



ANALYTICAL REPORT
3-MeO-PCMo (C₁₇H₂₅N₂O₂)

Acknowledgement

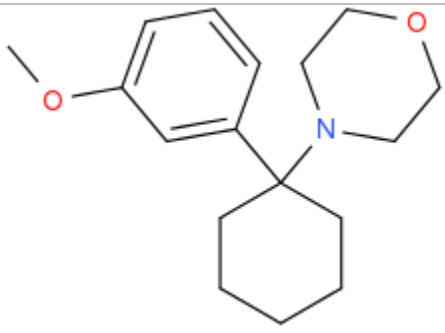
Analytically evaluated sample was kindly provided by the Forensic Science Institute (FSI) Zurich, Switzerland. NMR analyses were performed in ETH Zürich Institute of Pharmaceutical Sciences by Dr. Bernhard Pfeiffer and are enclosed in this report by the permission of Dr. Michael Bovens.

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

ANALYTICAL REPORT
3-MeO-PCMo (C₁₇H₂₅N₂O₂)
4-[1-(3-methoxyphenyl)cyclohexyl]morpholine

Remark – other active cpd. detected: **none**

Sample ID:	1431-16
Sample description:	crystallinic - white
Sample type:	collected/Kindly provided by Forensic Science Institute Zurich, Switzerland (NMR confirmed);
Comments ¹ :	
Date of entry:	1/15/2016

Substance identified-structure ² (base form)	
Systematic name:	4-[1-(3-methoxyphenyl)cyclohexyl]morpholine
Other names:	
Formula (per base form)	C ₁₇ H ₂₅ N ₂ O ₂
M _w (g/mol)	275,39
Salt form:	base
StdInChIKey	BOGOEDFWPOXWQE-UHFFFAOYSA-N
Compound Class	Arylcyclohexylamines
Other active cpd. detected	none
Add.info (purity..)	>98%

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): 8,17 BP(1): 232; BP(2): 121,BP(3) :275,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	

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 °C.

Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.

Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.

MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°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 °C.

Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.

Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.

Split MS : IR : (1:9)

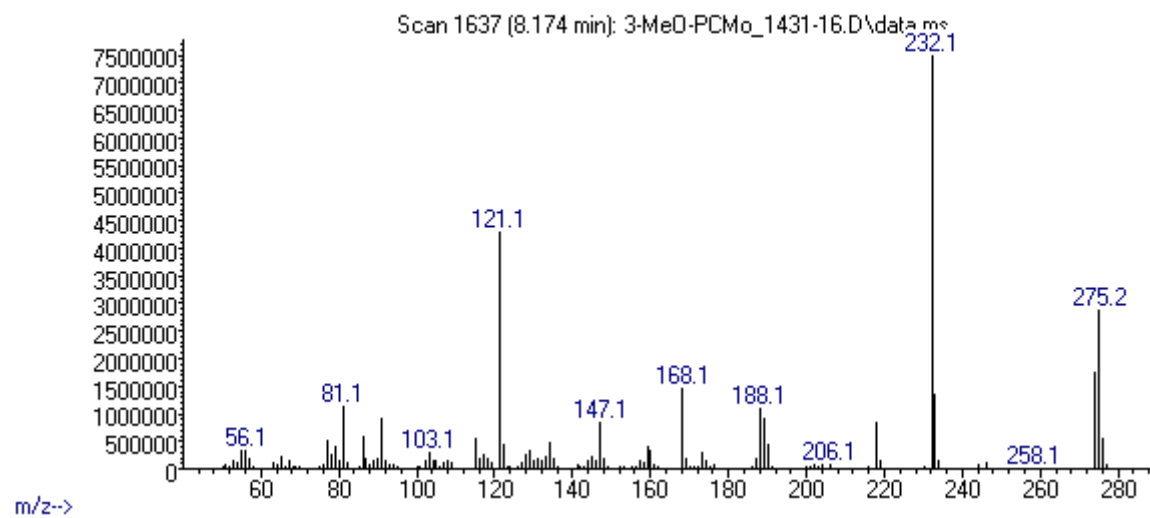
MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

