Supplementary Materials

3-(2-Chloroethoxy)-1-(4-methoxyphenyl)-1*H*-pyrazole-4-carbaldehyde

Gabrielė Varvuolytė[1,2], Aurimas Bieliauskas[2], Neringa Kleizienė[2], Asta Žukauskaitė[1,3*] and Algirdas Šačkus[1,2]

[1] Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania;
[2] Institute of Synthetic Chemistry, Kaunas University of Technology, Kaunas, Lithuania;
[3] Department of Chemical Biology, Faculty of Science, Palacký University, Olomouc, Czech Republic
* Correspondence: asta.zukauskaite@upol.cz

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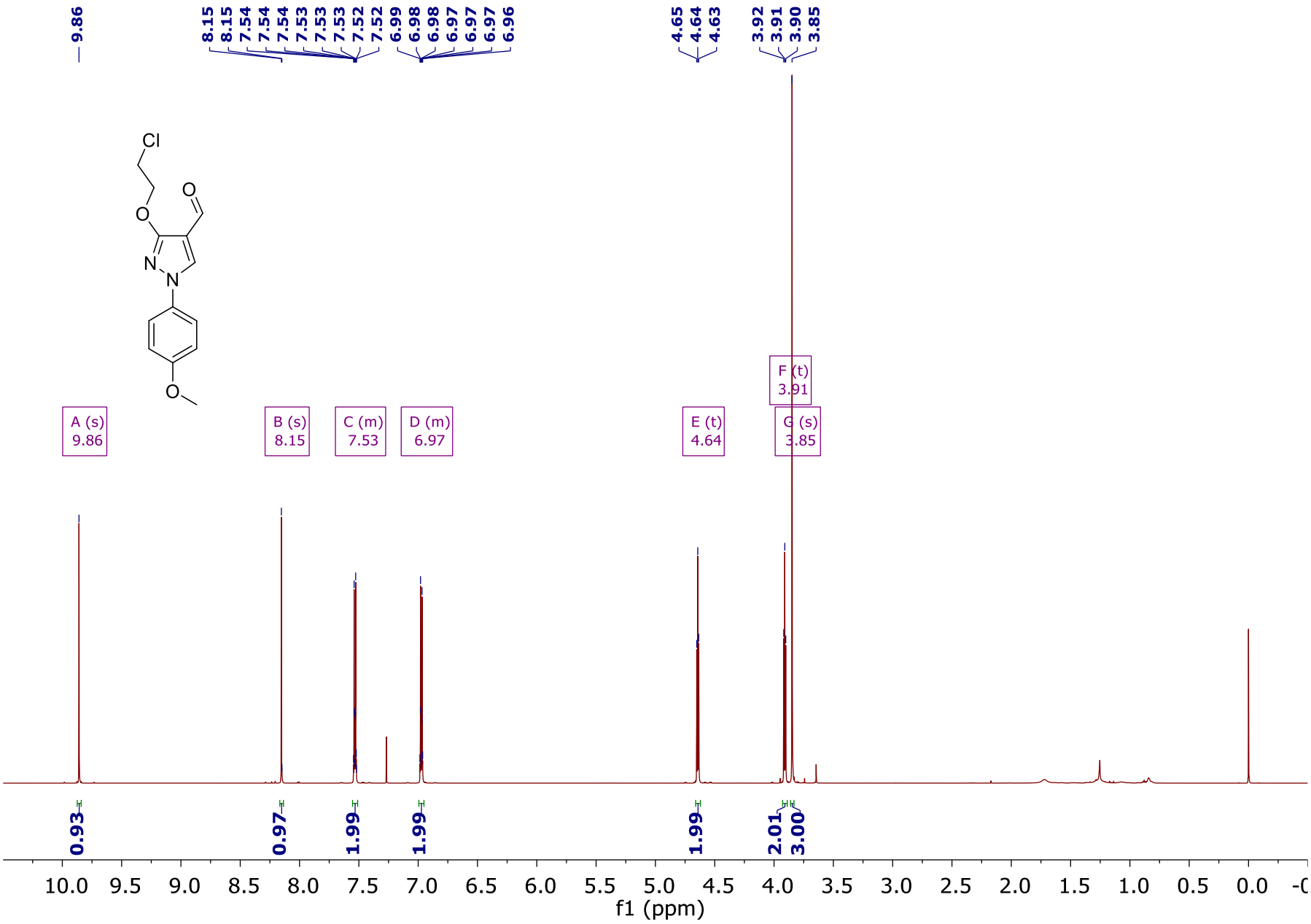


