NACIONALNI FORENZIČNI LABORATORIJ
NATIONAL FORENSIC LABORATORY

Vodovodna 95
1000 Ljubljana
SLOVENIJA

T: +386 (0)1 428 44 93
E: nfl@policija.si
www.policija.si

ANALYTICAL REPORT

N-Ethyl-norpentylone

Acknowledgement

Analytically evaluated sample was kindly provided by the Forensic Science Institute (FSI) Zurich, Switzerland. NMR analyses were performed in ETH Zürich Institute of Pharmaceutical Sciences by Dr. Bernhard Pfeiffer and are enclosed in this report by the permission of Dr. Michael Bovens.

MS and FTIR measurements shown in this report were done in NFL.

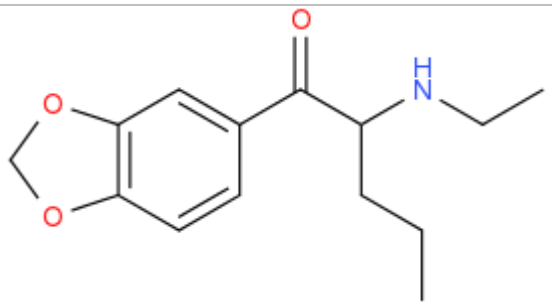
ANALYTICAL REPORT

N-Ethyl-norpentylone (C14H19NO3)

1-(2H-1,3-benzodioxol-5-yl)-2-(ethylamino)pentan-1-one

Remark – other active cpd. detected: alpha-PBP

Sample ID:	1437-16
Sample description:	powder - brown
Sample type:	collected/Kindly provided by Foresic Science Institute Zurich, Switzerland (NMR confirmed); mixture with a-PBP;
Comments[1]:	
Date of entry:	1/15/2016

Substance identified-structure[2] (base form)	
Systematic name:	1-(2H-1,3-benzodioxol-5-yl)-2-(ethylamino)pentan-1-one
Other names:	
Formula (per base form)	C14H19NO3
M_w (g/mol)	249,31
Salt form:	HCl
StdInChIKey	VERDHJIMZYXGIW-UHFFFAOYSA-N
Compound Class	Cathinones
Other active cpd. detected	alpha-PBP
Add.info (purity..)	(N-ethyl-norpentylone app. 40%) + alpha-PBP(cca 45%) + sort of sugar

[1] This report has been produced with the financial support of the Prevention of and fight against crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.

[2] Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ **DOI:** 10.1021/ci100384d

Report updates

date	comments (explanation)

Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 6,46 BP(1): 100; BP(2): 58,BP(3) :101,
FTIR-ATR	-	
GC-IR (condensed phase)	+	spectrum consistent by the one obtained in FSI Zurich (QM>0.98)

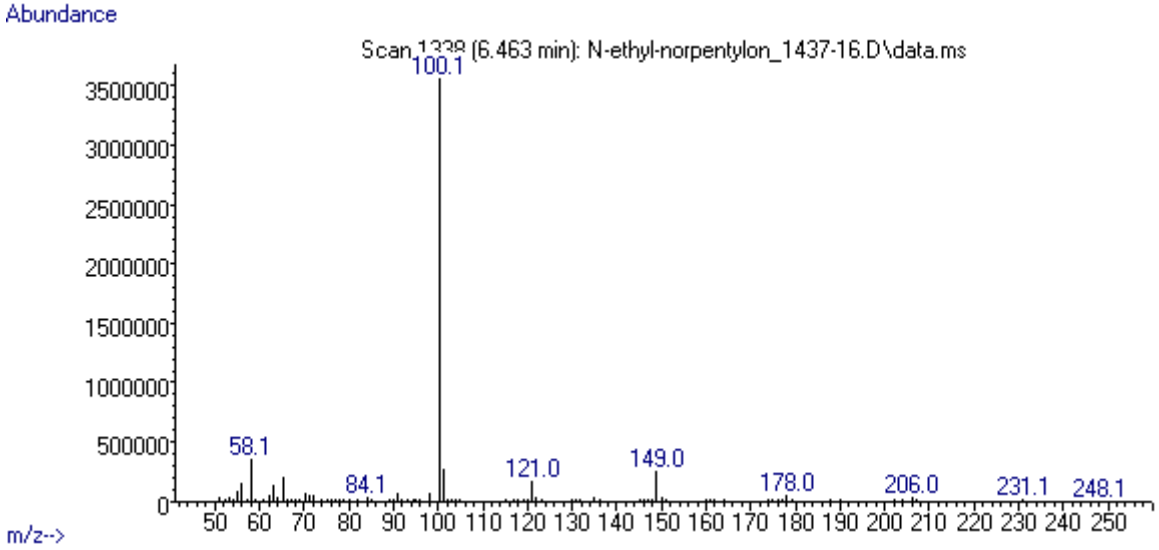
GC-MS (Agilent):
GC-method is RT locked to tetracosane (RT=9.53 min).
Injection volume 1 ml and split mode (1:50) .
Injector temperature: 280 ^{0}C.
Chromatographic separation
Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 293 ^{0}C at a rate of 18 ^{0}C/min, hold for 6.1 min, than heating at 50 ^{0}C/min up to 325 ^{0}C and finally 2.8 min isothermal.
MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

