

SUPPORTING INFORMATION

Methyl 2-amino-4-[1-(tert-butoxycarbonyl)azetidine-3-yl]-1,3-selenazole-5-carboxylate

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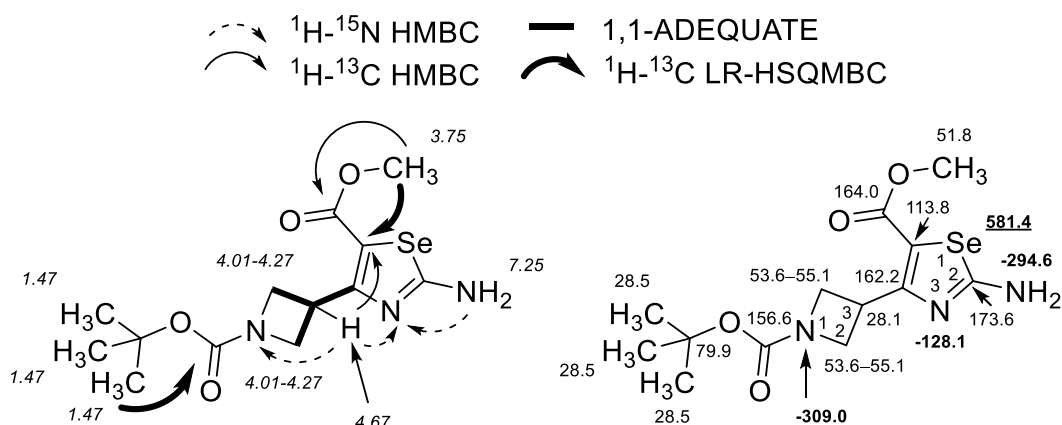
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Correlations:



Relevant 1,1-ADEQUATE, ¹H-¹³C HMBC, ¹H-¹⁵N HMBC, ¹H-¹³C LR-HSQC correlations and ¹H NMR (in italics), ¹⁵N NMR (in bold), ⁷⁷Se (in bold, underlined) and ¹³C NMR chemical shifts of Compound **4**.