Figure S1. ^{1}H NMR spectrum of compound **2**

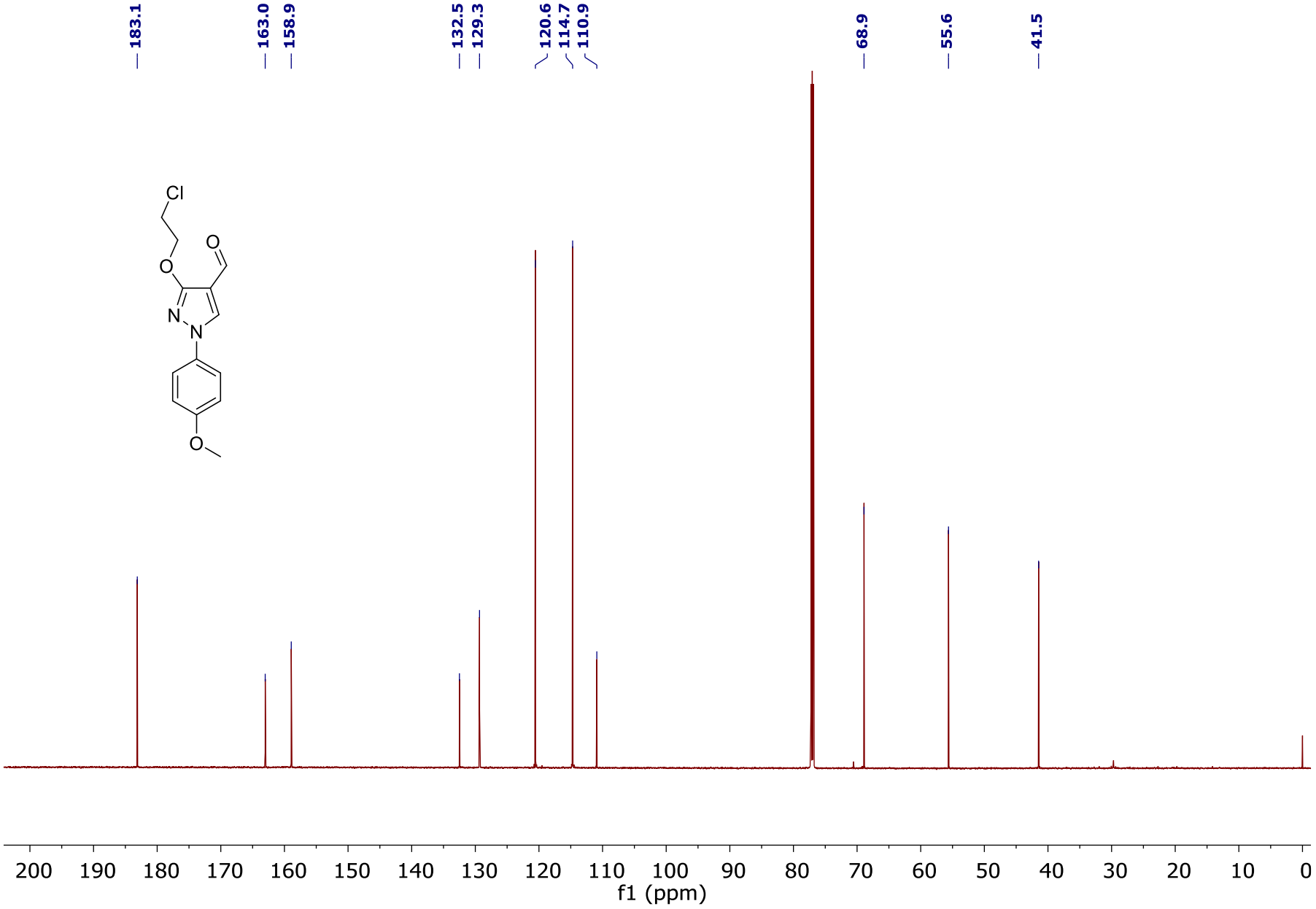


Figure S2. ^{13}C NMR spectrum of compound **2**

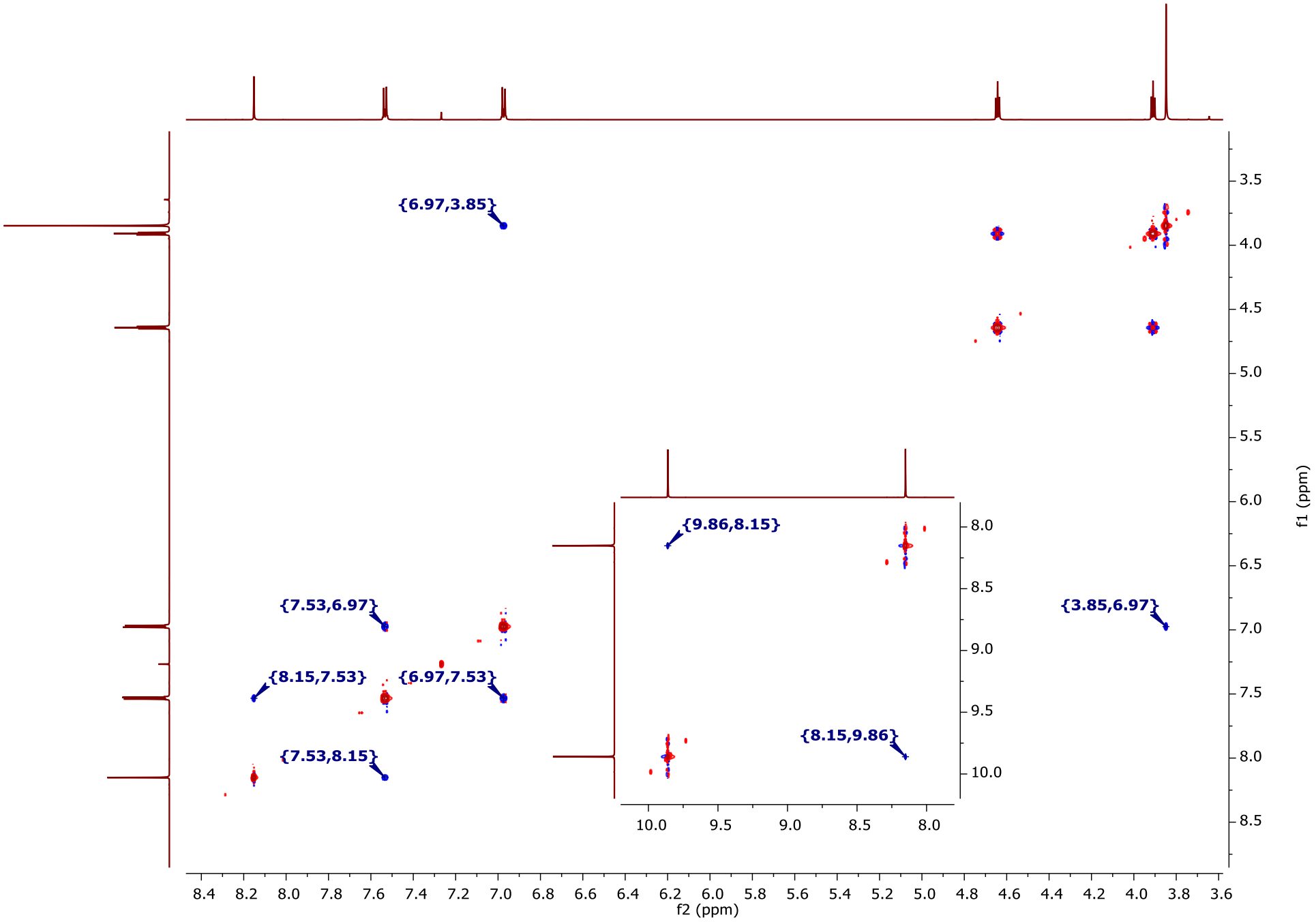


Figure S3. ^{1}H-^{1}H NOESY spectrum of compound **2**

