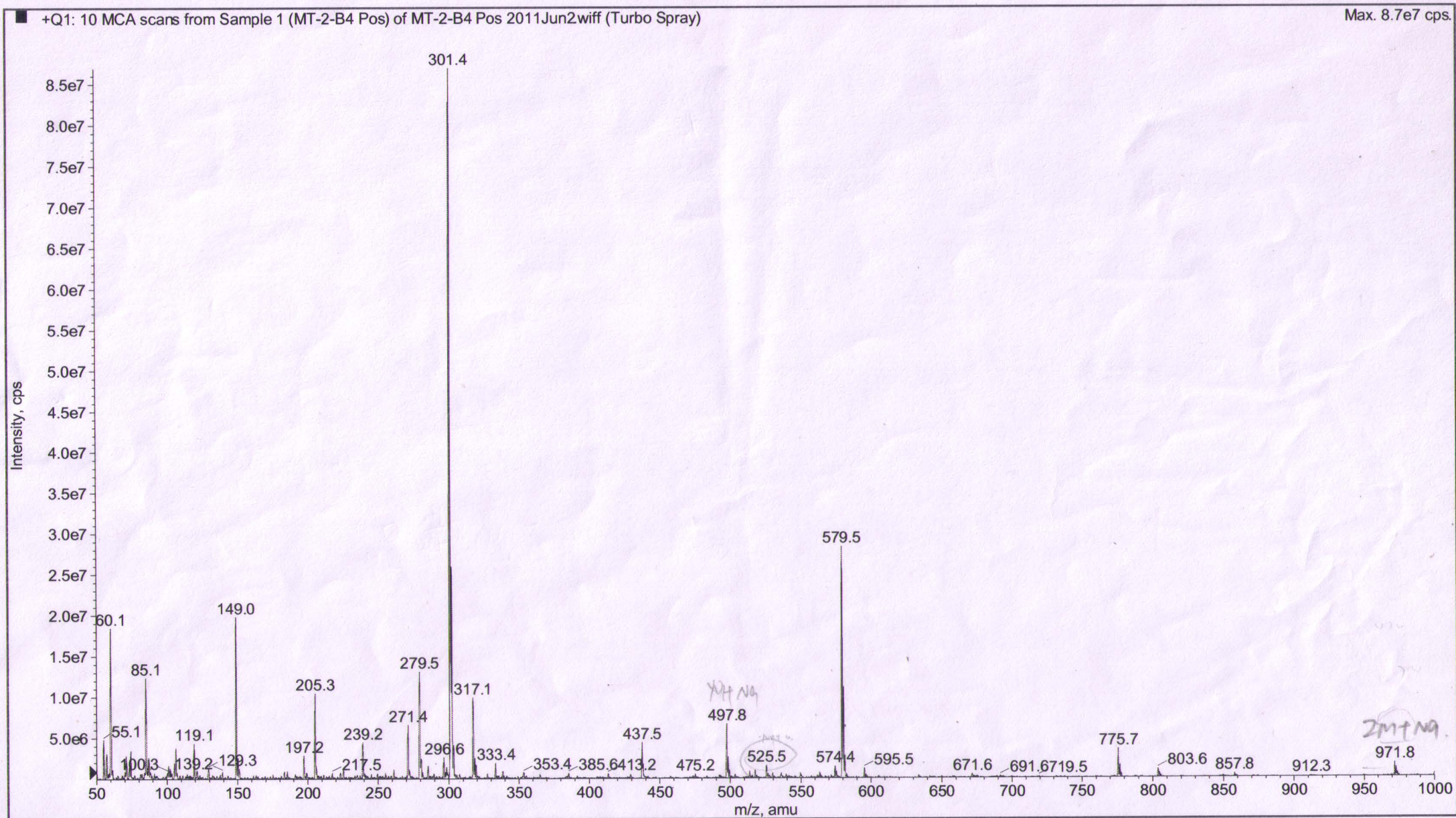
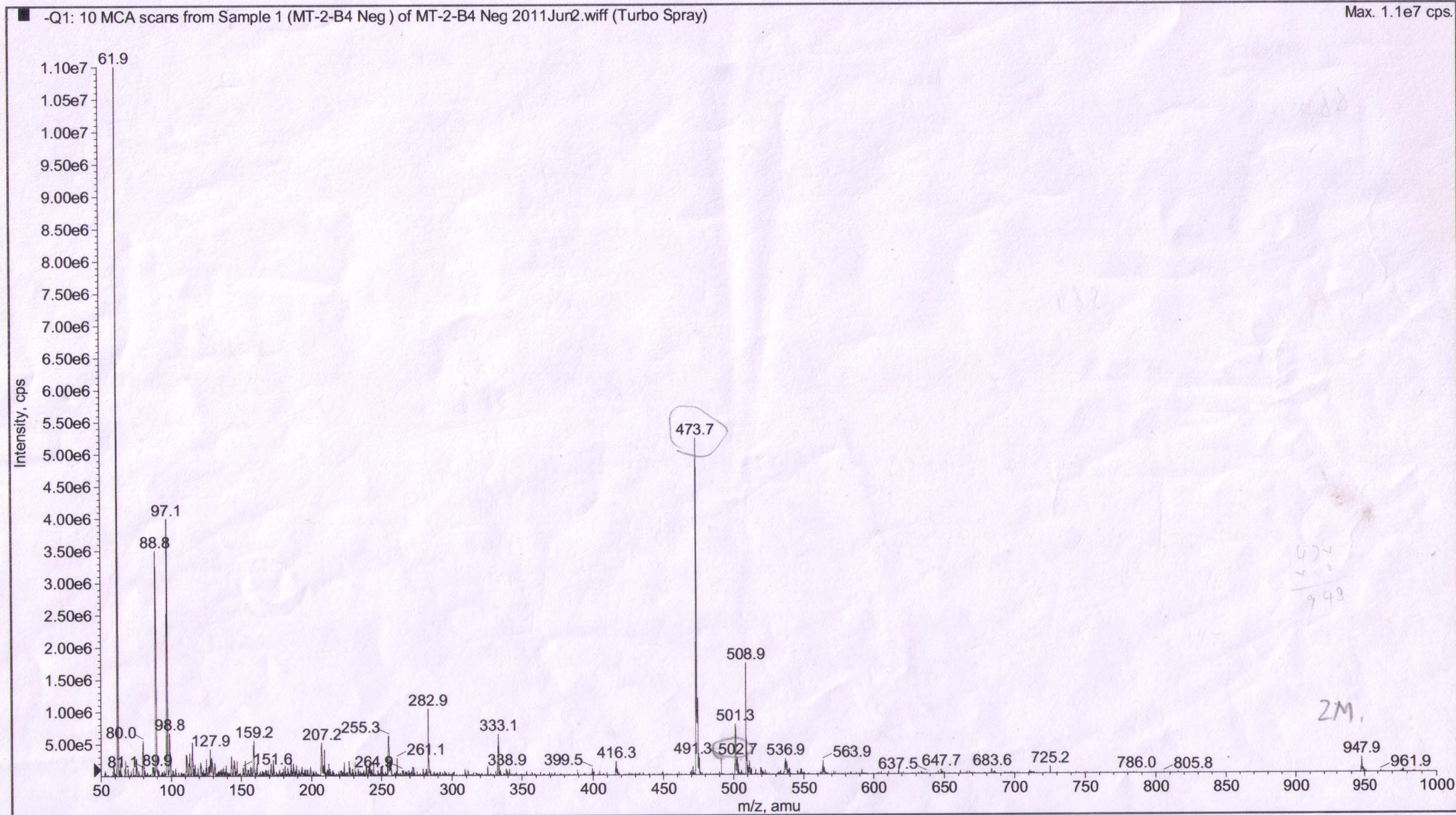