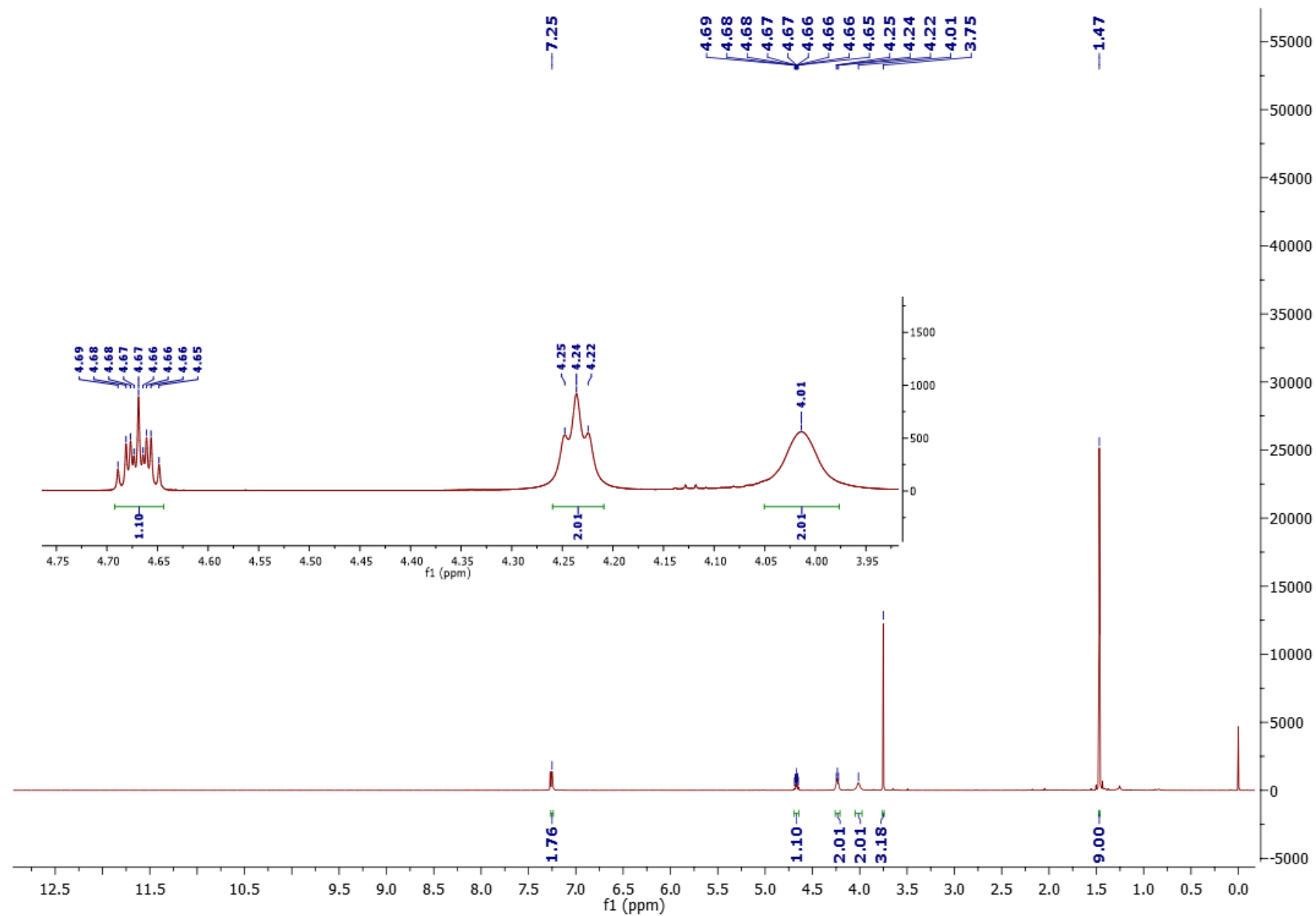


Figure S1. ^1H NMR spectrum of compound 4.