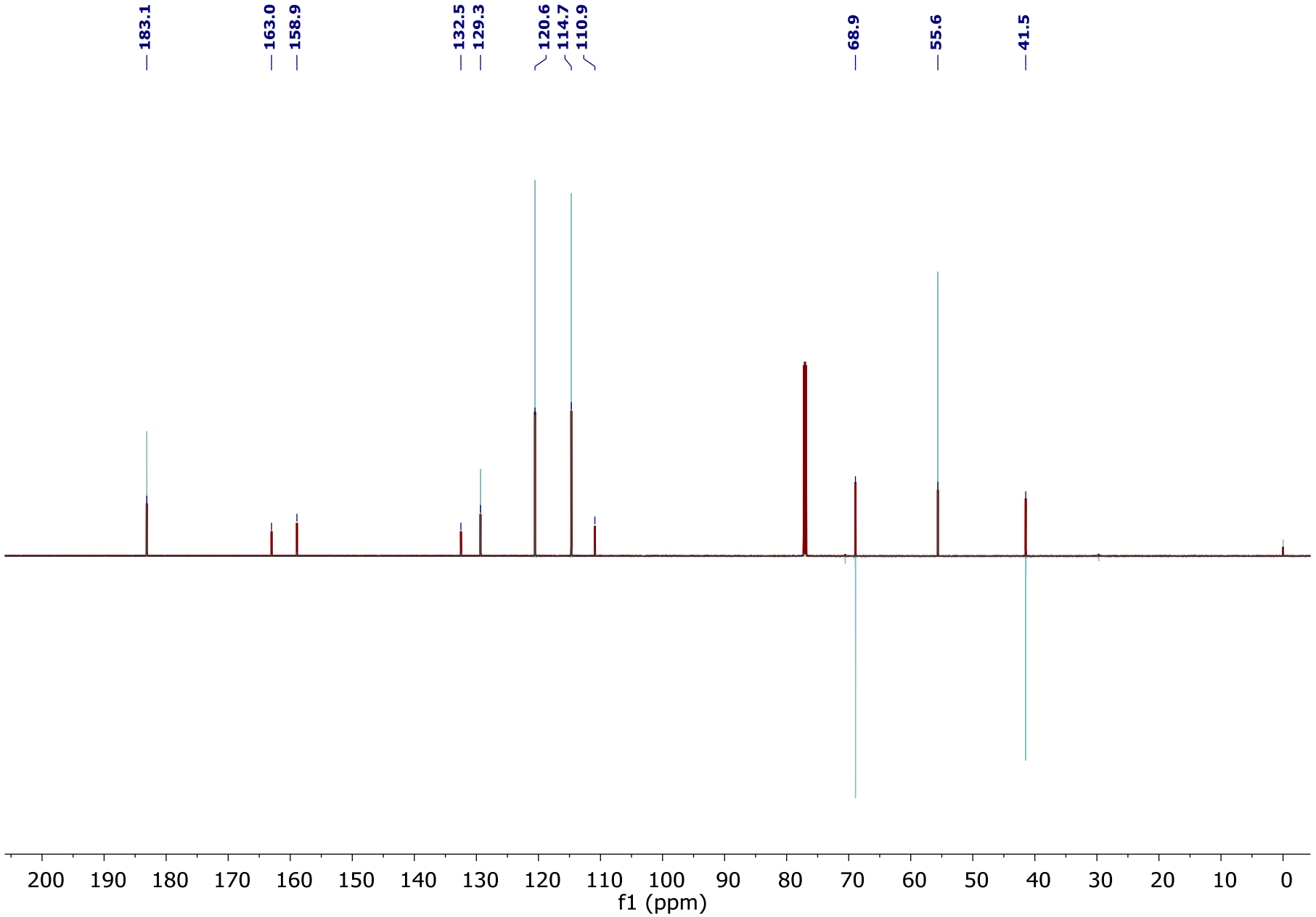


Figure S4. ^{13}C NMR/DEPT 135 spectra of compound **2**

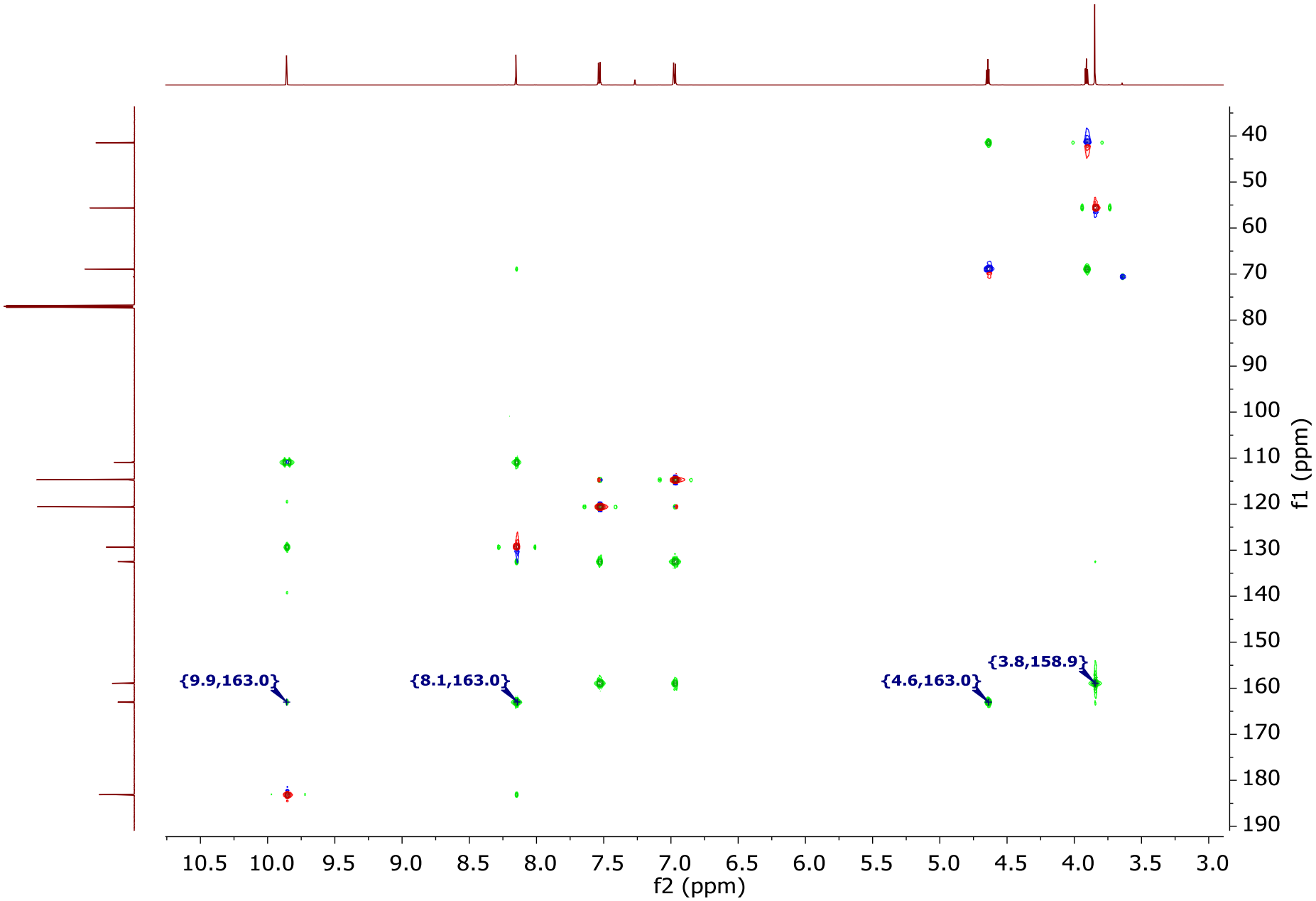


Figure S5. The overlaid ^{1}H-^{13}C HSQC/HMBC NMR spectra of compound **2**

