

58.34
53.31
50.76

32.65
28.90
25.97
23.97
18.95

5i



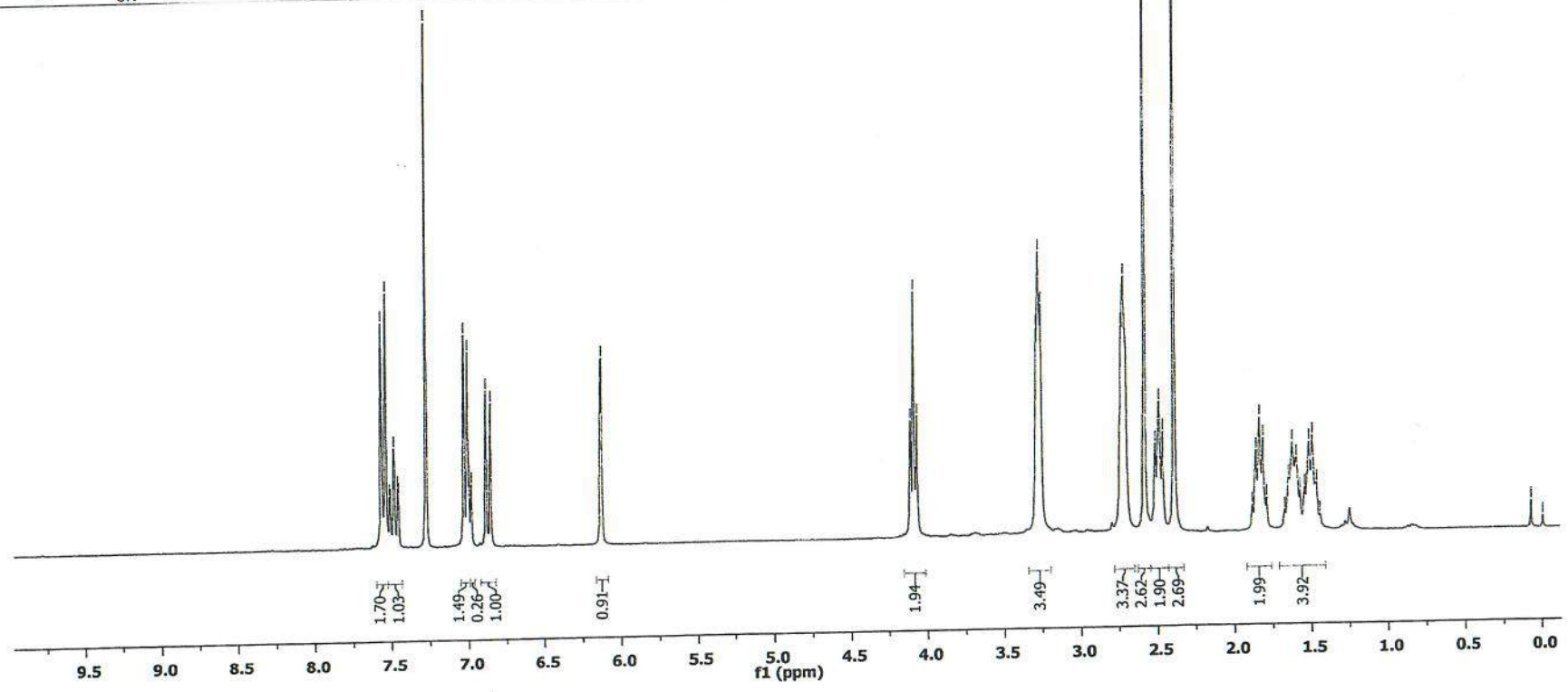
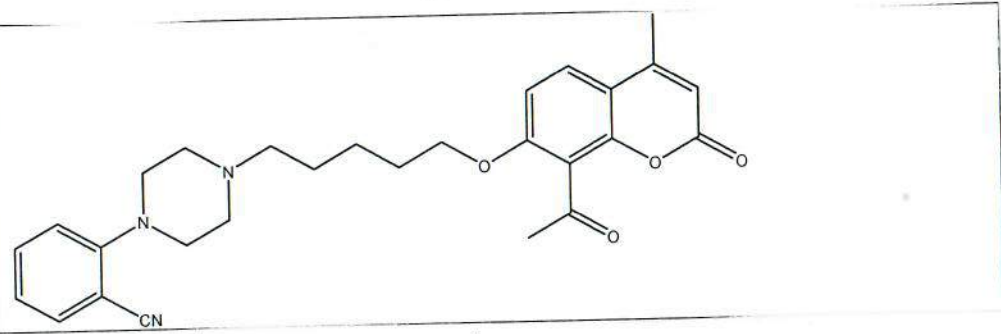
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

5j

KO-403-1H
KO-403 1H w CDCl3

7.567
7.537
7.512
7.507
7.485
7.459
7.454
7.276
7.030
7.004
6.981
6.886
6.857
6.128
4.112
4.091
4.070
3.290
3.275
3.260
2.736
2.722
2.586
2.515
2.492
2.466
2.391
1.885
1.863
1.839
1.815
1.793
1.674
1.650
1.624
1.600
1.575
1.541
1.516
1.494
1.466
1.446
0.069
-0.007

5j



5j

KO-403-13C

KO 403 13C w CDCl3

199.27

159.96

157.90

155.28

152.08

150.66

134.27

133.90

126.34

122.13

119.61

118.83

118.33

113.92

112.56

108.31

106.15

77.47

77.25

77.05

76.62

68.90

58.04

52.98

50.86

32.45

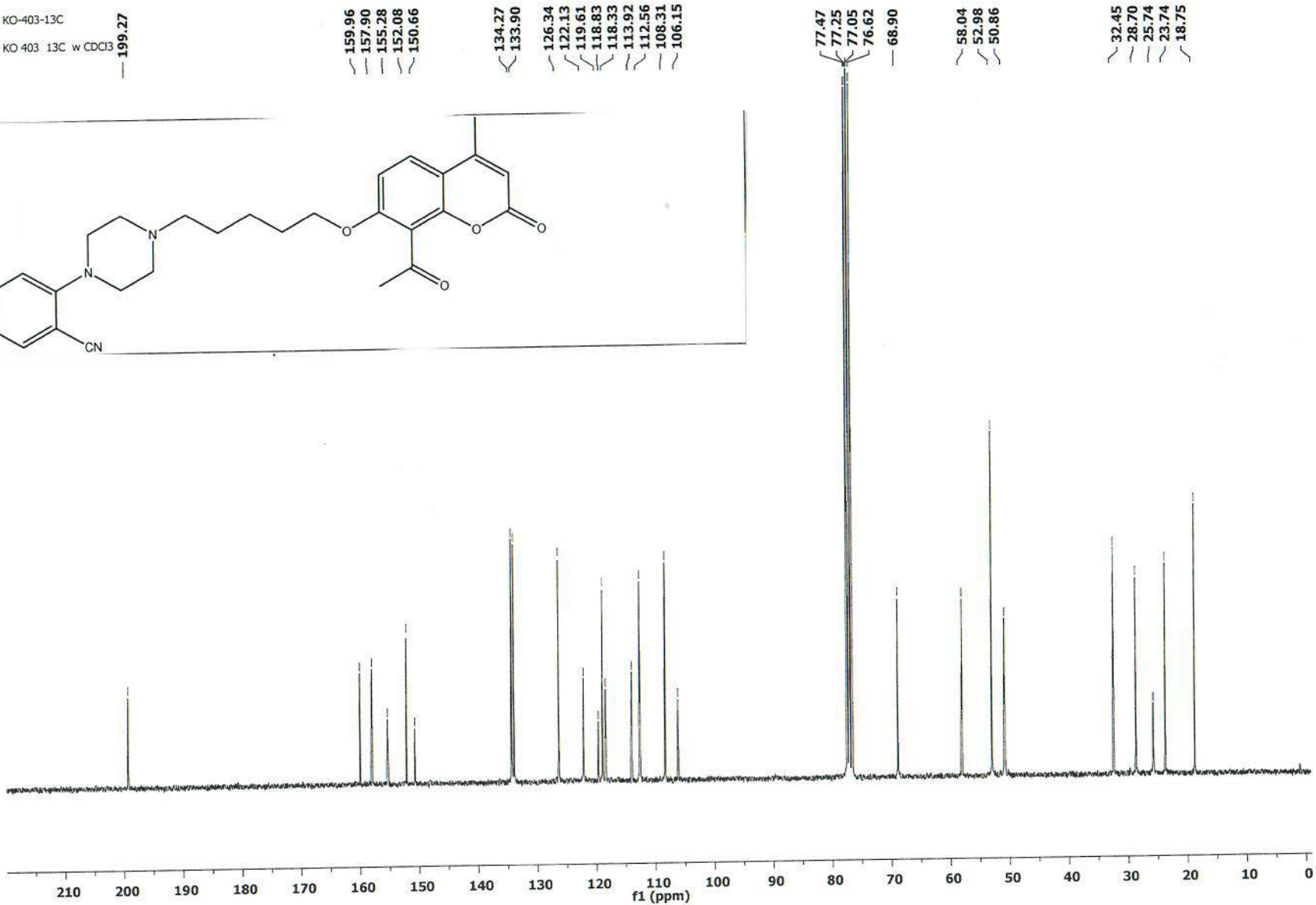
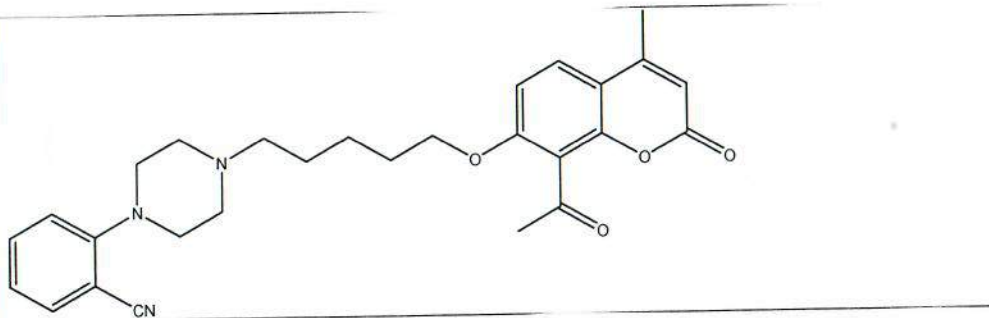
28.70

25.74

23.74

18.75

5j



KO-411b-1H-cdd3
KO411b w CDCl3 + TMS

7.58
7.56

7.27

6.87
6.84

6.17
6.17

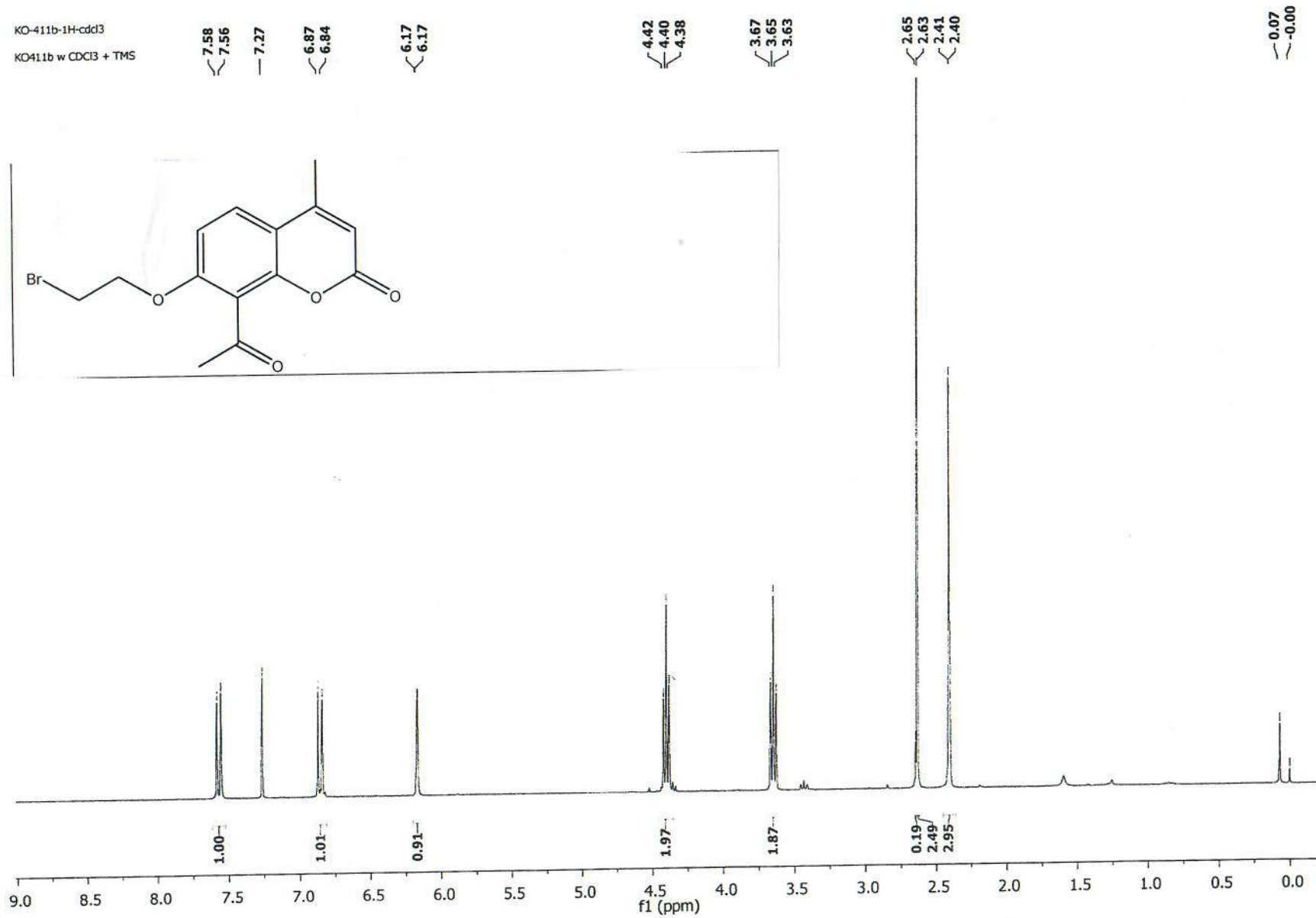
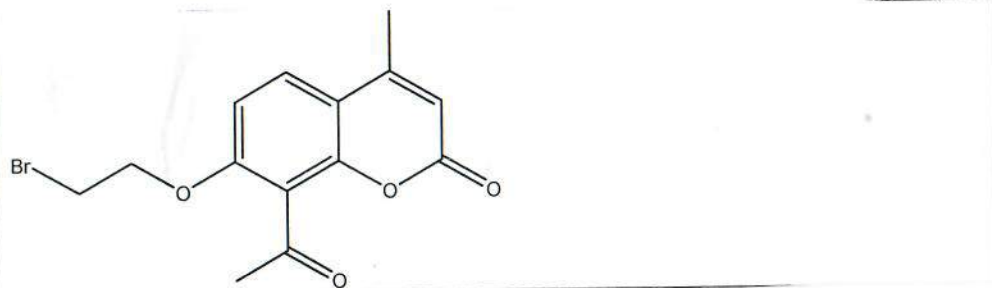
4.42
4.40
4.38

3.67
3.65
3.63

2.65
2.63
2.41
2.40

0.07
-0.00

6



KO-411b-13C-cdcl3
KO 411b 13C w CDCl3

— 199.19

— 159.92
— 156.98
— 152.05
— 150.91

— 126.55

— 120.30
— 114.87
— 113.29
— 108.60

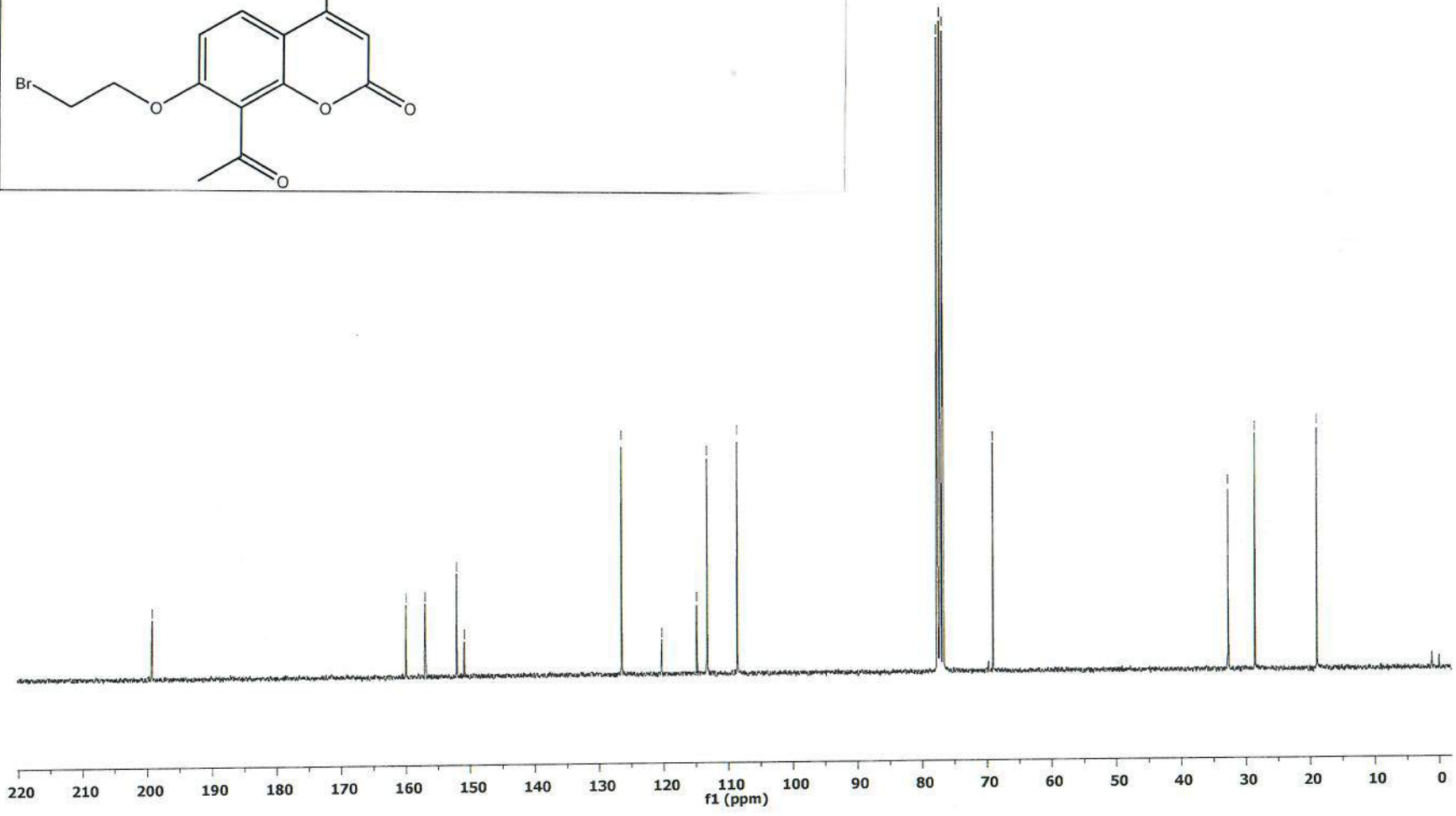
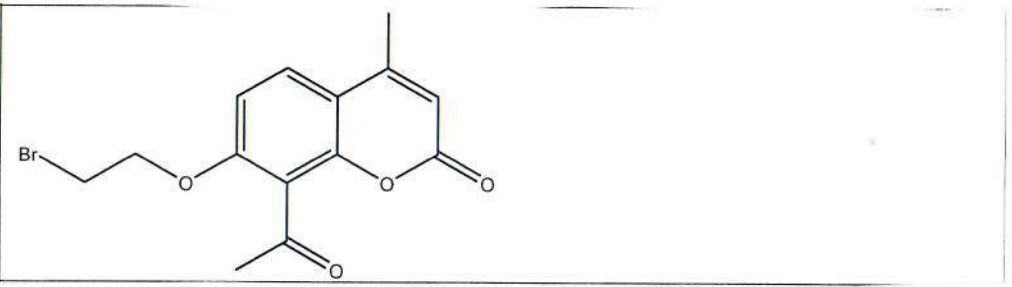
— 77.65
— 77.23
— 76.81

— 69.07

— 32.77
— 28.56

— 18.97

6



6a

KO-412-1H-cdcl3
KO-412 w CDCl3 + TMS

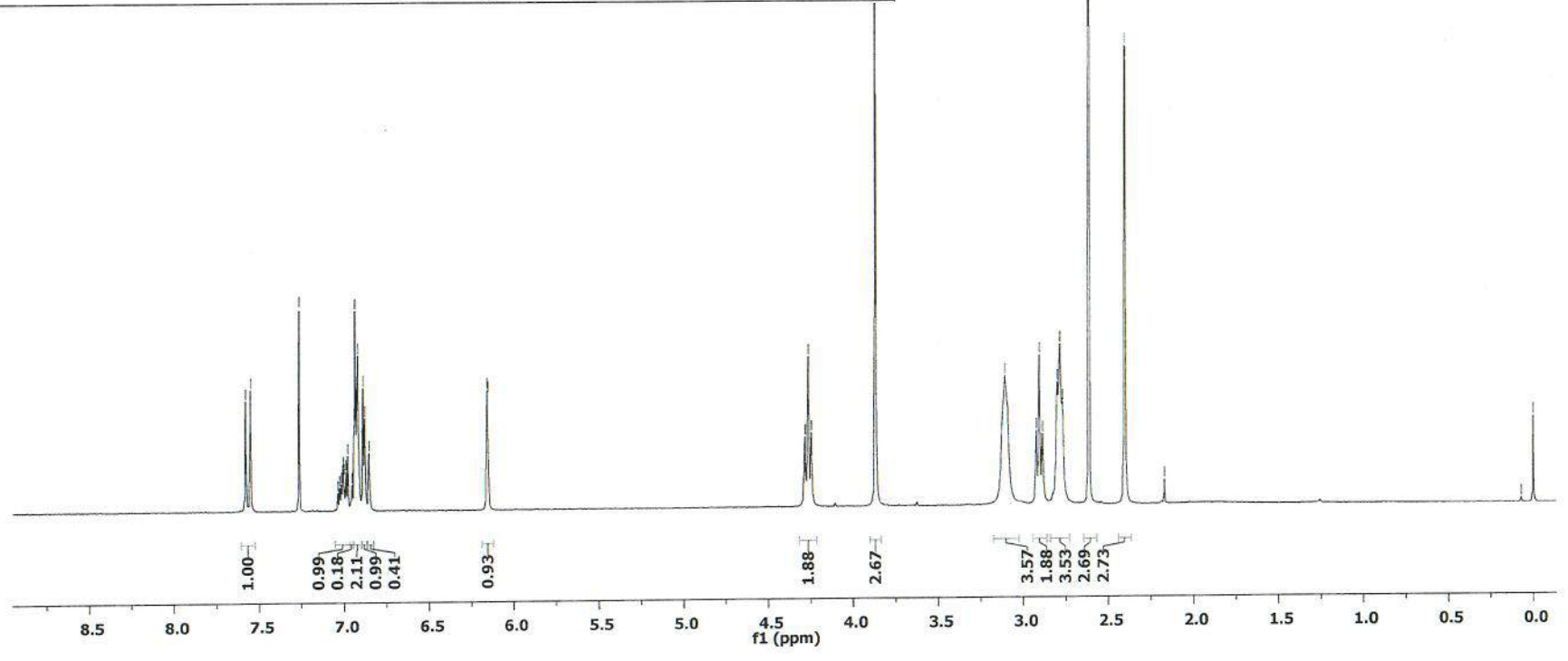
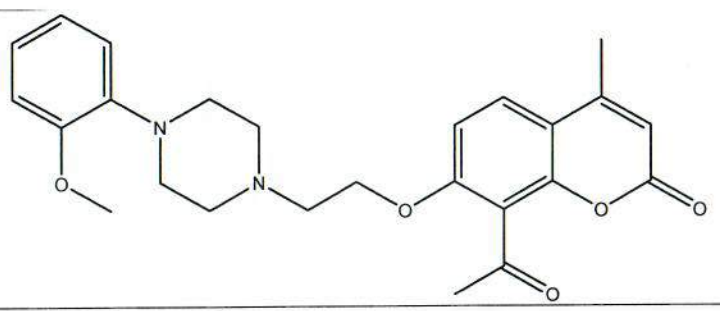
7.58
7.55
7.26
7.00
6.98
6.94
6.93
6.92
6.89
6.88
6.85
6.86
6.15