FTIR-ATR (Perkin Elmer): scan range 4000-400 cm-1; resolution 4cm-1

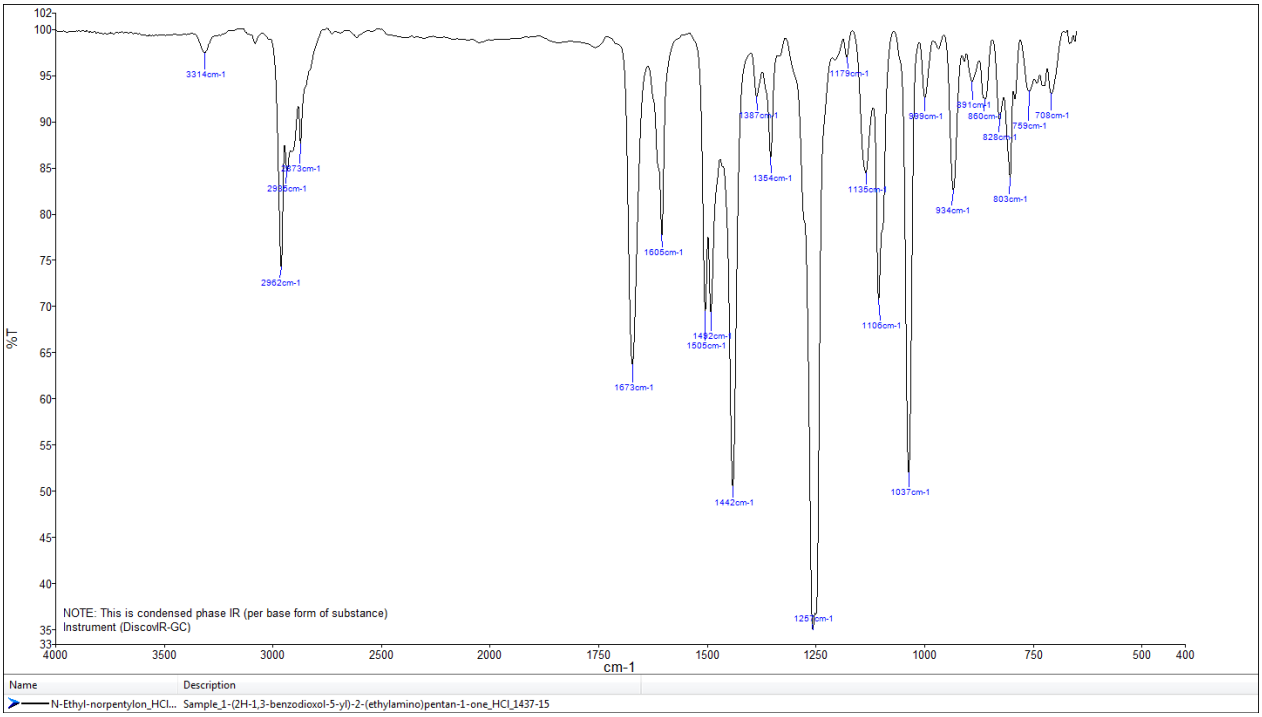
GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm-1
GC-method:
Injection volume 1 ml and split mode (1:5) .
Injector temperature: 280 ^{0}C.
Chromatographic separation
Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 293 ^{0}C at a rate of 18 ^{0}C/min, hold for 6.1 min, than heating at 50 ^{0}C/min up to 325 ^{0}C and finally 2.8 min isothermal.
Split MS : IR : (1:9)
MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.
IR (condesed phase): IR scan range 4000 to 700, resolution 4cm-1