IR (condensed phase): IR scan range 4000 to 700, resolution 4cm⁻¹

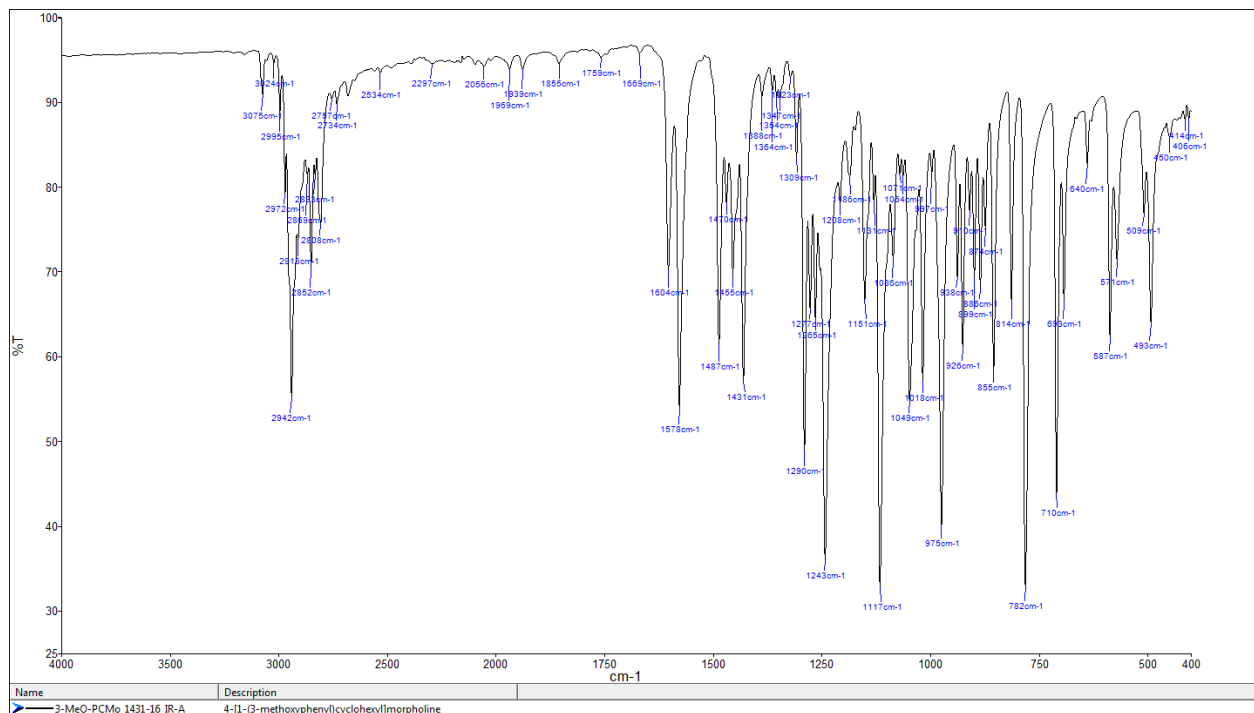
FIGURES OF SPECTRA

MS (EI)