4.28
4.26
4.25
3.87

3.11
2.92
2.90
2.89
2.80
2.79
2.77
2.61
2.40
2.17

0.07
0.00

6a



6a

KO-412-13C-cdcl3
KO 412 13C

— 199.28

~ 160.00
~ 157.41
~ 152.43
~ 152.18
~ 150.98

— 140.71

~ 126.69
~ 123.62
~ 121.24
~ 119.97
~ 118.60
~ 114.57
~ 113.09
~ 111.45
~ 108.72

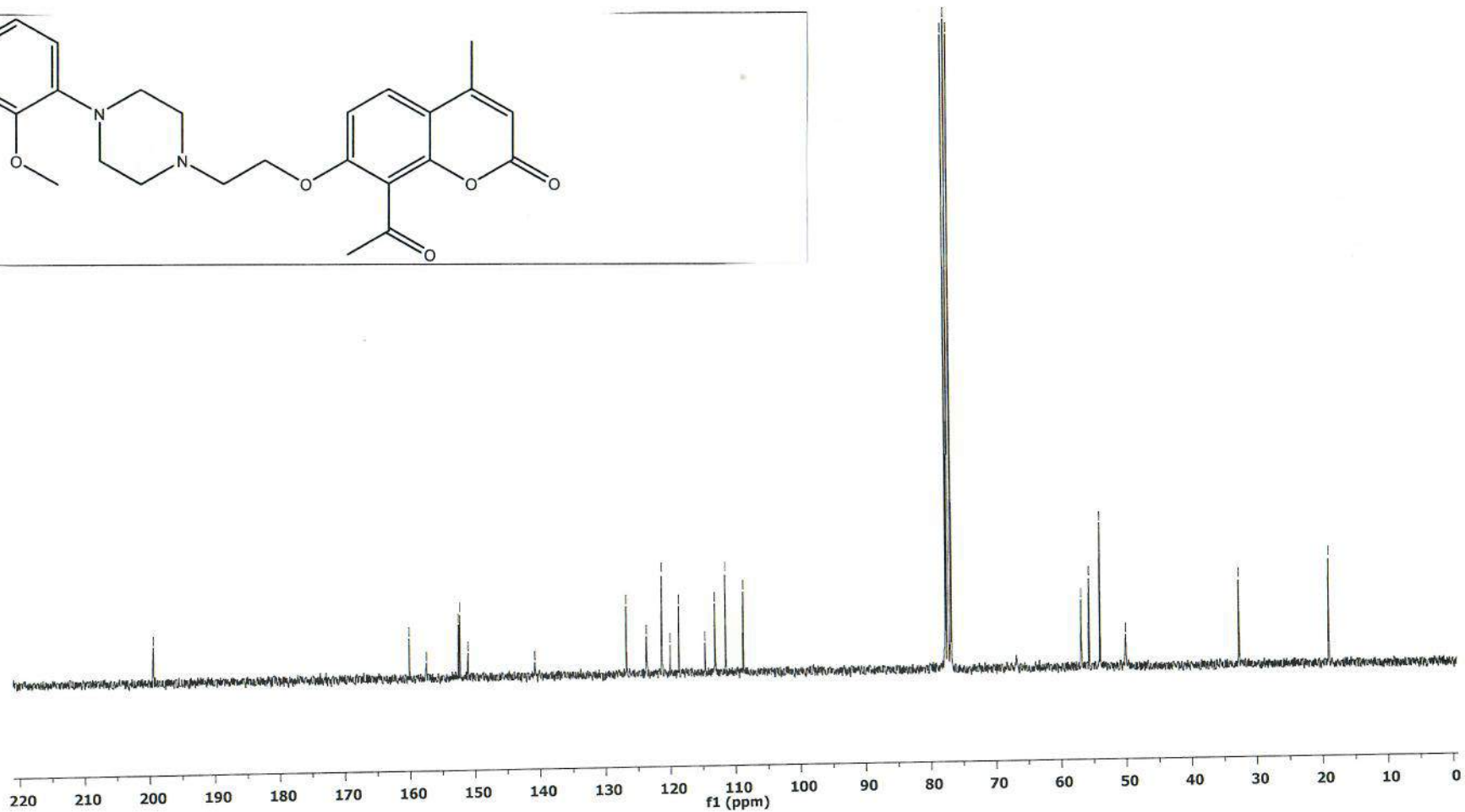
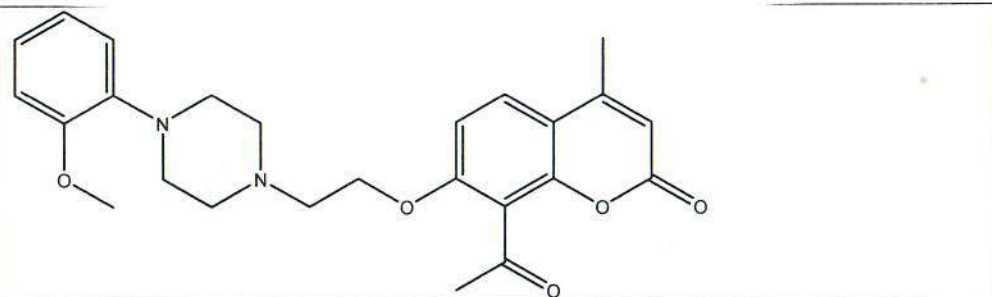
~ 77.65
~ 77.23
~ 76.81

~ 56.82
~ 55.63
~ 53.99
~ 50.03

— 32.71

— 18.99

6a



6b

KO-416-1H-cdcl3
KO-416 w CDCl3 + TMS

7.58
7.55
7.27
7.05
7.03
7.01
6.98
6.96
6.94
6.92
6.89
6.85
6.14

4.27
4.25
4.24

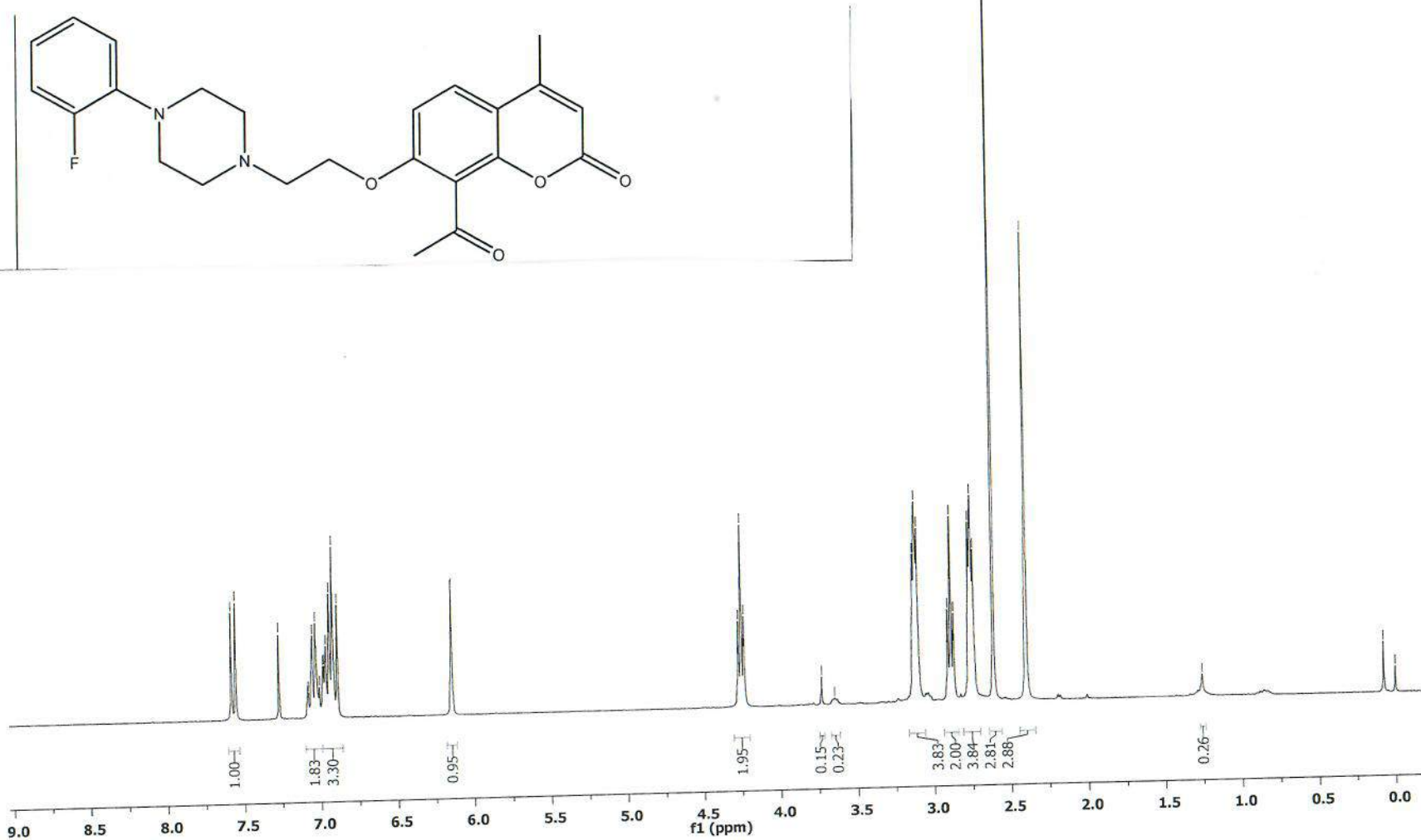
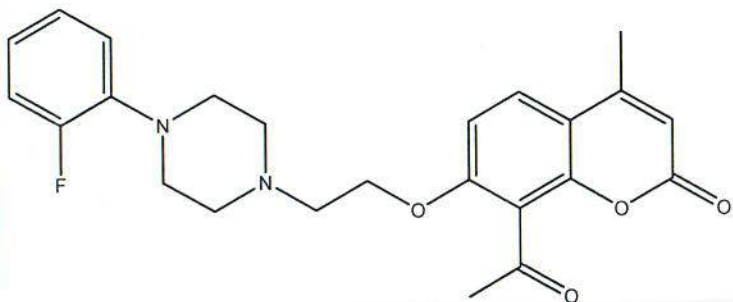
3.73
3.65

3.13
3.12
3.10
2.91
2.89
2.87
2.77
2.75
2.74
2.61
2.40

1.26

0.08
-0.00

6b



KO-416-13C-cdcl3
KO 416 13C in CDCl3

— 199.34

160.04
157.70
157.50
154.24
152.20
150.88
140.06
139.95
126.58
124.67
124.63
122.85
122.75
119.96
119.16
119.12
116.43
116.16
114.38
112.93
108.62

77.65
77.23
76.81

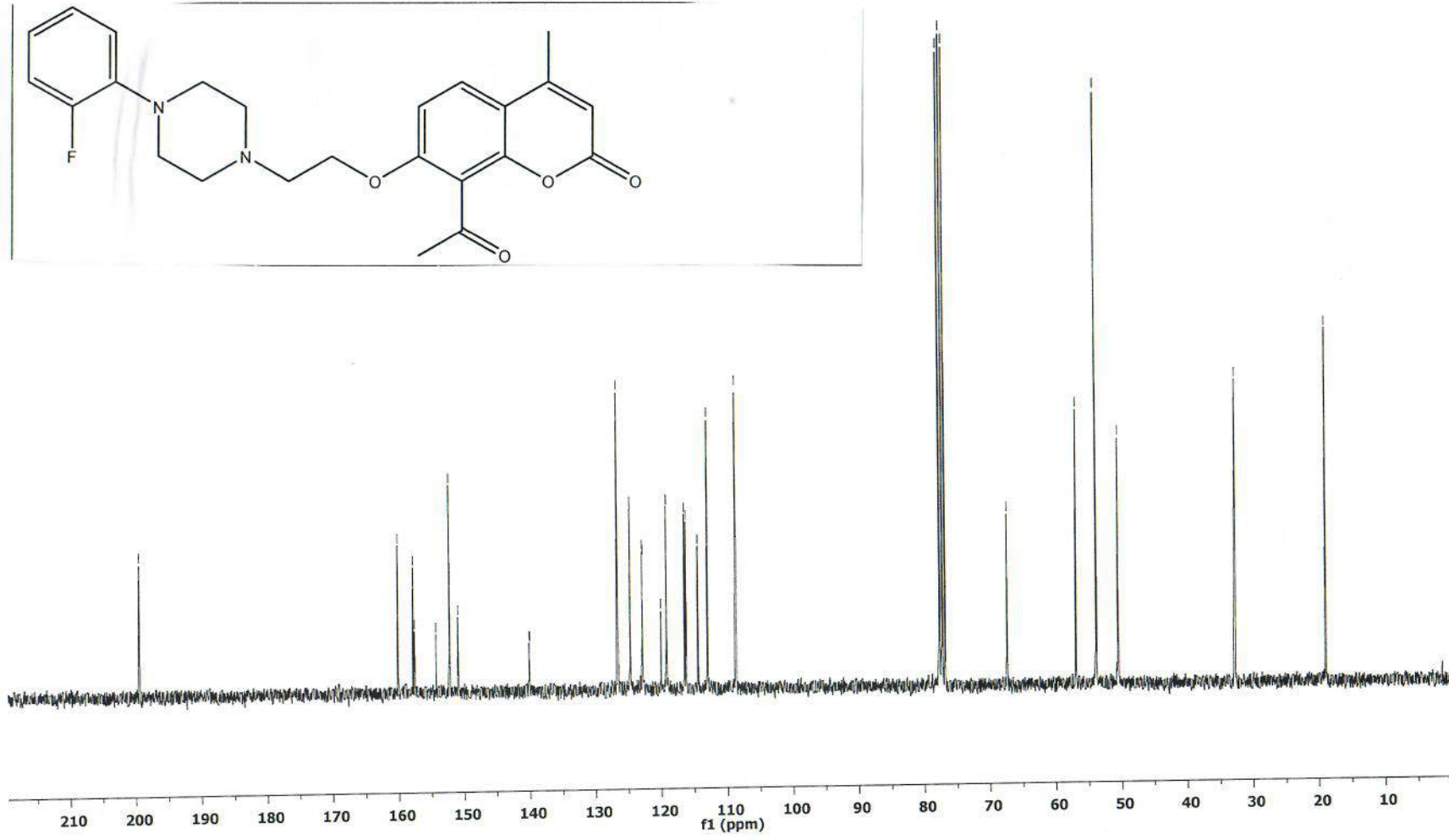
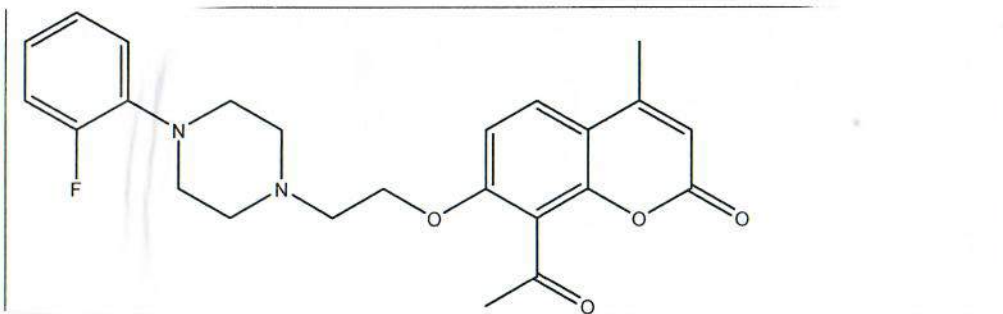
— 67.40

56.87
53.85
50.51

— 32.65

— 18.94

6b



6c

KO-415-1H-cdcl3
KO-415 w CDCl3 + TMS

7.58
7.55
7.27
7.17
7.14
6.92
6.89
6.46
6.45
6.43
6.14

4.27
4.25
4.23

3.78
3.73

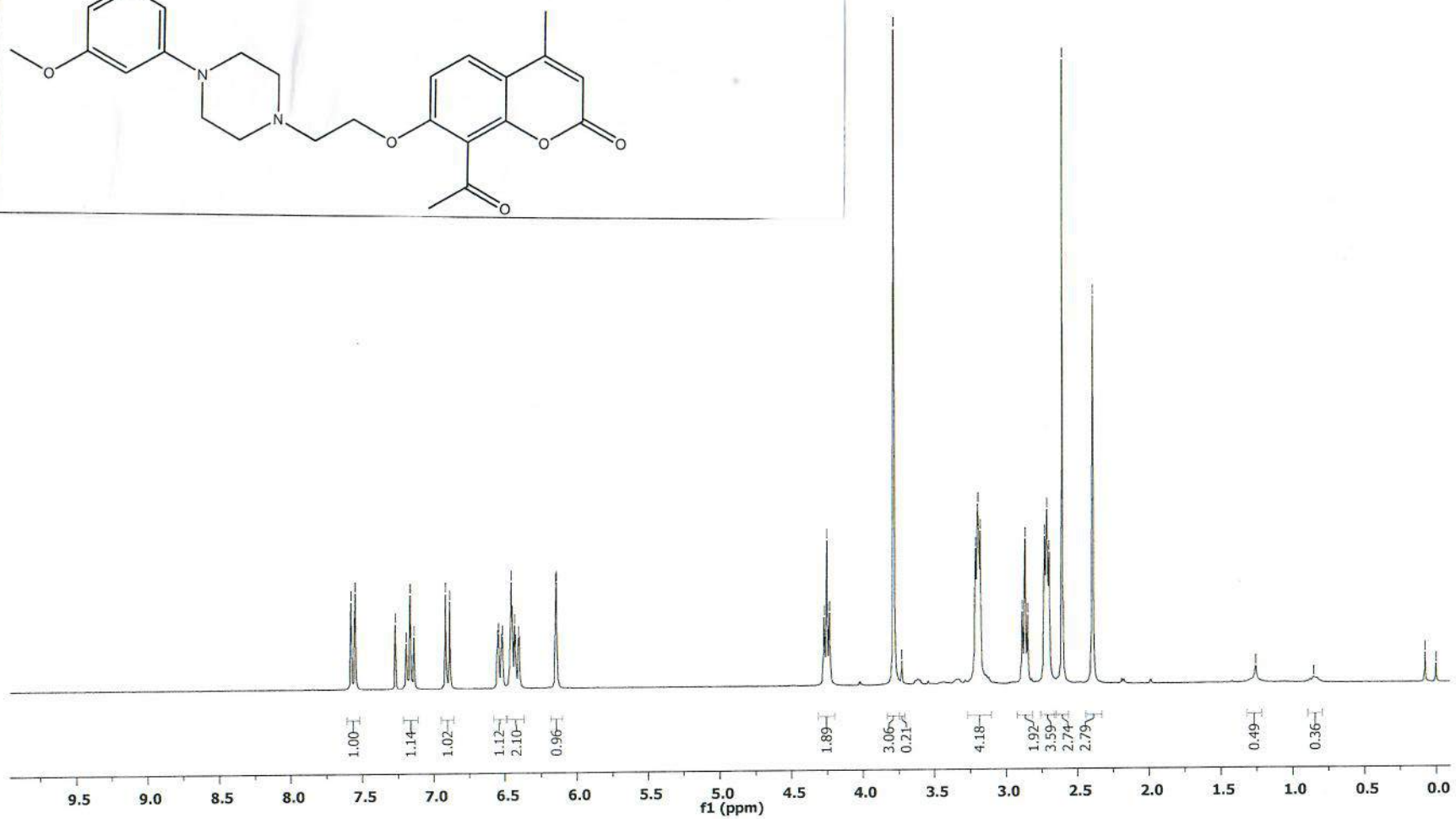
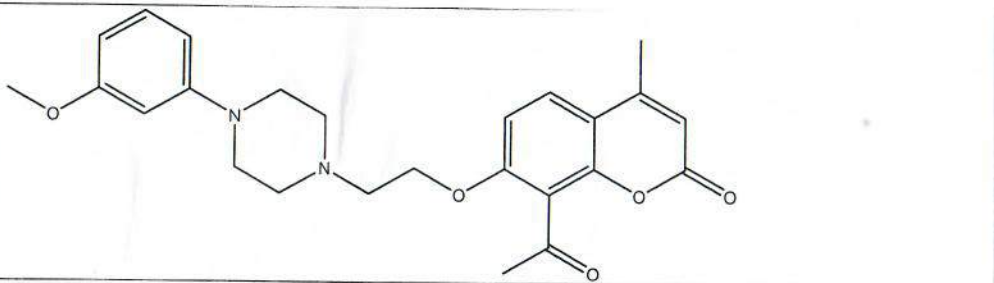
3.21
3.20
3.18
2.89
2.87
2.85
2.73
2.71
2.70
2.61
2.39