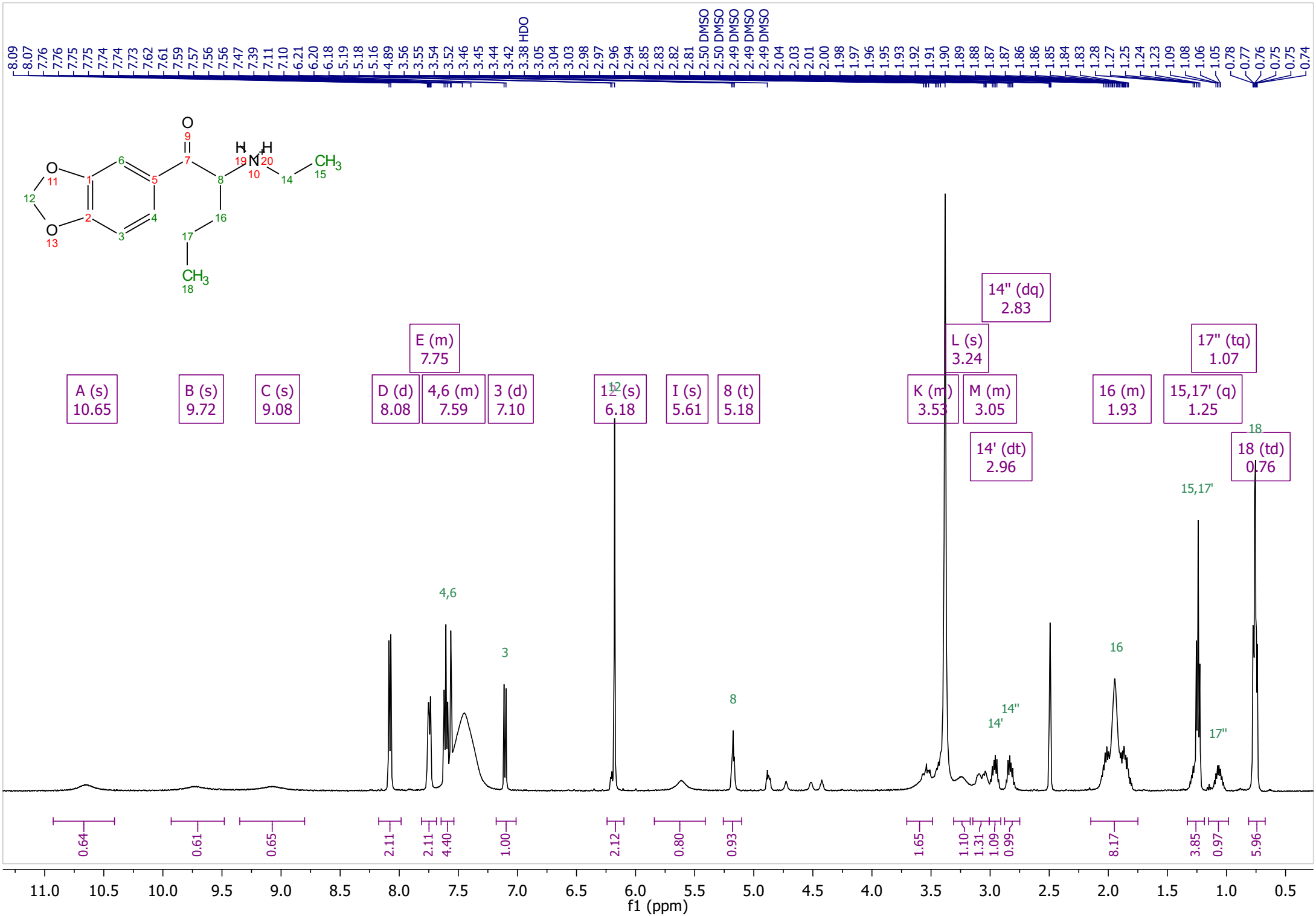
FIGURES OF SPECTRA

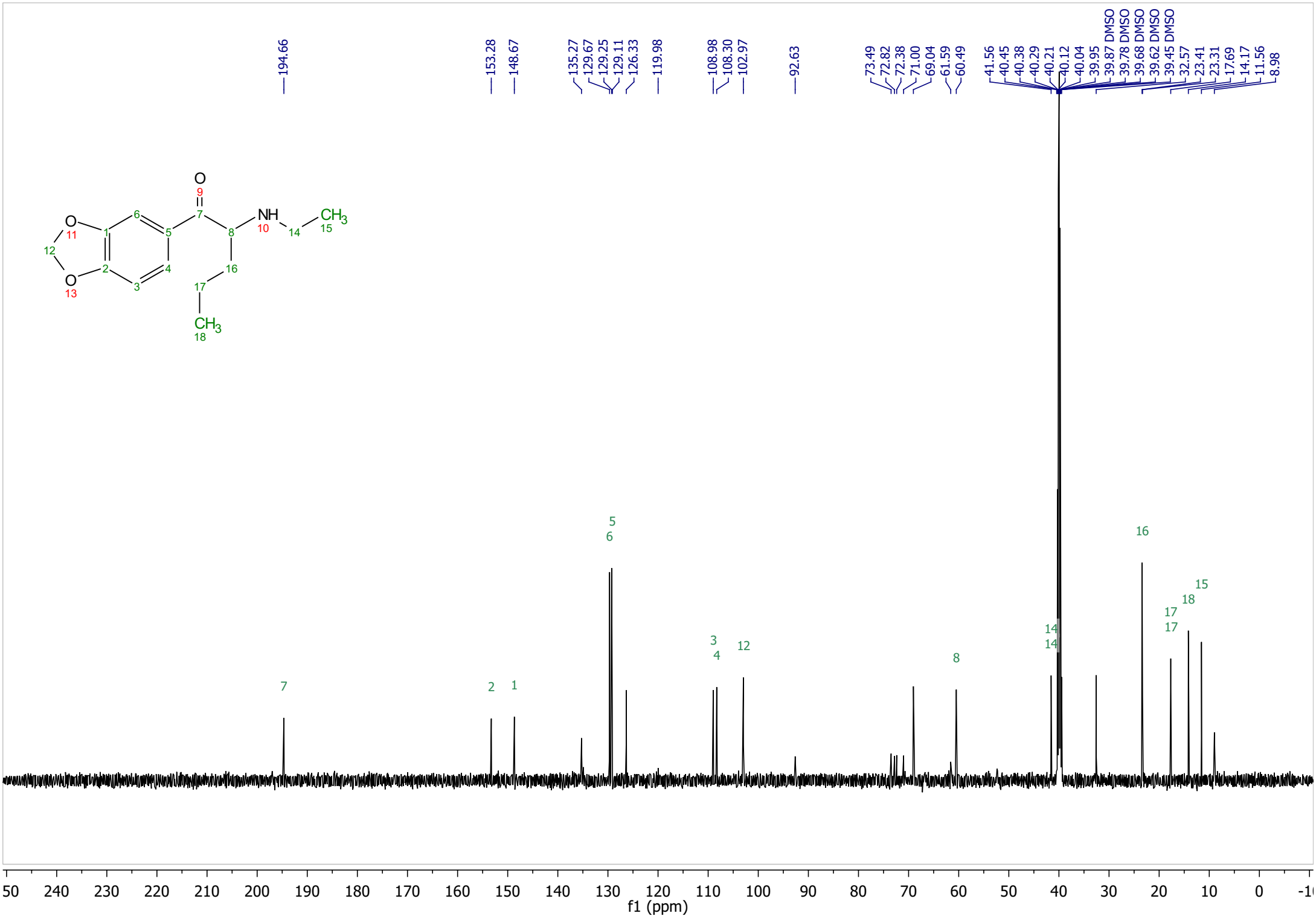
MS (EI)