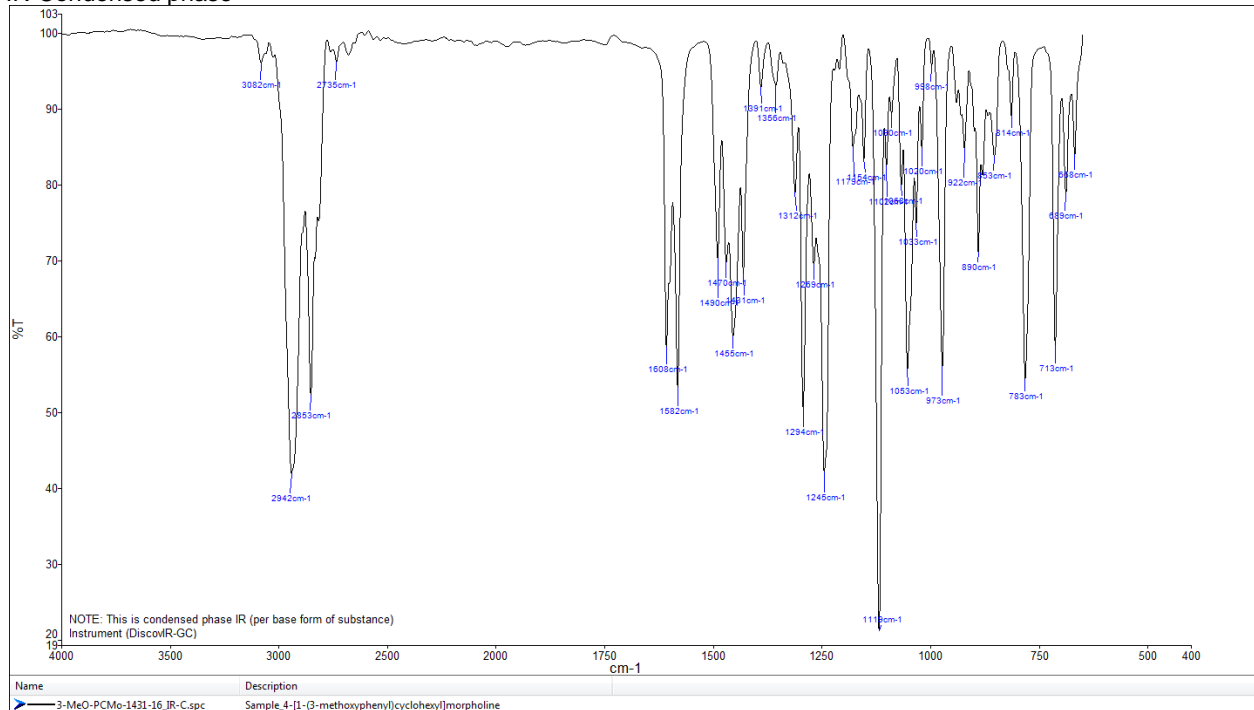
Abundance



FTIR-ATR

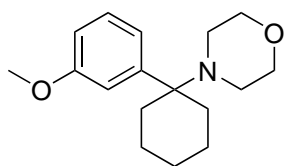


IR-Condensed phase



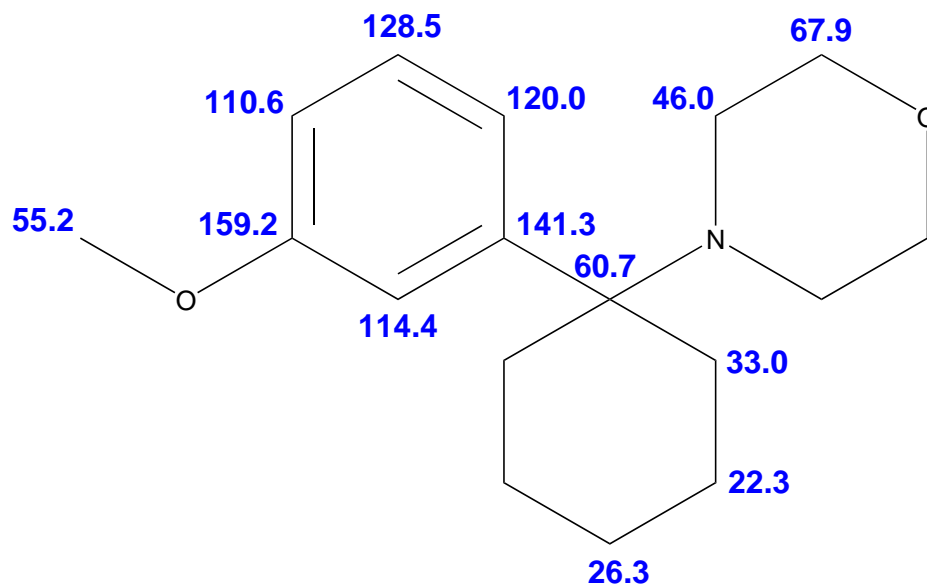
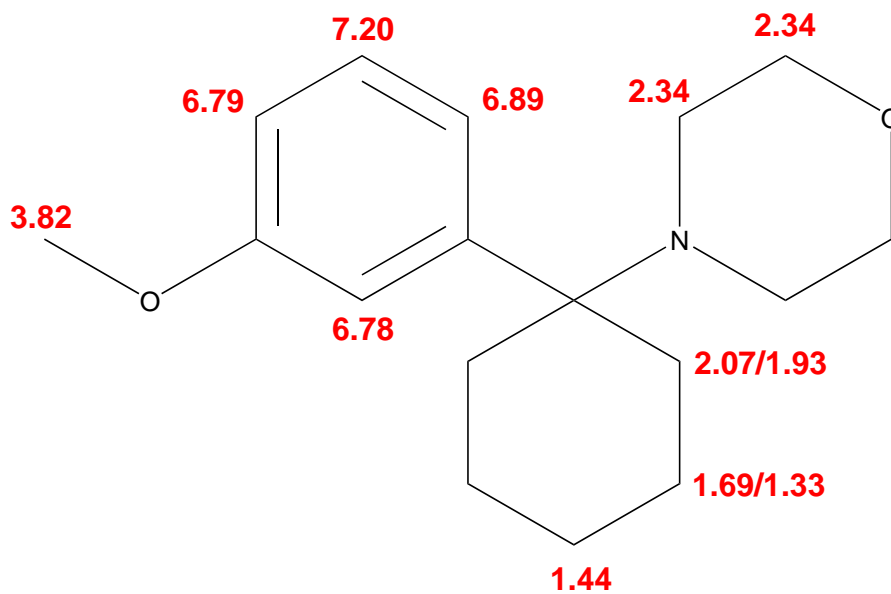
END OF NFL data.