1.26

0.85

0.08
0.00

6c



6c

KO-415-13C-cdcl3
KO 415 13C in CDCl3

— 199.41

160.78
160.06
157.70
152.64
152.24
150.89

— 130.01
— 126.62

— 119.95
114.41
112.95
109.08
108.64
104.88
102.75

77.69
77.26
76.84

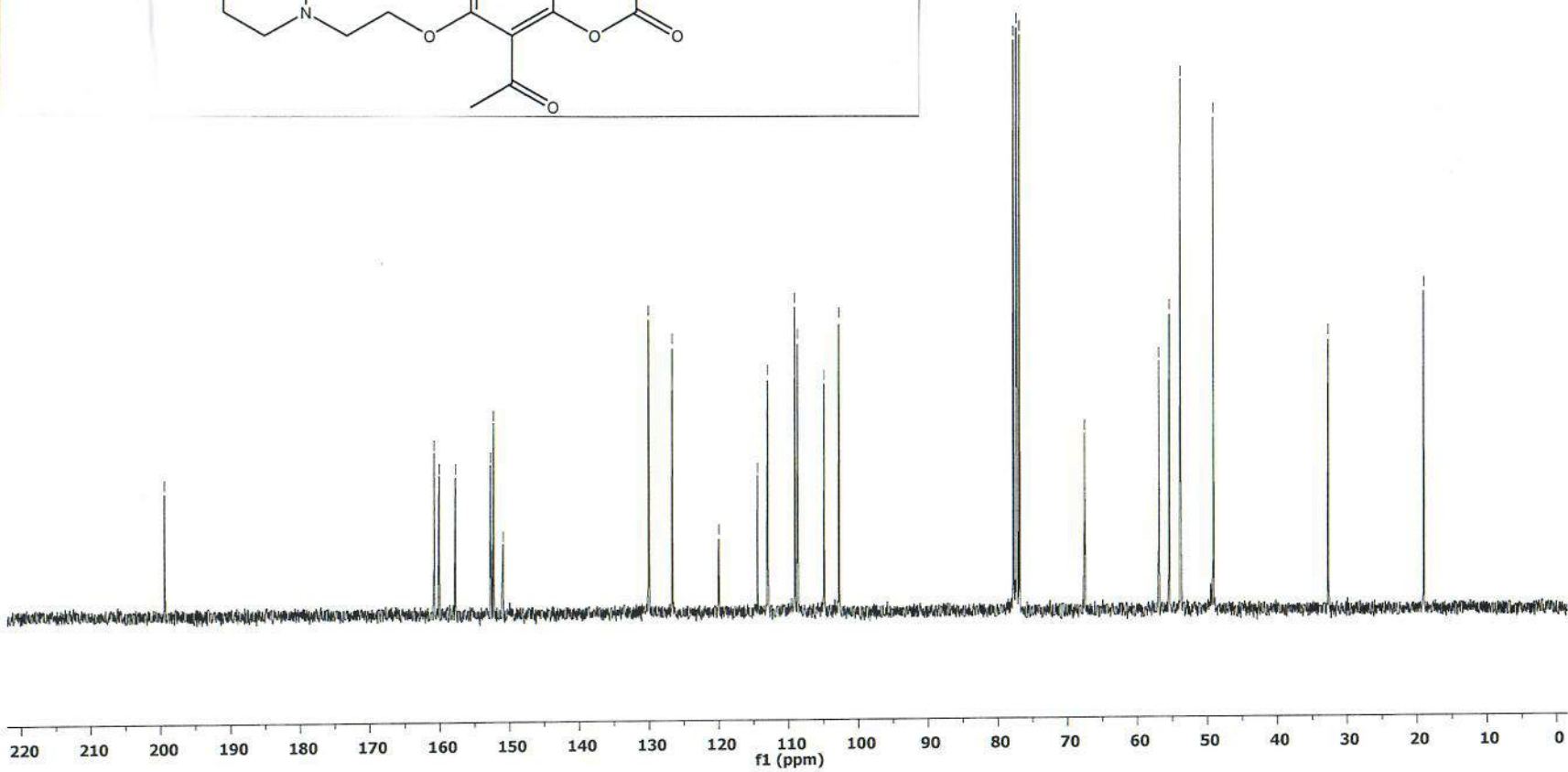
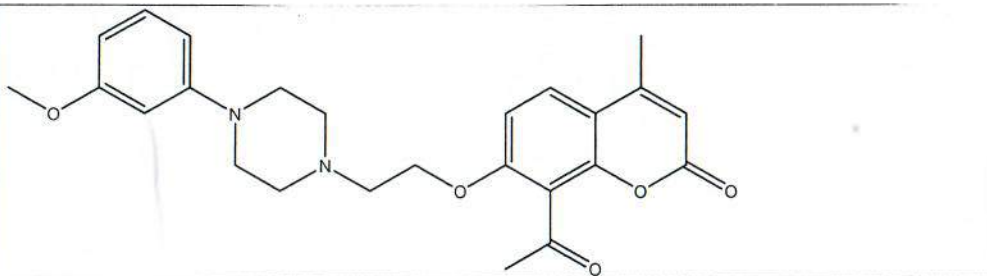
— 67.55

56.88
55.40
53.79
49.12

— 32.68

— 18.96

6c



6d

KO-418-1H-cdcl3
KO-418 w CDCB + TMS

7.58
7.55
7.26
7.06
7.04
6.93
6.90
6.81
6.78

6.14
6.14

4.28
4.26
4.24

3.73

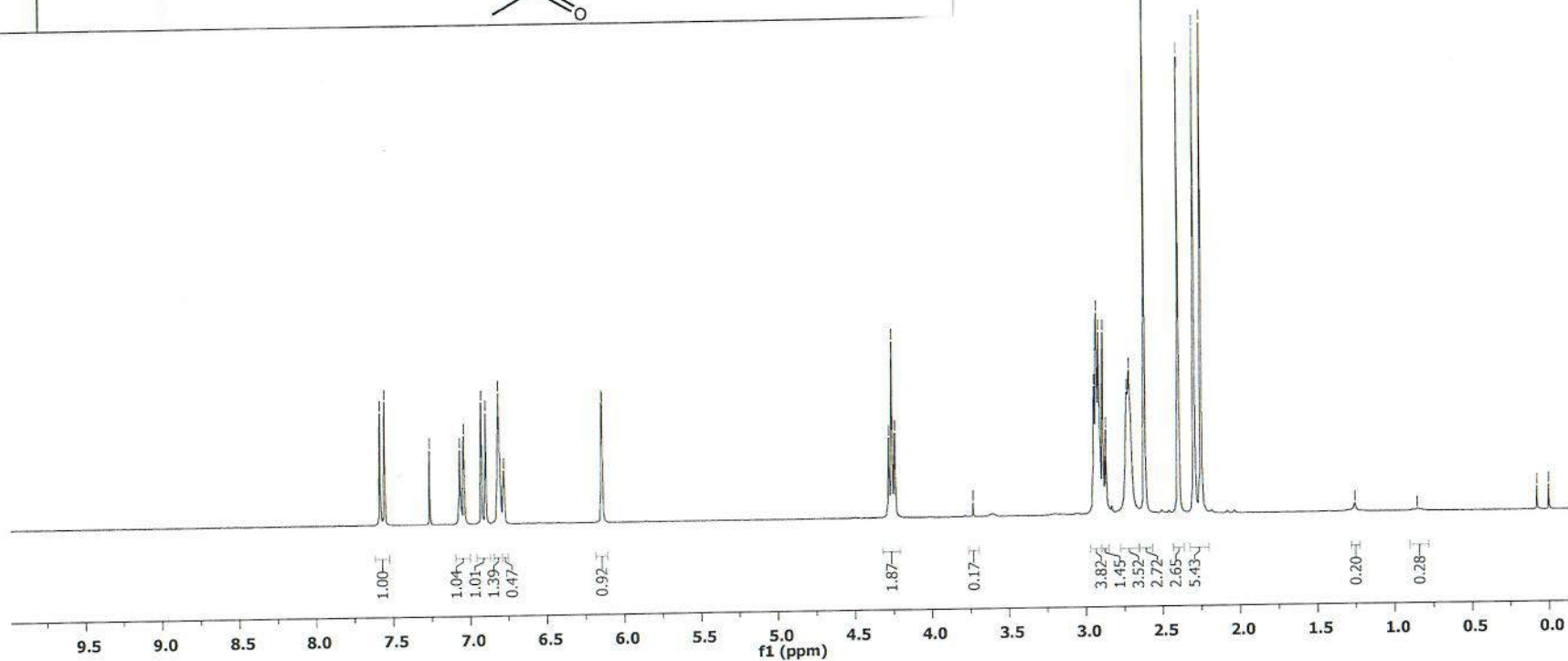
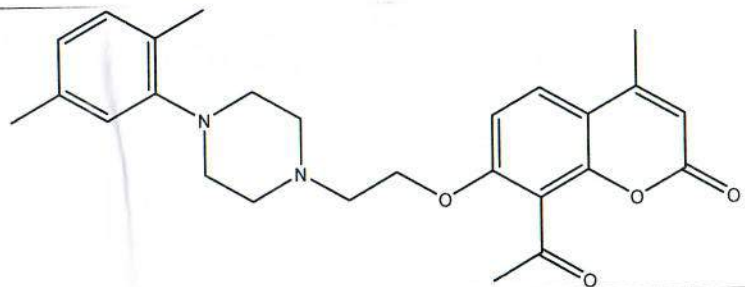
2.94
2.93
2.91
2.89
2.87
2.73
2.72
2.62
2.40
2.40
2.30
2.25

1.26

0.85

0.08
-0.00

6d



6d

KO-418-13C
KO 418 13C in CDCl3

199.36

160.04
157.75
152.21
151.19
150.86

136.27
131.06
129.43
126.58
124.07
119.90

114.34
112.89
108.64

77.65
77.23
76.81

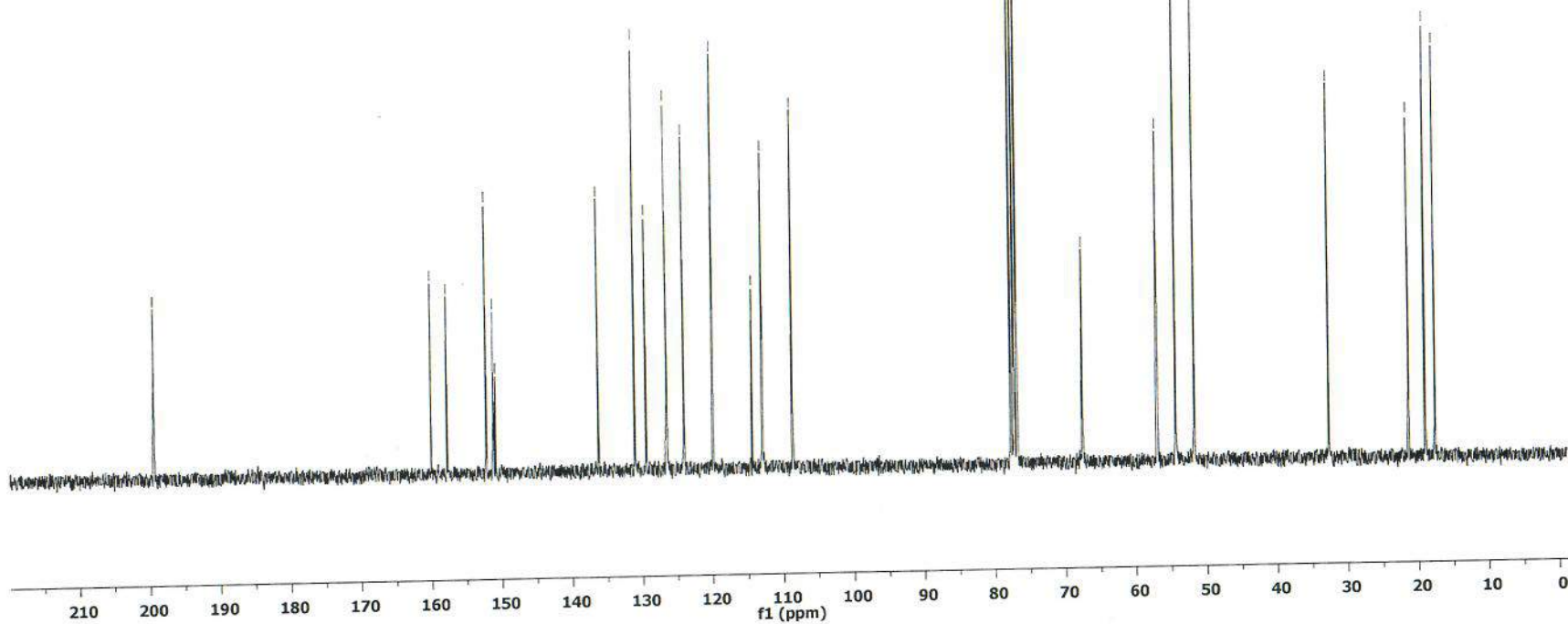
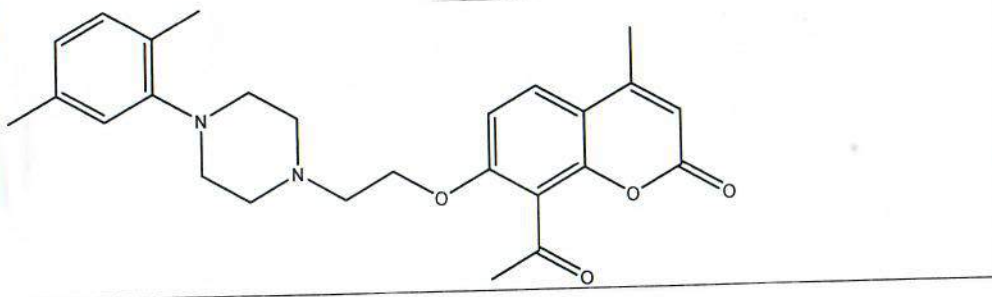
67.52

56.93
54.34
51.69

32.64

21.36
18.93
17.62

6d



6e

KO-419-1H-cdcl3
KO-419 w CDCl3 + TMS

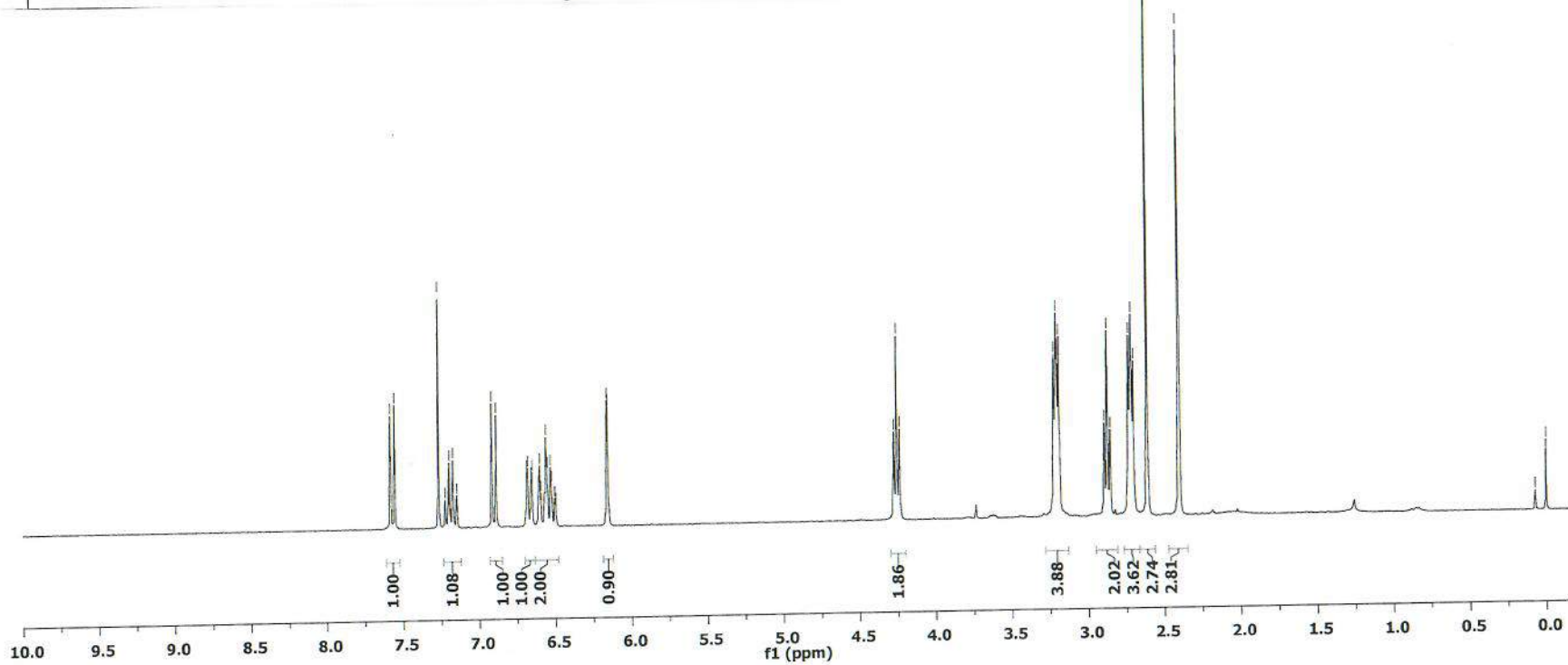
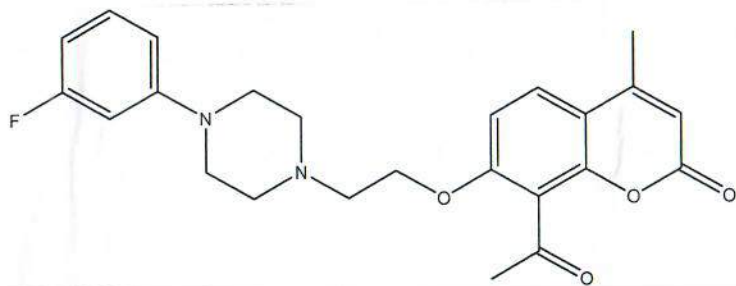
7.58
7.55
7.26
7.20
7.17
6.92
6.89
6.68
6.60
6.56
6.53
6.18
6.15

4.27
4.26
4.24

3.22
3.21
3.19
2.89
2.87
2.85
2.73
2.72
2.70
2.61
2.40
2.40

0.07
-0.00

6e



6e

KO-419-13C
KO 419 13C in CDCl3

— 199.35

165.63
162.40
160.00
157.51
152.80
152.66
152.17
150.97

130.46
130.33
126.66
119.97
114.53
113.07
111.52
111.49
108.65
106.60
106.32
103.26
102.93

77.65
77.23
76.81

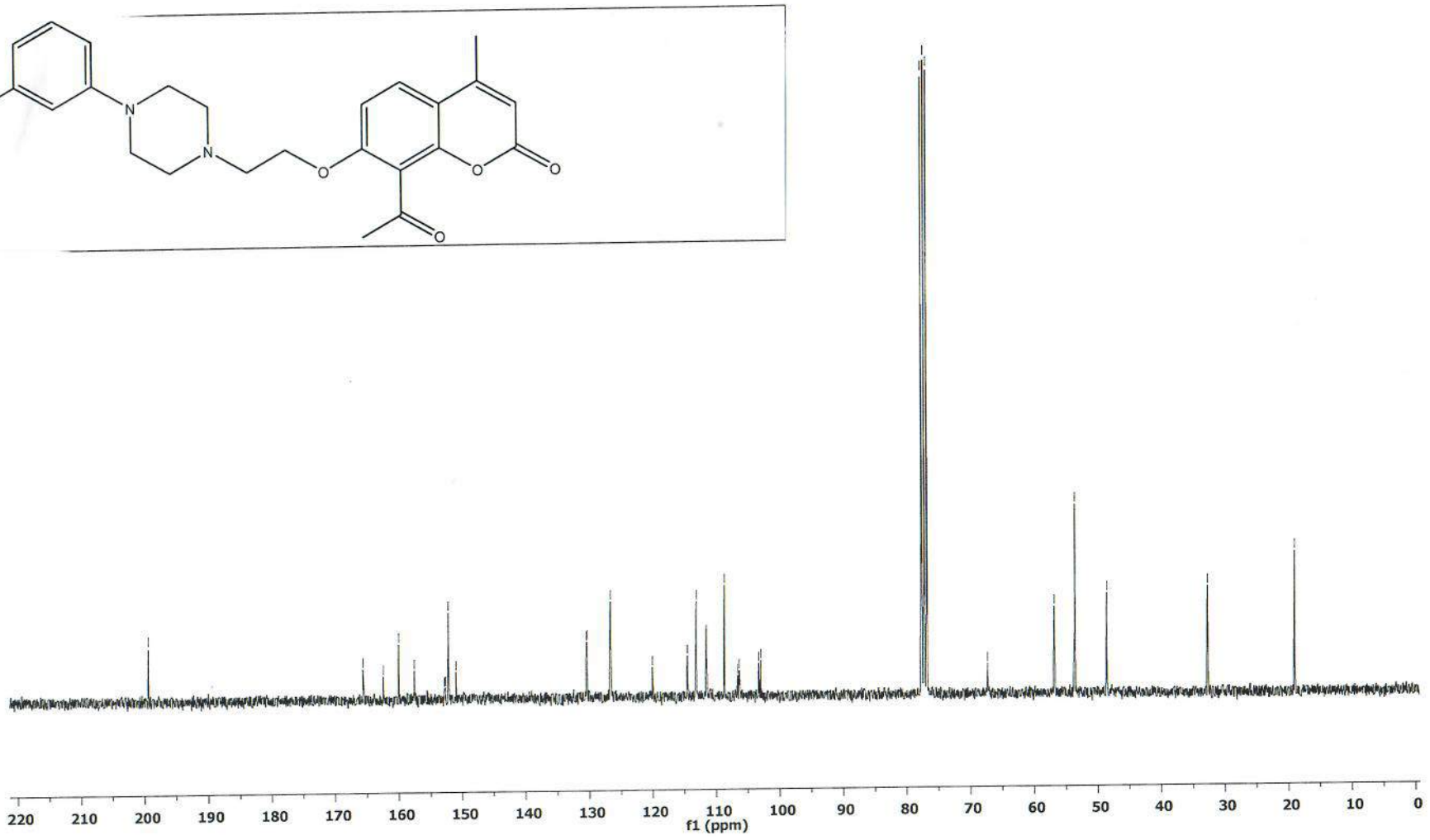
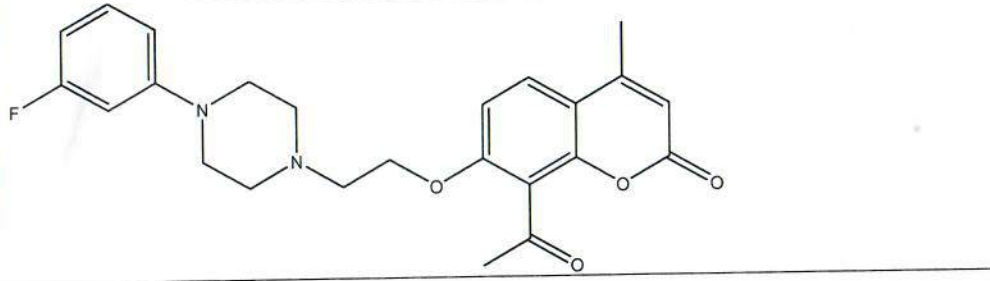
— 67.28