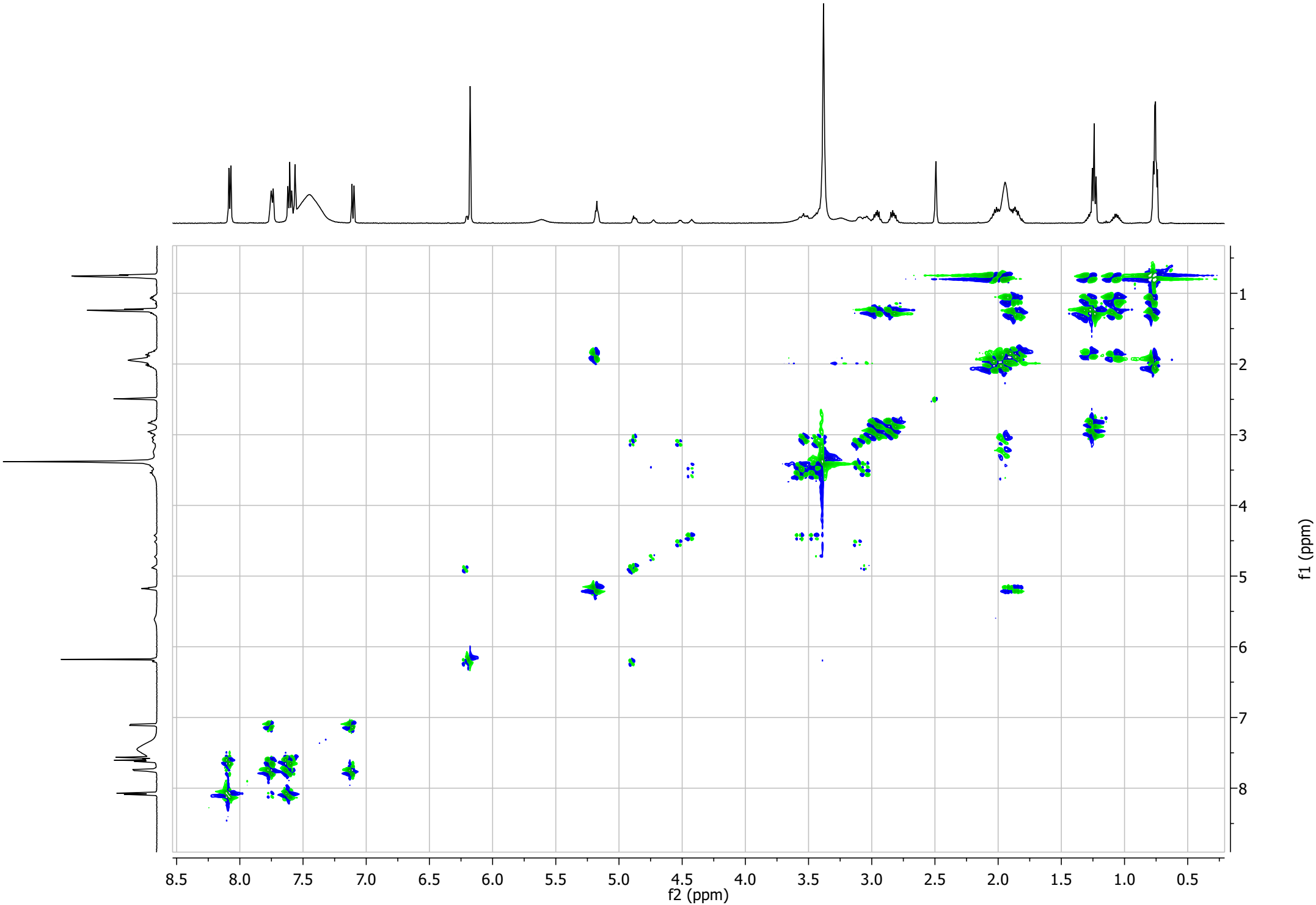


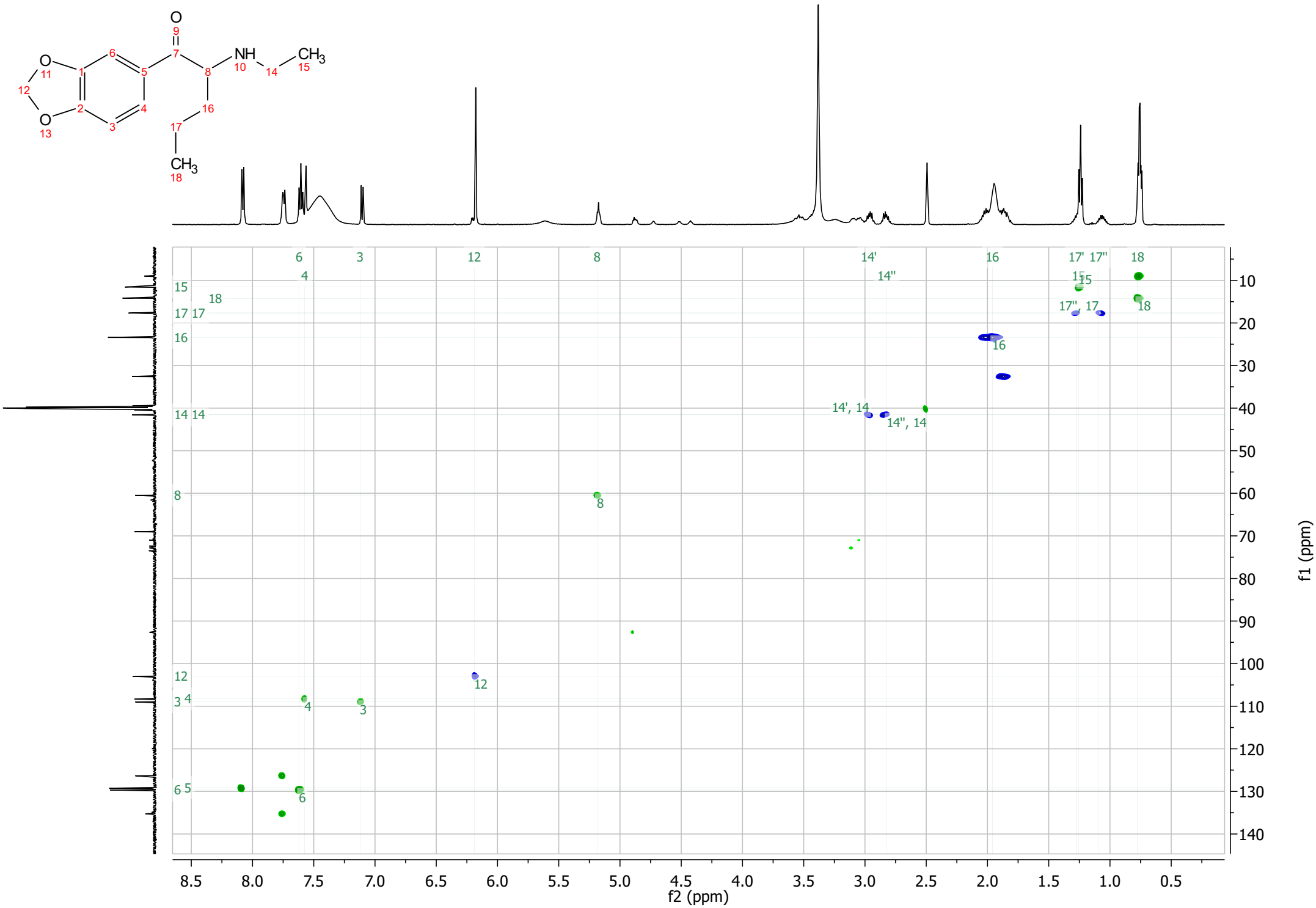
IR-Condensed phase

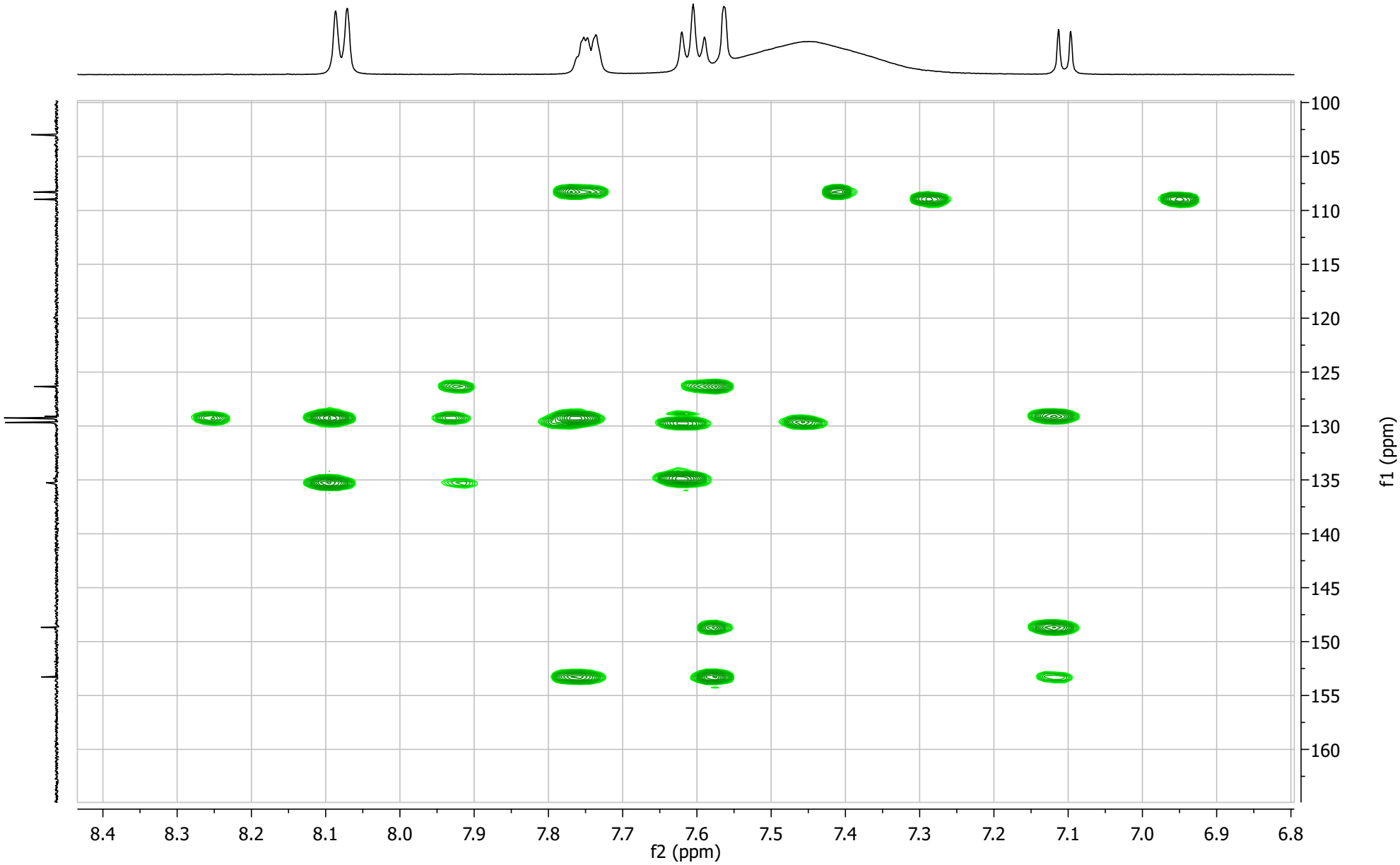


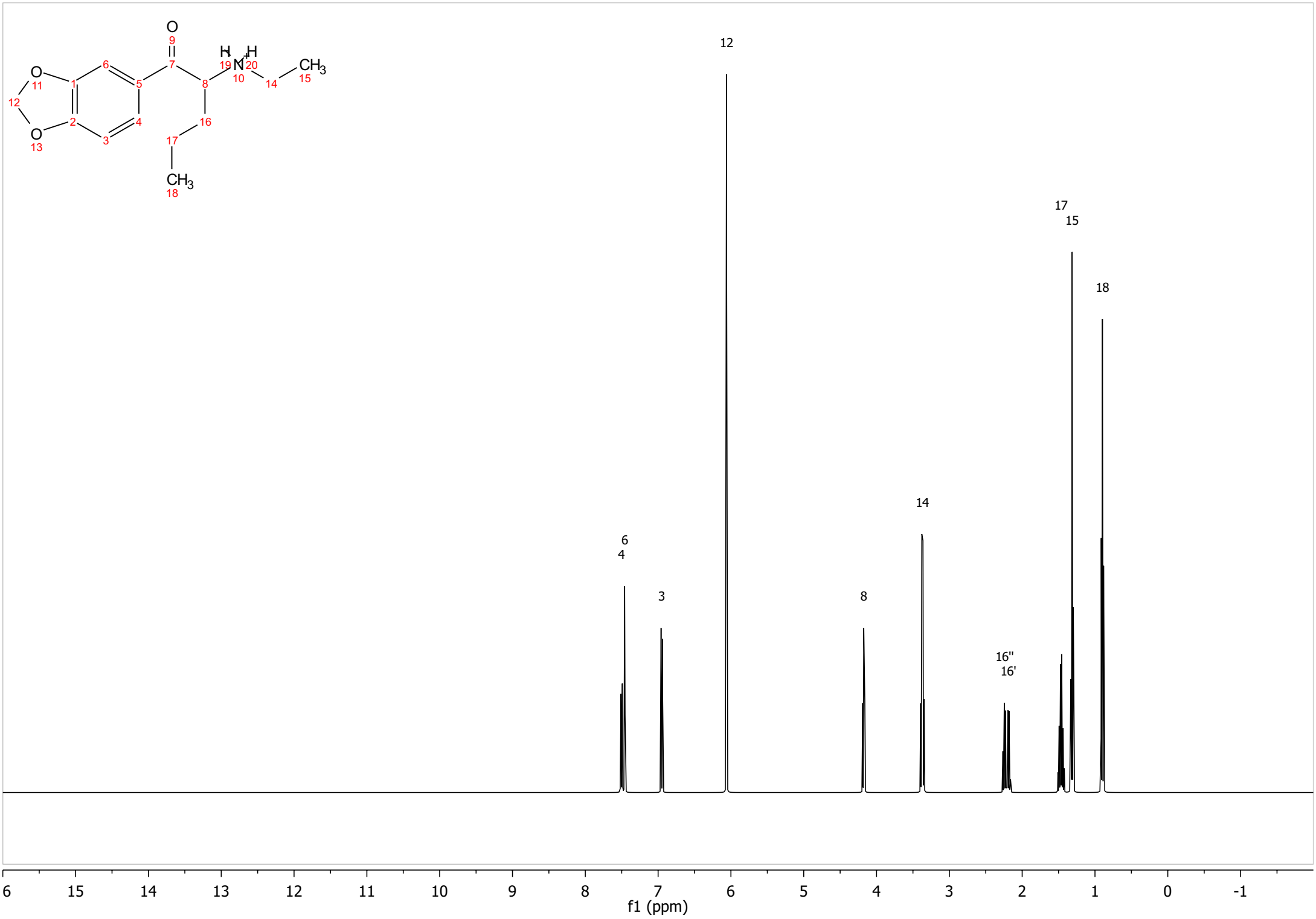

8.09 8.07 7.76 7.76 7.75 7.75 7.74 7.74 7.73 7.62 7.61 7.59 7.57 7.56 7.56 7.47 7.39 7.11 7.10 6.21 6.20 6.18 5.19 5.18 5.16 4.89 3.56 3.55 3.54 3.52 3.46 3.45 3.44 