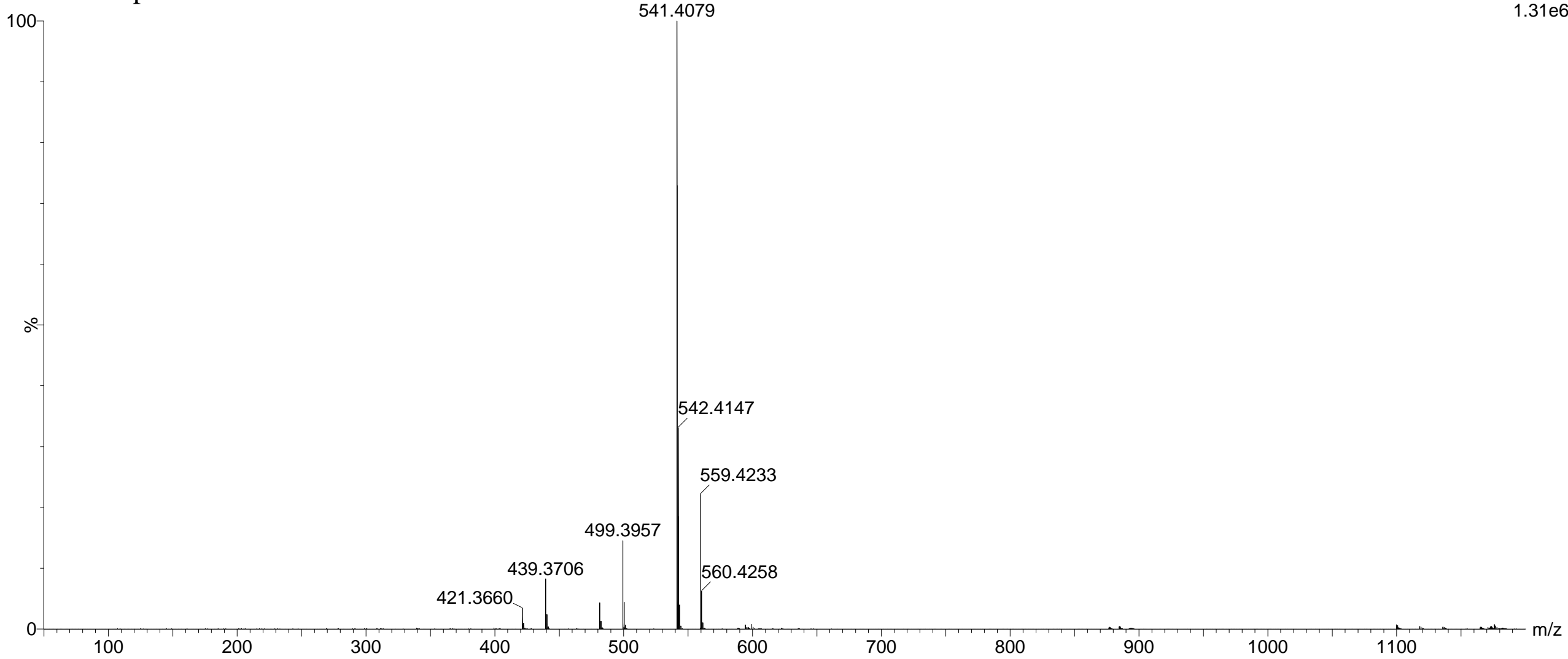


# Compound 1: Supplementary Data

## Mass Spectrum

LC-MS (Synapt) Facility

UP, Chemistry Dept.  
1: TOF MS ES+  
1.31e6



### Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

80 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
541.3894	541.3893	0.1	0.2	8.5	C34 H53 O5	44.8	0.053	94.79	34	53	5	
	541.3869	2.5	4.6	5.5	C32 H54 O5 Na	47.7	2.955	5.21	32	54	5	1

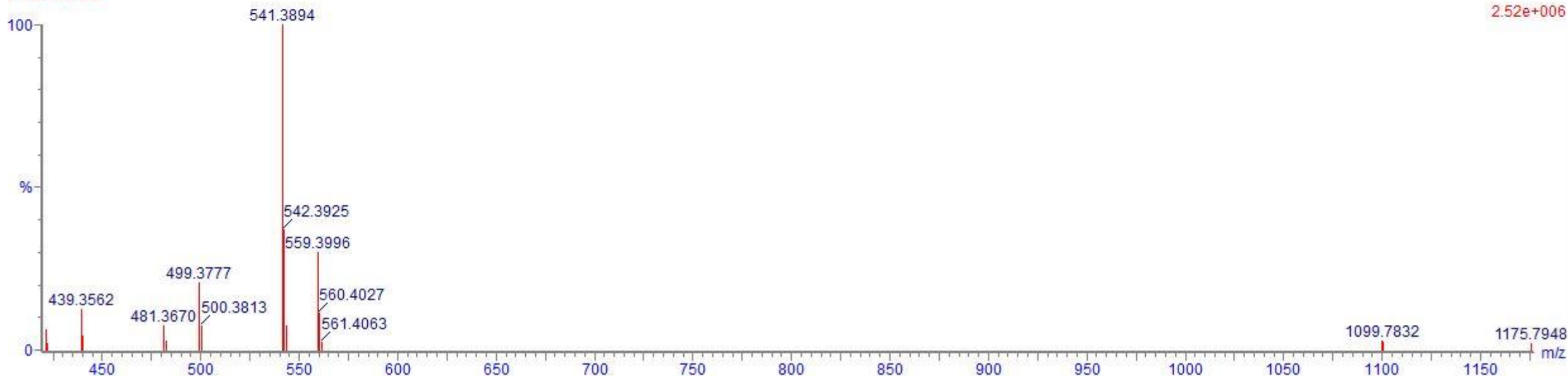
LC-MS (Synapt) Facility

UP, Chemistry Dept.

20191024\_PM\_1\_1F47T\_p 829 (9.436) AM2 (Ar,18000.0,556.28,0.00,LS 100); ABS

1: TOF MS ES+

2.52e+006



## Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

144 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
559.3996	559.3999	-0.3	-0.5	7.5	C34 H55 O6	15.6	0.000	99.95	34	55	6	
	559.3975	2.1	3.8	4.5	C32 H56 O6 Na	23.3	7.638	0.05	32	56	6	1

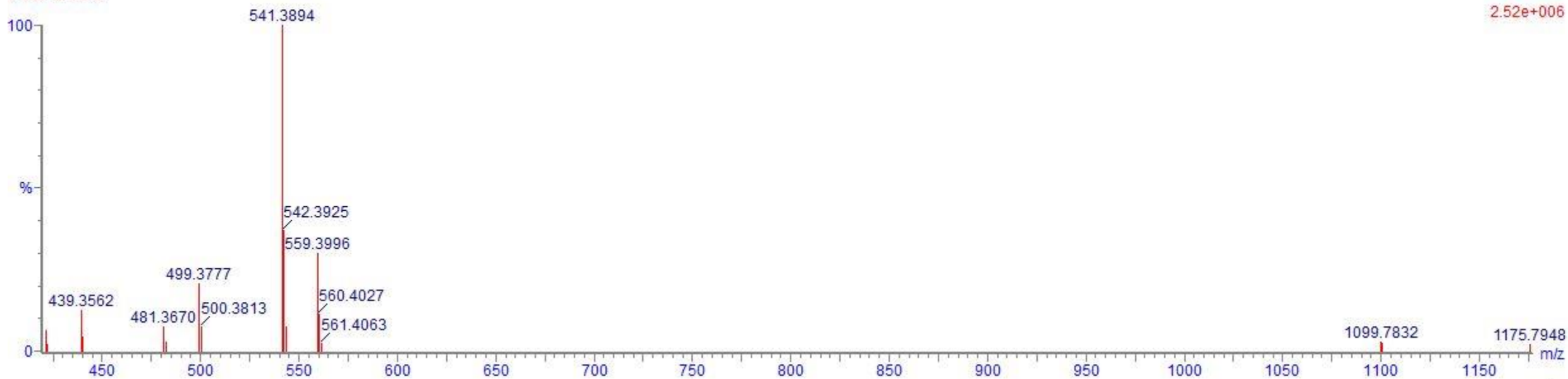
\_C-MS (Synapt) Facility

UP, Chemistry Dept.