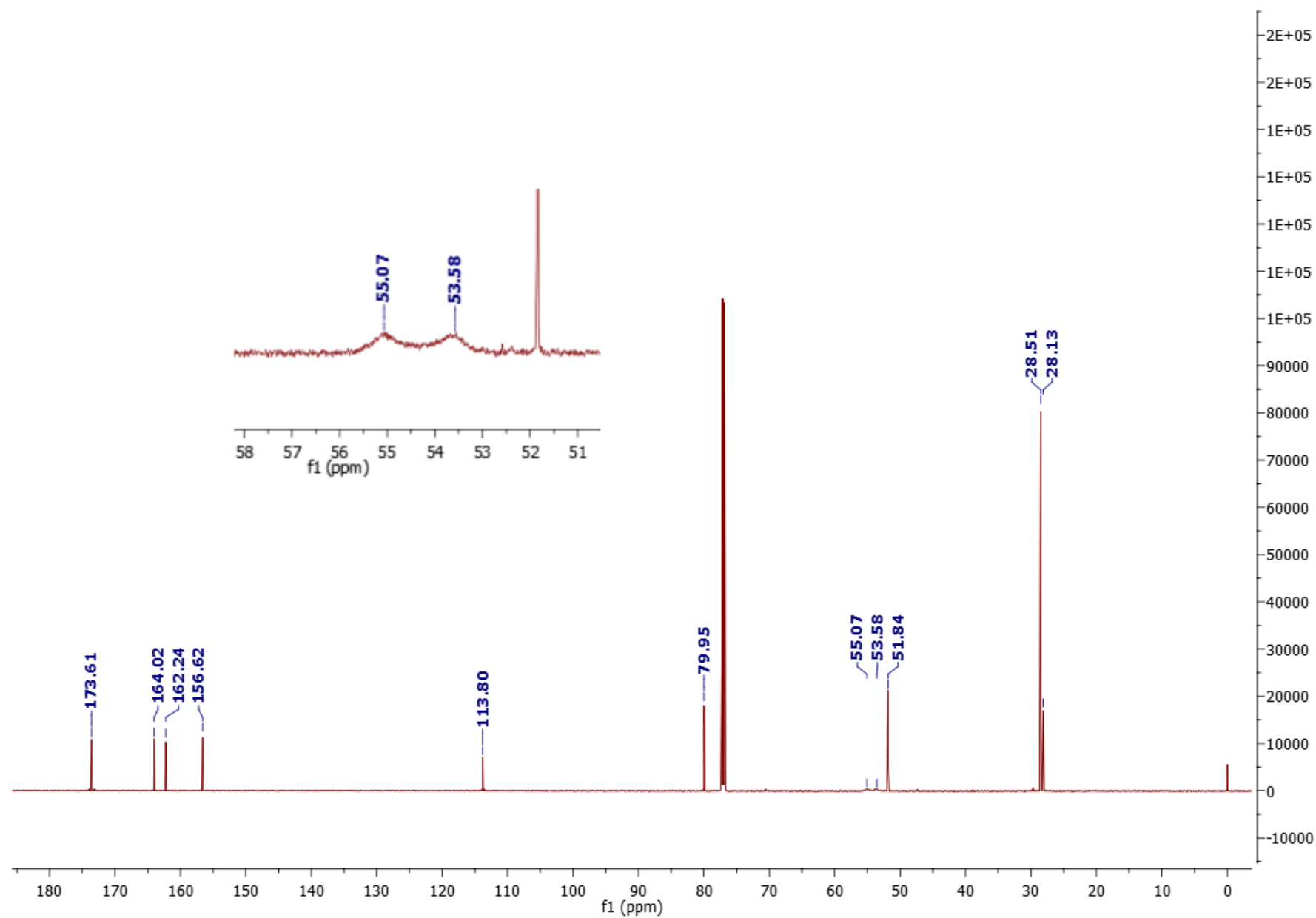


Figure S2. ^{13}C NMR spectrum of Compound 4.