3.42 3.38 HDO 3.05 3.04 3.03 2.98 2.97 2.96 2.94 2.85 2.83 2.82 2.81 2.50 DMSO 2.50 DMSO 2.49 DMSO 2.49 DMSO 2.49 DMSO 2.04 2.03 2.01 2.00 1.98 1.97 1.96 1.95 1.93 1.92 1.91 1.90 1.89 1.88 1.87 1.87 1.86 1.86 1.85 1.84 1.83 1.28 1.27 1.25 1.24 1.23 1.09 1.08 1.06 1.05 0.78 0.77 0.76 0.75 0.75 0.74
A (s) 10.65
B (s) 9.72
C (s) 9.08
D (d) 8.08
E (m) 7.75
4,6 (m) 7.59
3 (d) 7.10
12 (s) 6.18
I (s) 5.61
8 (t) 5.18
K (m) 3.53
L (s) 3.24
M (m) 3.05
14" (dq) 2.83
14' (dt) 2.96
16 (m) 1.93
15,17' (q) 1.25
17" (tq) 1.07
18 (td) 0.76
4,6
3
8
14'
14"
16
15,17'
17"
18
0.64
0.61
0.65
2.11
2.11
4.40
1.00
2.12
0.80
0.93
1.65
1.10
1.31
1.09
0.99
8.17
3.85
0.97
5.96
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