56.82
53.58
48.51

— 32.72

— 18.98

6e

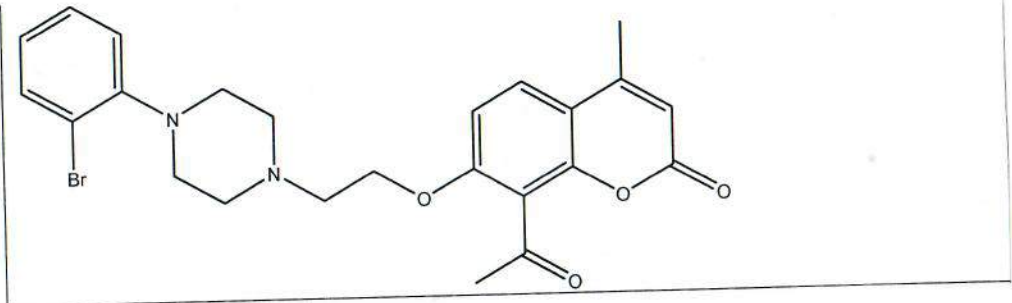


6f

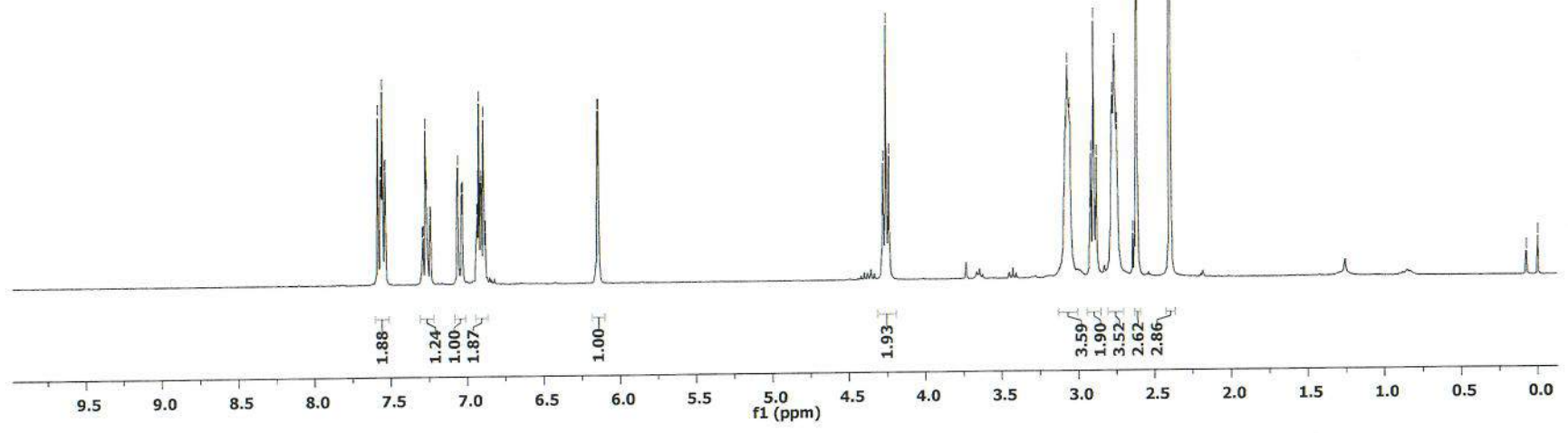
KO-420-1H-cdcl3
KO-420 w CDCl3

7.58	7.57	7.56	7.55	7.54	7.53	7.29	7.27	7.27	7.26	7.24	7.24	7.06	7.06	7.04	7.03	6.94	6.93	6.92	6.91	6.91	6.89	6.89	6.88	6.15	6.14
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

6f



4.28	4.26	4.24	3.08	3.07	3.06	2.92	2.90	2.88	2.78	2.76	2.75	2.64	2.63	2.62	2.40	2.40	0.08	-0.00
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------



6f

KO-420-13C
KO 420 13C in CDCl3

— 199.33

— 160.03
— 157.70
— 152.20
— 150.86
— 150.45

— 134.00
— 128.47
— 126.58
— 124.71
— 121.11
— 120.02
— 119.95
— 114.37
— 112.91
— 108.64

— 77.65
— 77.23
— 76.81

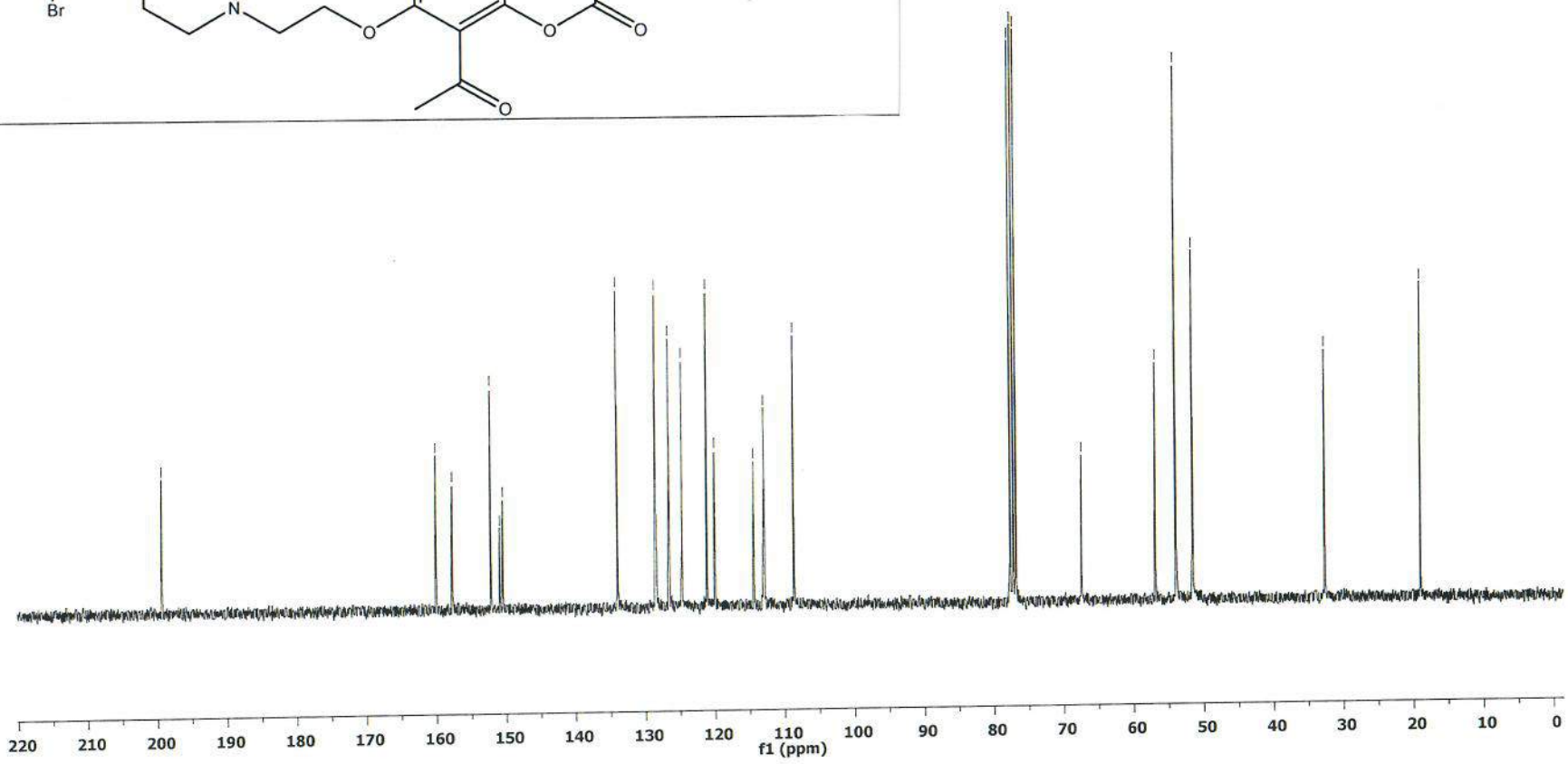
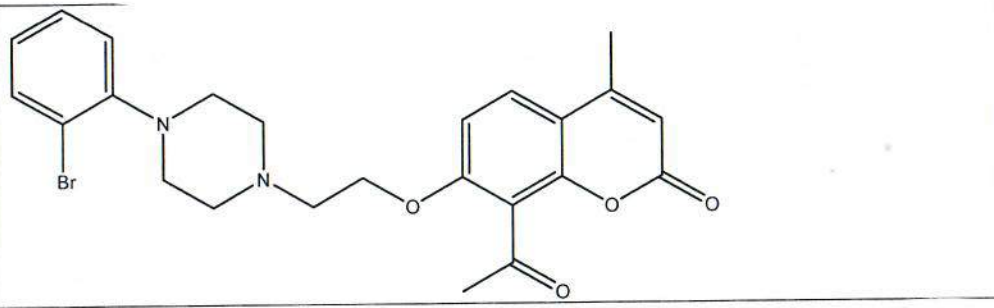
— 67.40

— 56.84
— 53.94
— 51.55

— 32.65

— 18.94

6f



6g

KO-417-1H-cdd3
KO-417 w CDCl3 + TMS

7.58
7.55
7.27
7.10
7.07
7.03
7.02
7.02
6.97
6.92
6.89
6.16
6.15

4.27
4.26
4.24

3.73

3.21
3.20
3.18

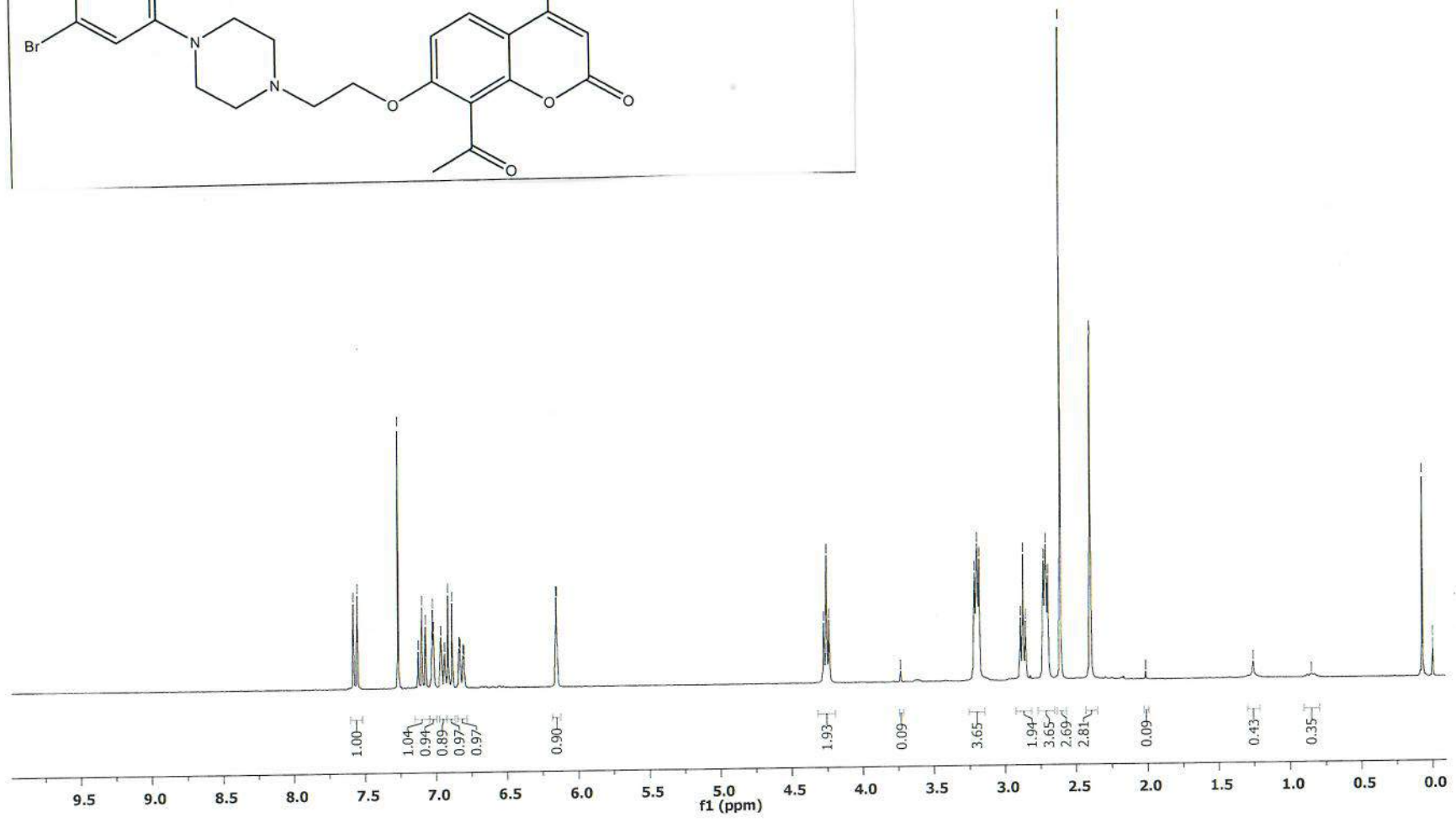
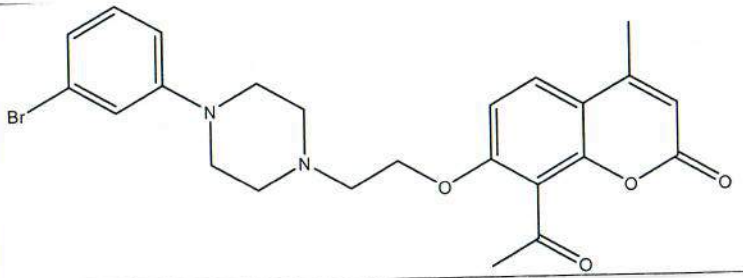
2.87
2.73
2.71
2.70
2.61
2.40
2.01

1.26

0.85

0.07
-0.00

6g



KO-417-13C
KO 417 13C in CDCl3

— 199.36

~ 160.01
~ 157.58
~ 152.36
~ 152.19
~ 150.92

~ 130.55
~ 126.63
~ 123.42
~ 122.70
~ 119.95
~ 119.00
~ 114.67
~ 114.46
~ 113.00
~ 108.63

~ 77.65
~ 77.23
~ 76.81

— 67.42

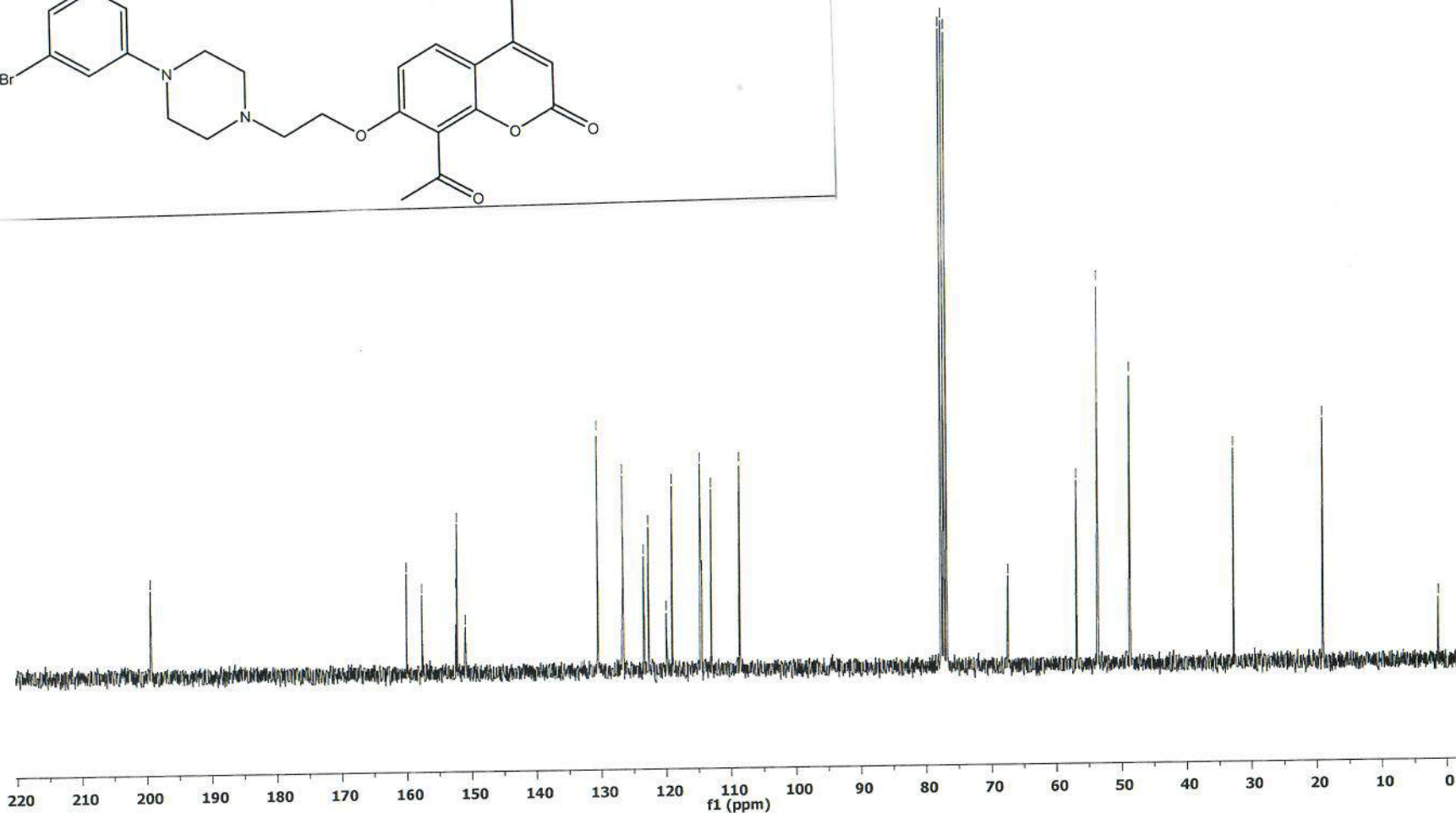
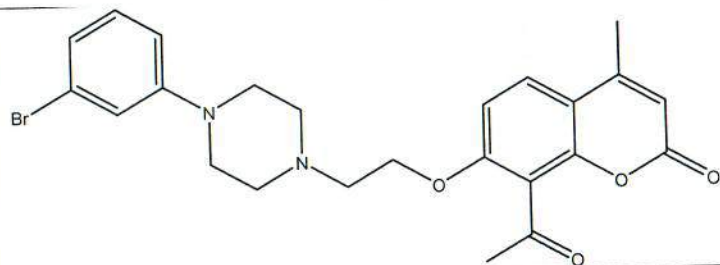
~ 56.81
~ 53.59
~ 48.64

— 32.69

— 18.96

— 1.21

6g



6g

KO-421-1H-cdcl3
KO-421 w CDCl3 + TMS

7.58
7.55

7.26

6.92
6.89

6.55
6.52

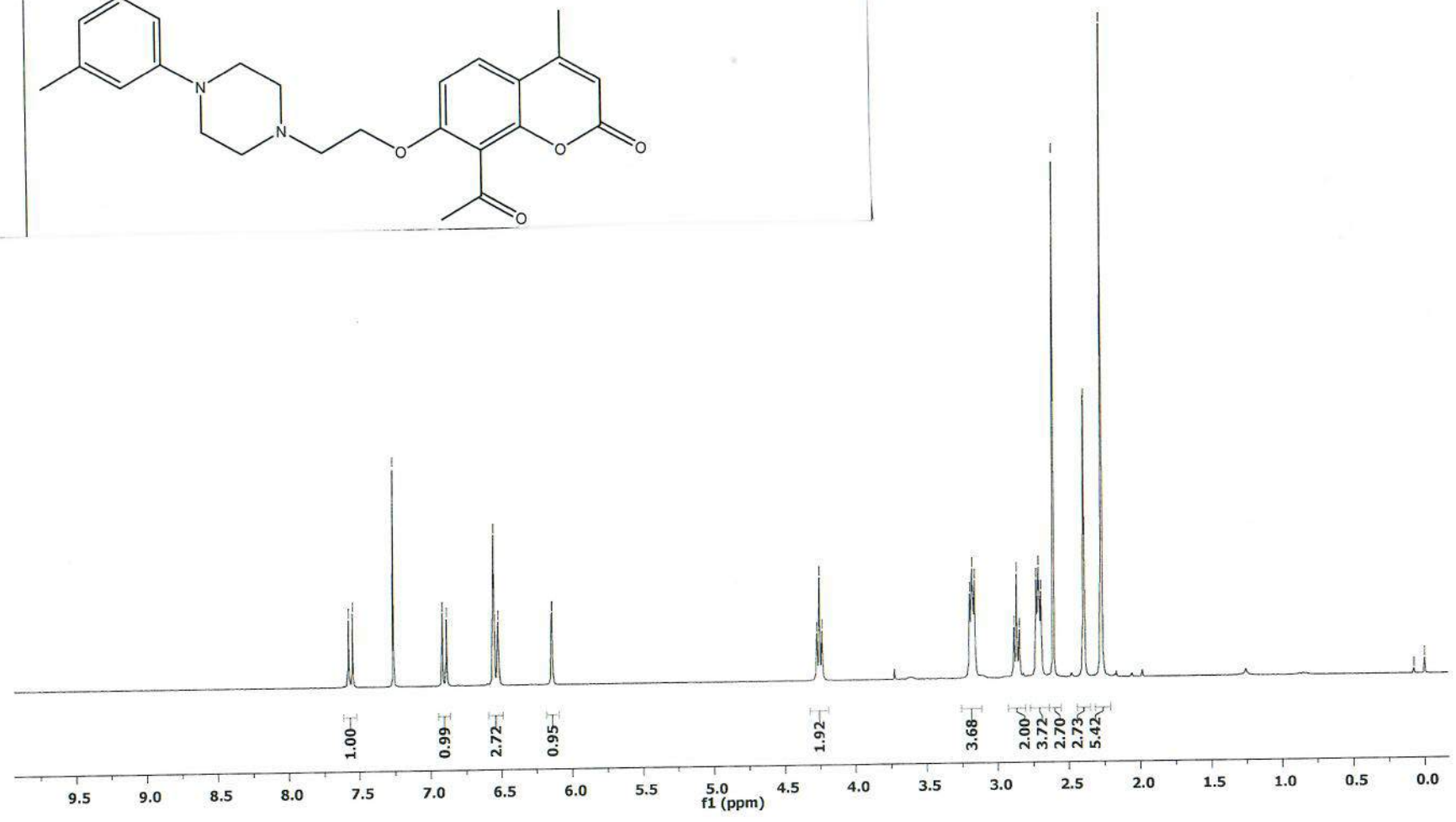
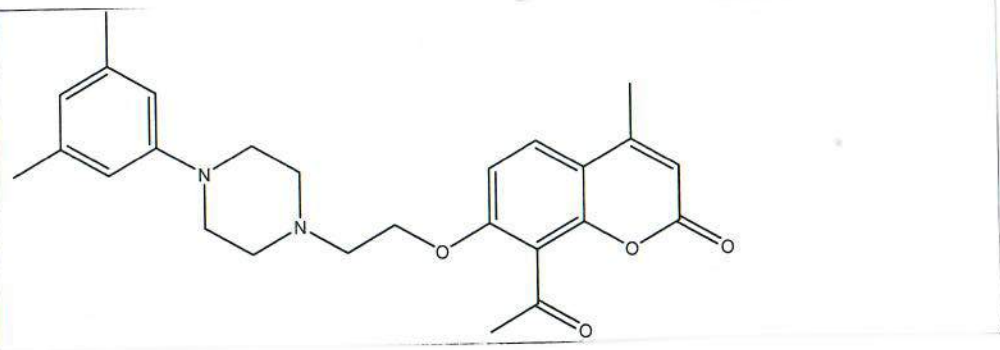
6.14
6.14