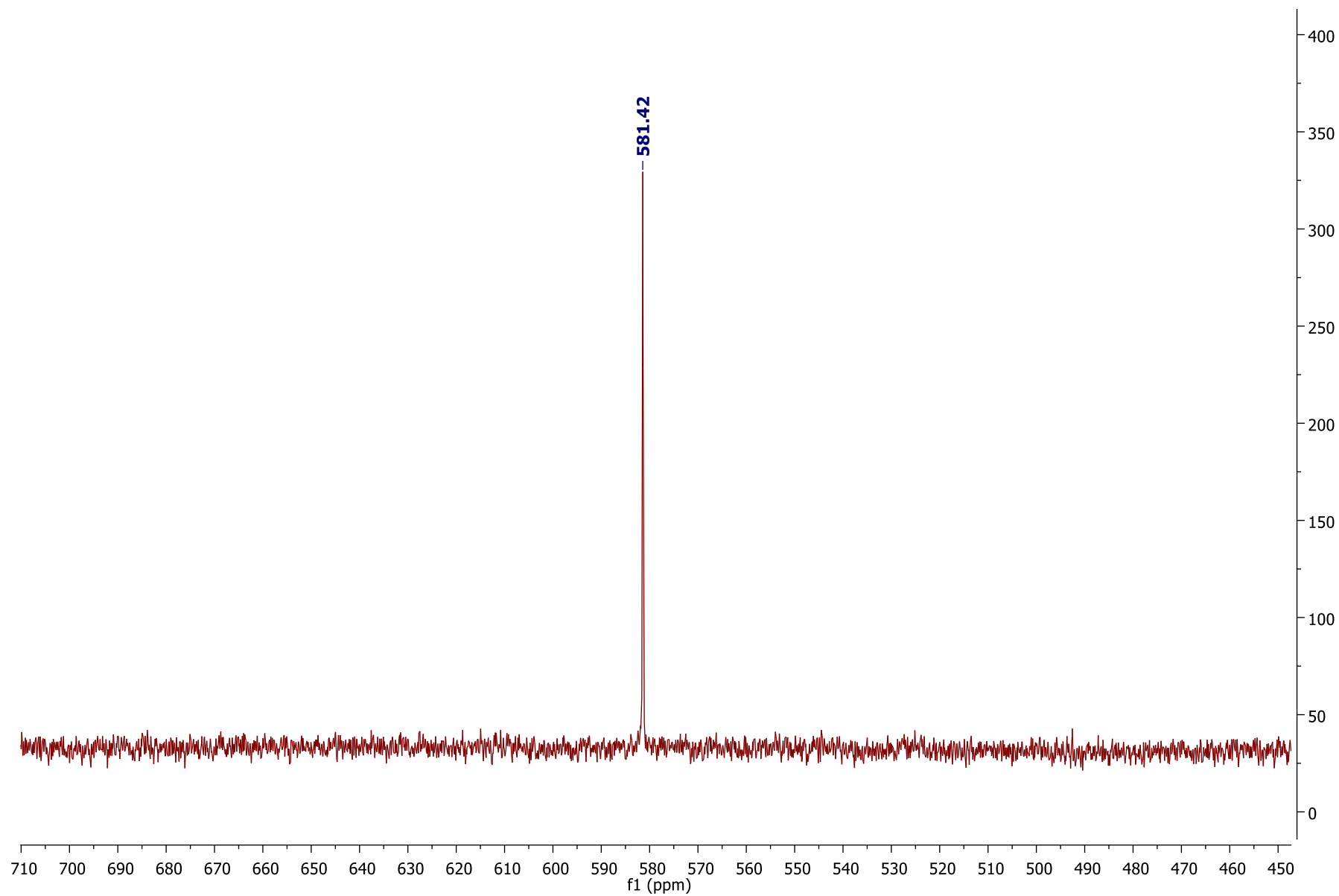


Figure S3. ^{77}Se NMR spectrum of Compound **4**.

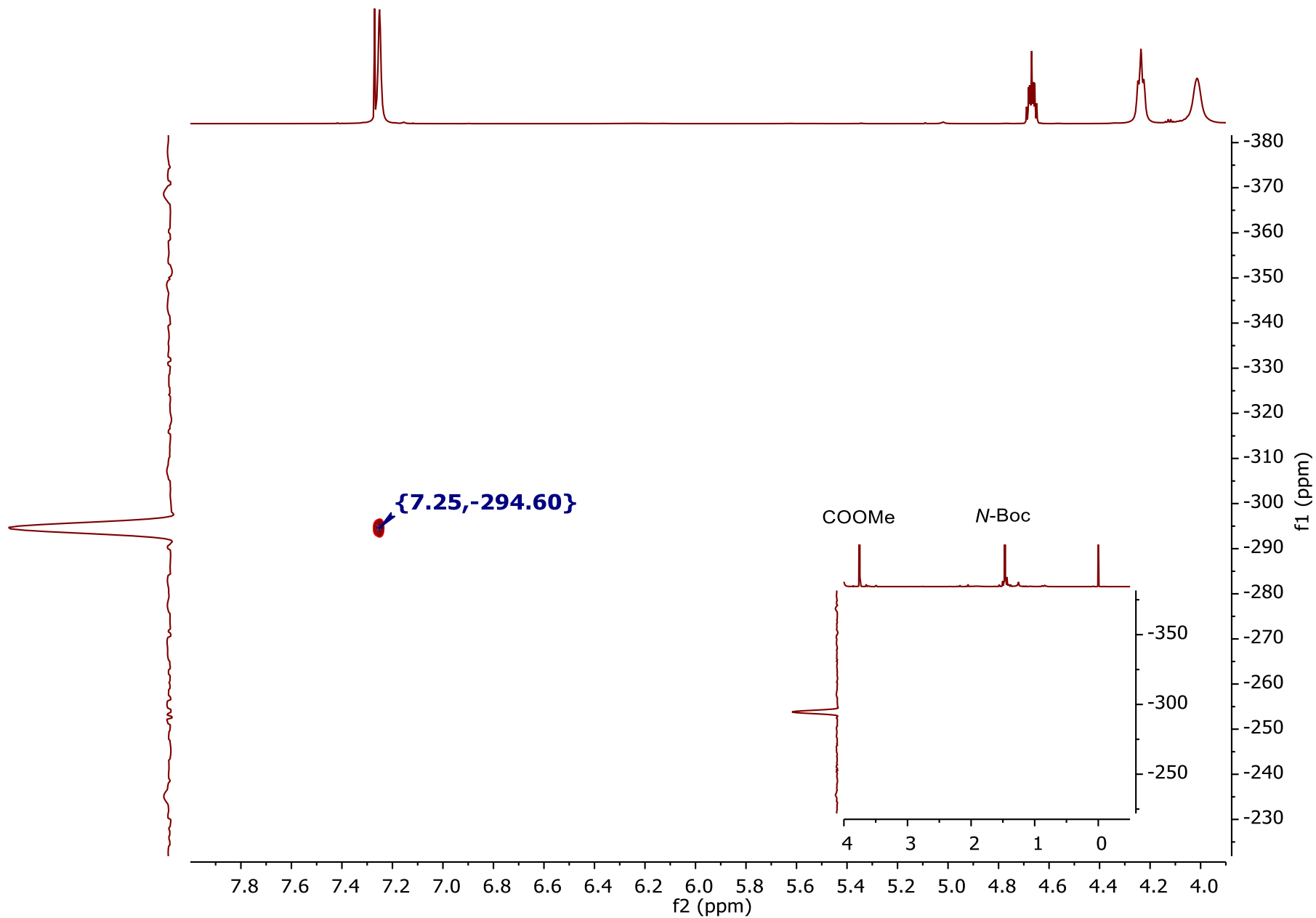


Figure S4. ^1H - ^{15}N HSQC NMR spectrum of compound 4.