ESIMS(+) of Compound 1



ESIMS(-) of Compound 1



Mass Spectrum SmartFormula Report

Analysis Info

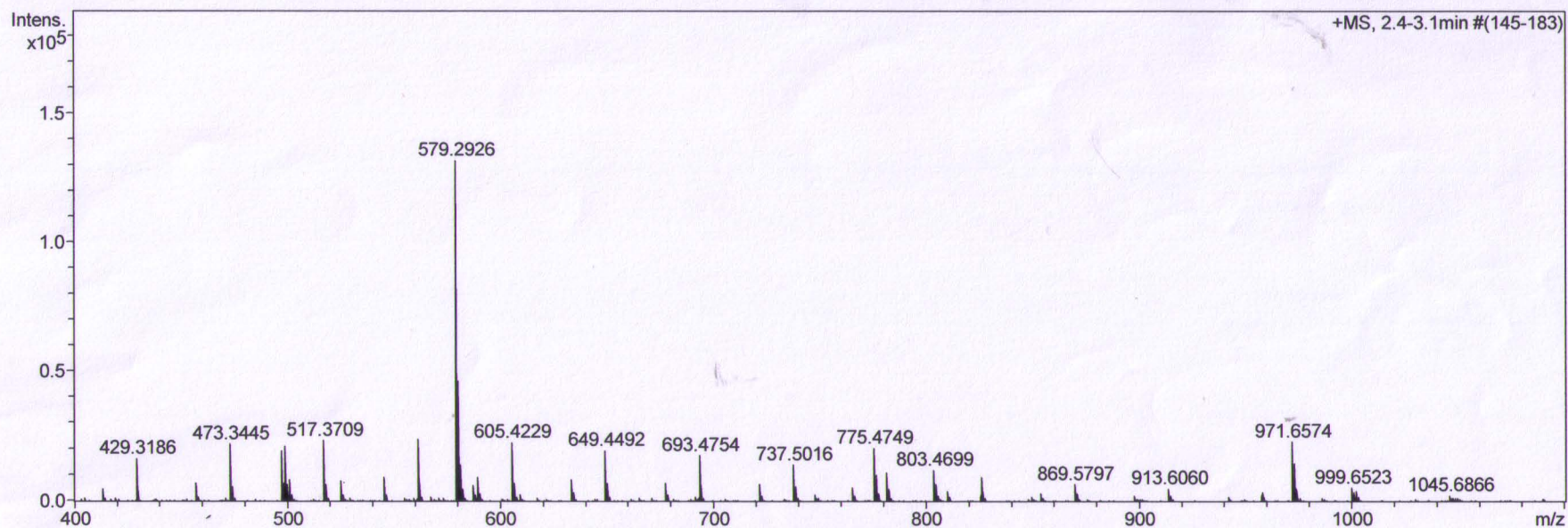
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Method POS_100-2000_Dirrect Infusion.m
Sample Name
Comment

Acquisition Date 11/21/2012 11:20:44 AM

Operator SCSIO
Instrument / Ser# maXis 29

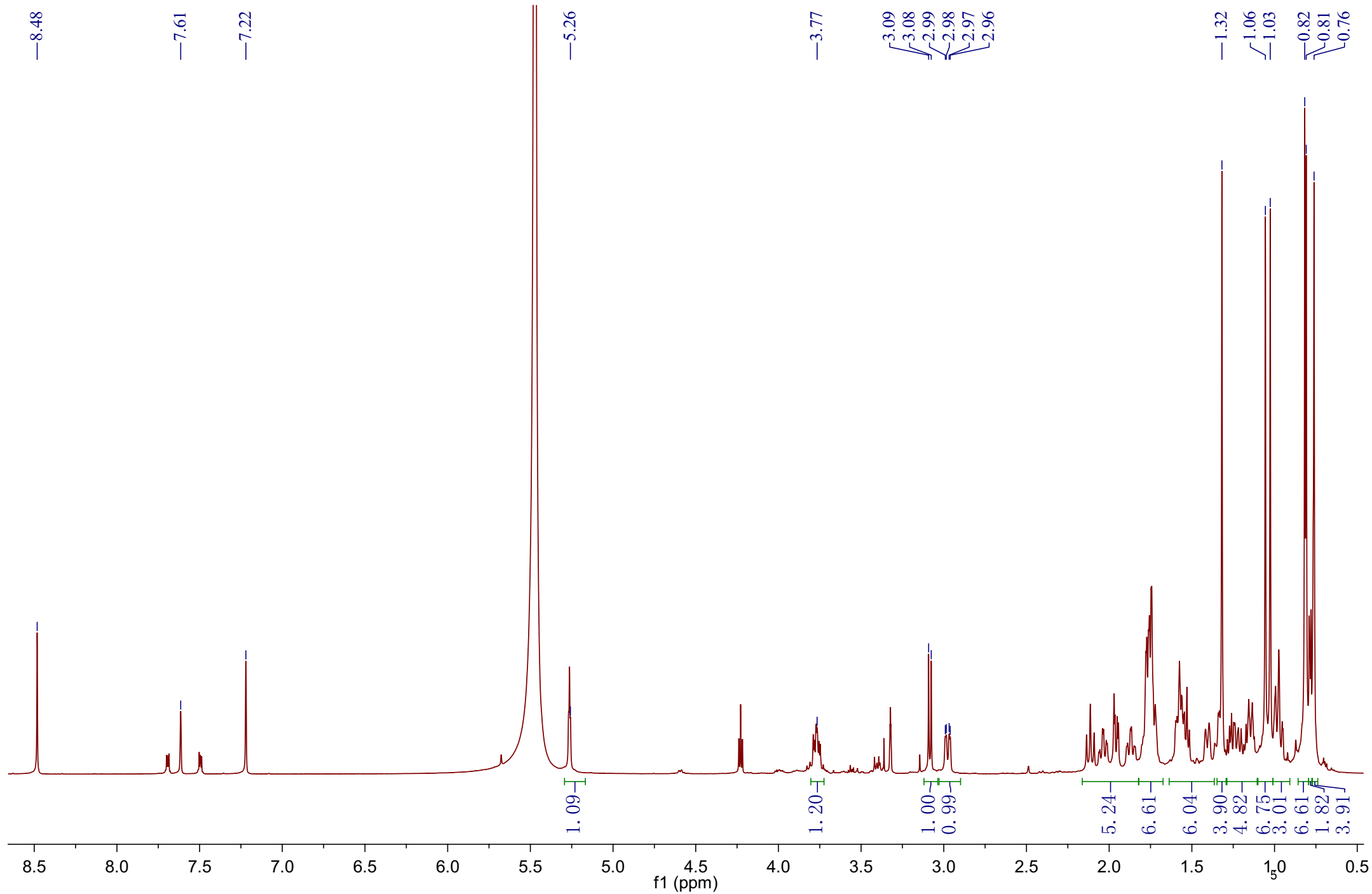
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste