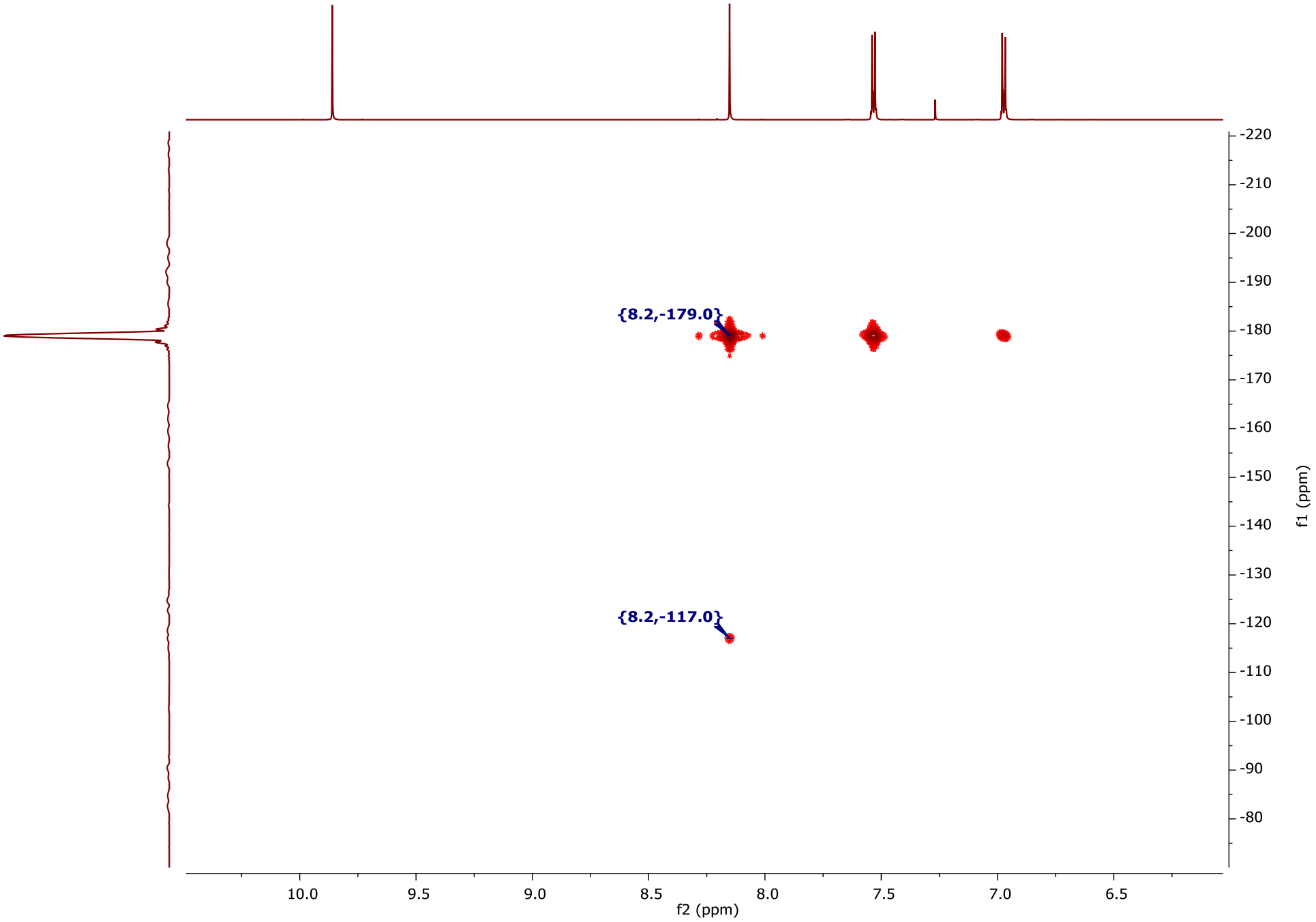


Figure S6. ^{1}H-^{15}N HMBC spectrum of compound **2**

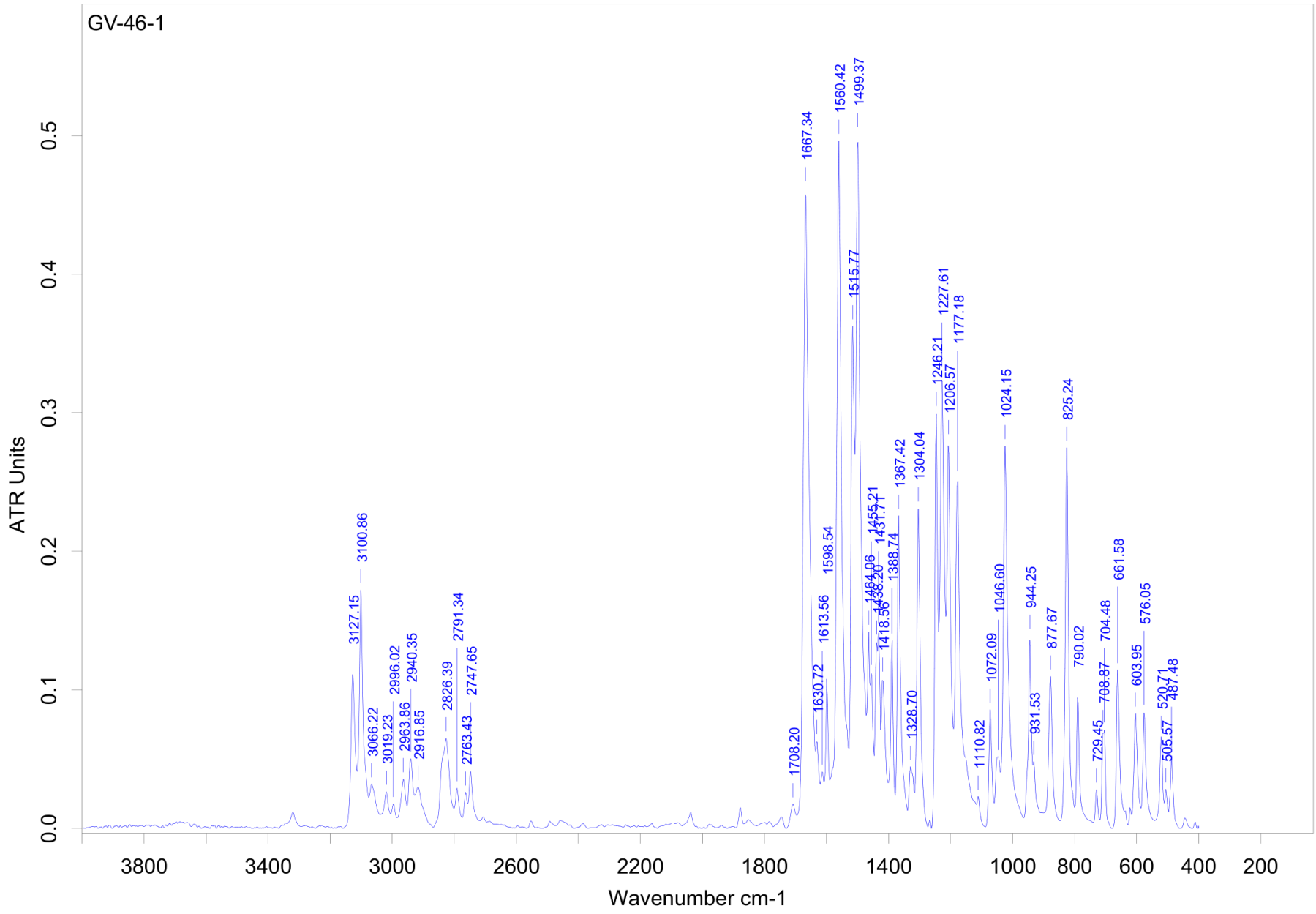


Figure S7. FT-IR spectrum of compound **2**