20191024\_PM\_I\_1F47T\_p 829 (9.436) AM2 (Ar,18000.0,556.28,0.00,LS 100); ABS

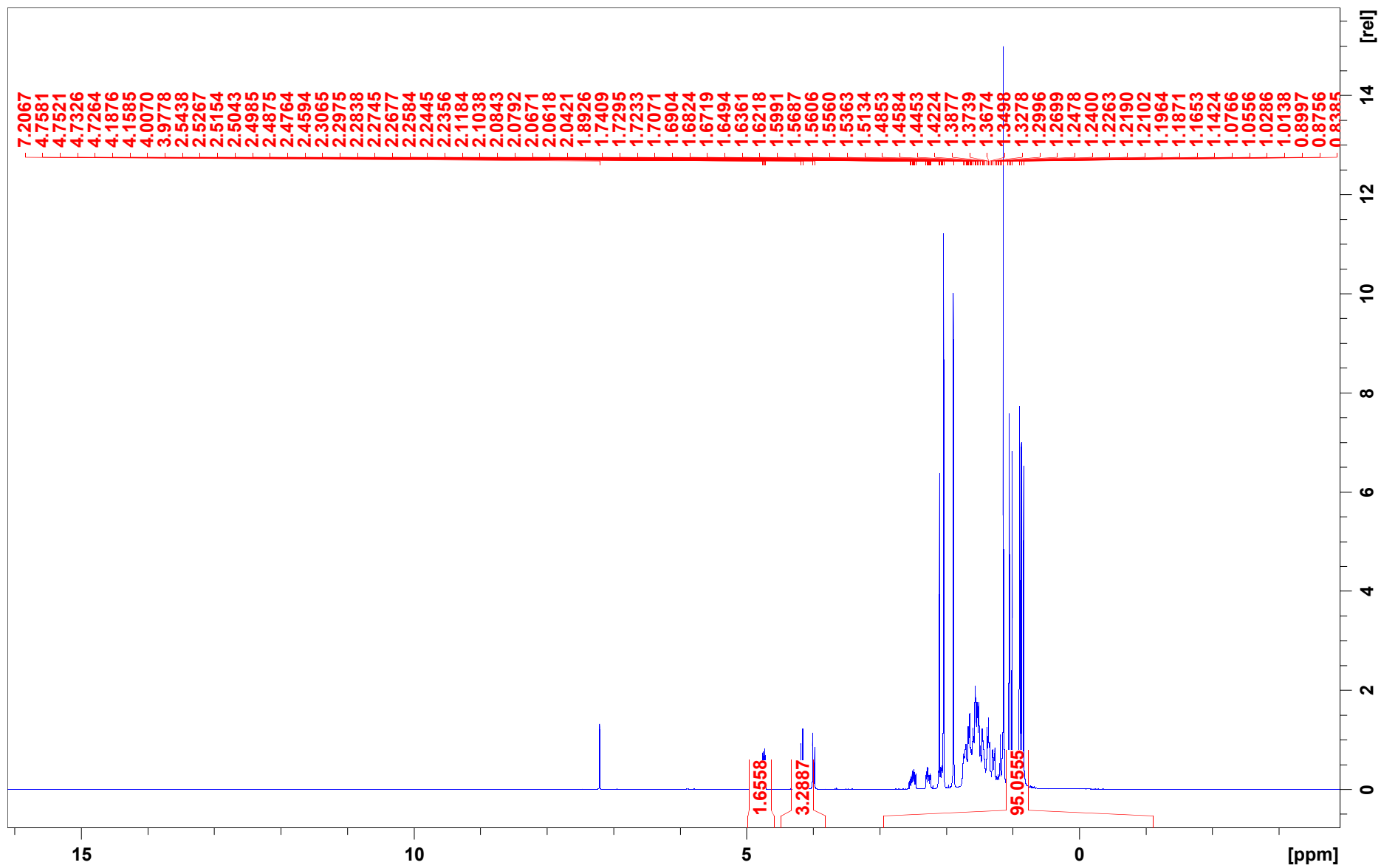
1: TOF MS ES+

2.52e+006



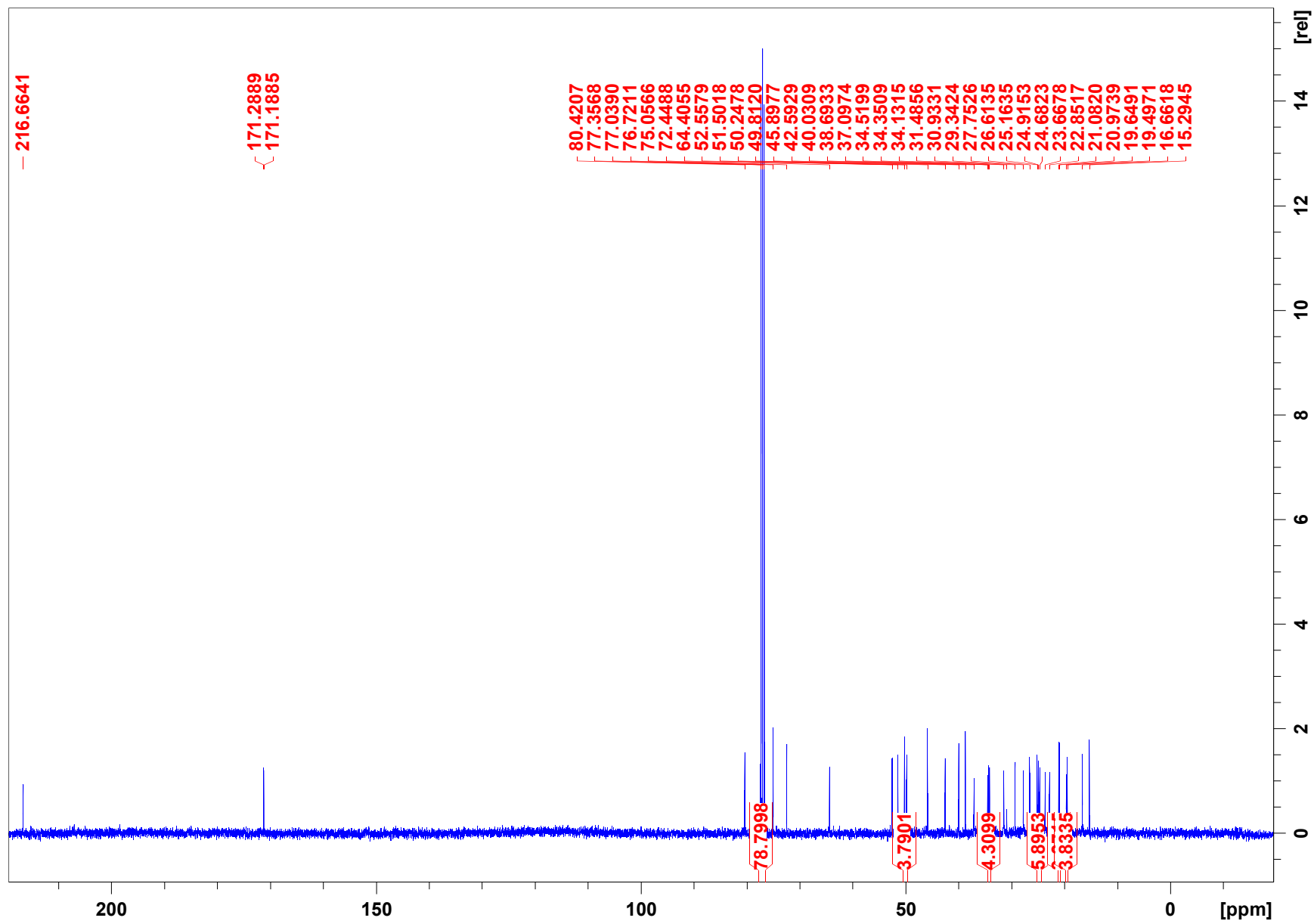
Compound 1

Proton NMR



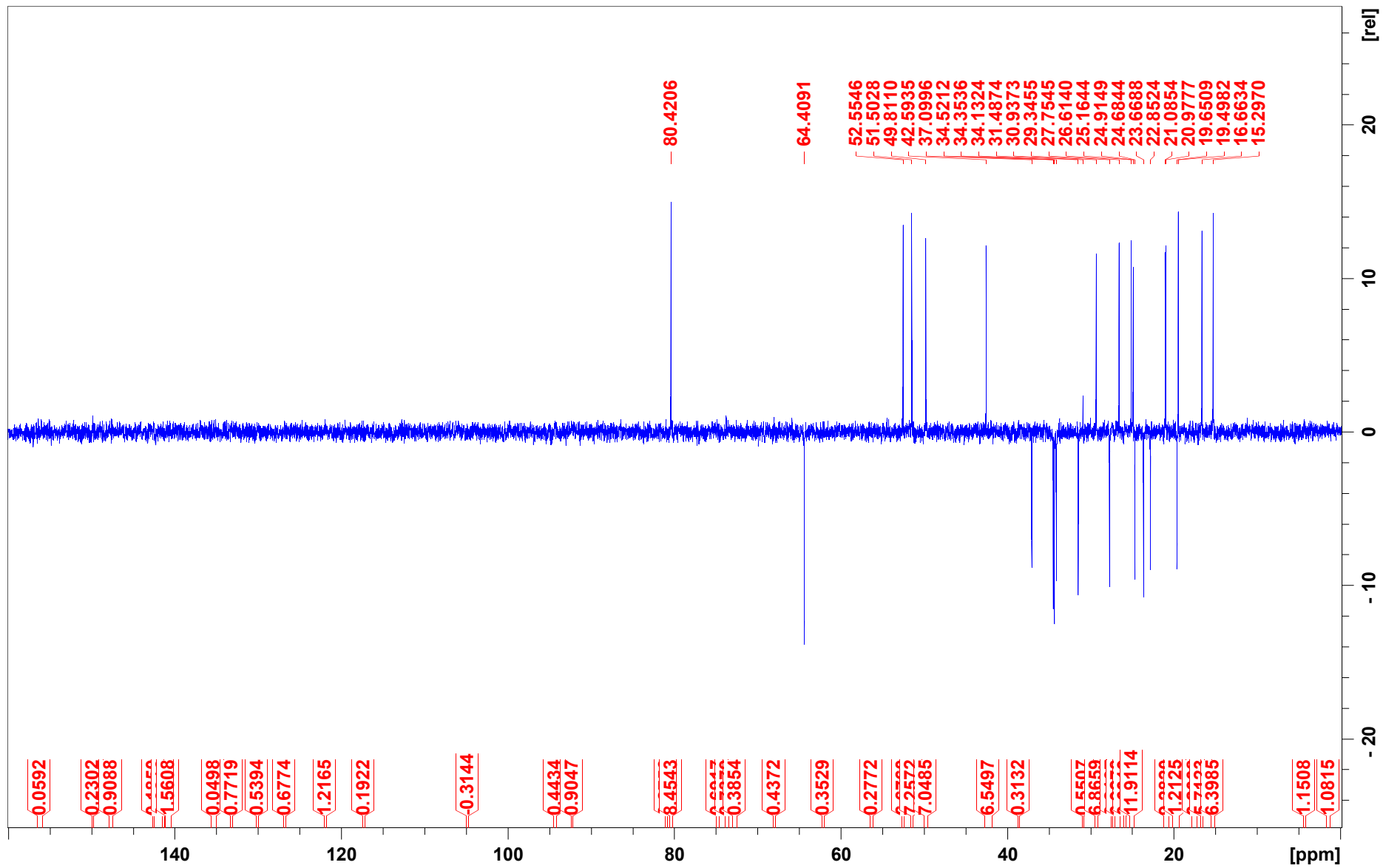