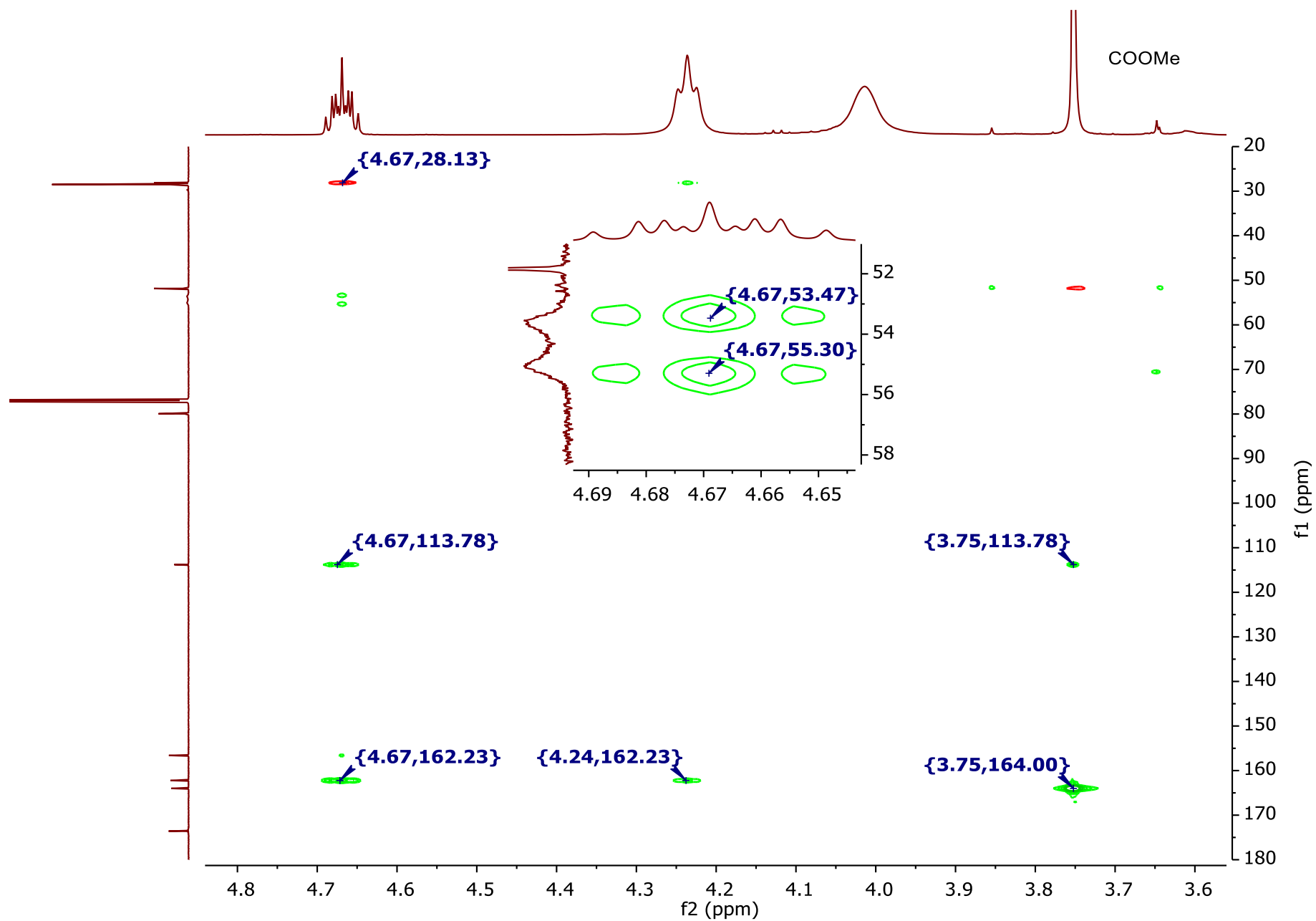


Figure S5. The overlaid ^1H - ^{13}C gs-HSQC and gs-HMBC NMR spectra of compound 4.