4.27
4.25
4.24

3.20
3.18
3.16
2.88
2.87
2.85
2.73
2.71
2.70
2.61
2.40
2.39
2.27

0.07
-0.00

6h



6h

KO-421-13C
KO 421 13C

— 199.37

— 160.03
— 157.68
— 152.19
— 151.34
— 150.87

— 138.83

— 126.57
— 122.08
— 119.94
— 114.36
— 114.31
— 112.93
— 108.62

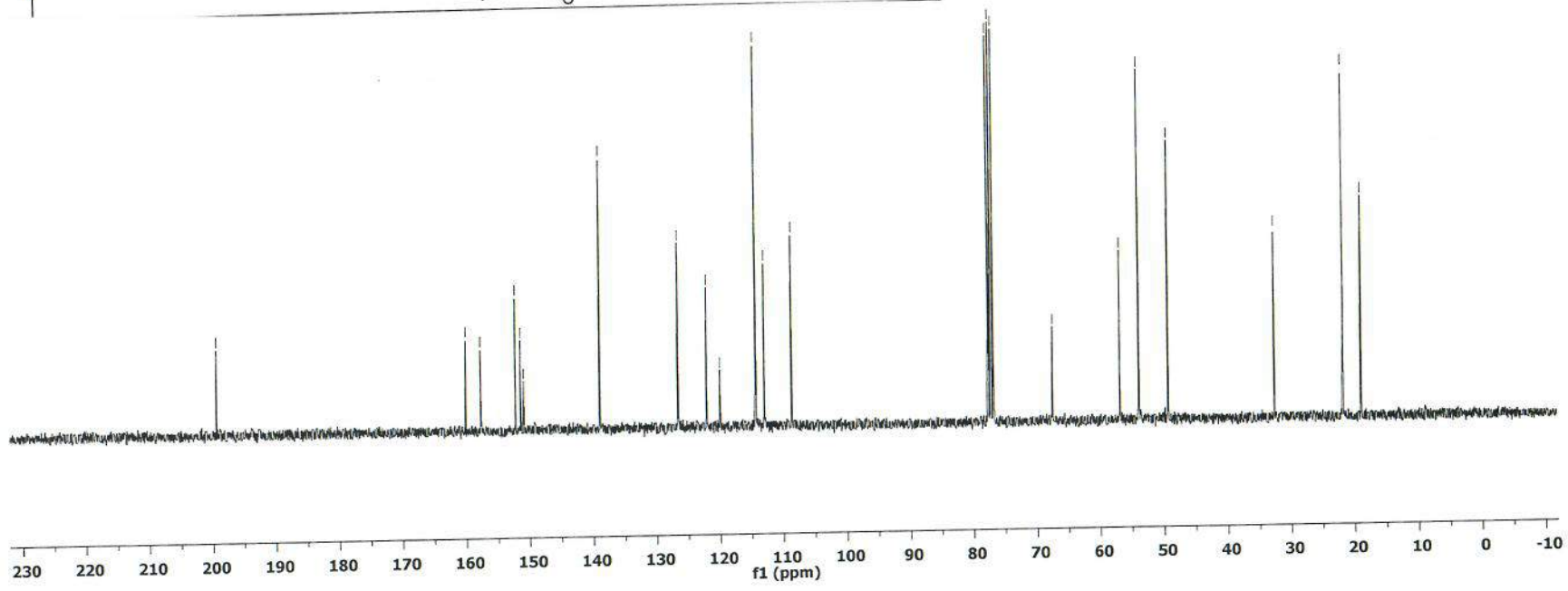
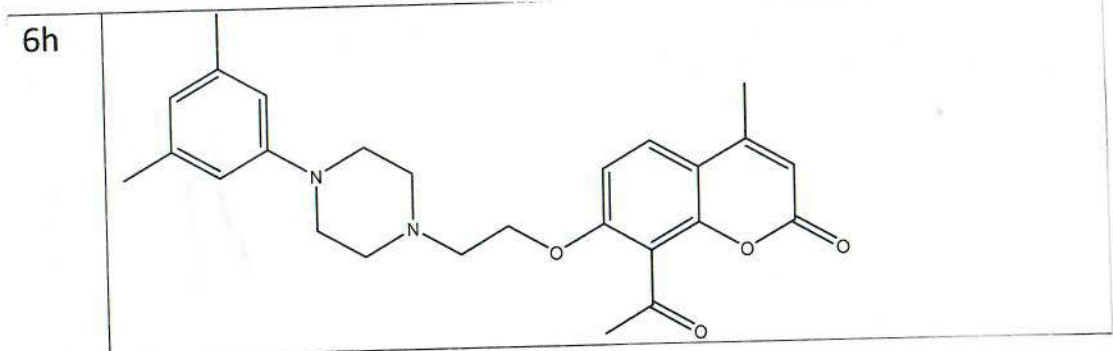
— 77.65
— 77.23
— 76.81

— 67.50

— 56.88
— 53.89
— 49.31

— 32.66

— 21.81
— 18.94



6i

KO-413-1H-cdcl3
KO-413 w CDCl3 + TMS

7.59
7.56
7.28
7.16
7.14
7.14
6.96
6.95
6.93
6.92
6.89

4.27
4.26
4.24

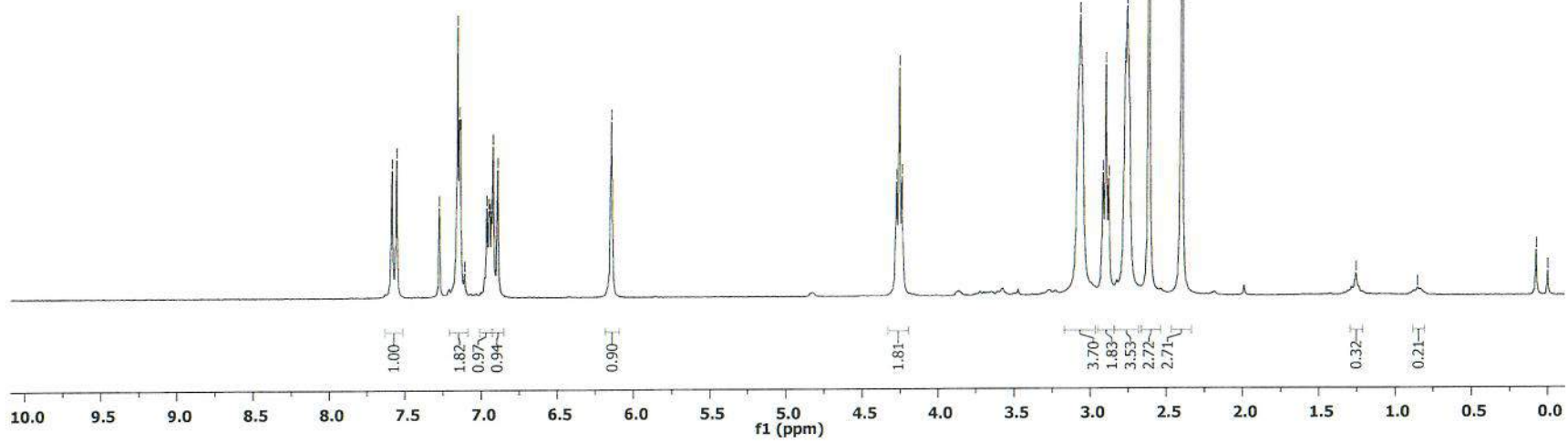
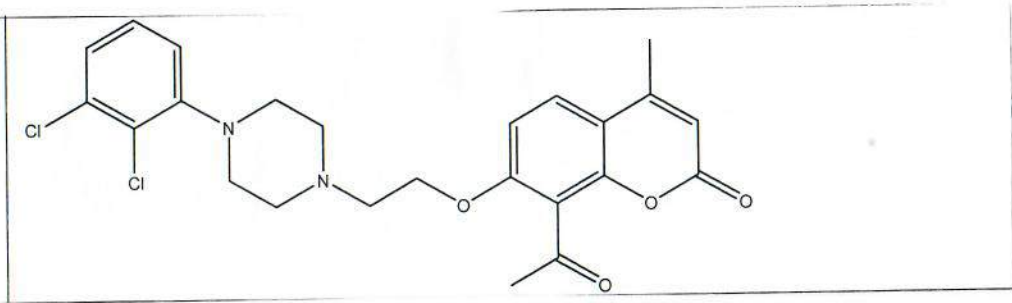
3.07
2.92
2.90
2.88
2.77
2.76
2.61
2.40

1.26

0.85

0.08
-0.00

6i



6i

KO-413-13C-cdd3
KO 413 13C in CDCl3

— 199.33

— 160.02
— 157.67
— 152.19
— 151.09
— 150.89

— 134.22
— 127.67
— 126.60
— 124.96
— 119.96
— 118.83
— 114.41
— 112.95
— 108.64

— 77.65
— 77.23
— 76.81

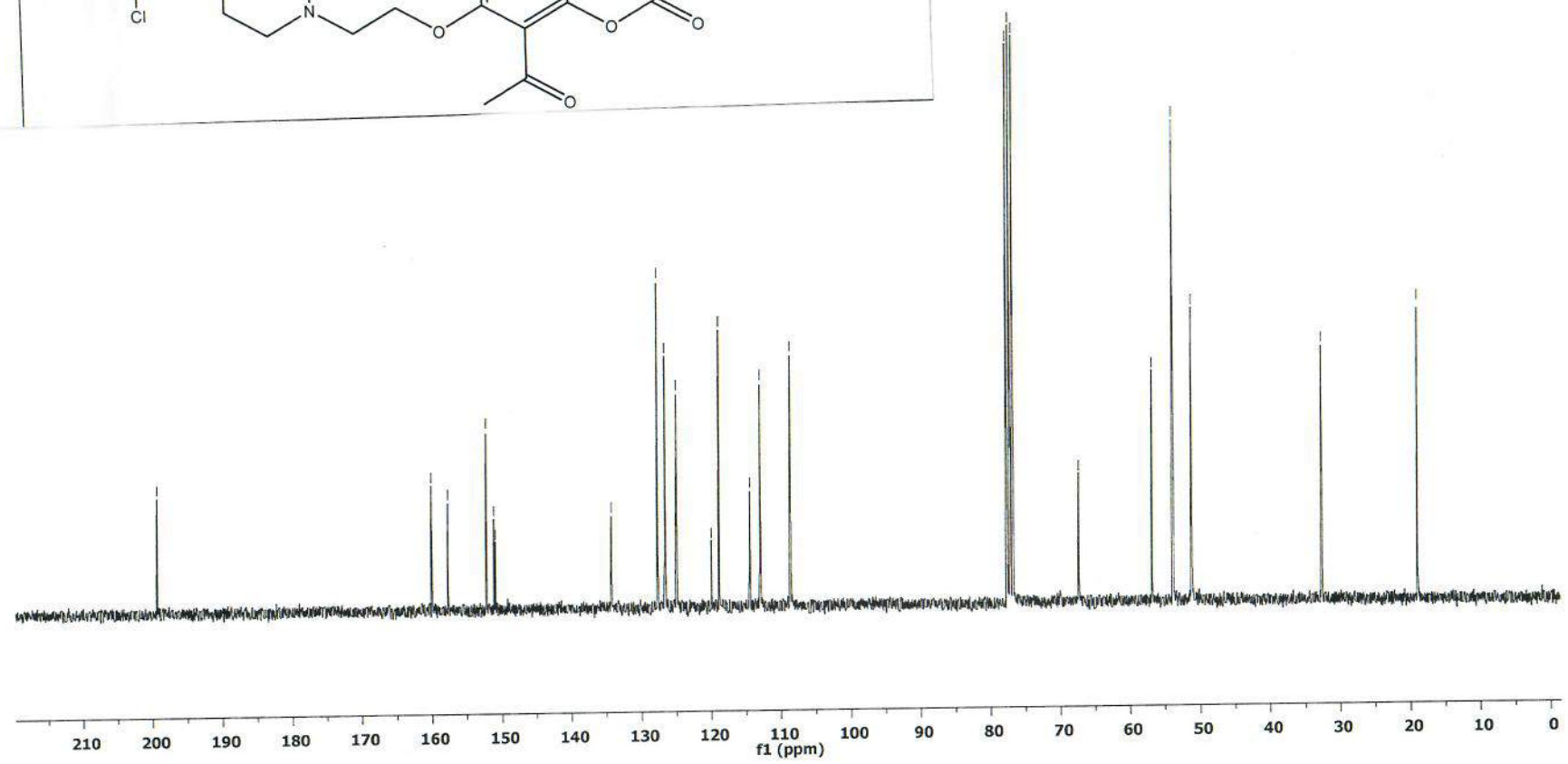
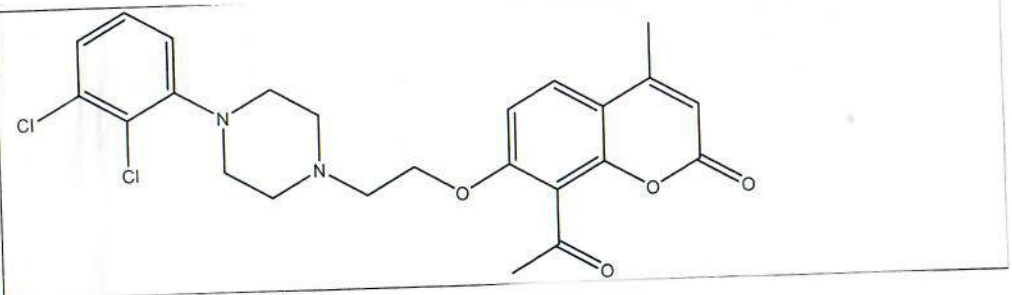
— 67.36

— 56.81
— 53.85
— 51.20

— 32.66

— 18.95

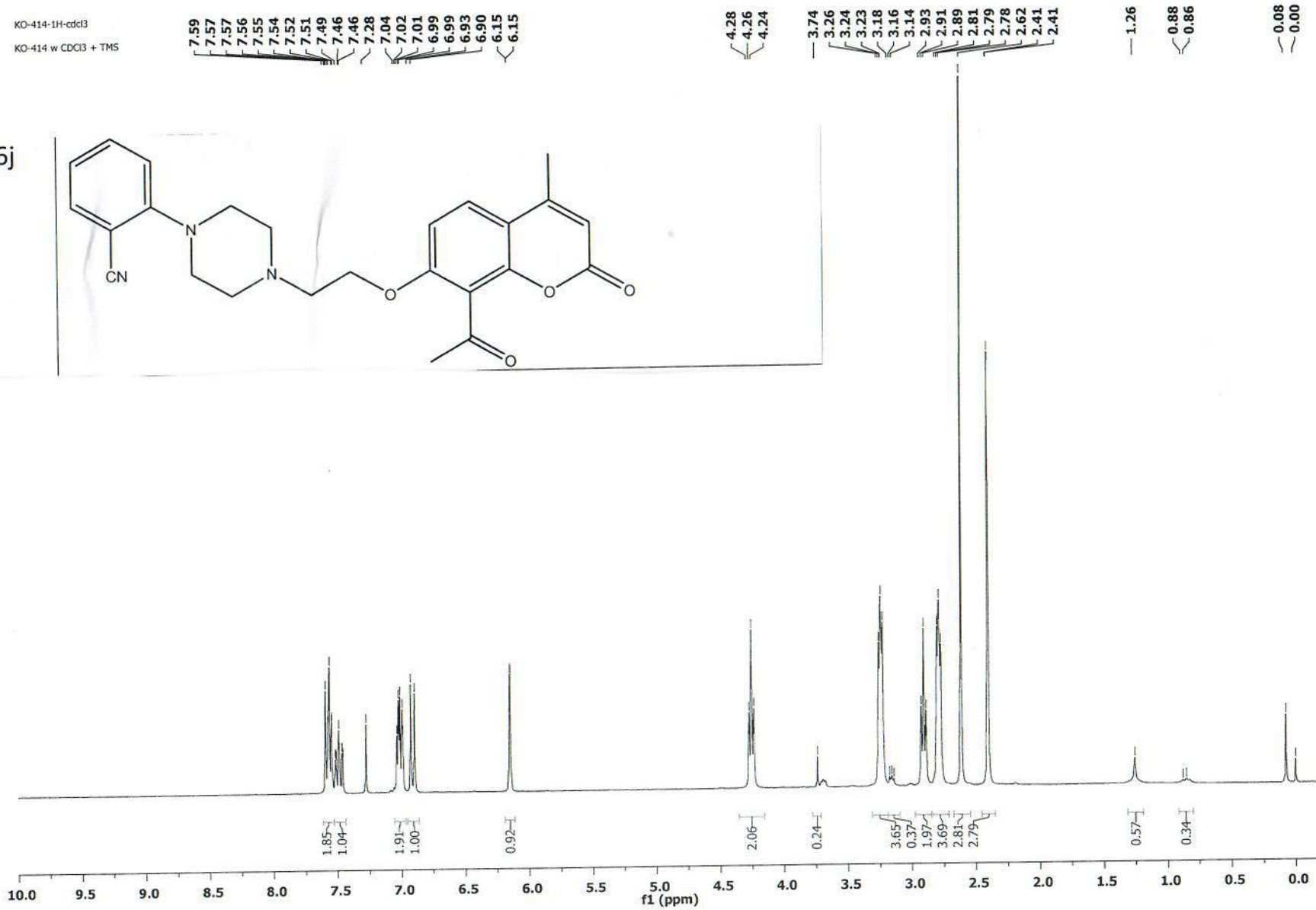
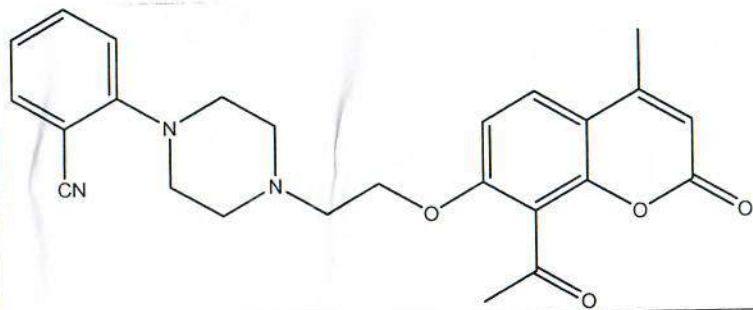
6i



6j

KO-414-1H-cdcl3
KO-414 w CDCl3 + TMS

6j



6j

KO-414-13C-cdcl3
KO 414 13C in CDCl3

— 199.34

~ 160.02
~ 157.62
~ 155.53
~ 152.19
~ 150.90

~ 134.48
~ 134.04
~ 126.60
~ 122.23
~ 119.99
~ 118.96
~ 118.53
~ 114.44
~ 112.97
~ 108.67
~ 106.28

~ 77.65
~ 77.23
~ 76.81

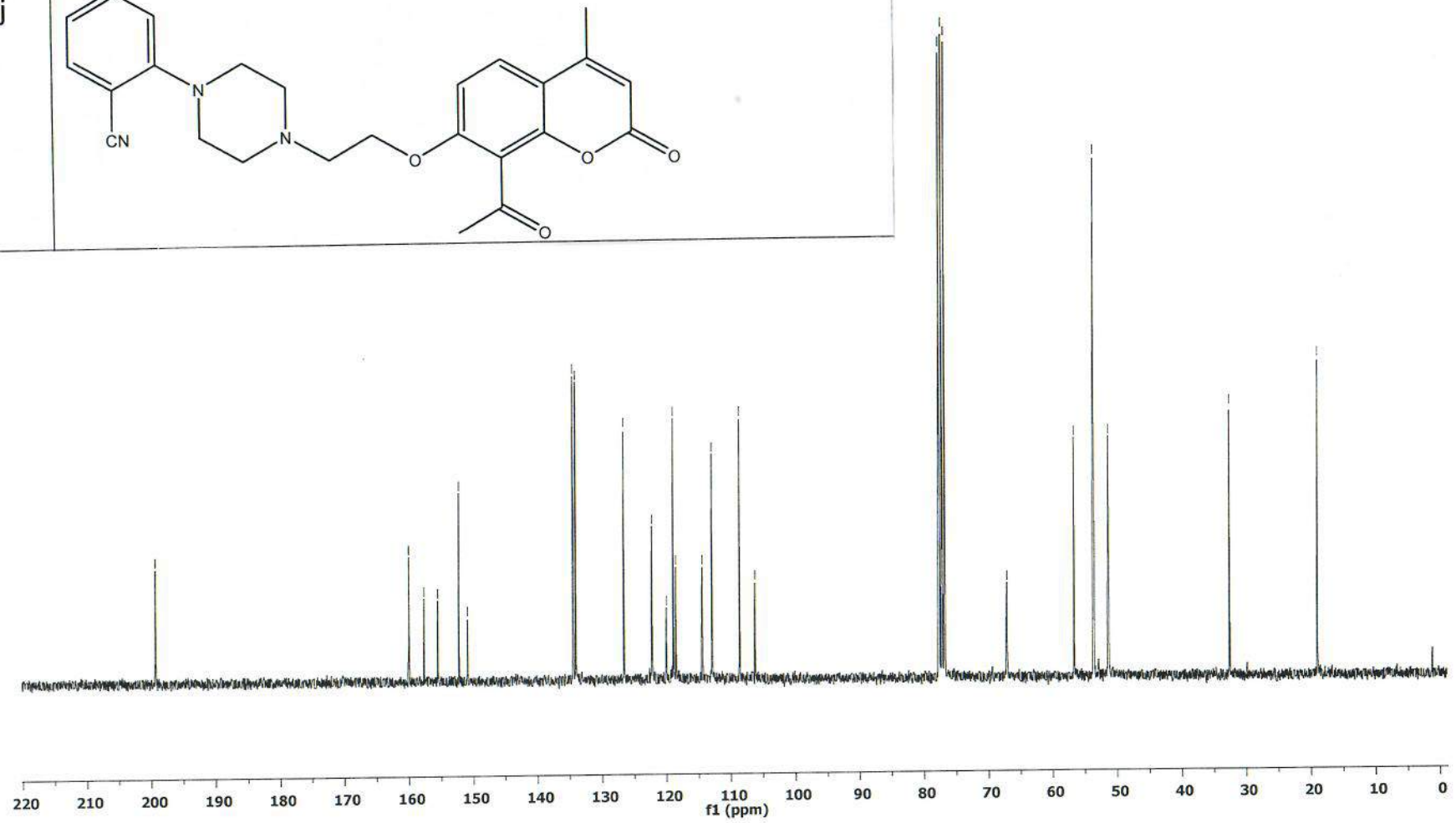
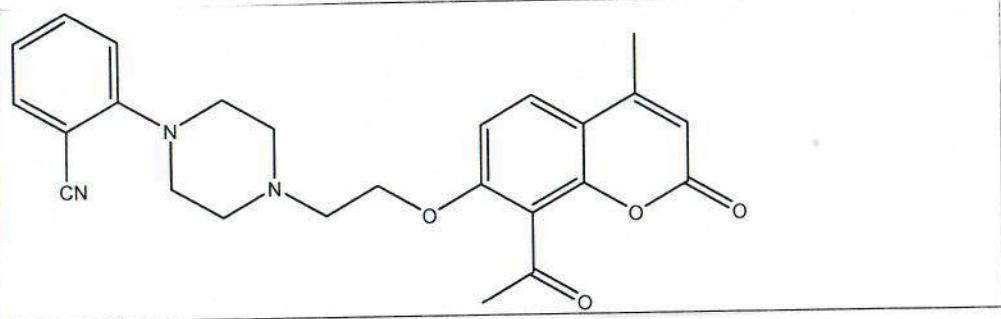
— 67.16

~ 56.70
~ 53.67
~ 51.39

— 32.67

— 18.95

6j



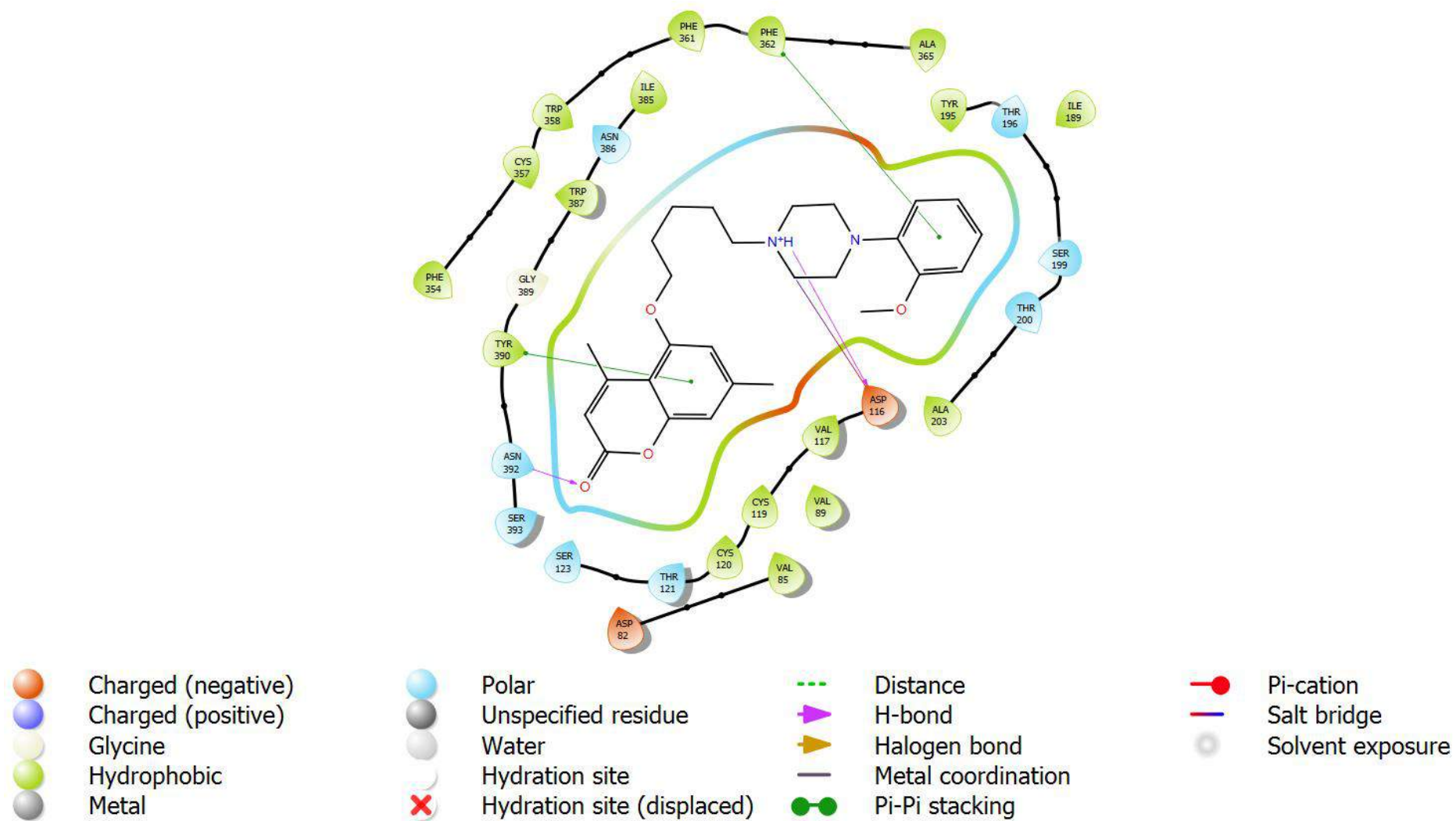


Figure S2. Ligand interaction diagram for compound **1a** docked to 5HT_{1A} receptor.