Compound 1

Carbon NMR



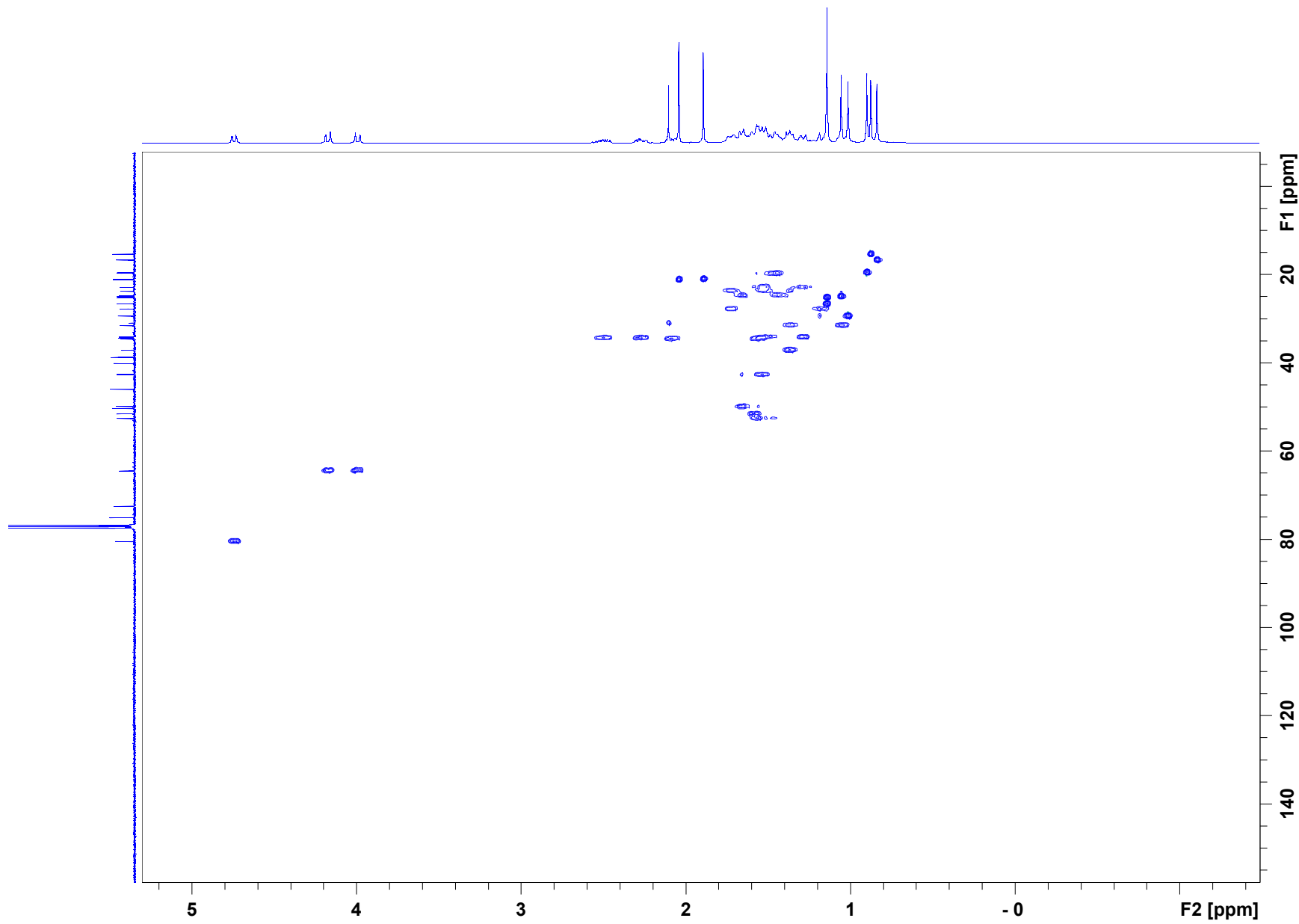
Compound 1

DEPT



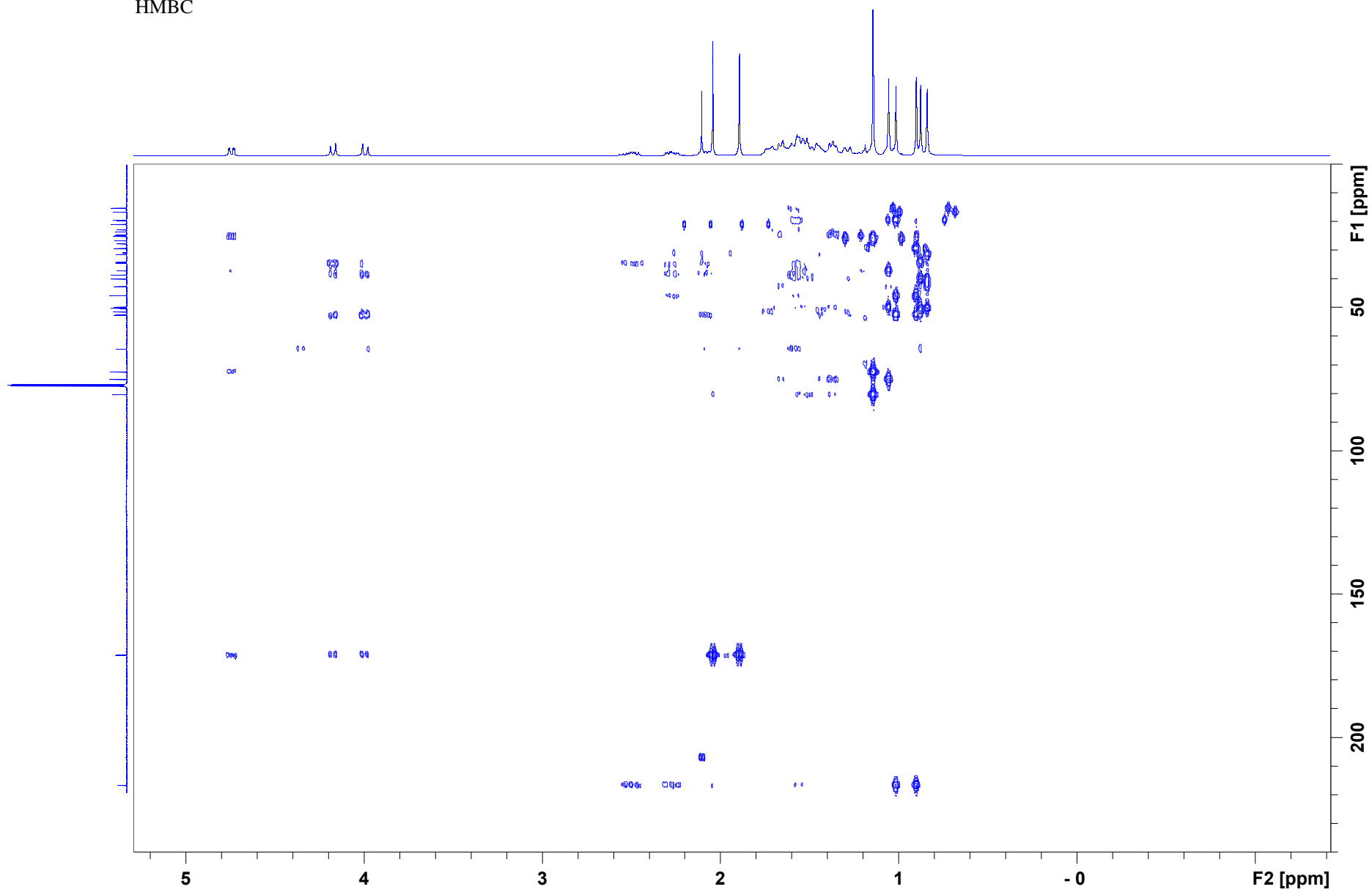
Compound 1

HSQC



Compound 1

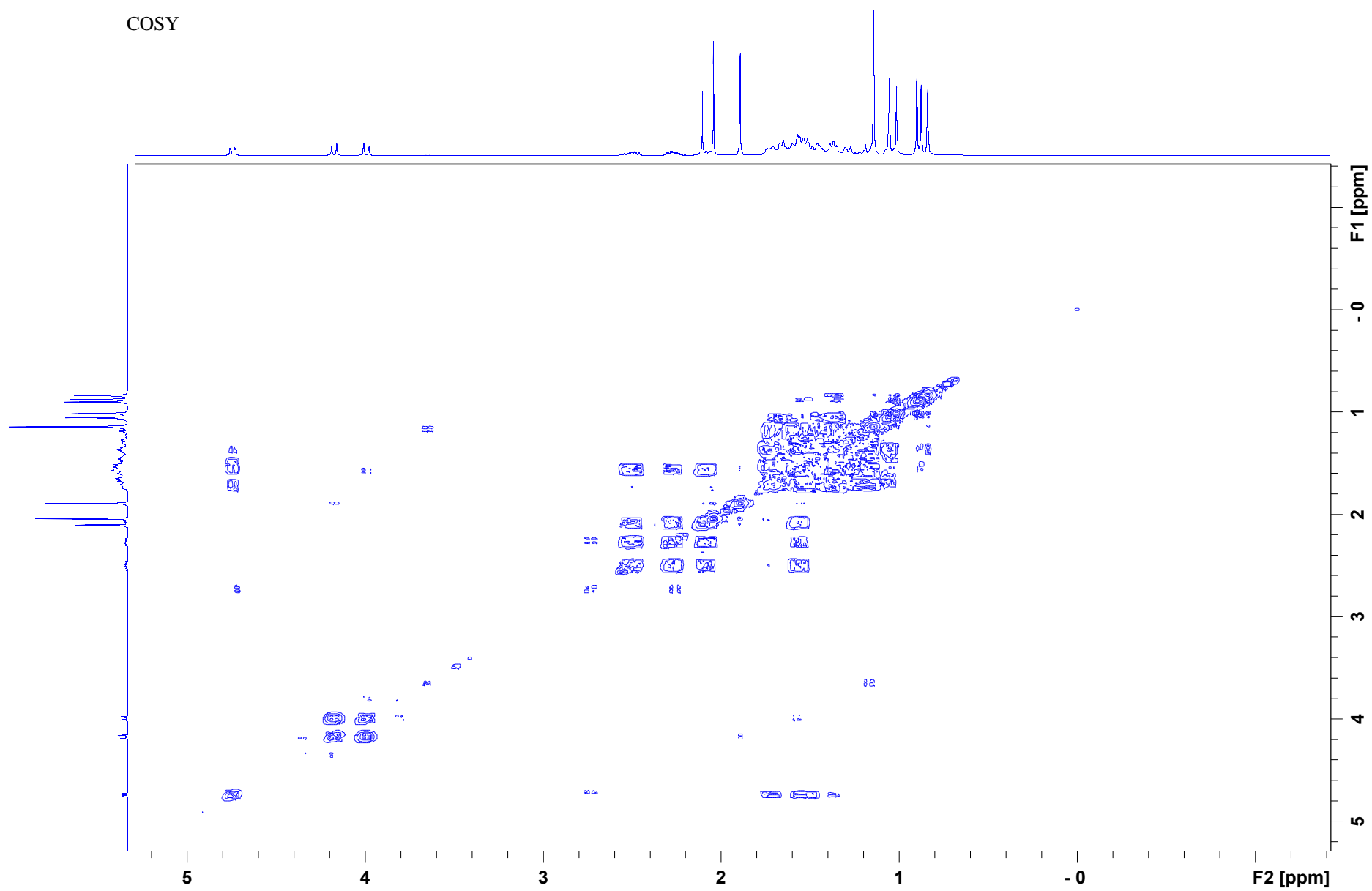
HMBC





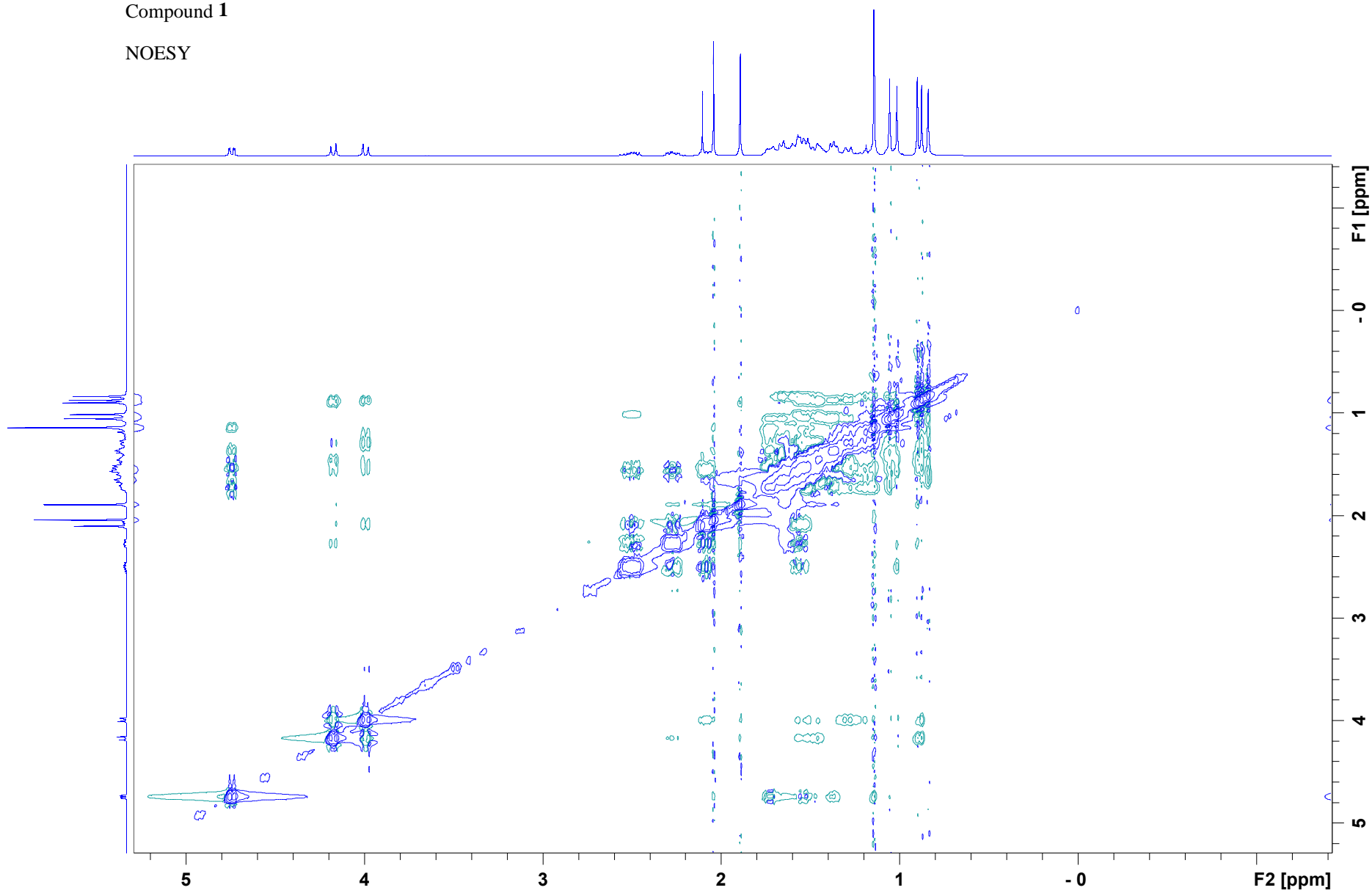
Compound 1