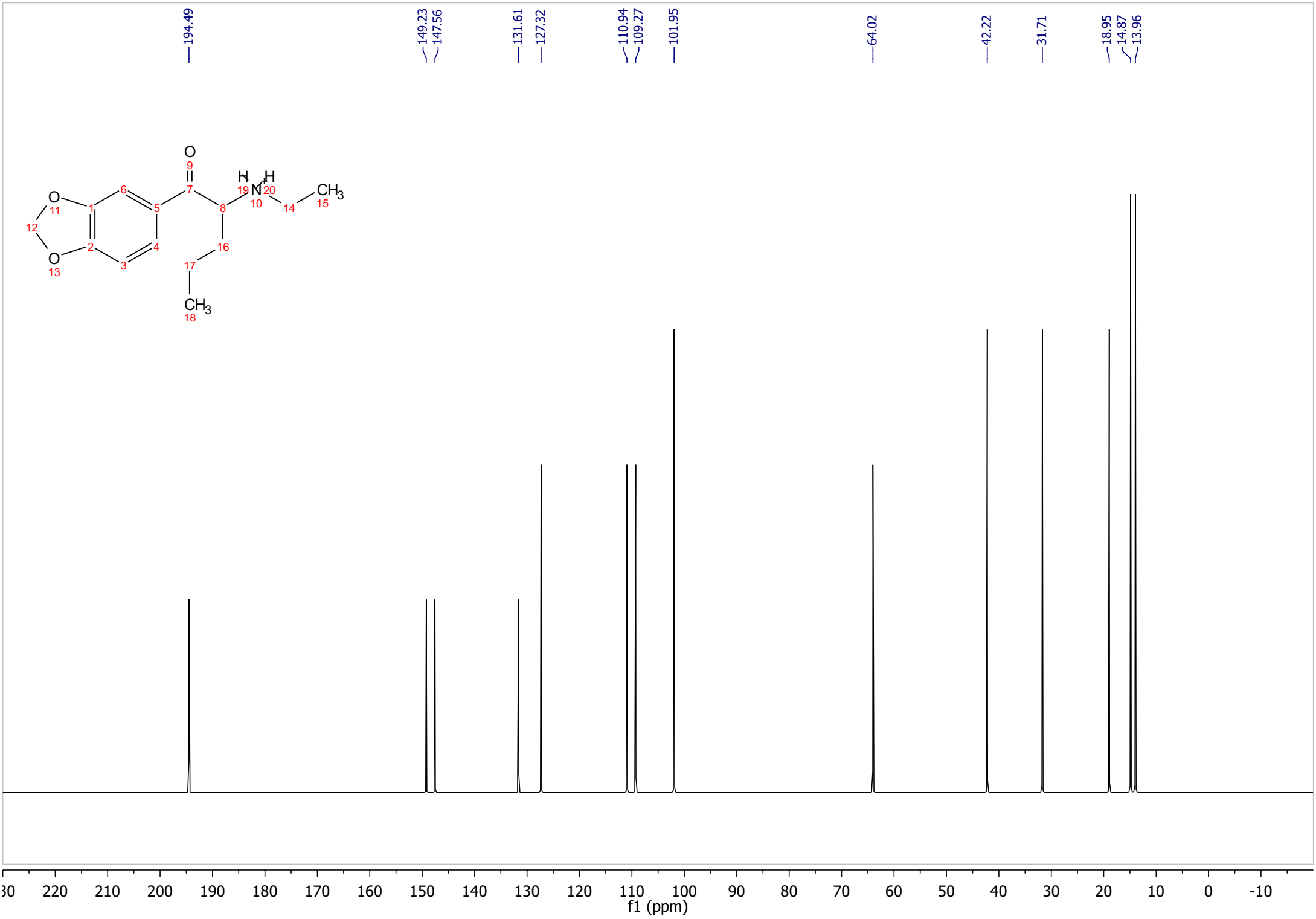

194.66
153.28
148.67
135.27
129.67
129.25
129.11
126.33
119.98
108.98
108.30
102.97
92.63
73.49
72.82
72.38
71.00
69.04
61.59
60.49
41.56
40.45
40.38
40.29
40.21
40.12
40.04
39.95
39.87 DMSO
39.78 DMSO
39.68 DMSO
39.62 DMSO
39.45 DMSO
32.57
23.41
23.31
17.69
14.17
11.56
8.98
O
9
O
11
NH
10
CH3
15
14
12
O
13
CH3
18
17
16
7
2
1
5
6
3
4
12
8
14
14
16
17
17
18
15
50 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

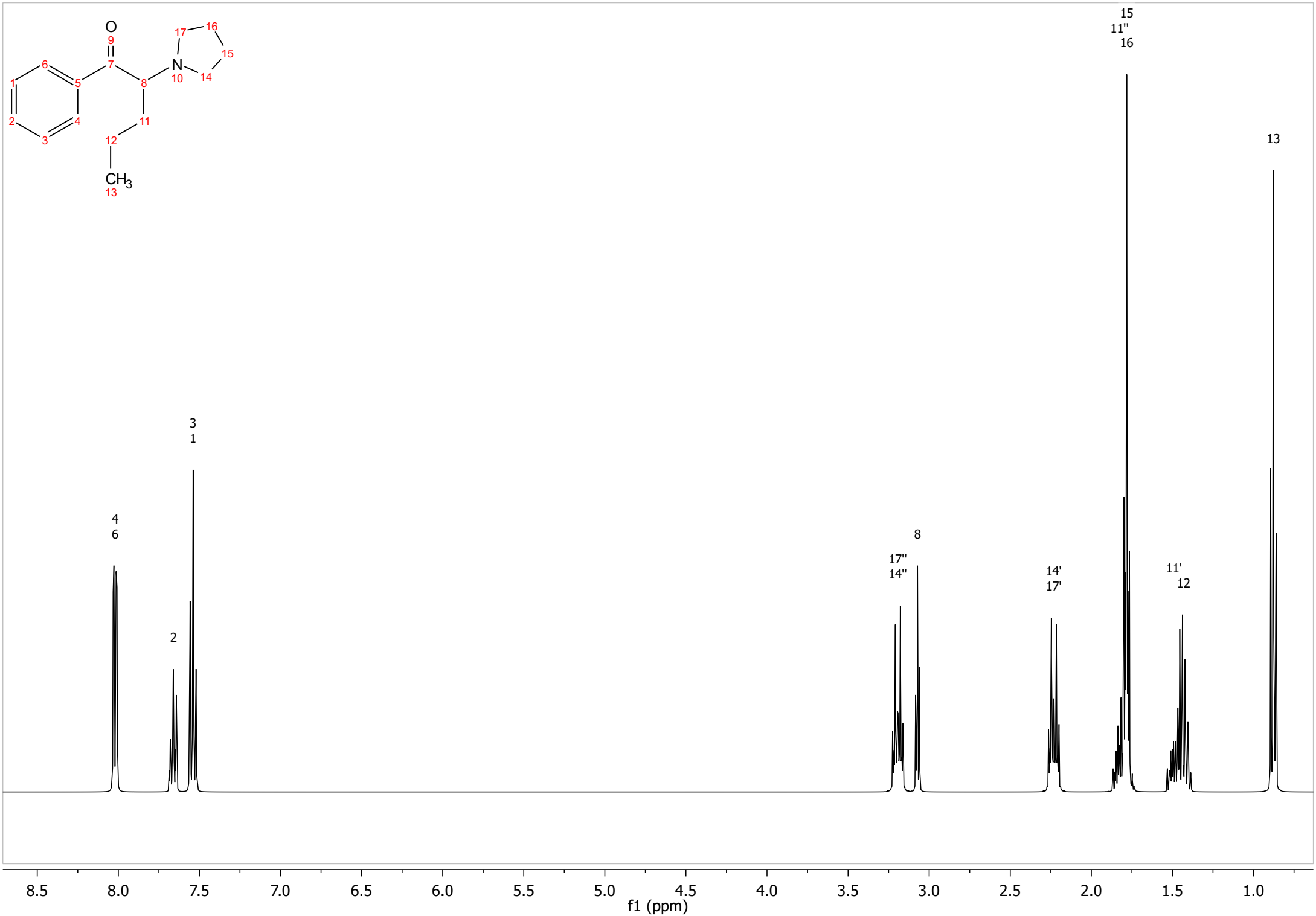

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)
1
2
3
4
5
6
7
8
f1 (ppm)