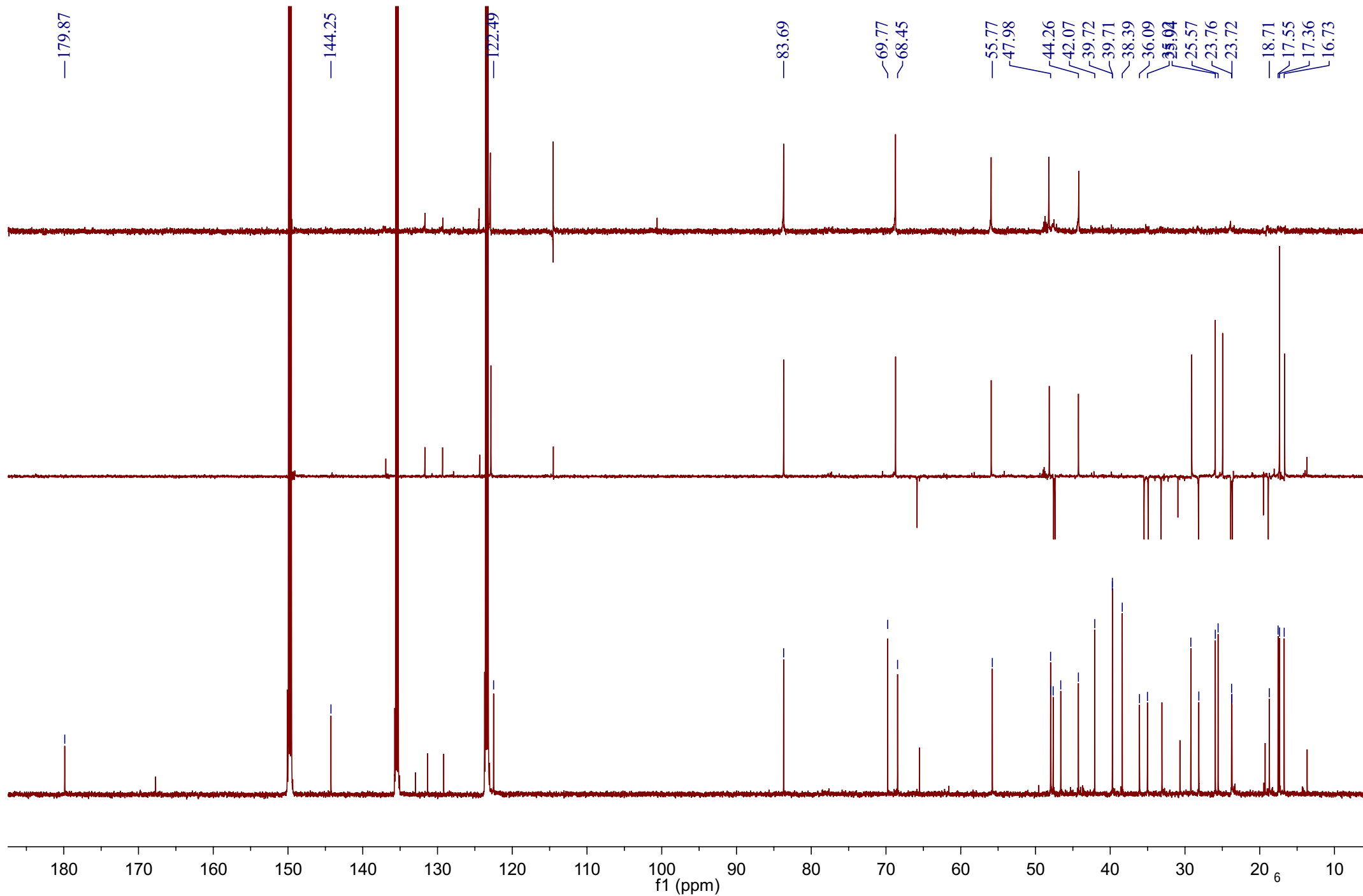


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
497.3235	1	C 29 H 46 Na O 5	100.00	497.3237	0.3	0.6	497.5	6.5	even	ok
971.6574	1	C 58 H 92 Na O 10	100.00	971.6583	0.9	0.9	6.3	12.5	even	ok