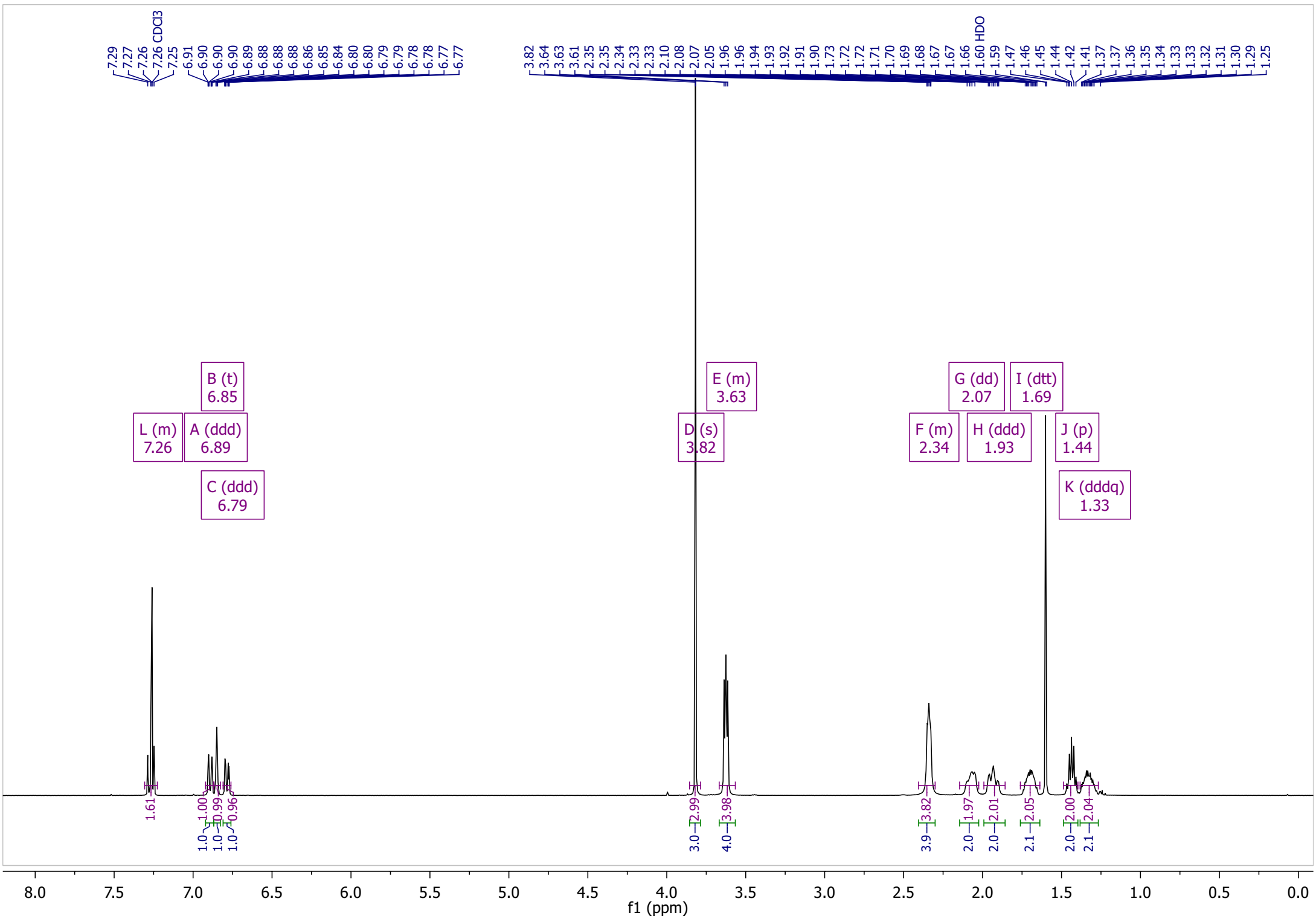
3-MeO-PCMo

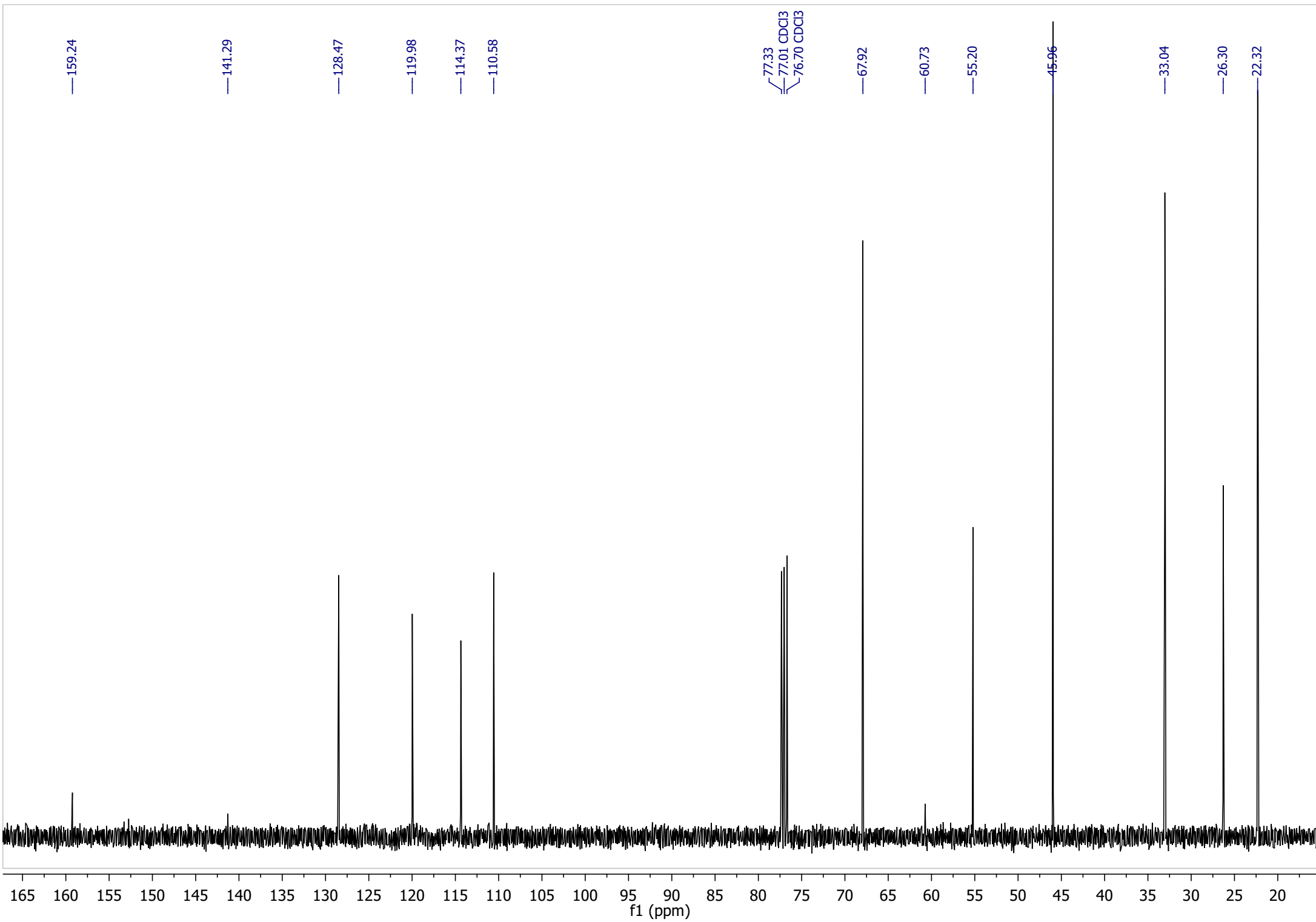