Compound Spectrum SmartFormula Report

Analysis Info

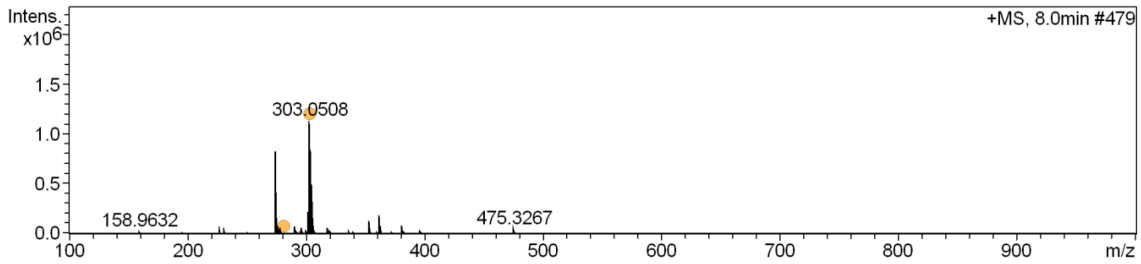
Analysis Name	D:\Data\GV-46-1.d	Acquisition Date	2/5/2024 10:06:03 AM
Method	DirectInfusion_TuneLow_pos.m	Operator	hplc
Sample Name	GV-46-1	Instrument	micrOTOF-Q III 8228888.20448
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.7	n.a.	Single spectrum	n.a.	n.a.	n.a.	304.2610	n.a.
n.a.	8.0	n.a.	Single spectrum	n.a.	n.a.	n.a.	303.0508	n.a.

+MS, 8.0min #479



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
281.0691	1	C13H14ClN2O3	281.0687	1.4	71.2	1	100.00	7.5	even	ok
303.0508	1	C13H13ClN2NaO3	303.0507	-0.3	52.2	1	100.00	7.5	even	ok

Figure S8. HRMS spectrum of compound **2**