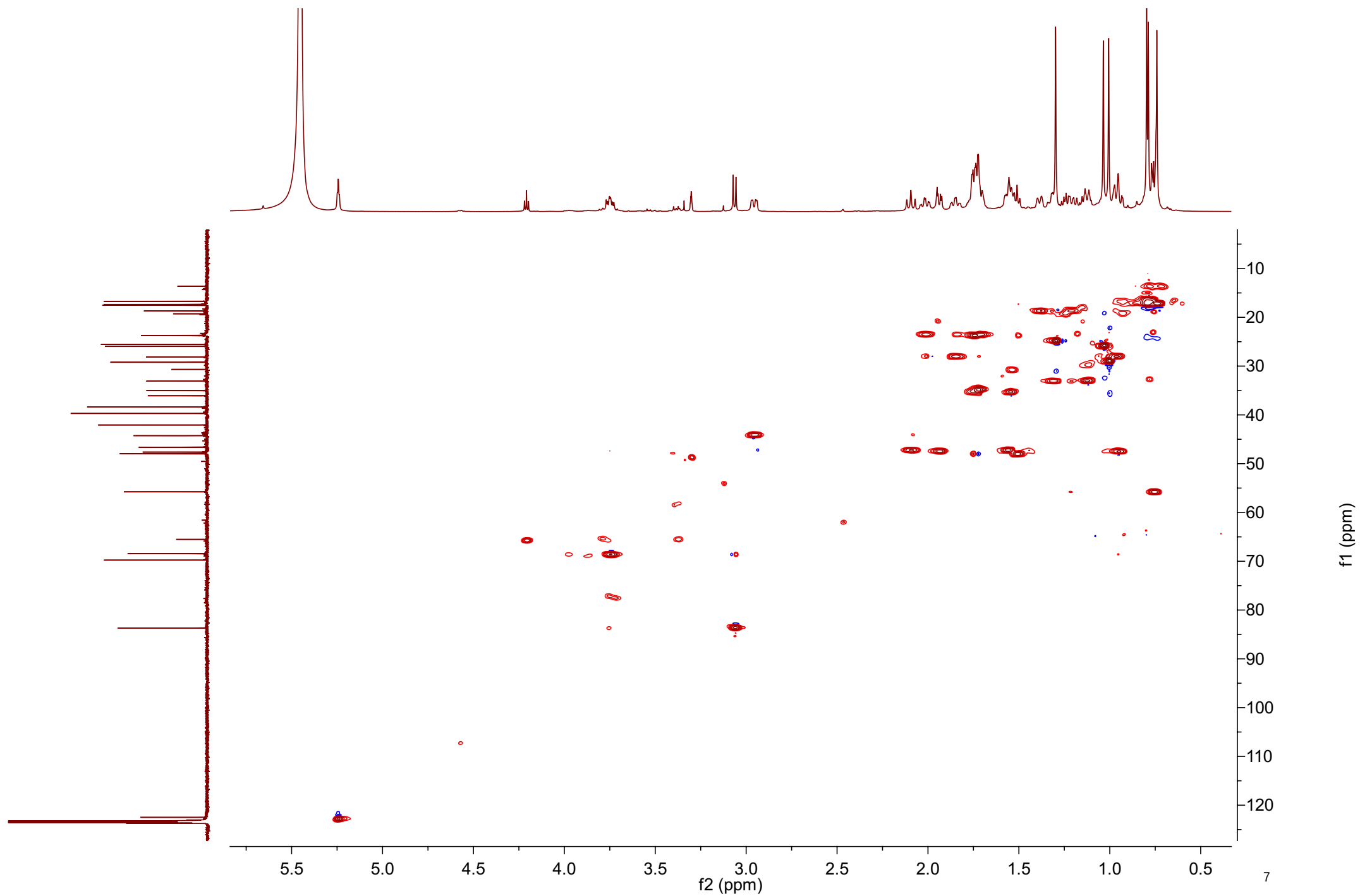
^1H NMR spectrum of compound **1**



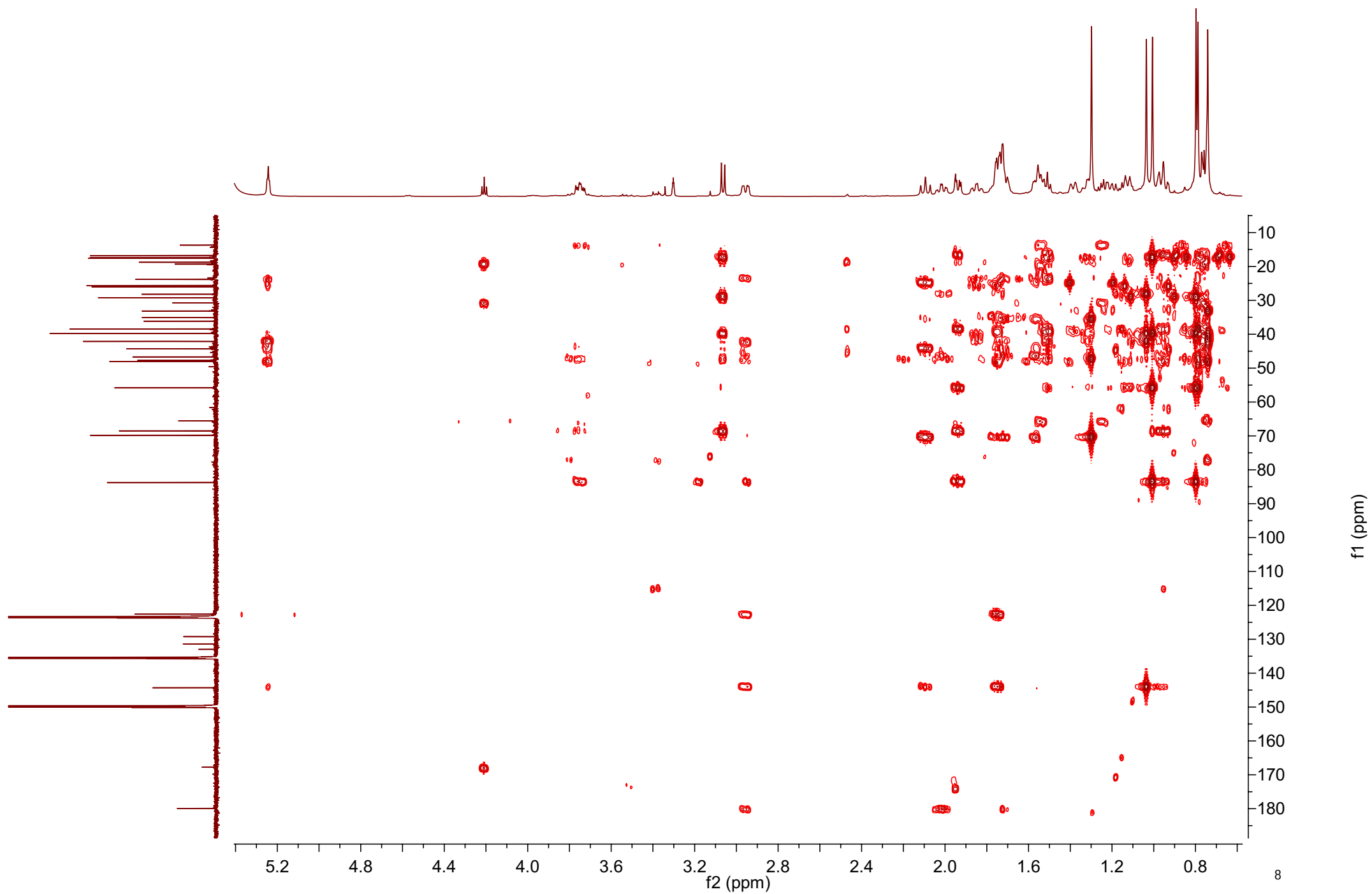
^{13}C NMR and DEPT spectra of compound 1