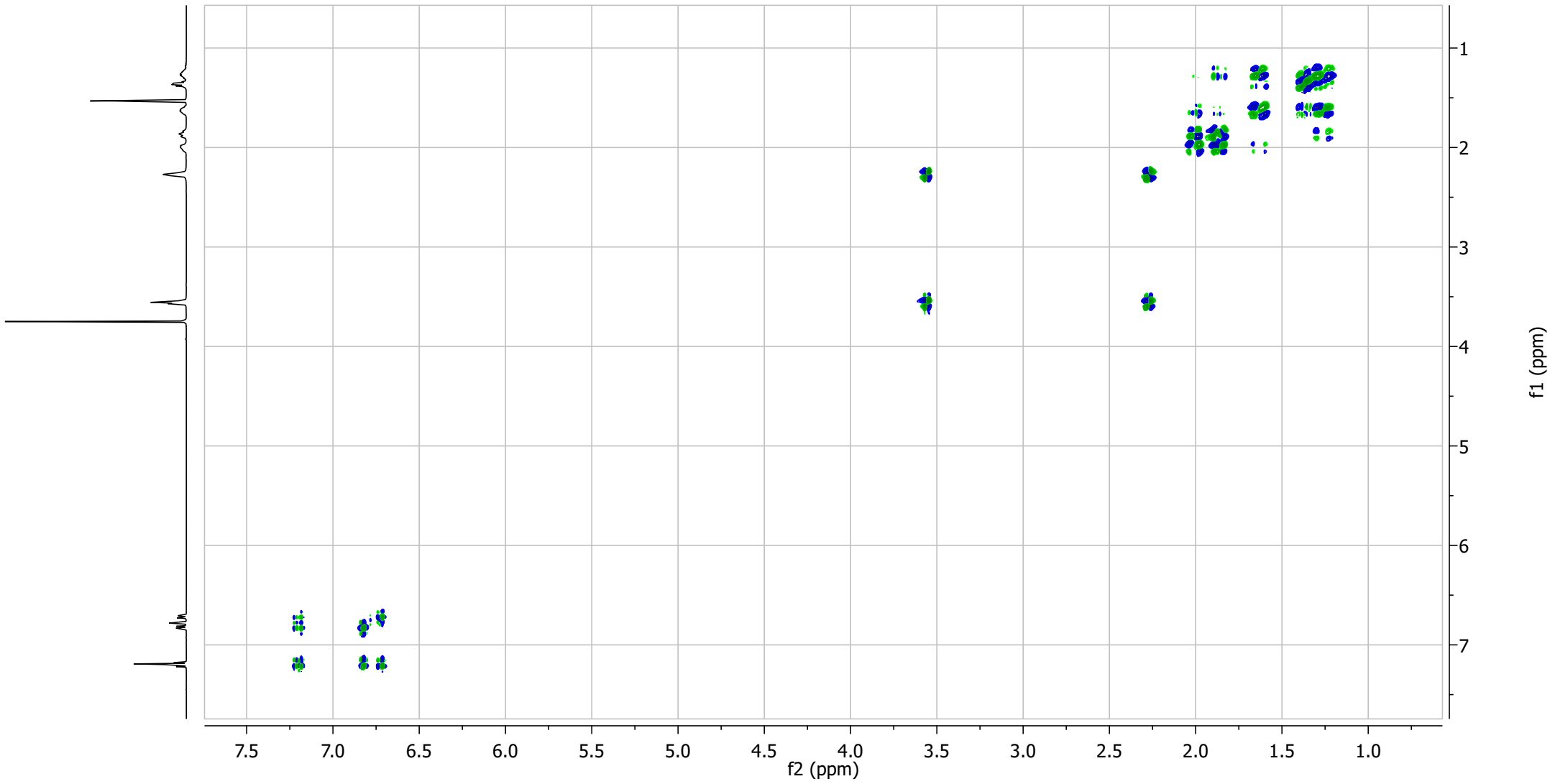
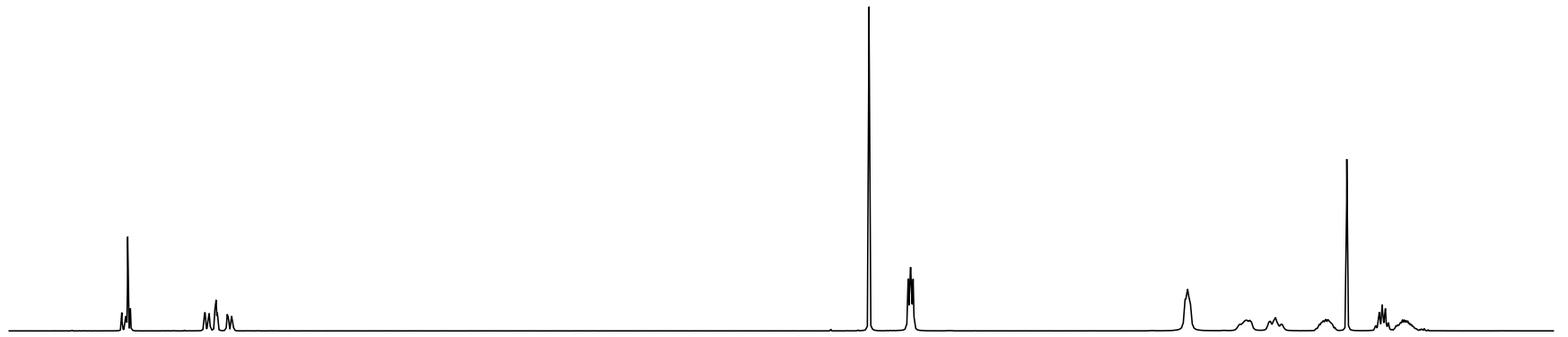
ESI-MS: 276.4 [M+H⁺] (100%)