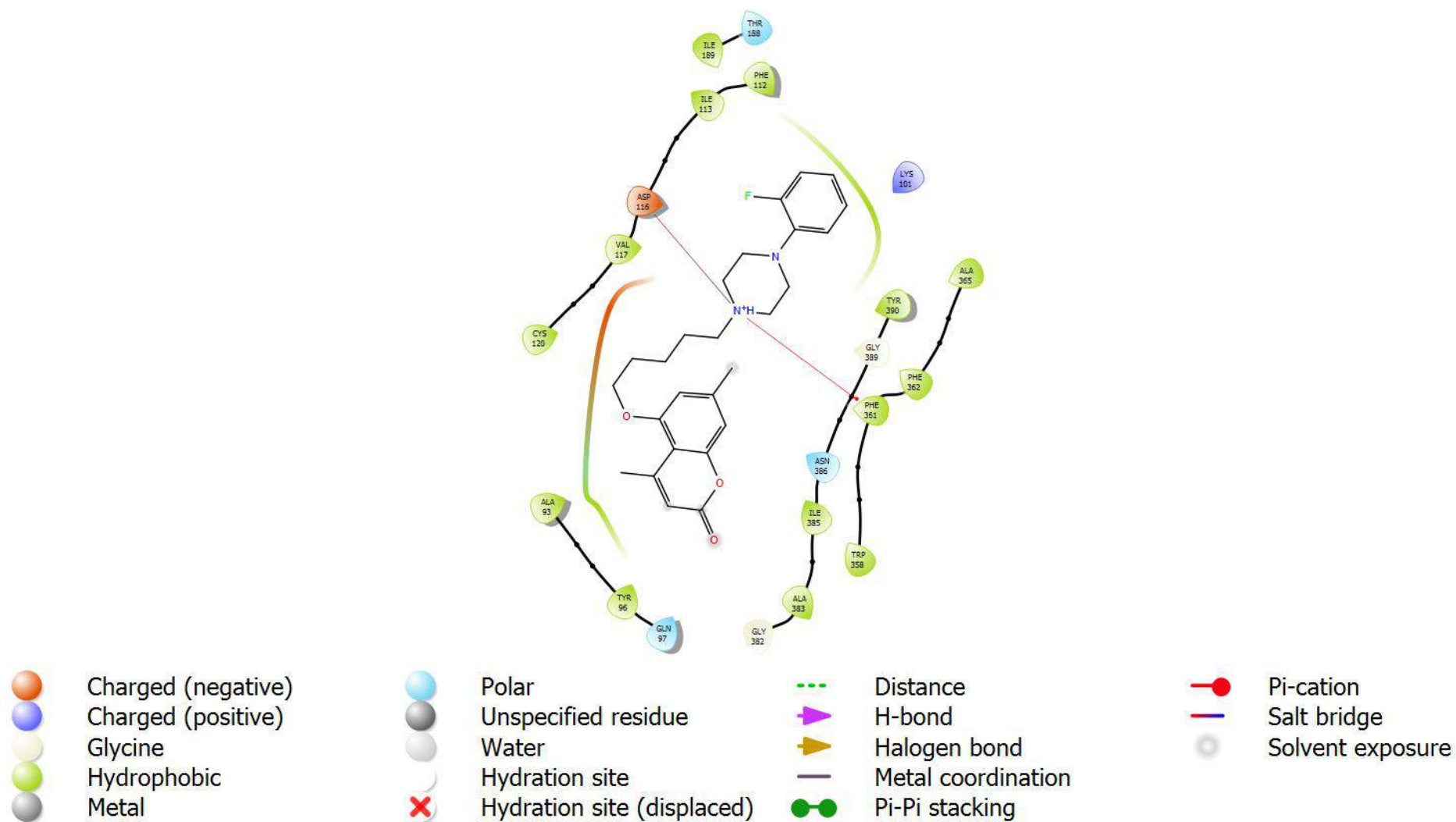


Figure S3. Ligand interaction diagram for compound **1b** docked to 5HT_{1A} receptor.

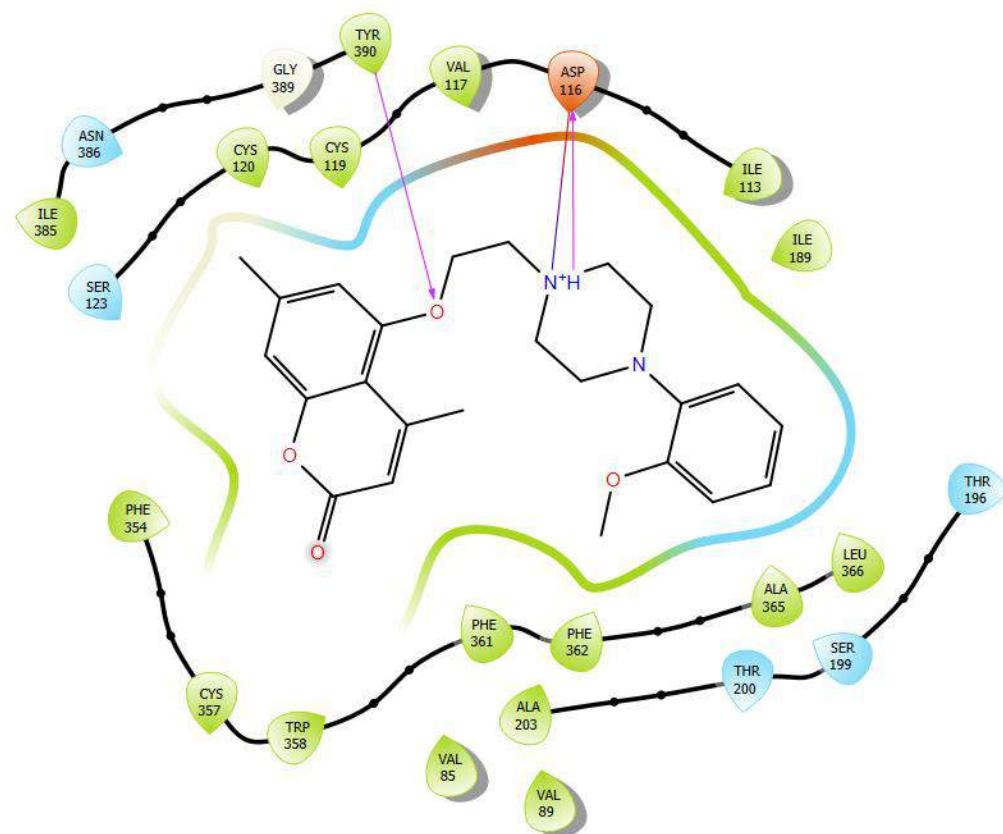


Figure S4. Ligand interaction diagram for compound **2a** docked to 5HT_{1A} receptor.

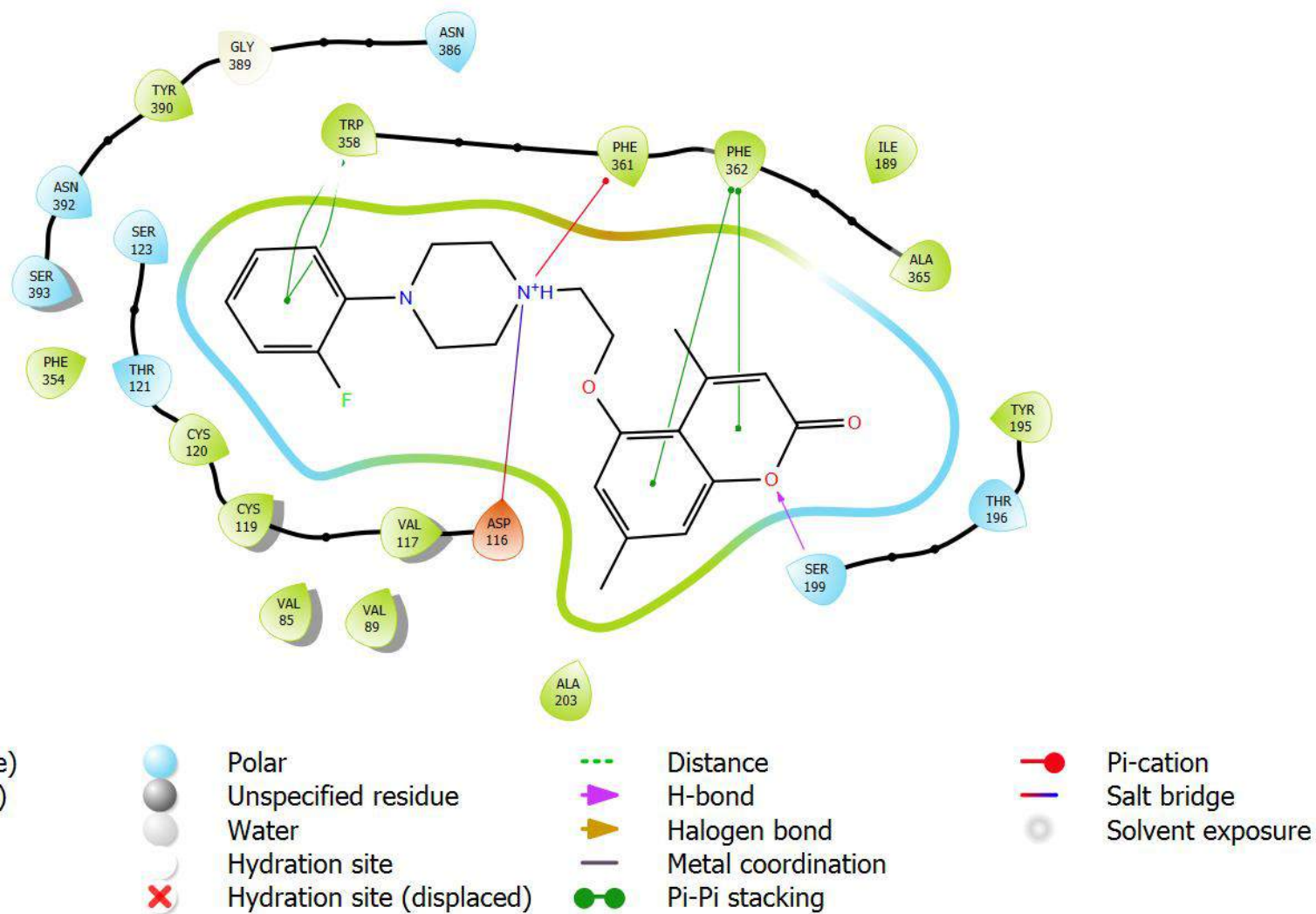


Figure S5. Ligand interaction diagram for compound **2b** docked to 5HT_{1A} receptor.

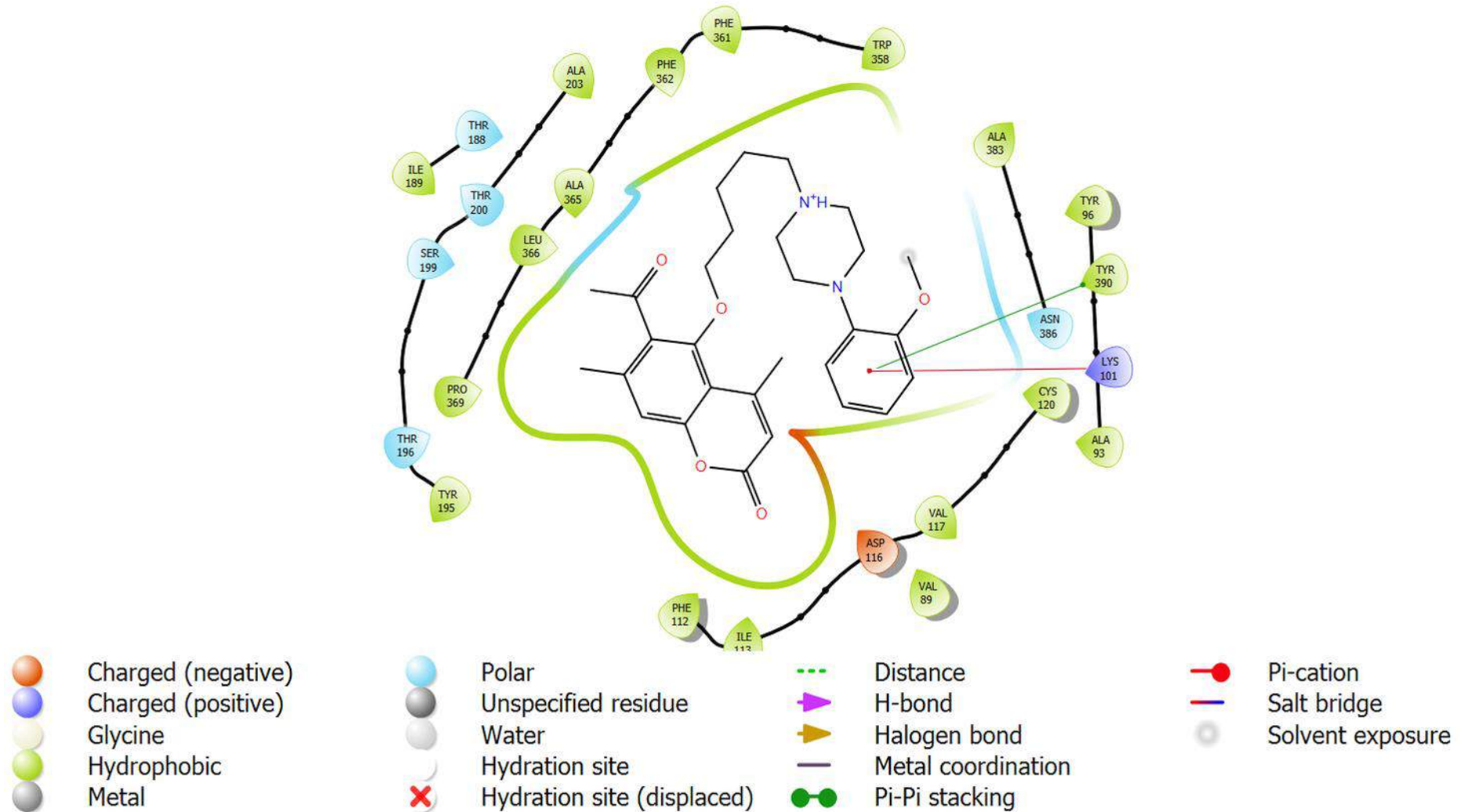


Figure S6. Ligand interaction diagram for compound **3a** docked to 5HT_{1A} receptor.

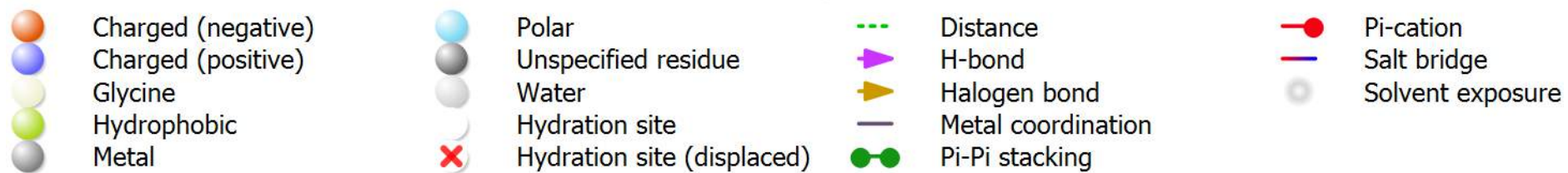
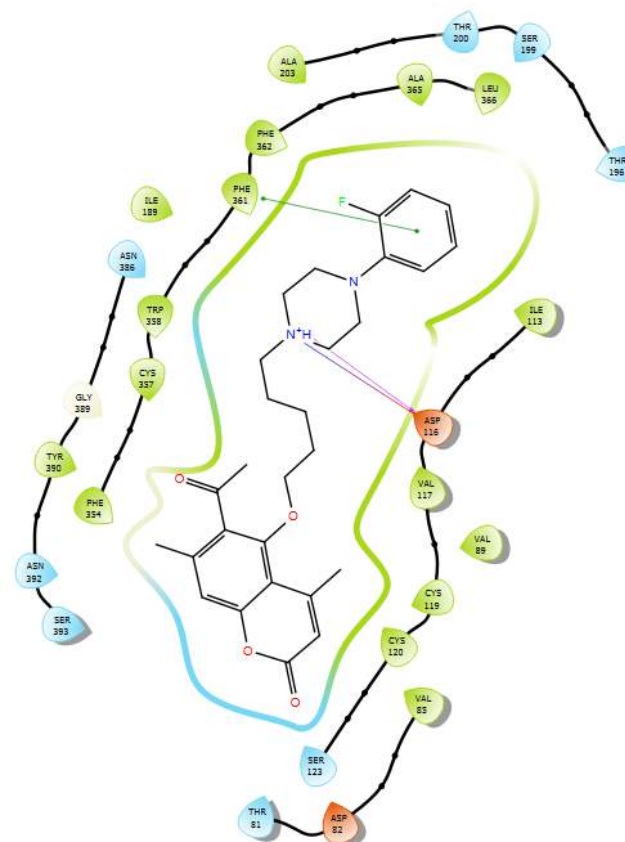


Figure S7. Ligand interaction diagram for compound **3b** docked to 5HT_{1A} receptor.

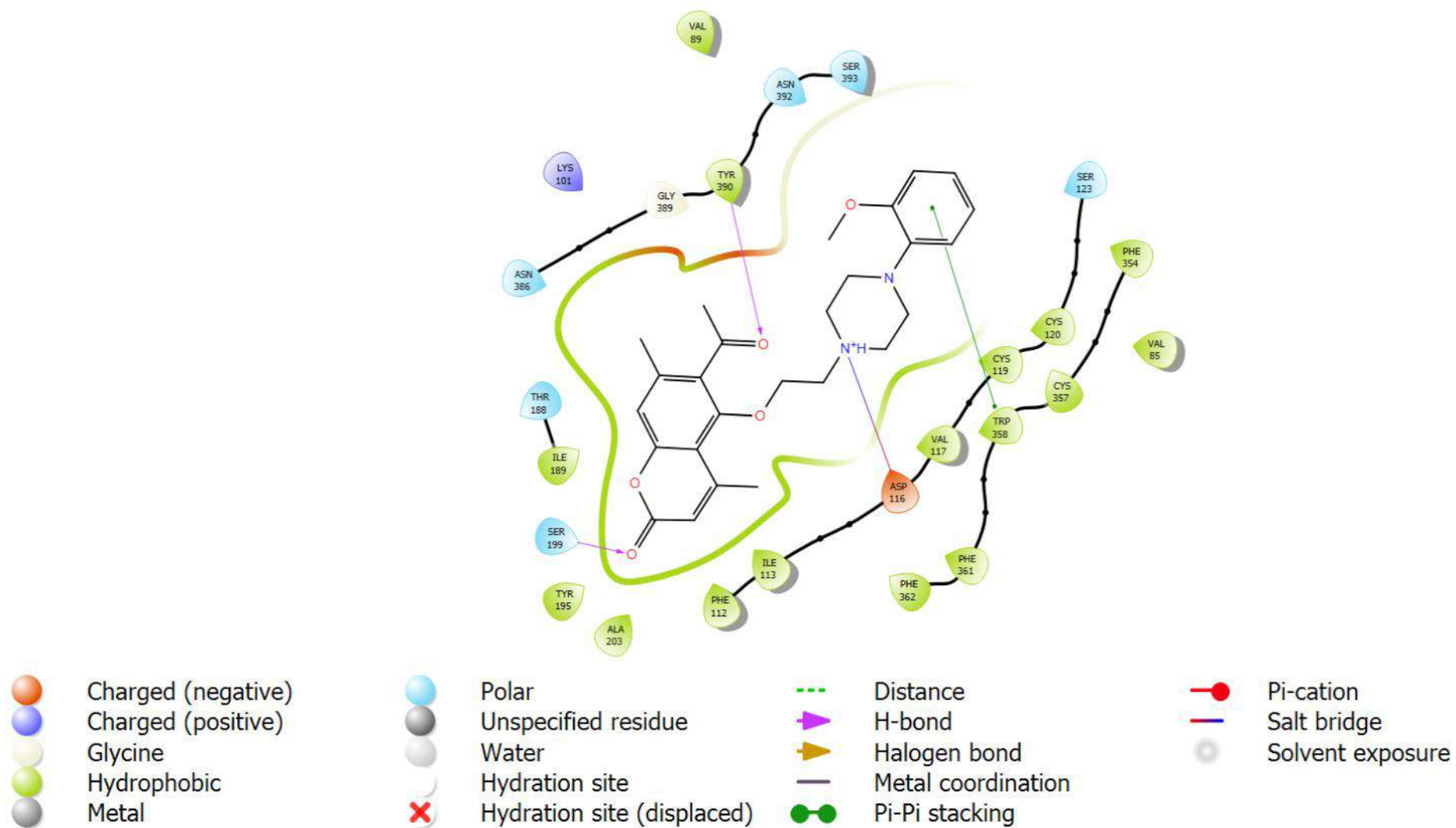


Figure S8. Ligand interaction diagram for compound **4a** docked to 5HT_{1A} receptor.