COSY



Compound 1

NOESY

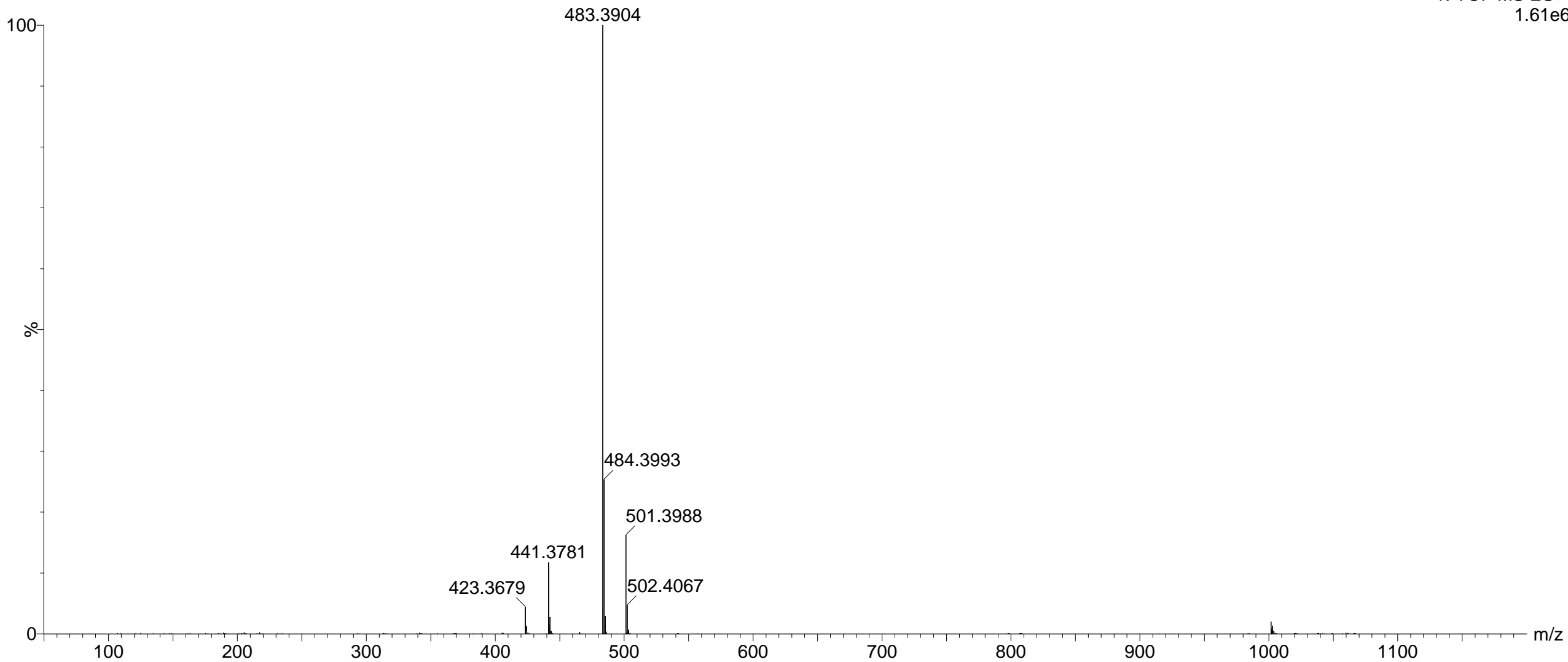


# Compound 2: Supplementary Data

## Mass Spectrum

LC-MS (Synapt) Facility

UP, Chemistry Dept.  
1: TOF MS ES+  
1.61e6



## Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