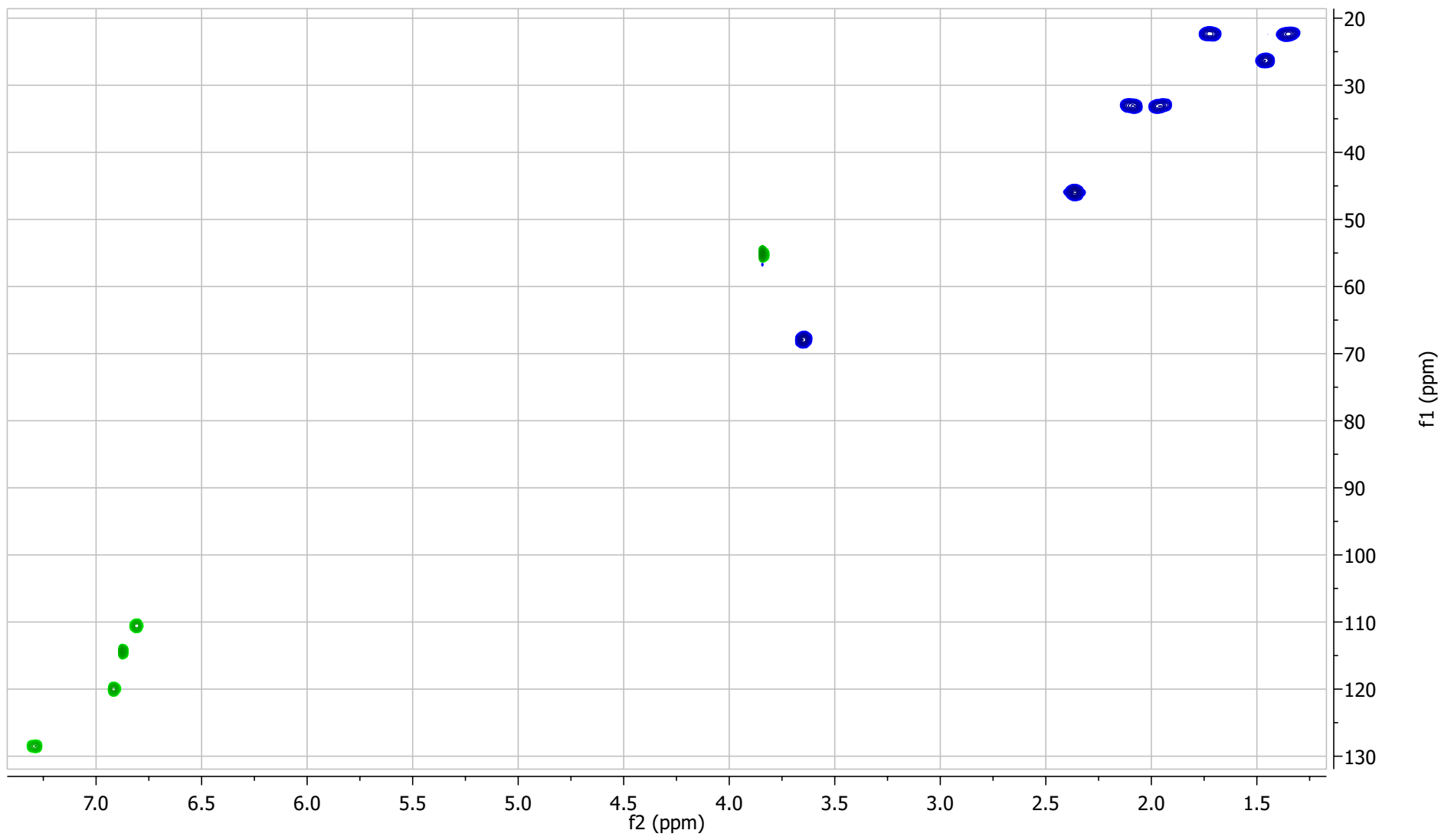
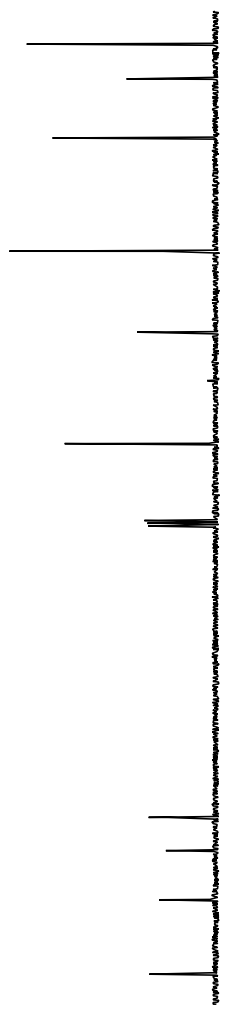
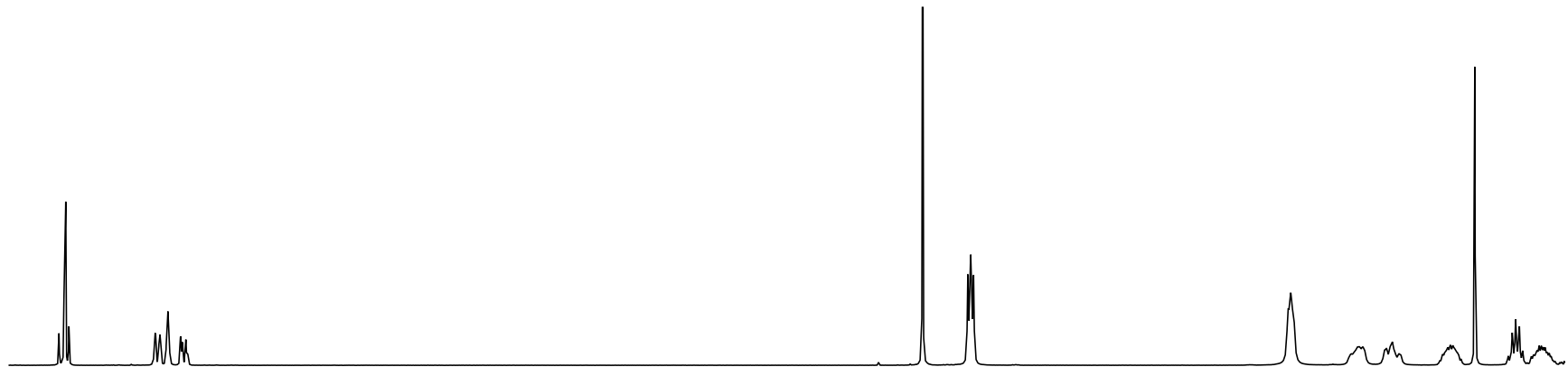
Chemical Formula: C₁₇H₂₅NO₂
Exact Mass: 275.1885