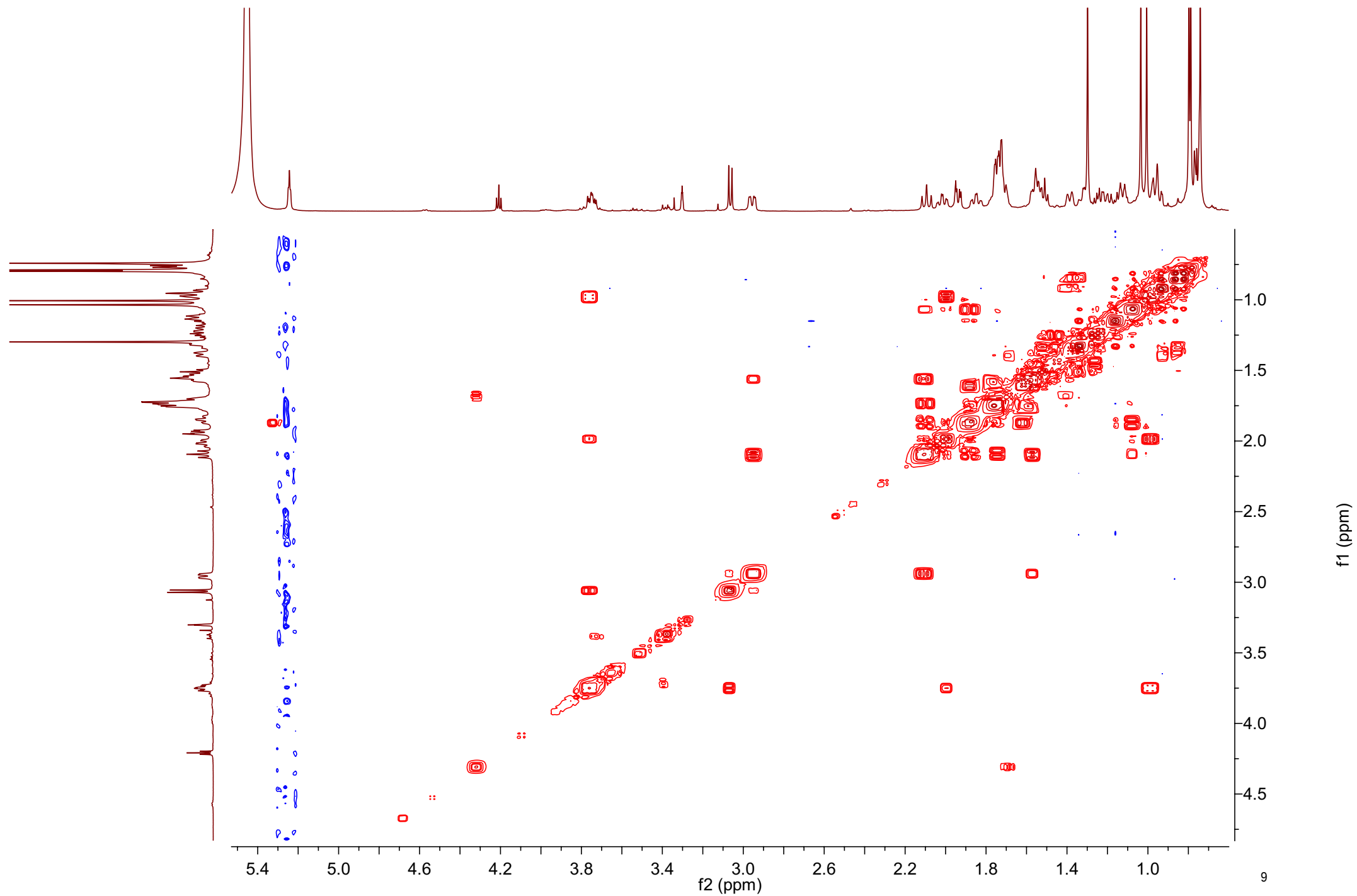


HSQC spectrum of compound 1

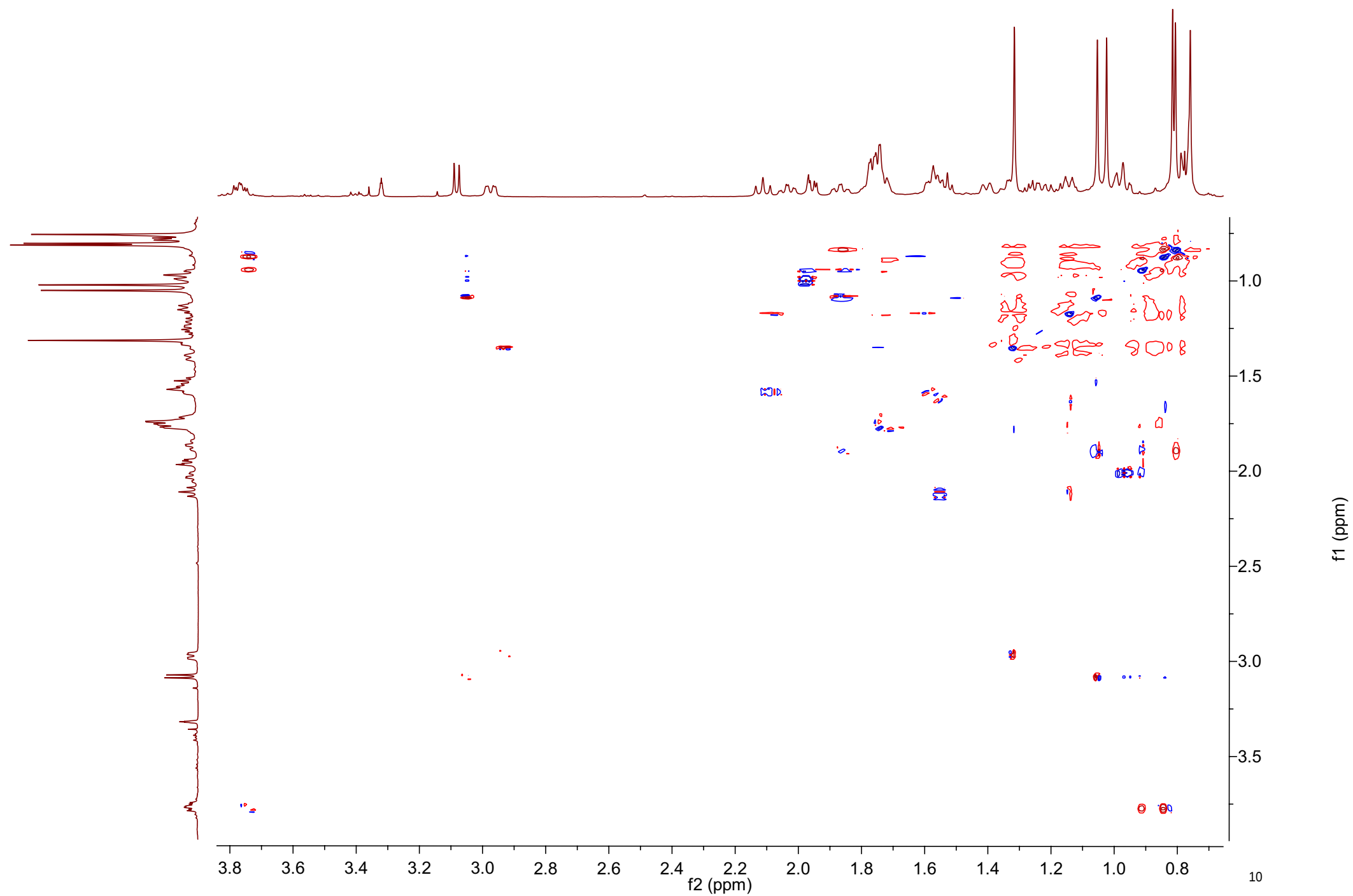


HMBC spectrum of compound 1

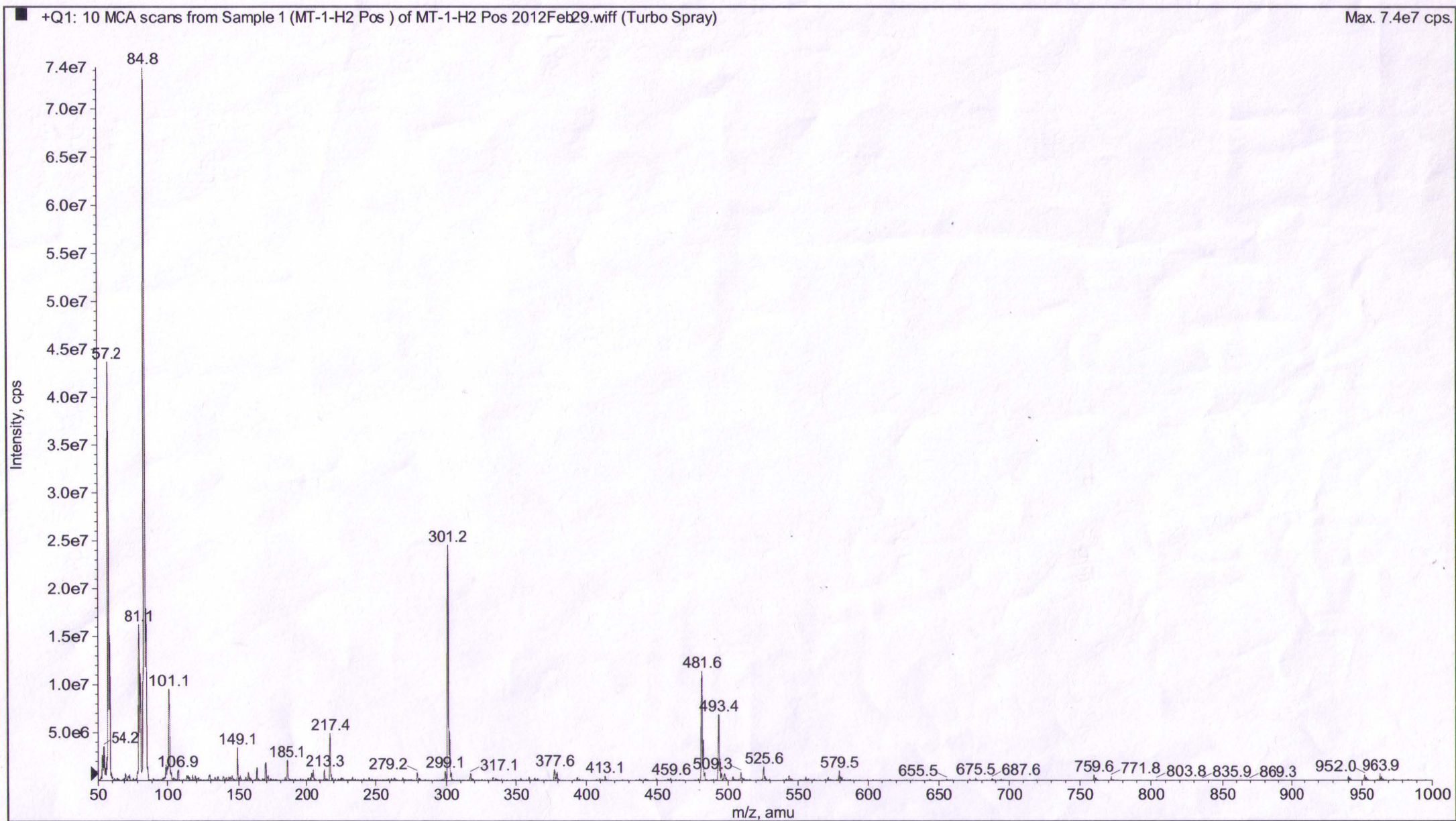


¹H-¹H COSY spectrum of compound 1

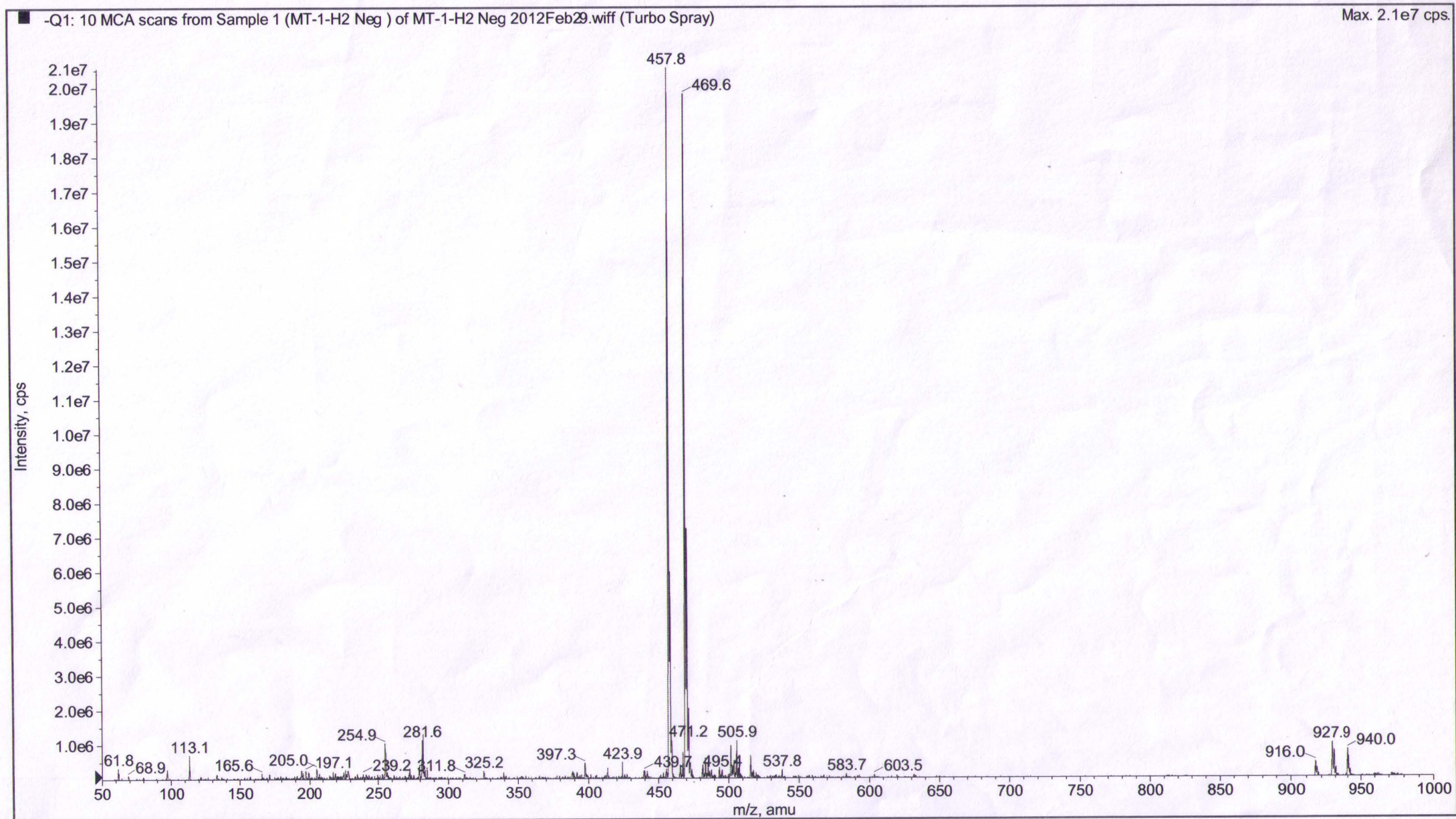