126 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
483.3871	483.3838	3.3	6.8	7.5	C32 H51 O3	49.3	0.008	99.18	32	51	3	
	483.3897	-2.6	-5.4	-1.5	C25 H55 O8	54.1	4.800	0.82	25	55	8	

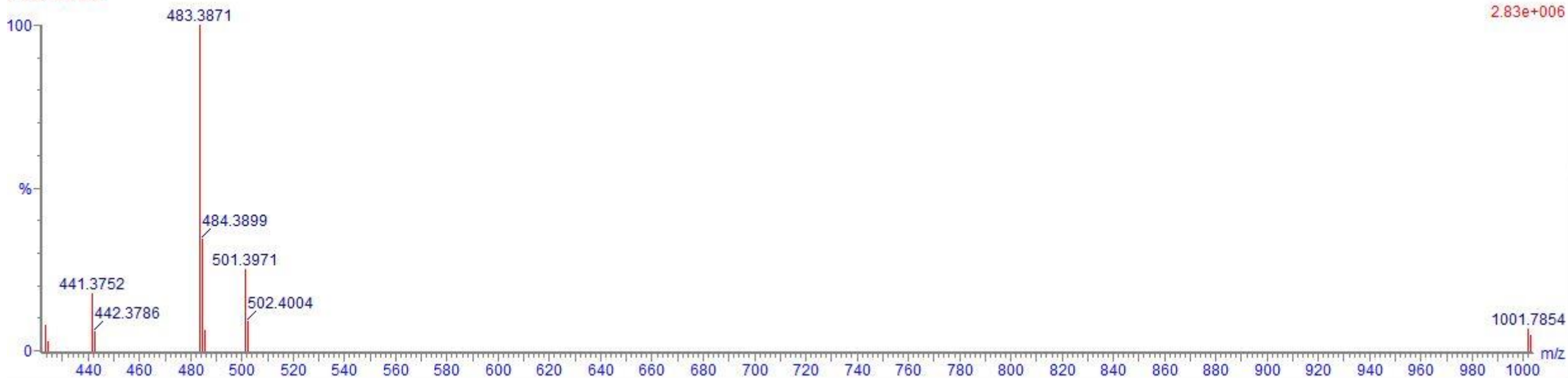
\_C-MS (Synapt) Facility

UP, Chemistry Dept.