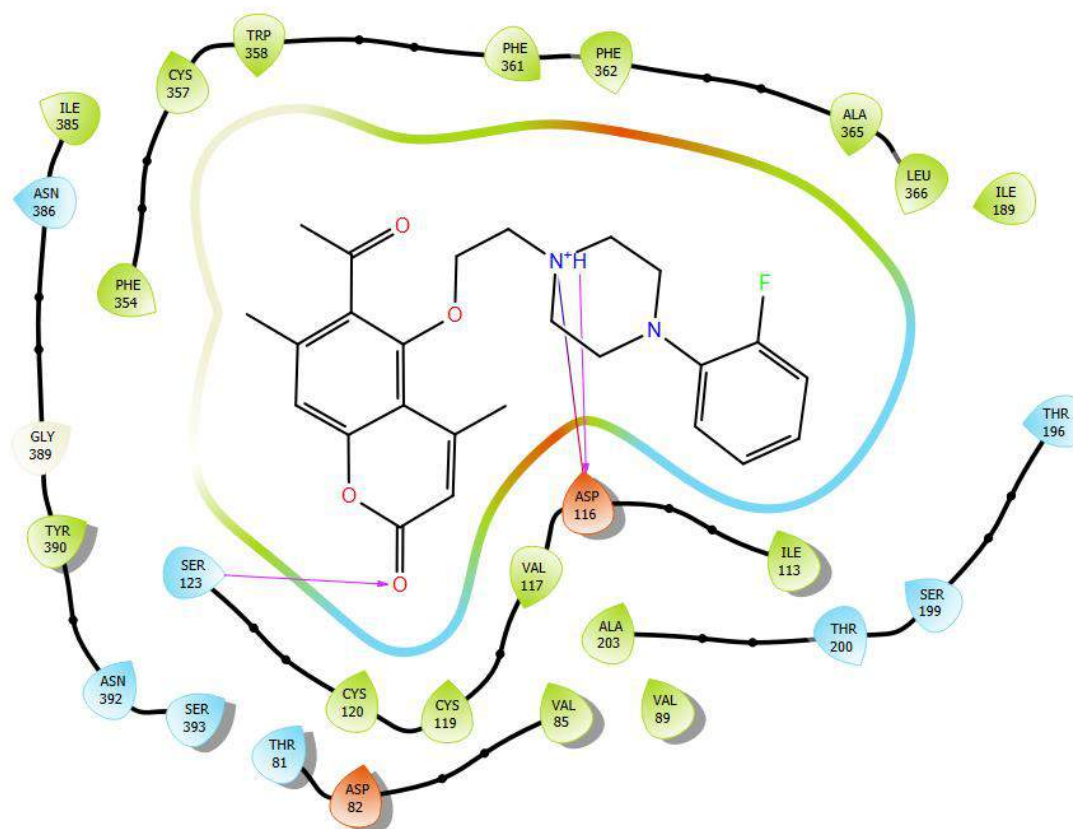


Figure S9. Ligand interaction diagram for compound **4b** docked to 5HT_{1A} receptor.

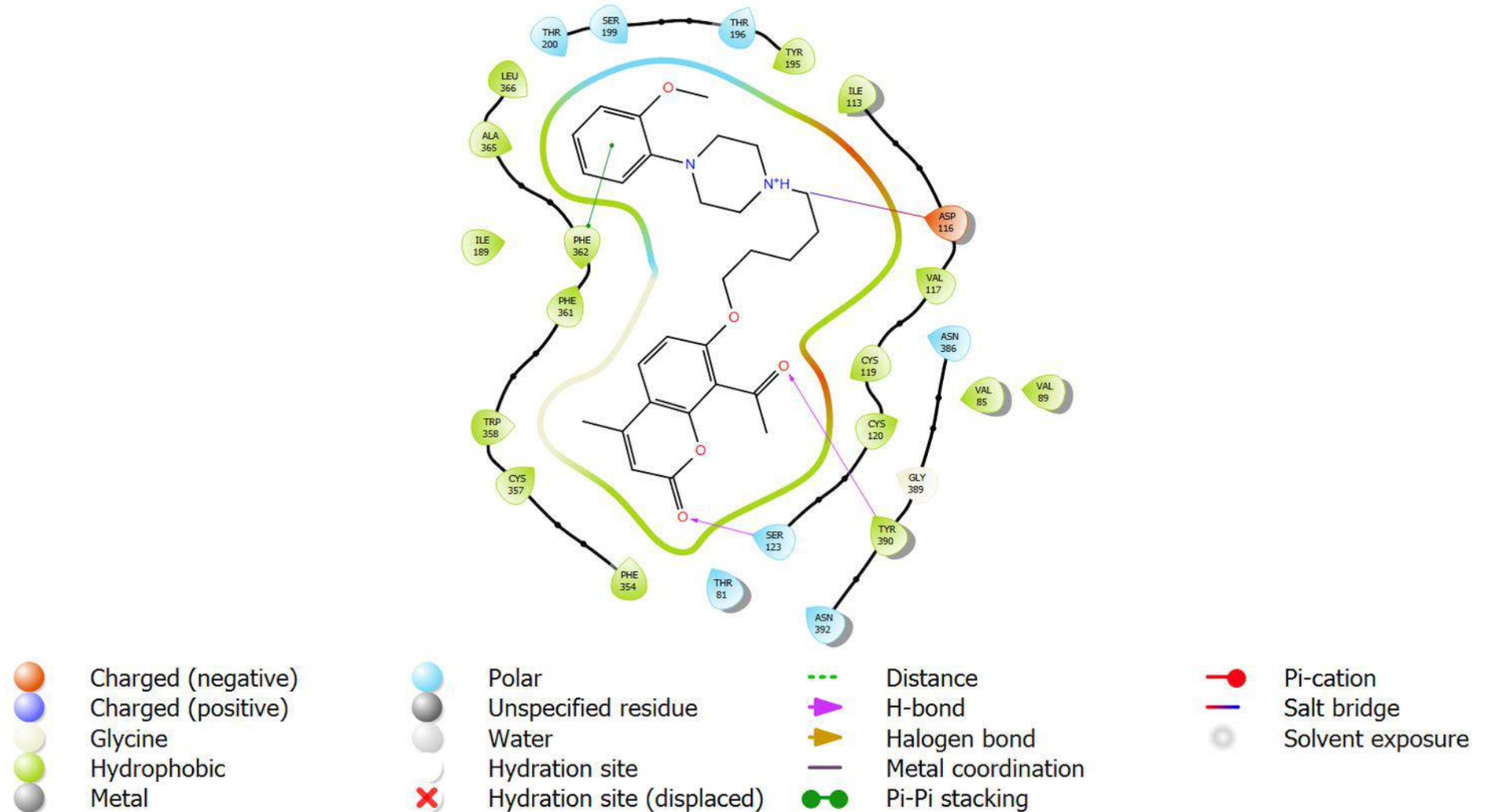
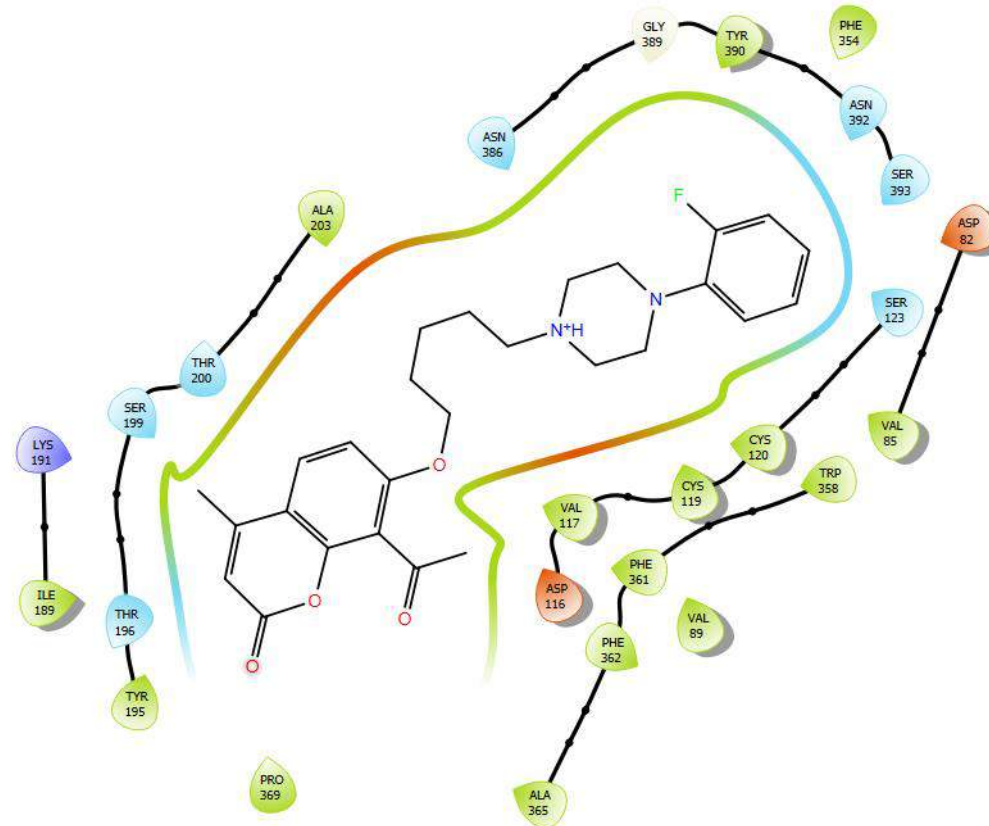


Figure S10. Ligand interaction diagram for compound **5a** docked to 5HT_{1A} receptor.




















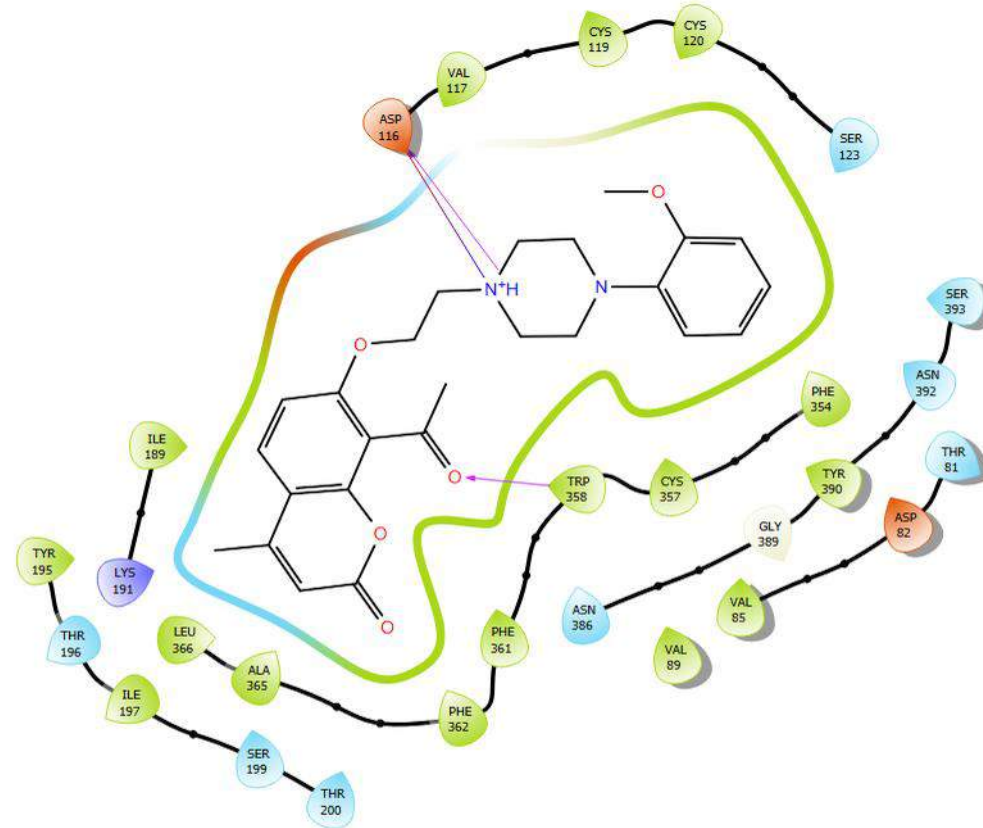
- | | | | | | | | |
|---|--------------------|---|----------------------------|---|--------------------|---|------------------|
|  | Charged (negative) |  | Polar |  | Distance |  | Pi-cation |
|  | Charged (positive) |  | Unspecified residue |  | H-bond |  | Salt bridge |
|  | Glycine |  | Water |  | Halogen bond |  | Solvent exposure |
|  | Hydrophobic |  | Hydration site (displaced) |  | Metal coordination | | |
|  | Metal | | |  | Pi-Pi stacking | | |

Figure S11. Ligand interaction diagram for compound **5b** docked to 5HT_{1A} receptor.



- Charged (negative)
- Charged (positive)
- Glycine
- Hydrophobic
- Metal

- Polar
- Unspecified residue
- Water
- Hydration site
- ✗ Hydration site (displaced)

- Distance
- ▶ H-bond
- ▶ Halogen bond
- Metal coordination
- Pi-Pi stacking

- Pi-cation
- Salt bridge
- Solvent exposure

Figure S12. Ligand interaction diagram for compound **6a** docked to 5HT_{1A} receptor.

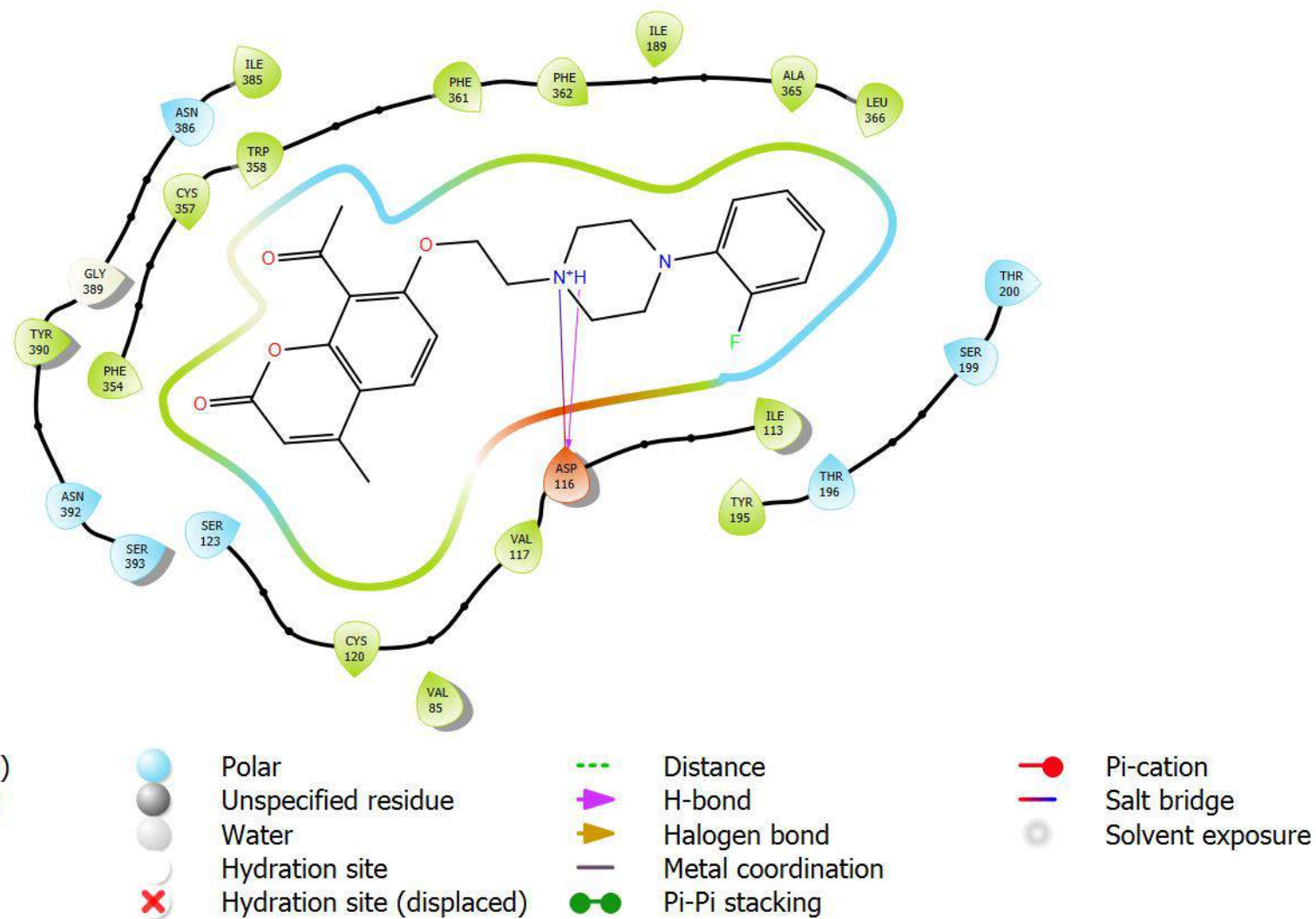


Figure S13. Ligand interaction diagram for compound **6b** docked to 5HT_{1A} receptor.

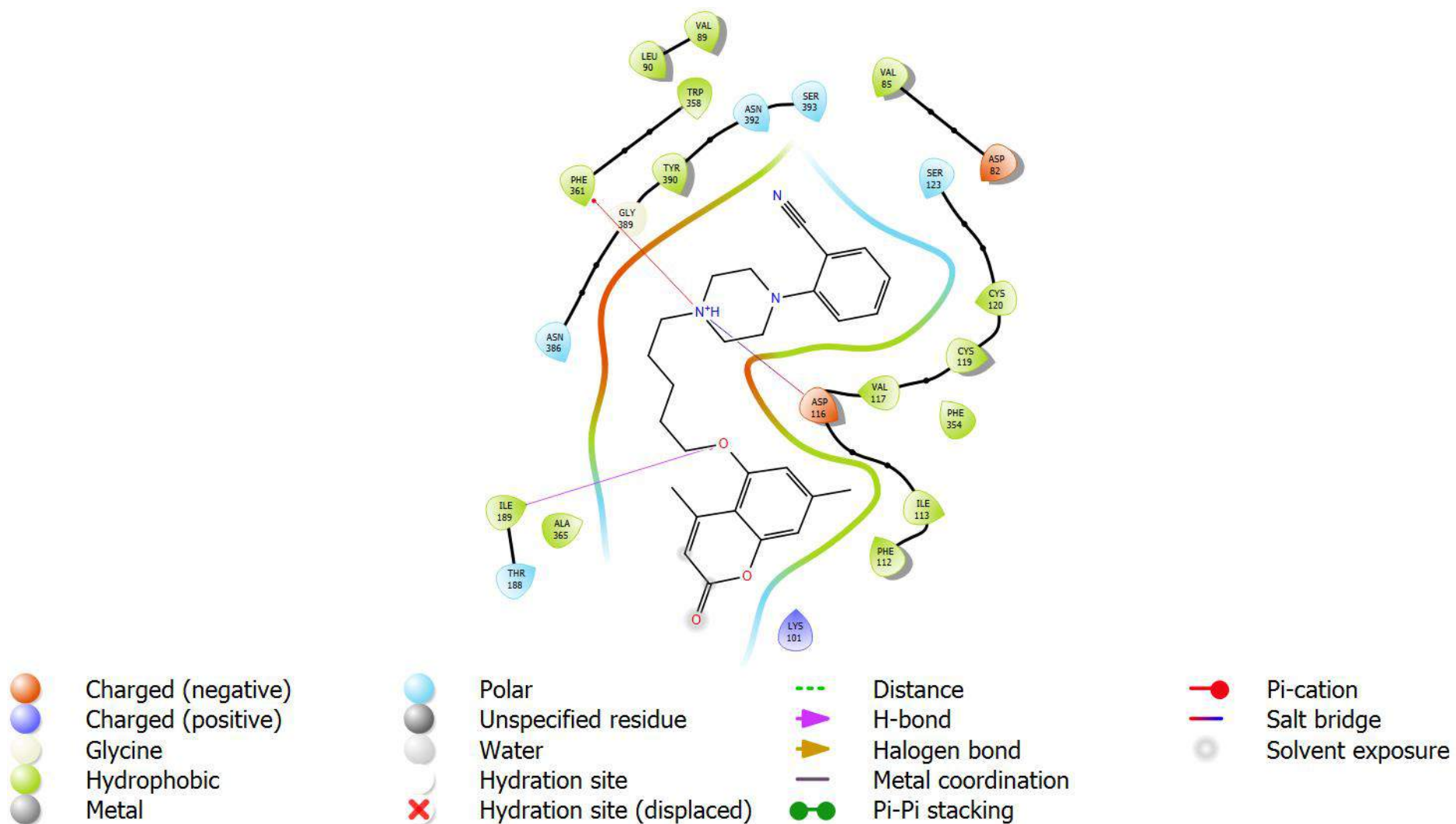


Figure S14. Ligand interaction diagram for compound **1j** docked to 5HT_{1A} receptor.

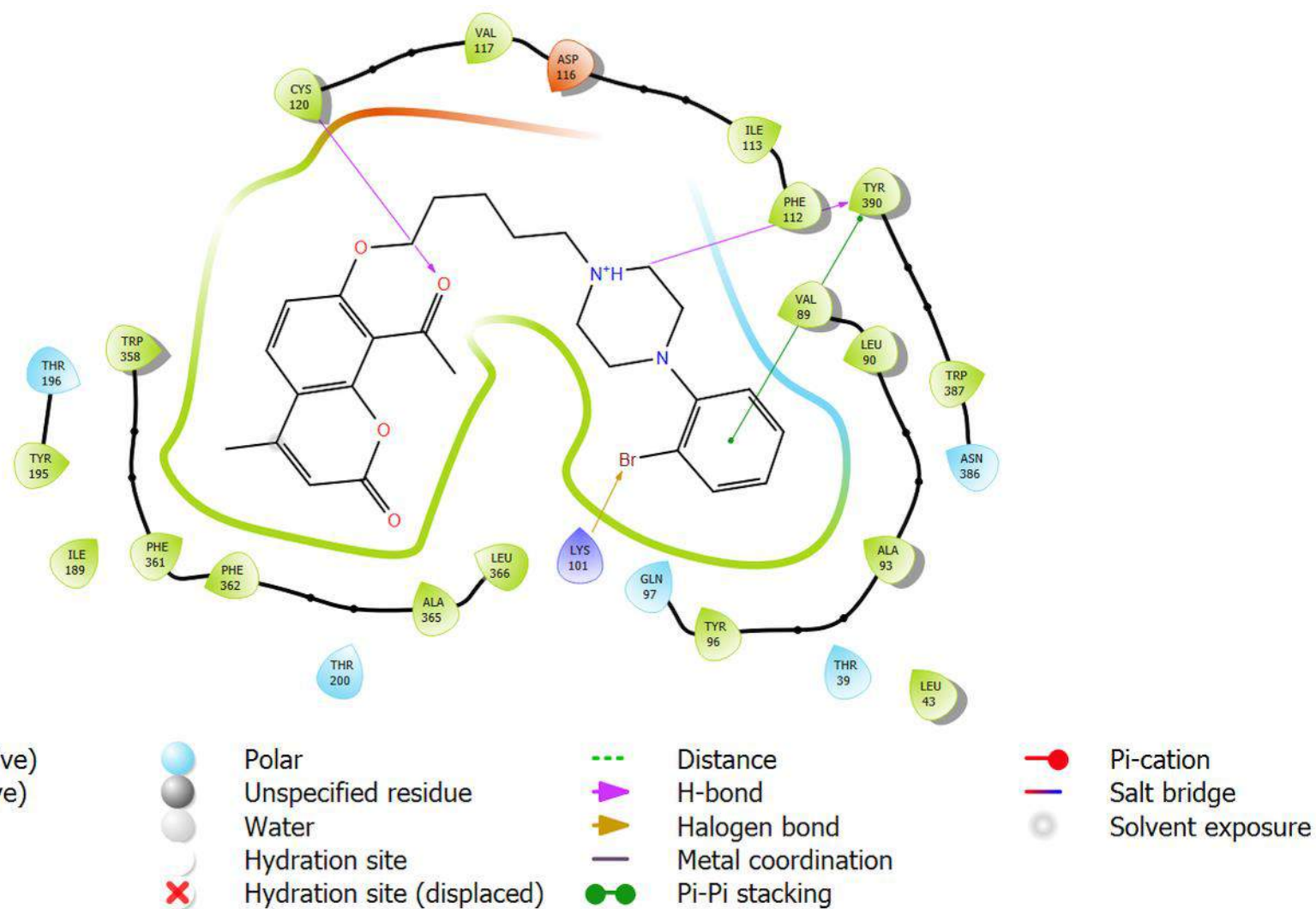


Figure S15. Ligand interaction diagram for compound **5f** docked to 5HT_{1A} receptor.