NOESY spectrum of compound 1



ESIMS(+) of Compound 2



ESIMS(-) of Compound 2



Mass Spectrum SmartFormula Report

Analysis Info

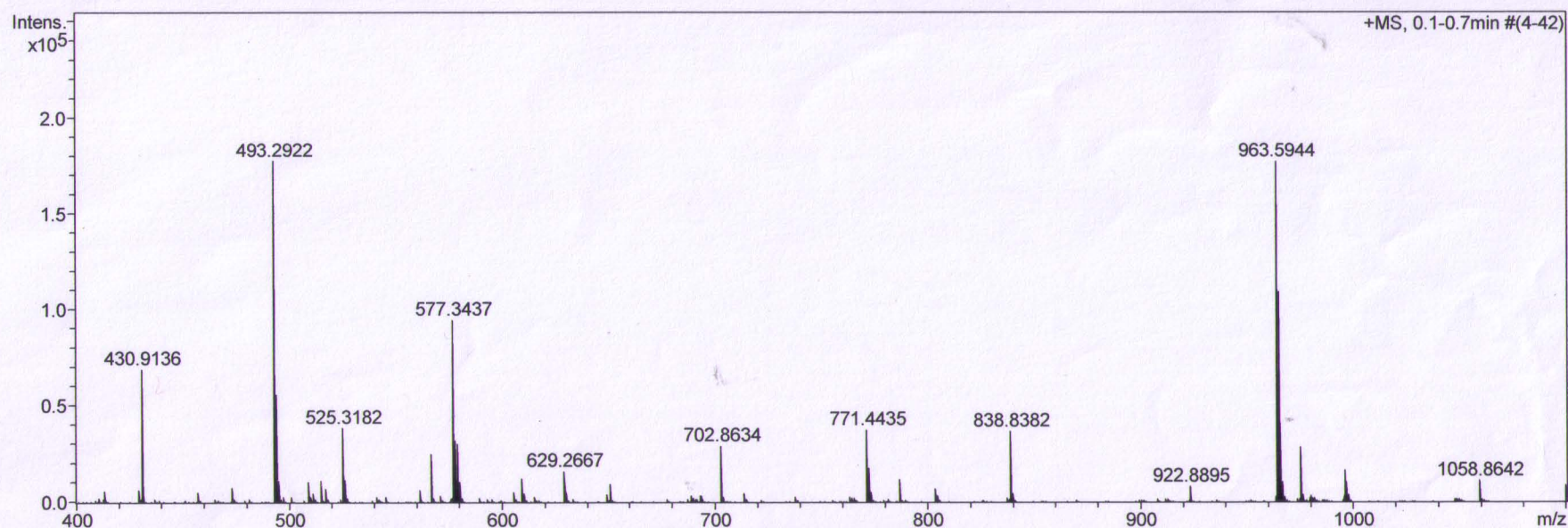
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Sample Name
Comment