20191015\_PM\_I\_1F73T\_p 1052 (11.967) AM2 (Ar,18000.0,556.28,0.00,LS 100); ABS

1: TOF MS ES+

2.83e+006



## Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

126 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
501.3971	501.3944	2.7	5.4	6.5	C32 H53 O4	40.8	n/a	n/a	32	53	4	

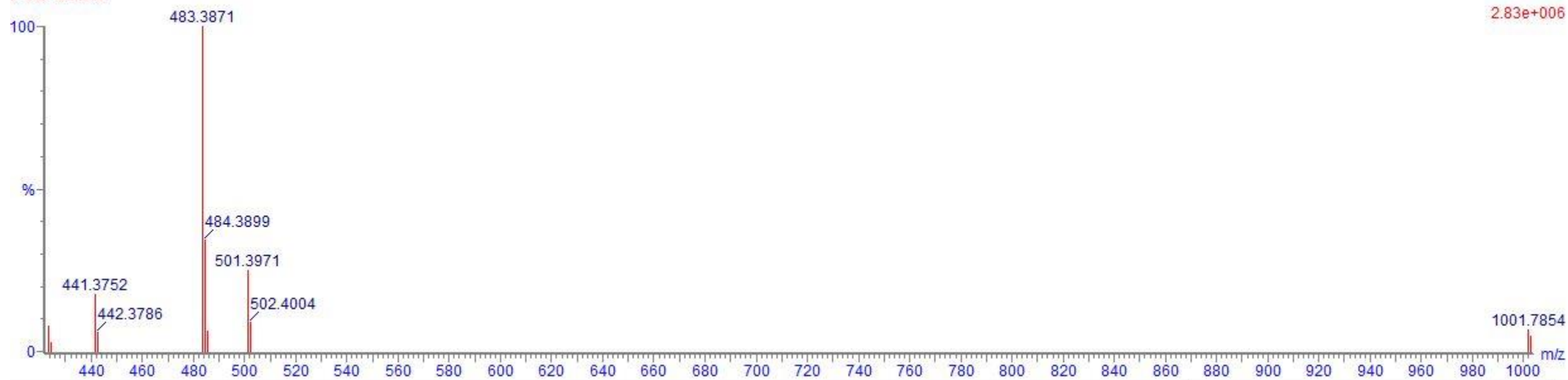
\_C-MS (Synapt) Facility

UP, Chemistry Dept.