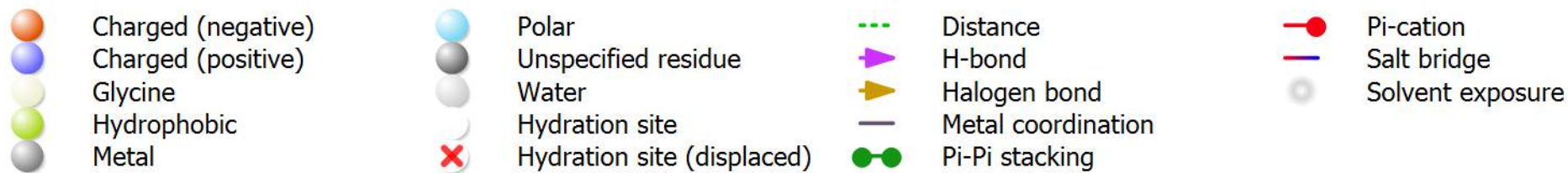
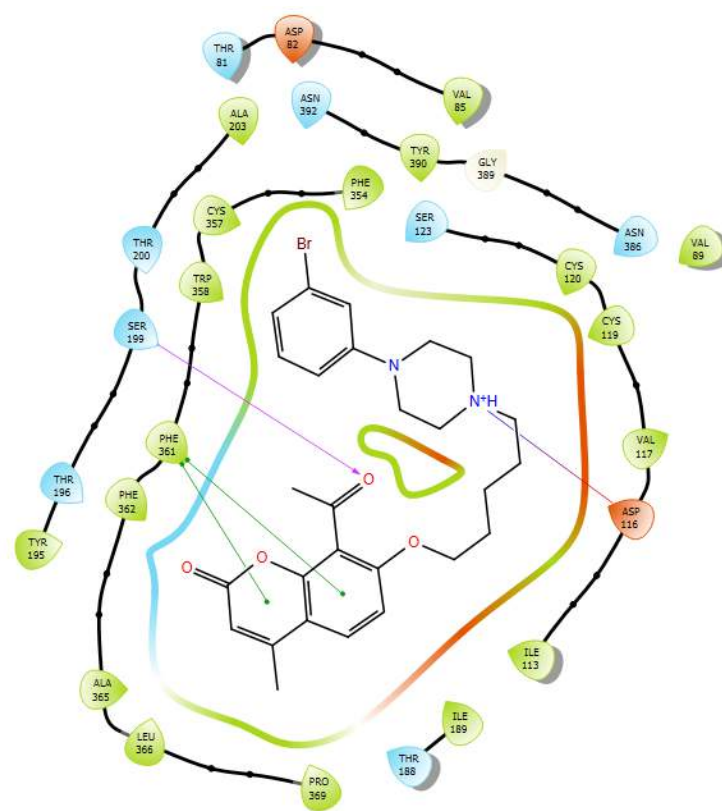


Figure S16. Ligand interaction diagram for compound **5g** docked to 5HT_{1A} receptor.

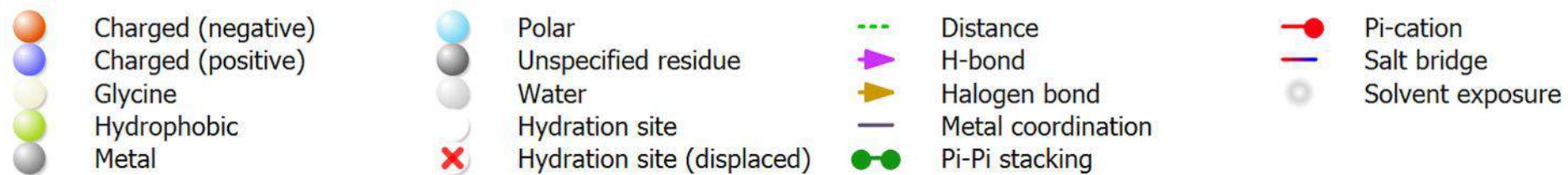
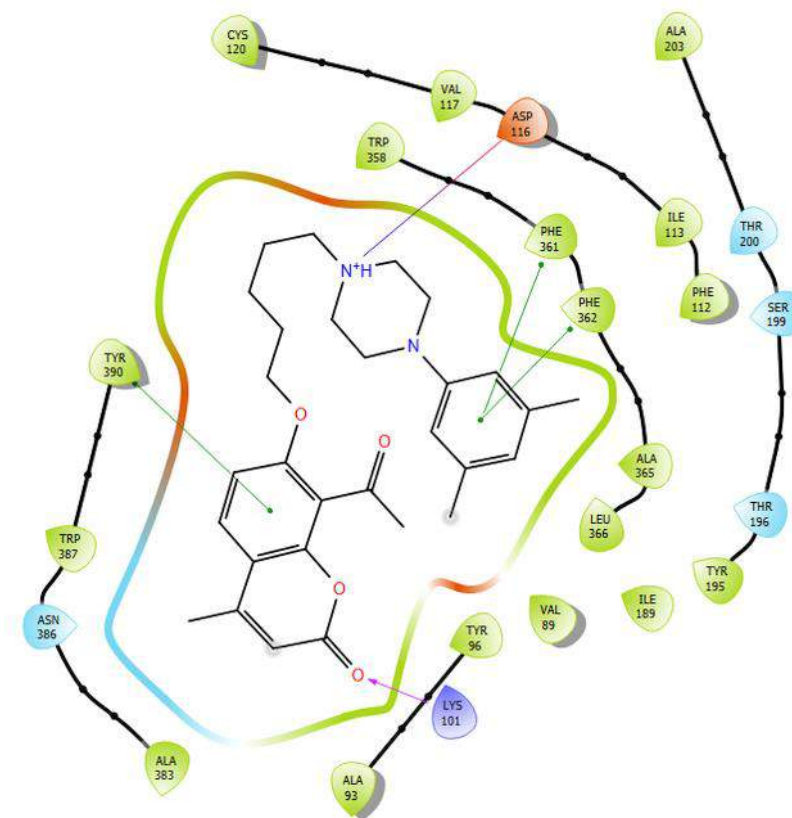


Figure S17. Ligand interaction diagram for compound **5h** docked to 5HT_{1A} receptor.

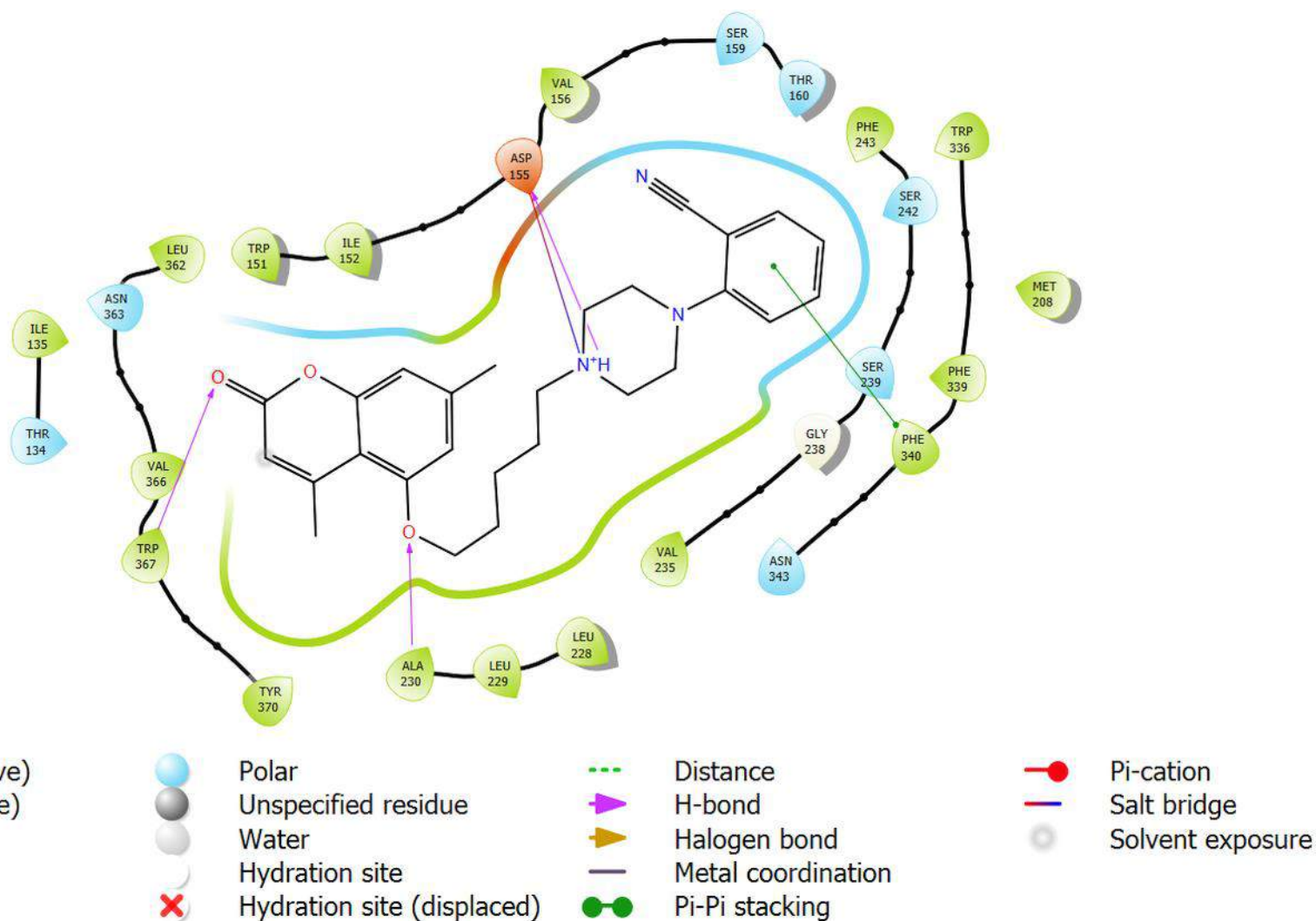


Figure S18. Ligand interaction diagram for compound **1j** docked to 5HT_{2A} receptor.

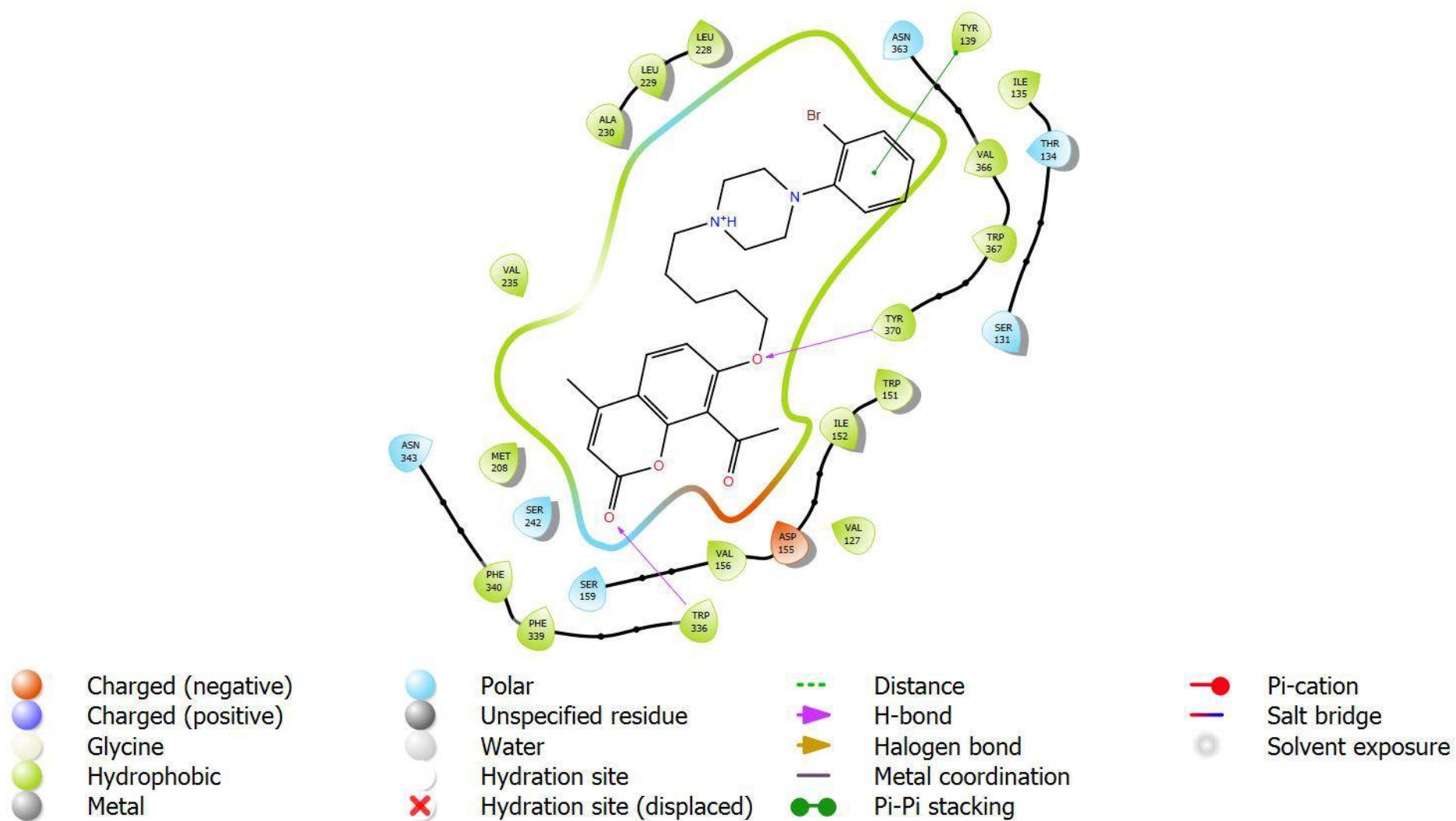


Figure S19. Ligand interaction diagram for compound **5f** docked to 5HT_{2A} receptor.

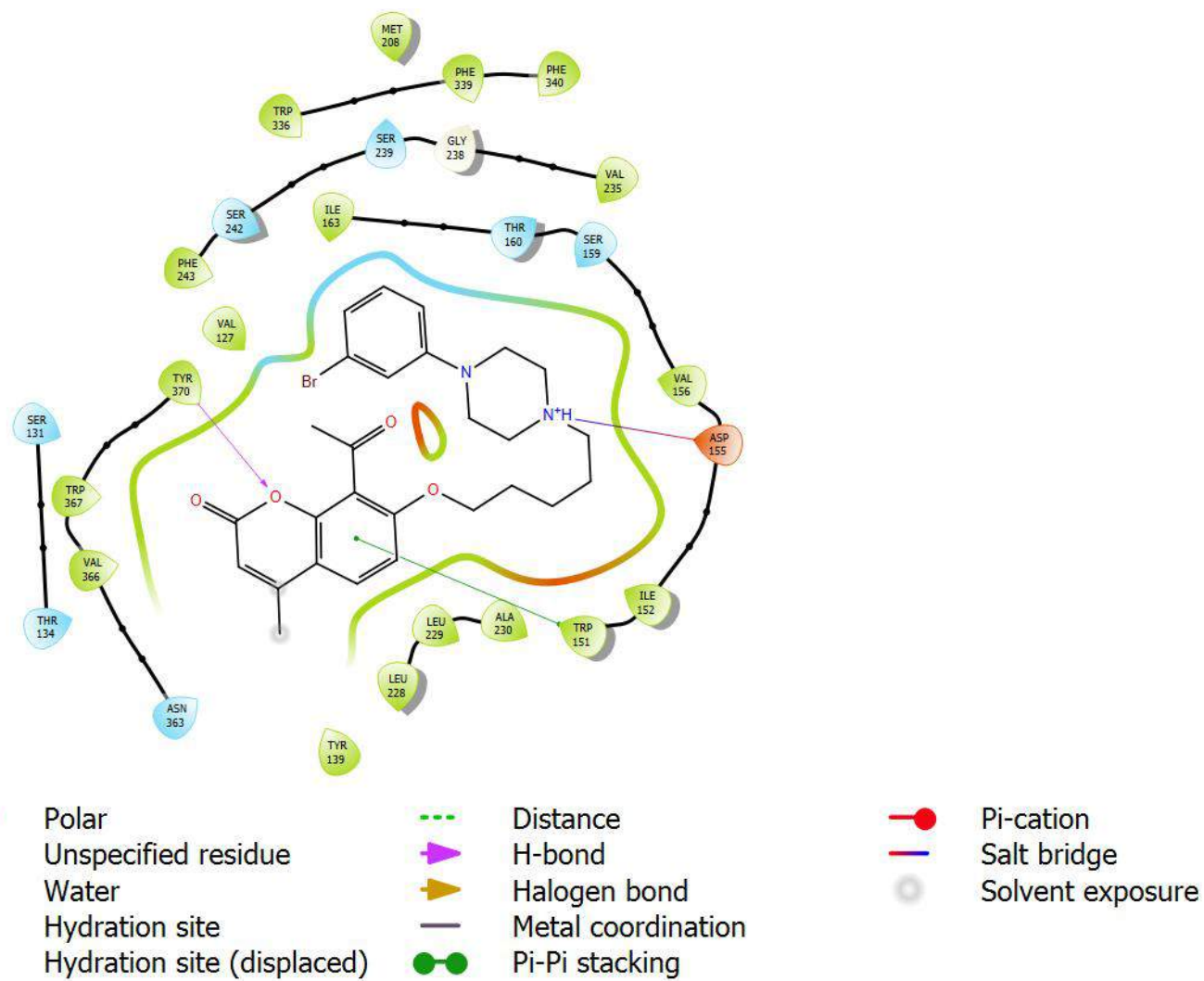


Figure S20. Ligand interaction diagram for compound **5g** docked to 5HT_{2A} receptor.

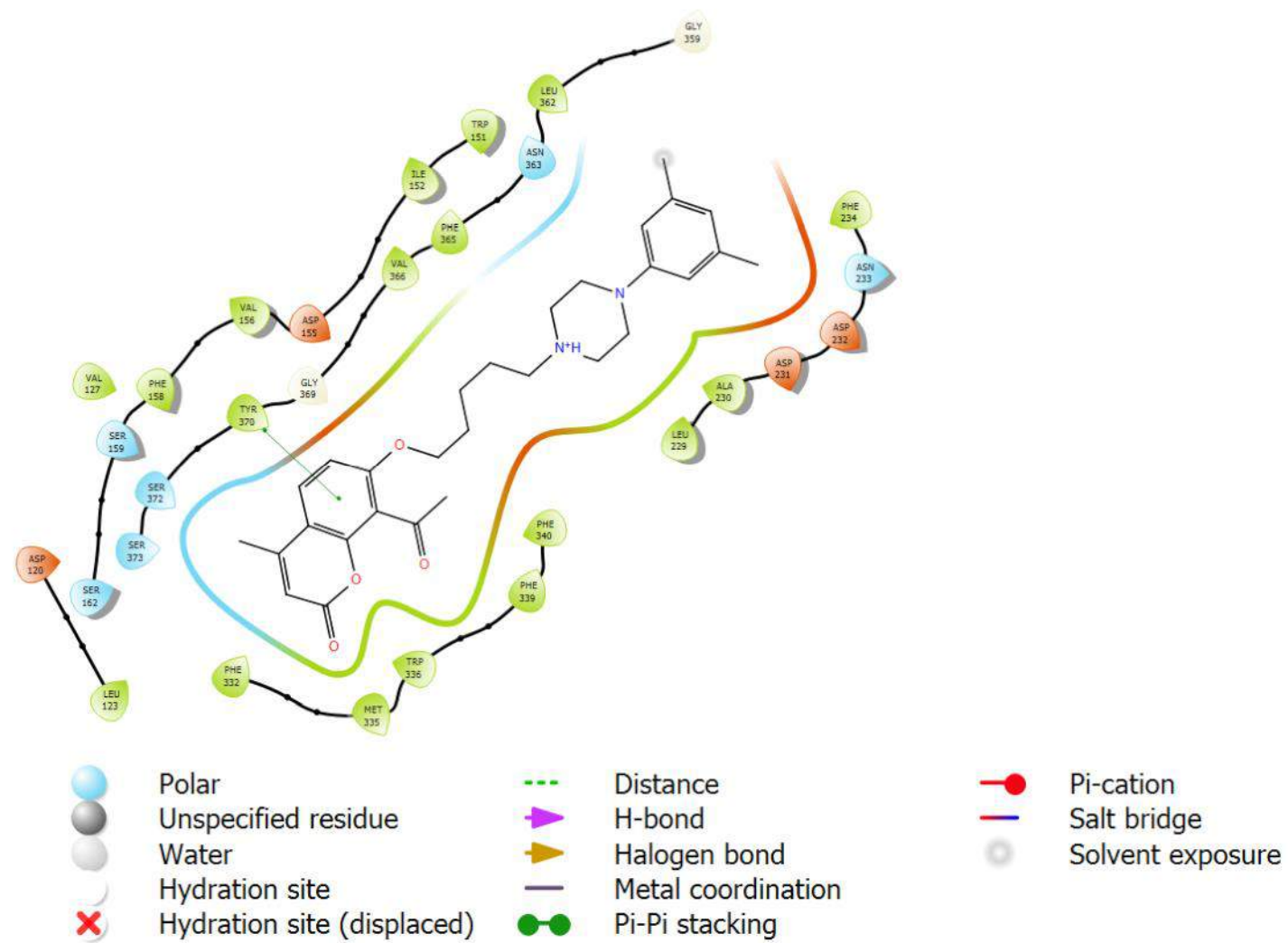


Figure S21. Ligand interaction diagram for compound **5h** docked to 5HT_{2A} receptor.