Acquisition Date 11/21/2012 11:09:43 AM

Operator SCSIO
Instrument / Ser# maXis 29

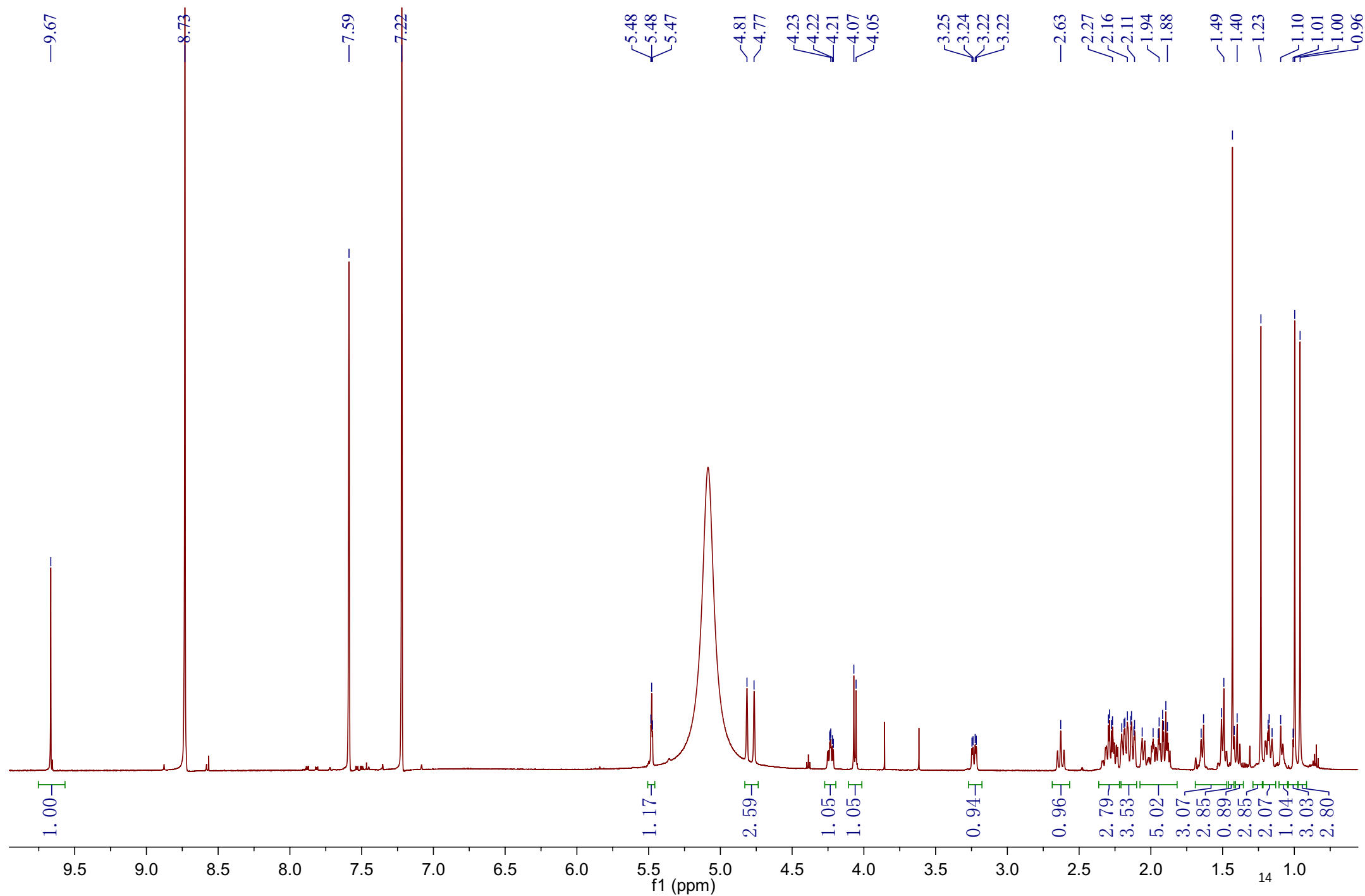
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste

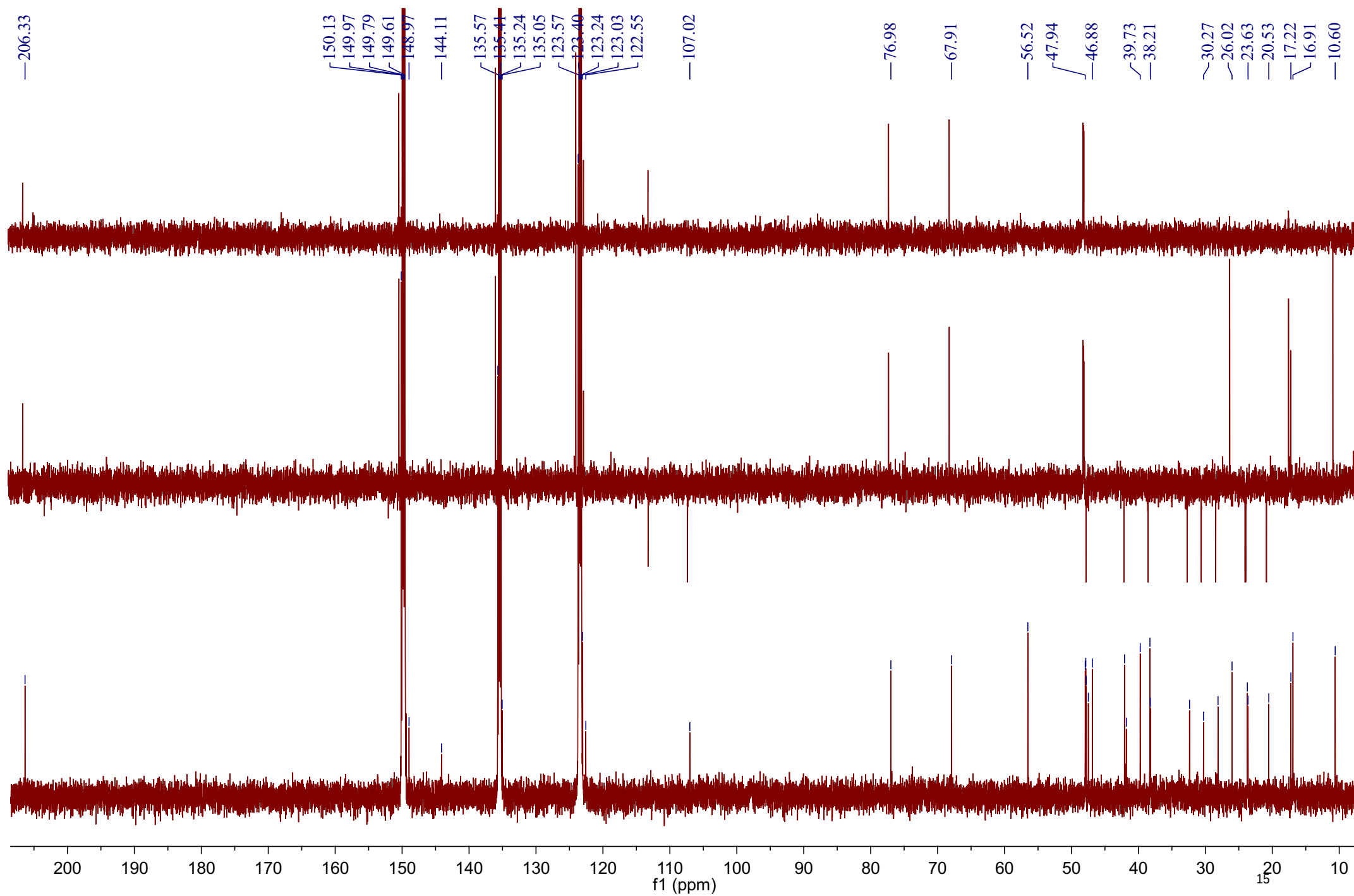


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
493.2922	1	C 29 H 42 Na O 5	100.00	493.2924	0.2	0.5	3.2	8.5	even	ok
963.5944	1	C 58 H 84 Na O 10	100.00	963.5957	1.3	1.4	12.6	16.5	even	ok