20191015\_PM\_I\_1F73T\_p 1052 (11.967) AM2 (Ar,18000.0,556.28,0.00,LS 100); ABS

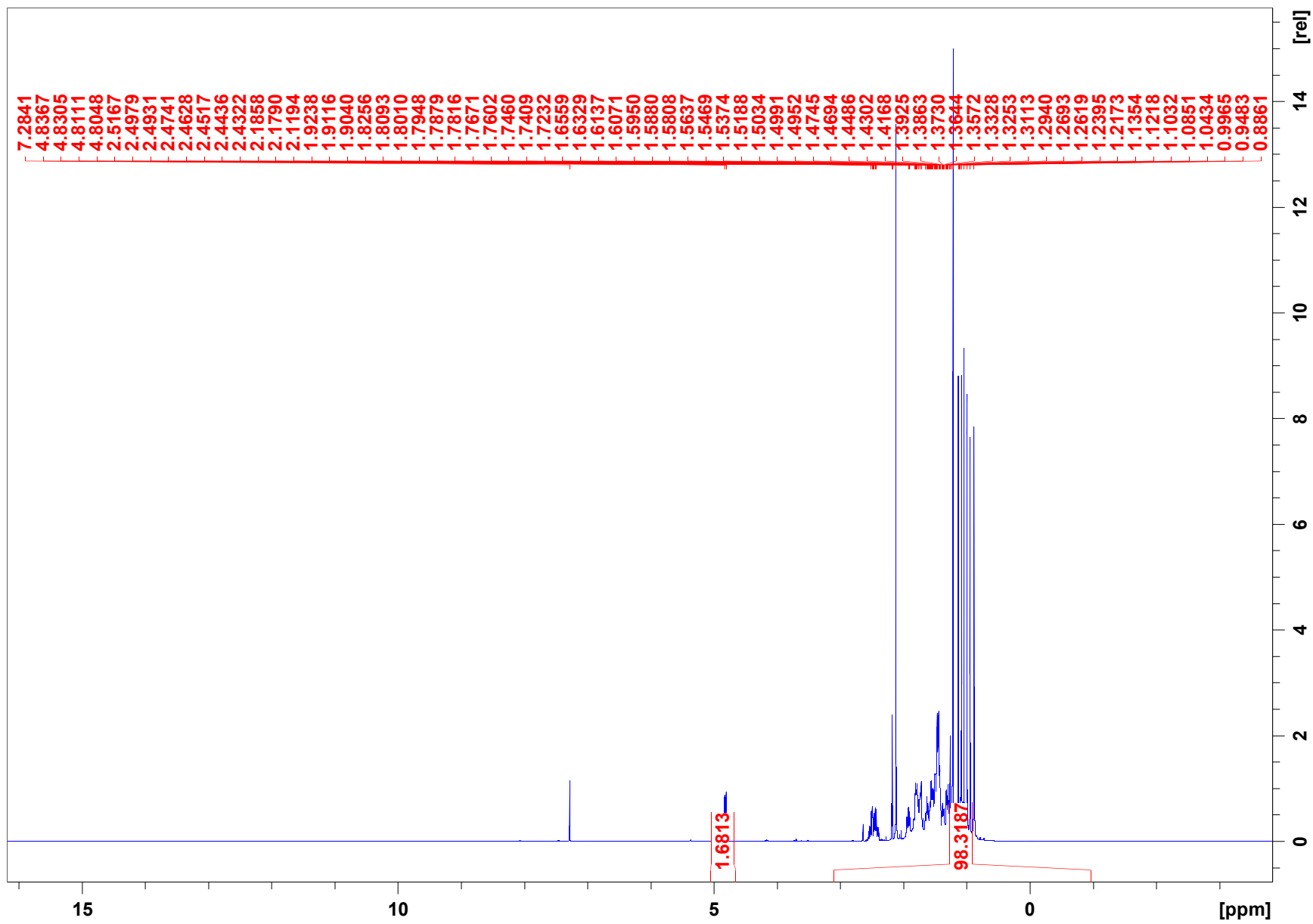
1: TOF MS ES+

2.83e+006



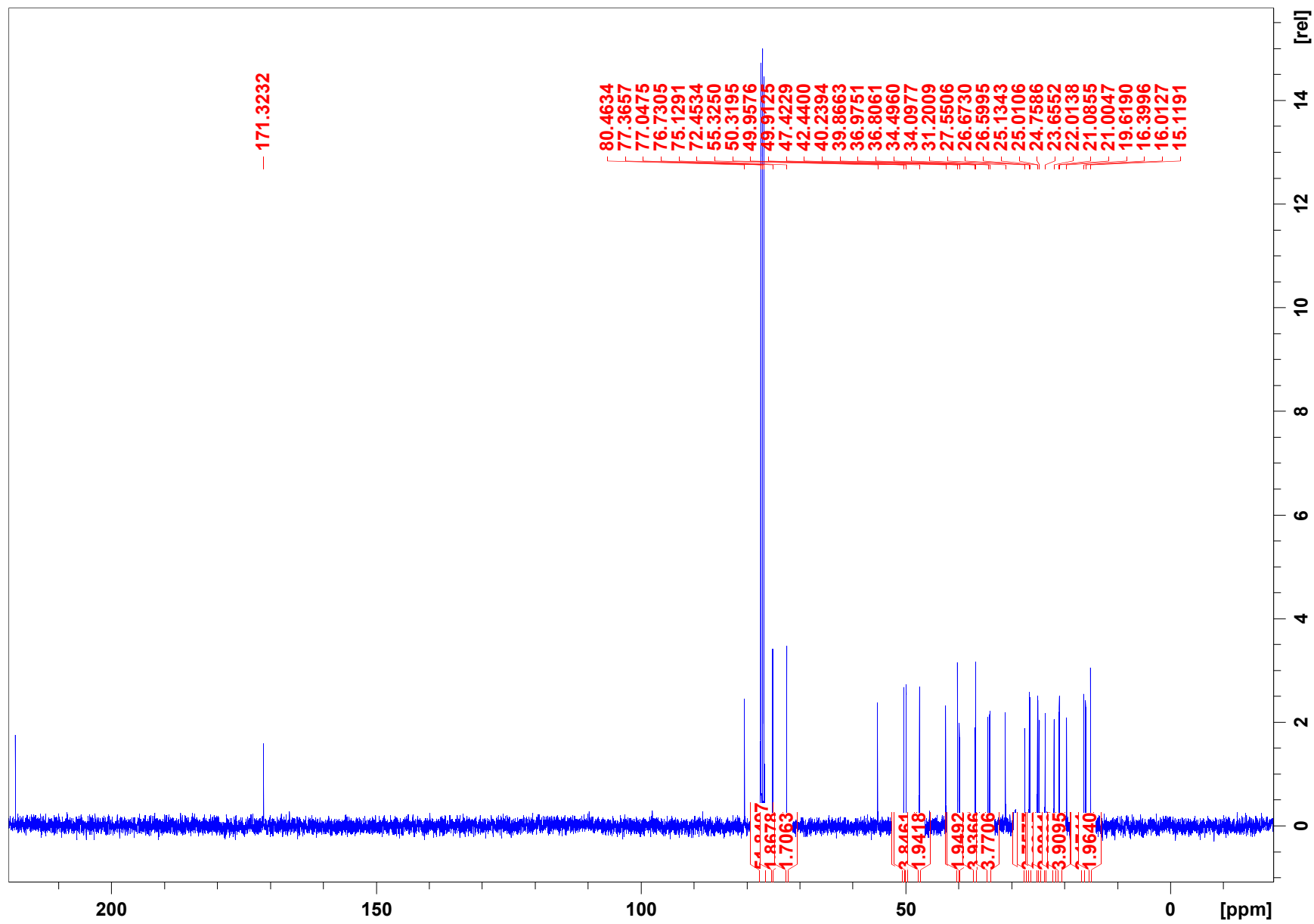
Compound 2

Proton NMR



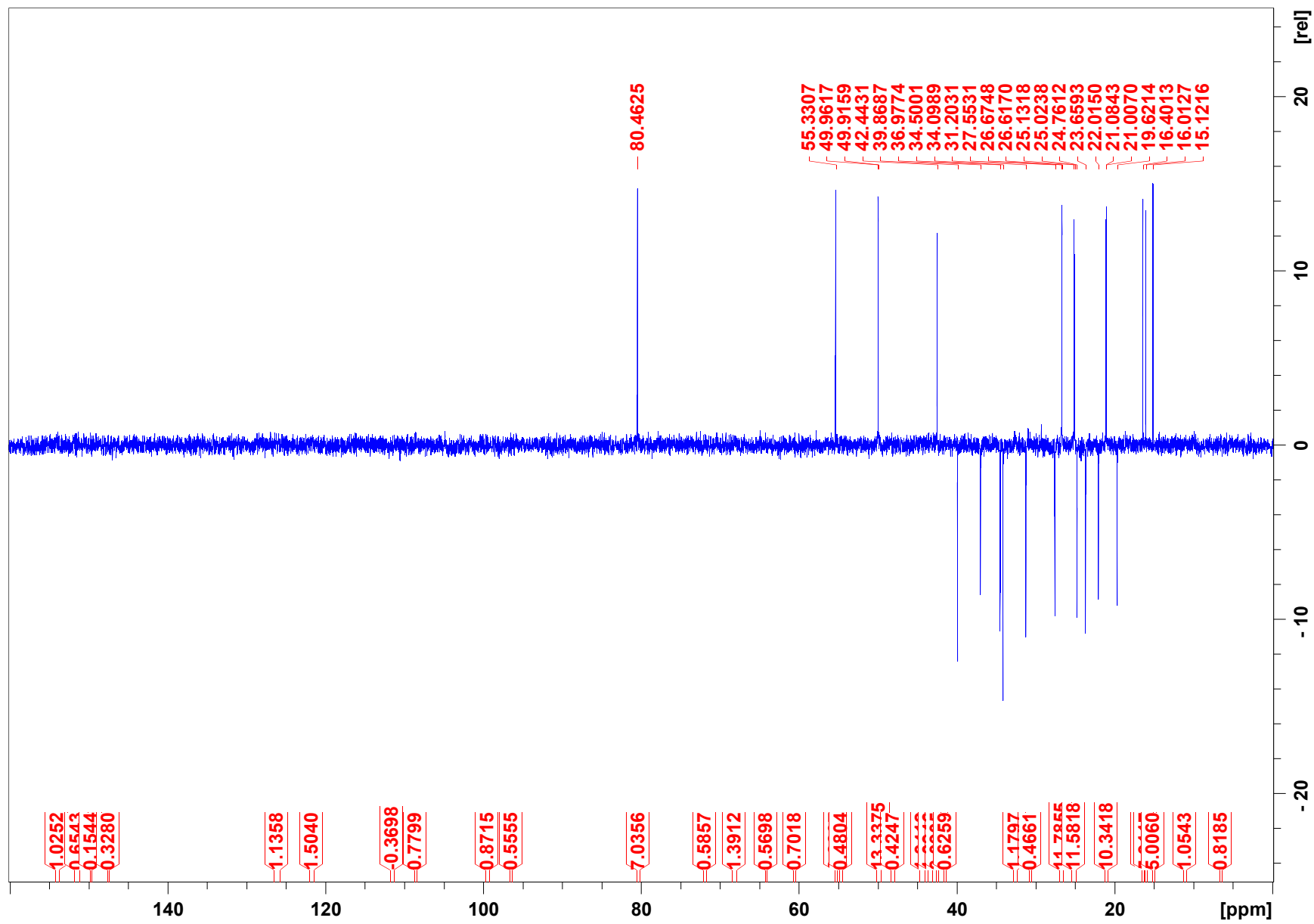