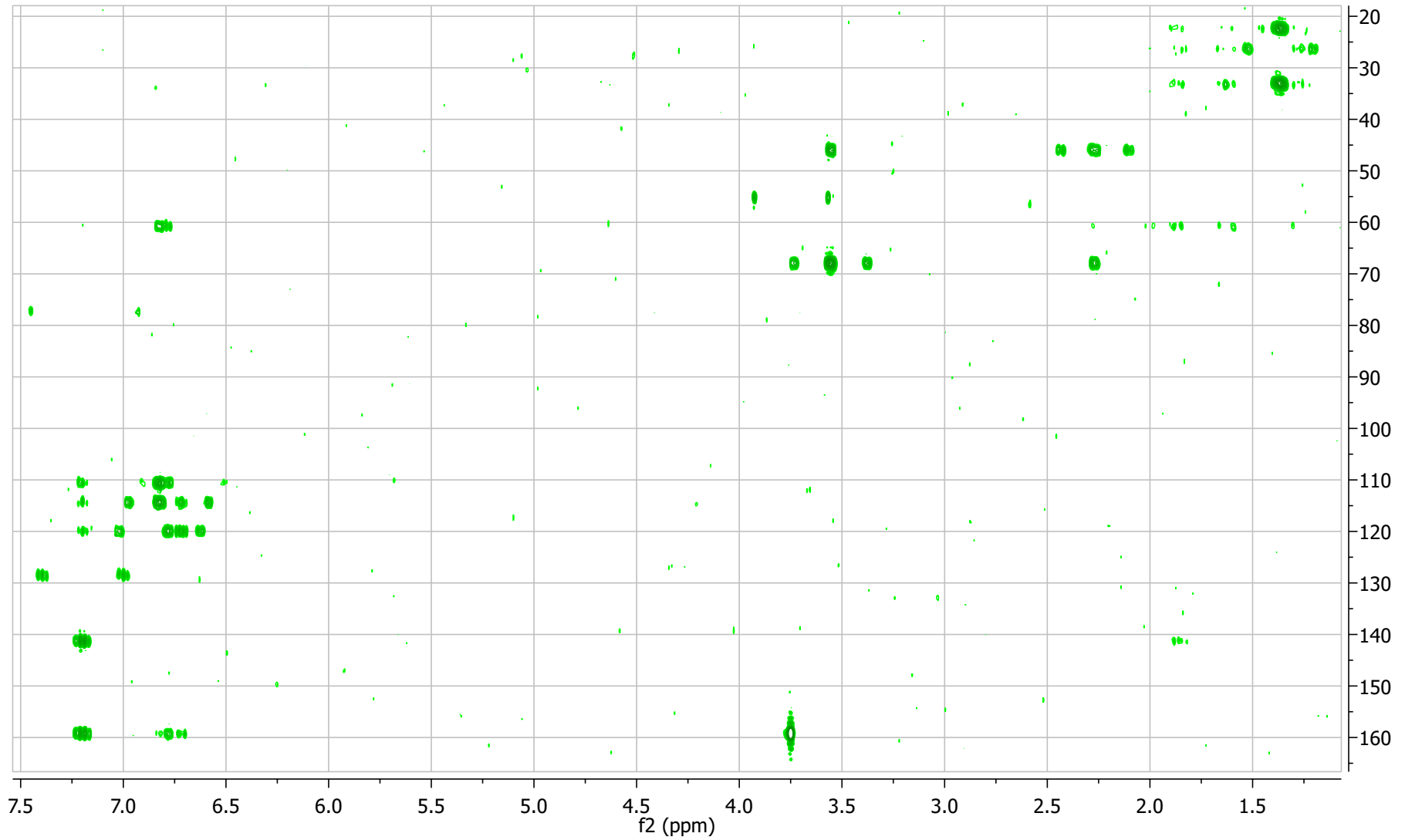
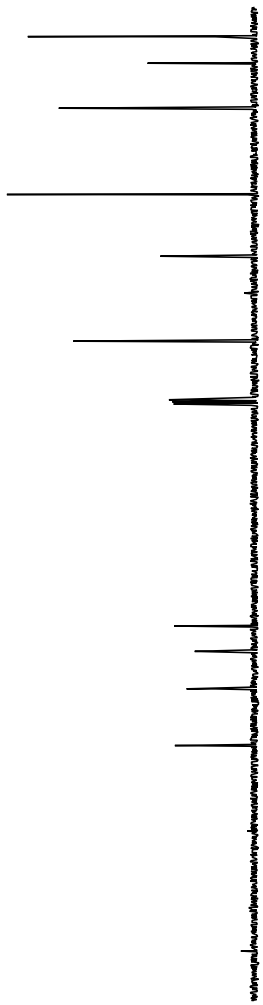
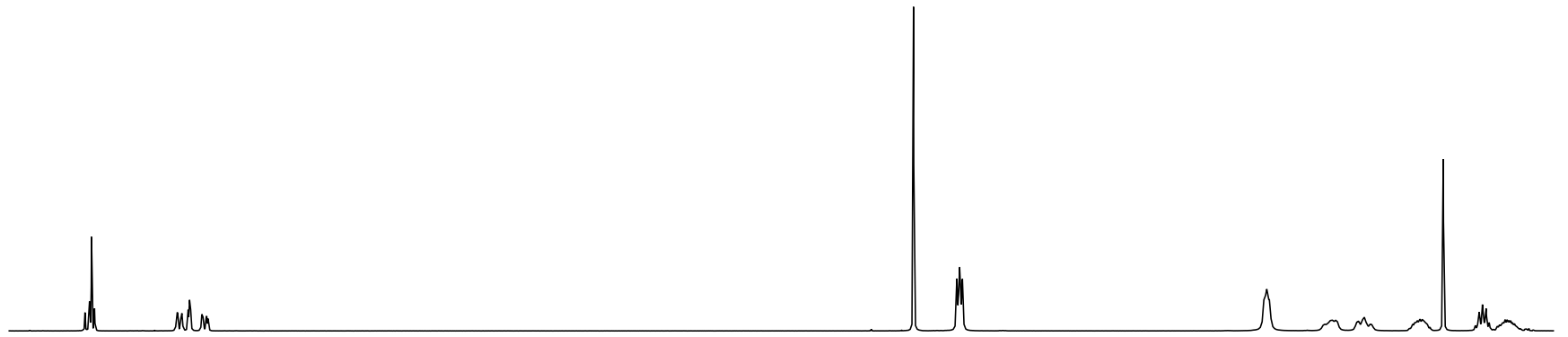












f1 (ppm)

f2 (ppm)