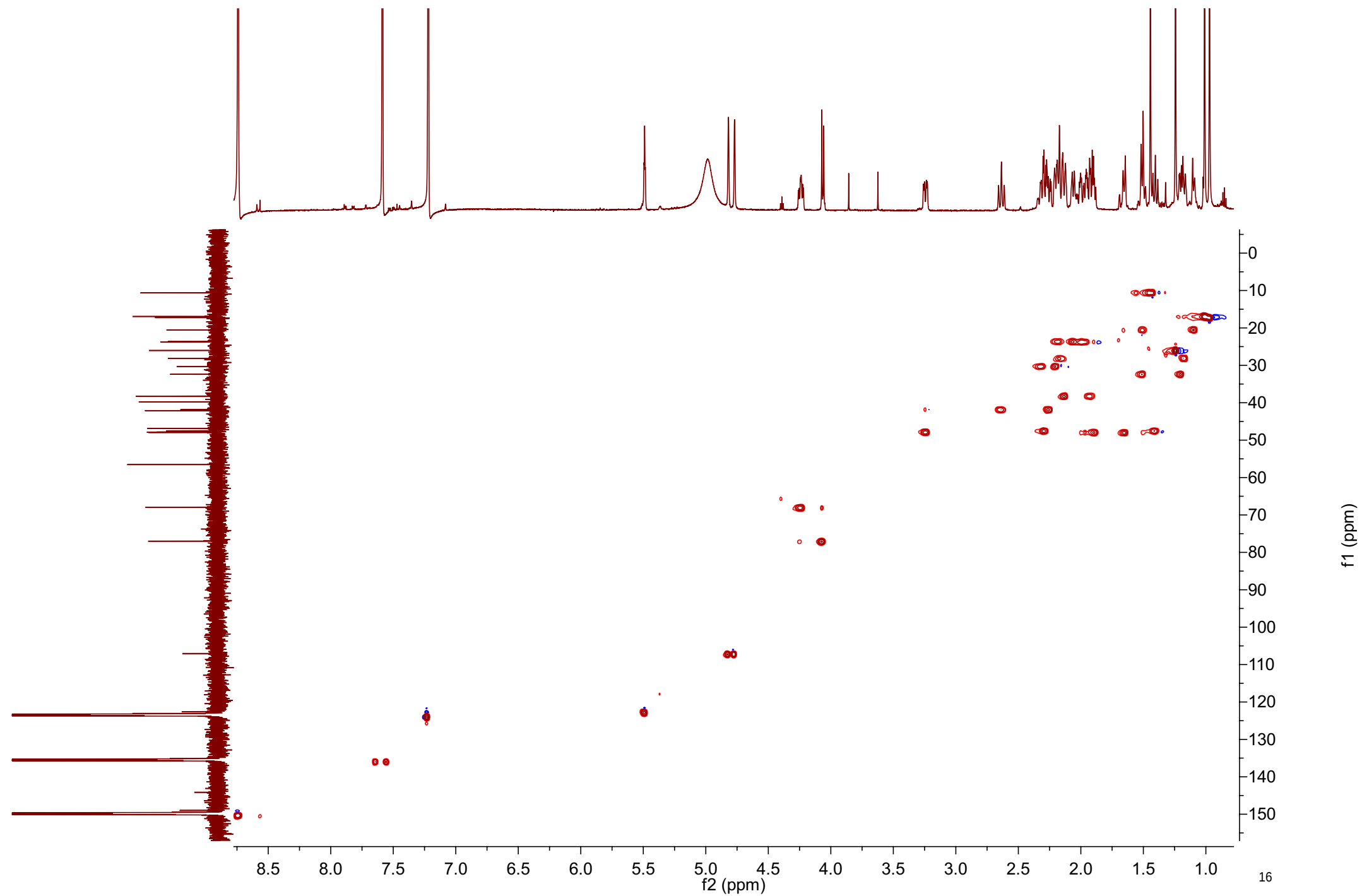
^1H NMR spectrum of compound 2



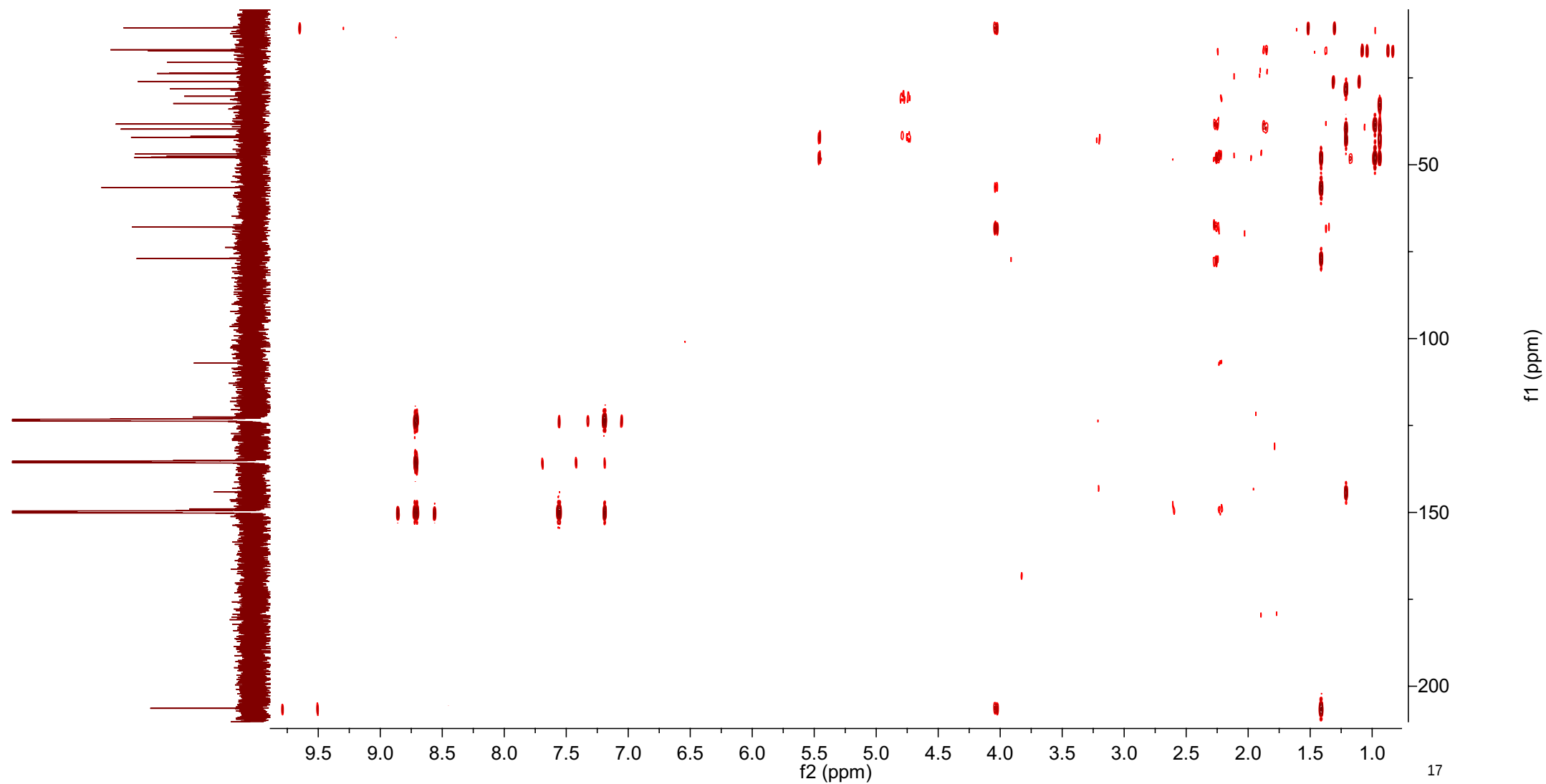
^{13}C NMR and DEPT spectra of compound 2



HSQC spectrum of compound 2



HMBC spectrum of compound 2



NOESY spectrum of compound 2