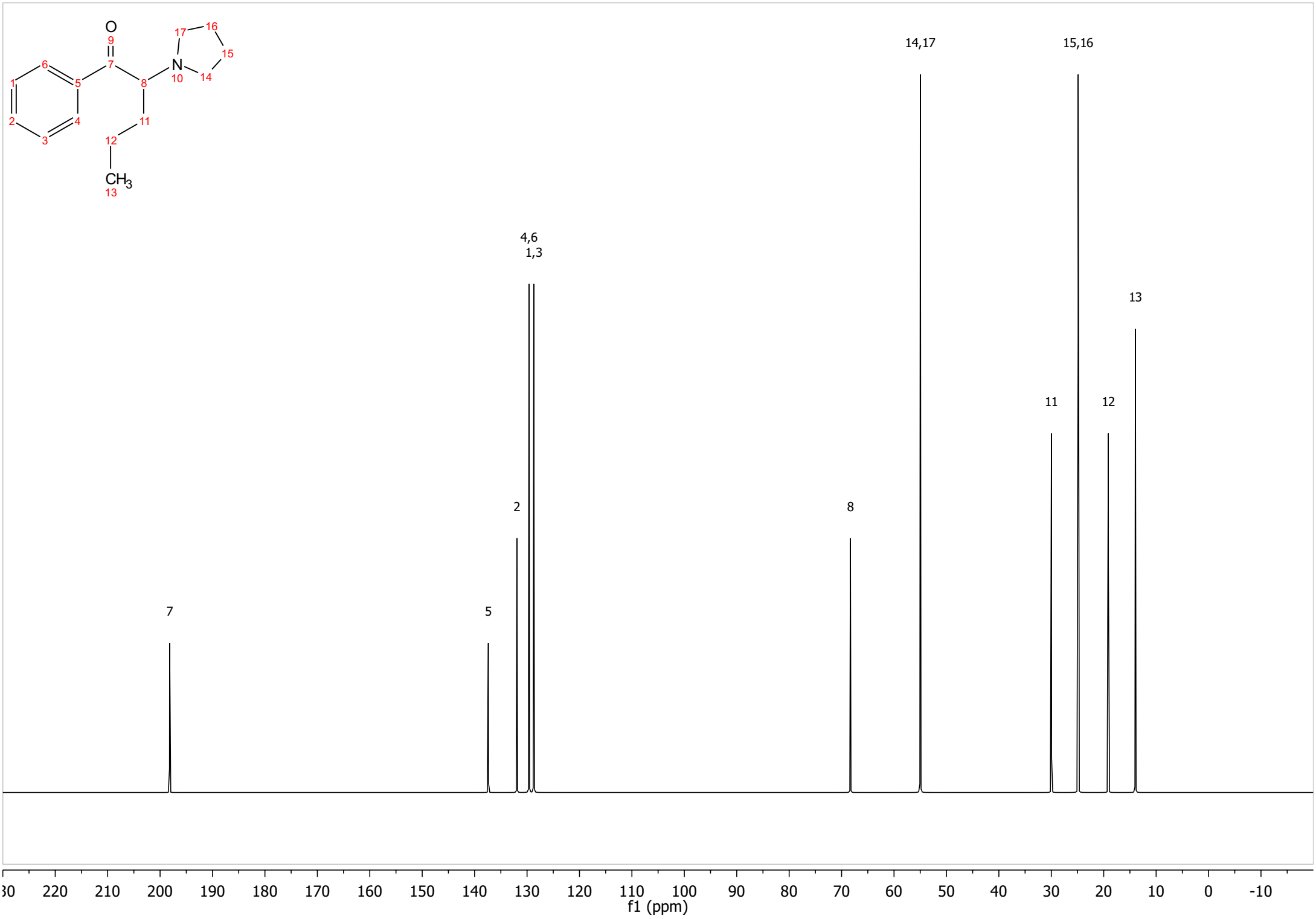

O
9
O
11
1
6
5
7
8
NH
10
14
CH3
15
12
2
4
16
O
13
3
17
CH3
18
6
4
3
12
8
14'
14''
16
17'
17''
18
15
18
17
17
16
14
14
8
12
3
4
6
5
14', 14
14'', 14
17'', 17
f2 (ppm)
f1 (ppm)


8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f2 (ppm)
100
105
110
115
120
125
130
135
140
145
150
155
160
f1 (ppm)


O
9
H
19
N
10
H
20
CH3
15
14
O
11
1
6
5
7
8
12
2
4
16
O
13
3
17
CH3
18
12
6
4
3
8
14
16"
16'
17
15
18
6
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


194.49
149.23
147.56
131.61
127.32
110.94
109.27
101.95
64.02
42.22
31.71
18.95
14.87
13.96
O
9
H
19
N
10
H
20
CH3
15
14
O
11
1
6
5
7
8
12
2
4
16
O
13
3
17
CH3
18
f1 (ppm)


O
9
17
16
15
6
7
N
10
14
1
5
8
2
4
11
3
12
CH3
13
15
11''
16
13
3
1
4
6
8
2
17''
14''
14'
17'
11'
12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)


O
9
17
16
15
6
7
N
10
14
1
5
8
2
4
11
3
12
CH3
13
14,17
15,16
4,6
1,3
13
11
12
2
8
7
5
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)