Sample: 1
File: Benny41-1_20150909
Description:

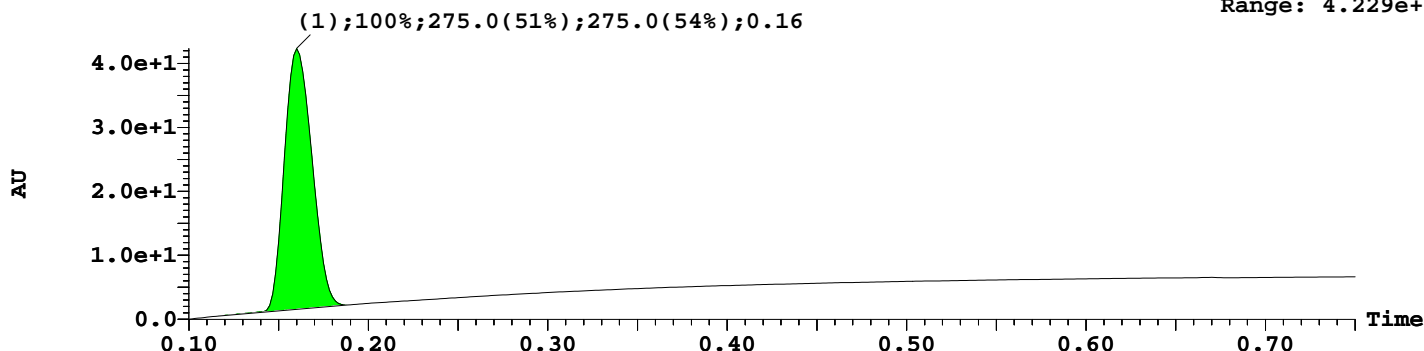
Vial: 2:6
Date: 09-Sep-2015

ID: 3-MeO-PCMo_20150909
Time: 10:24:03

Printed: Wed Sep 09 10:25:47 2015

4: UV Detector: TIC

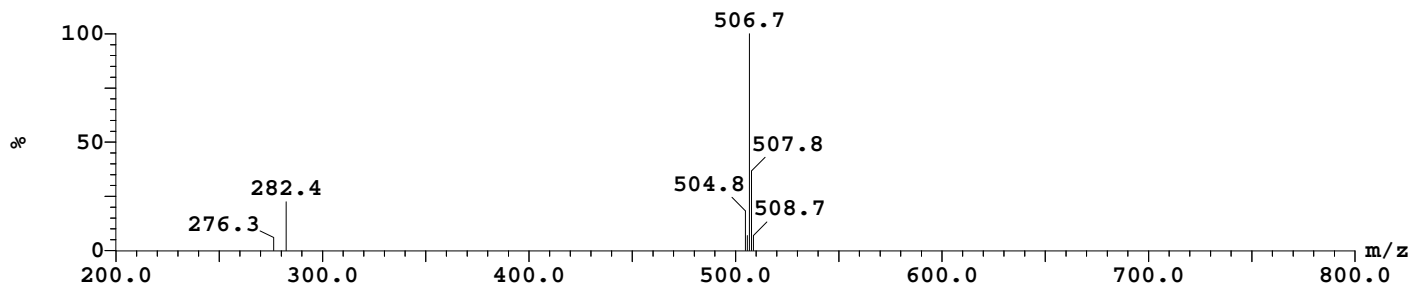
4.235e+1
Range: 4.229e+1



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	Found	0.16	7e+005	100.00	0	4e+007	275.00, 275.00

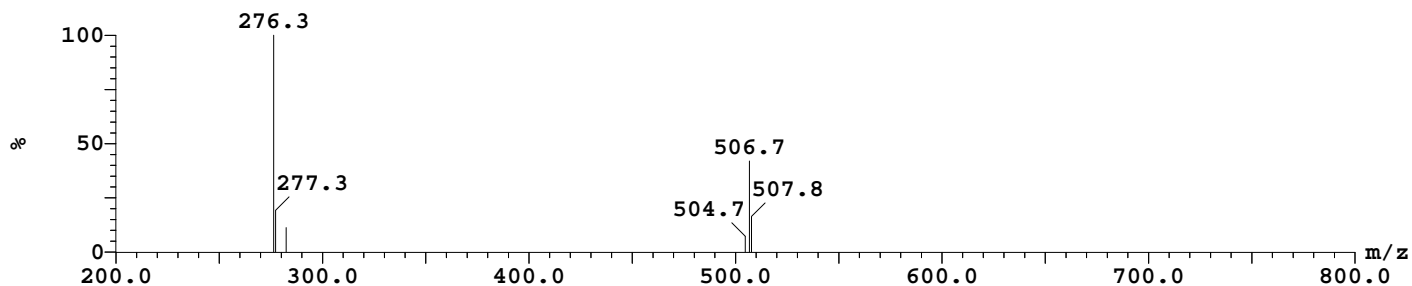
Peak ID	Compound	Time	Mass Found
1	Found	0.16	

1:MS ES+
5.9e+006



Peak ID	Compound	Time	Mass Found
1	Found	0.16	276.00

2:MS ES+
9.4e+006



Openlynx Report - Benny

Sample: 1
File: Benny41-1_20150909
Description:

Vial: 2:6
Date: 09-Sep-2015

ID: 3-MeO-PCMo_20150909
Time: 10:24:03

Printed: Wed Sep 09 10:25:47 2015

Peak ID	Compound	Time	Mass Found
1	Found	0.16	276.00

3:MS ES+
7.0e+006