Compound 2

Carbon NMR



Compound 2

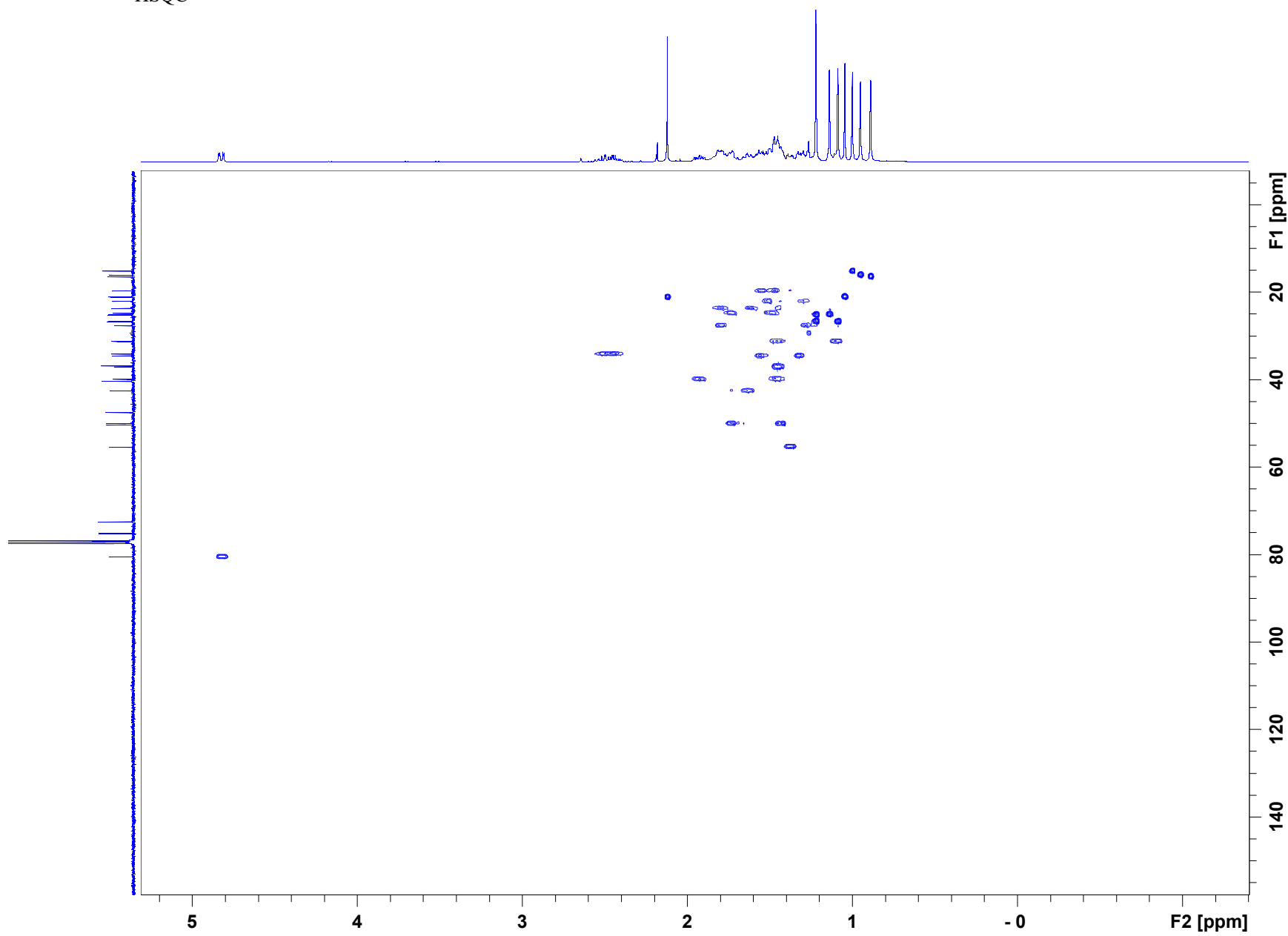
DEPT





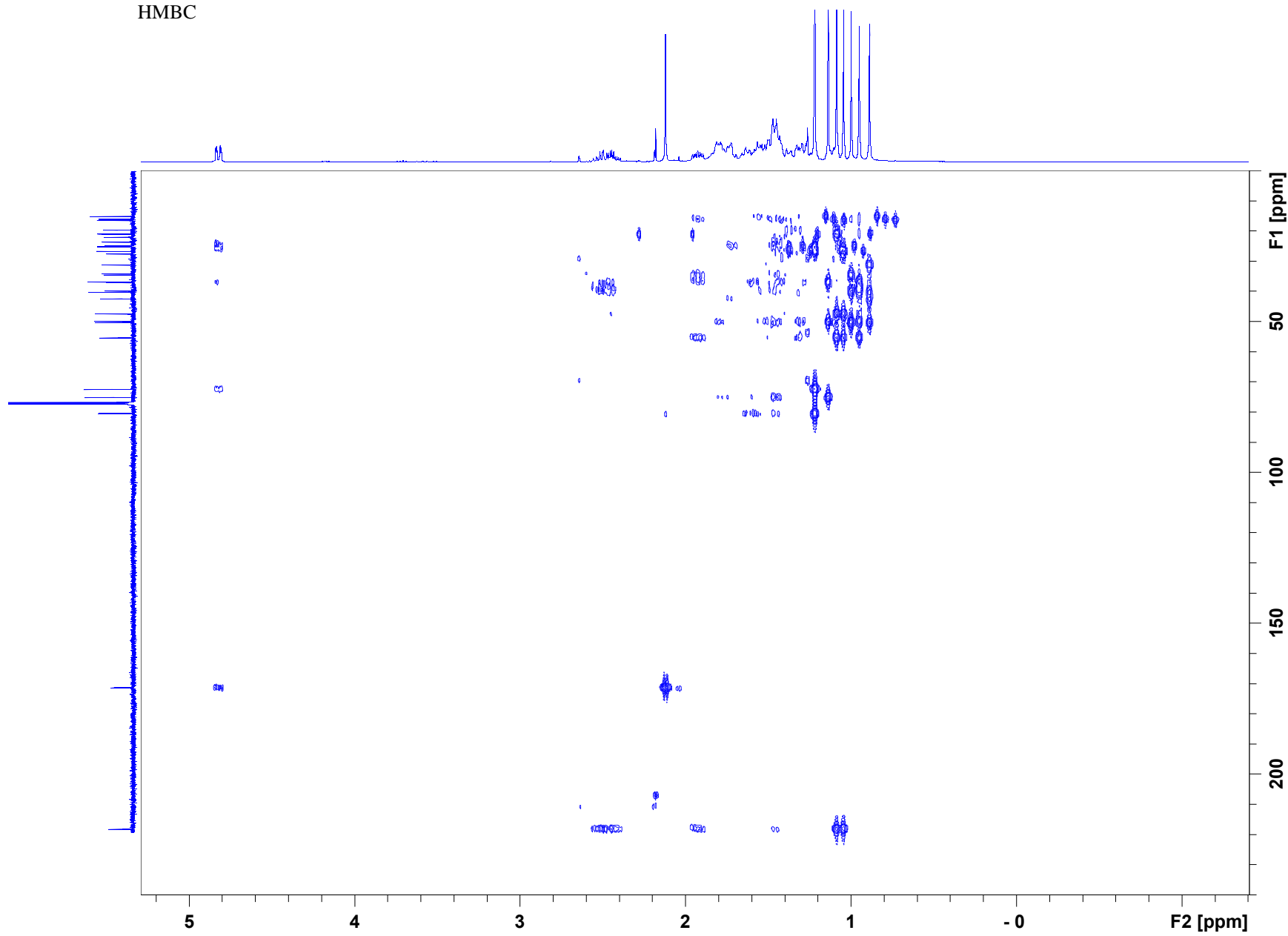
Compound 2

HSQC



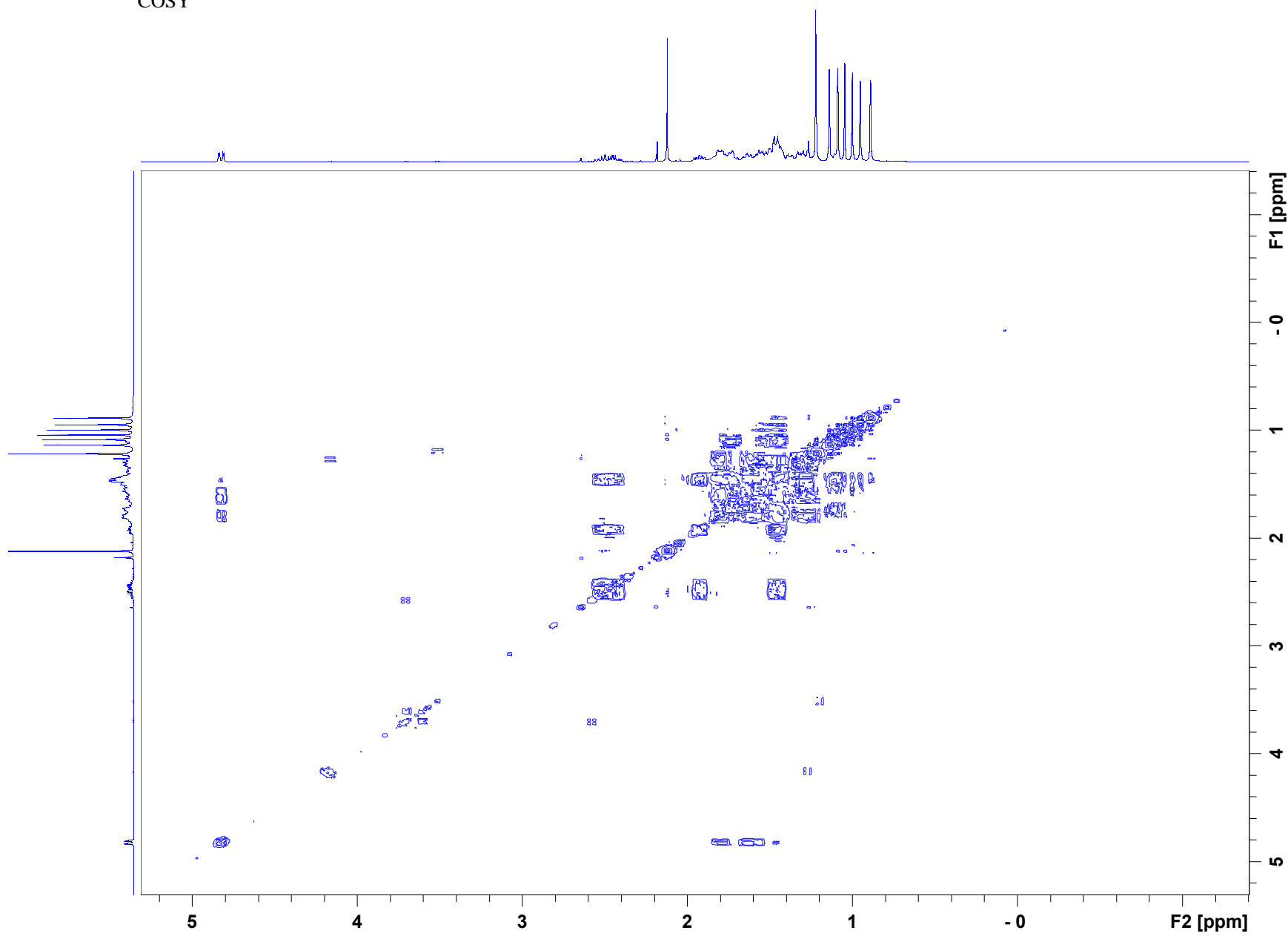
Compound 2

HMBC



Compound 2

COSY



Compound 2

NOESY