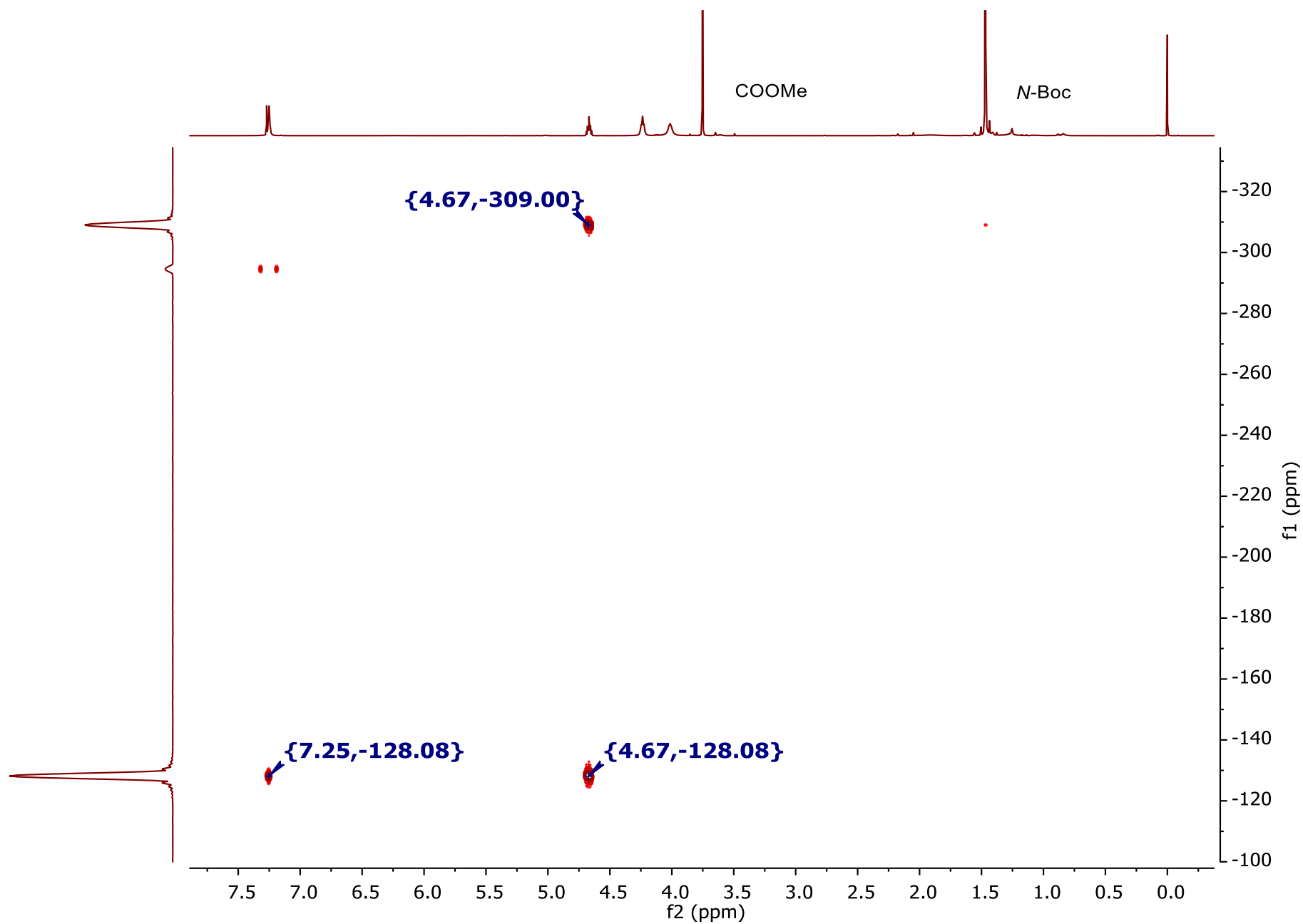


Figure S6. ¹H-¹⁵N HMBC NMR spectrum of compound 4.

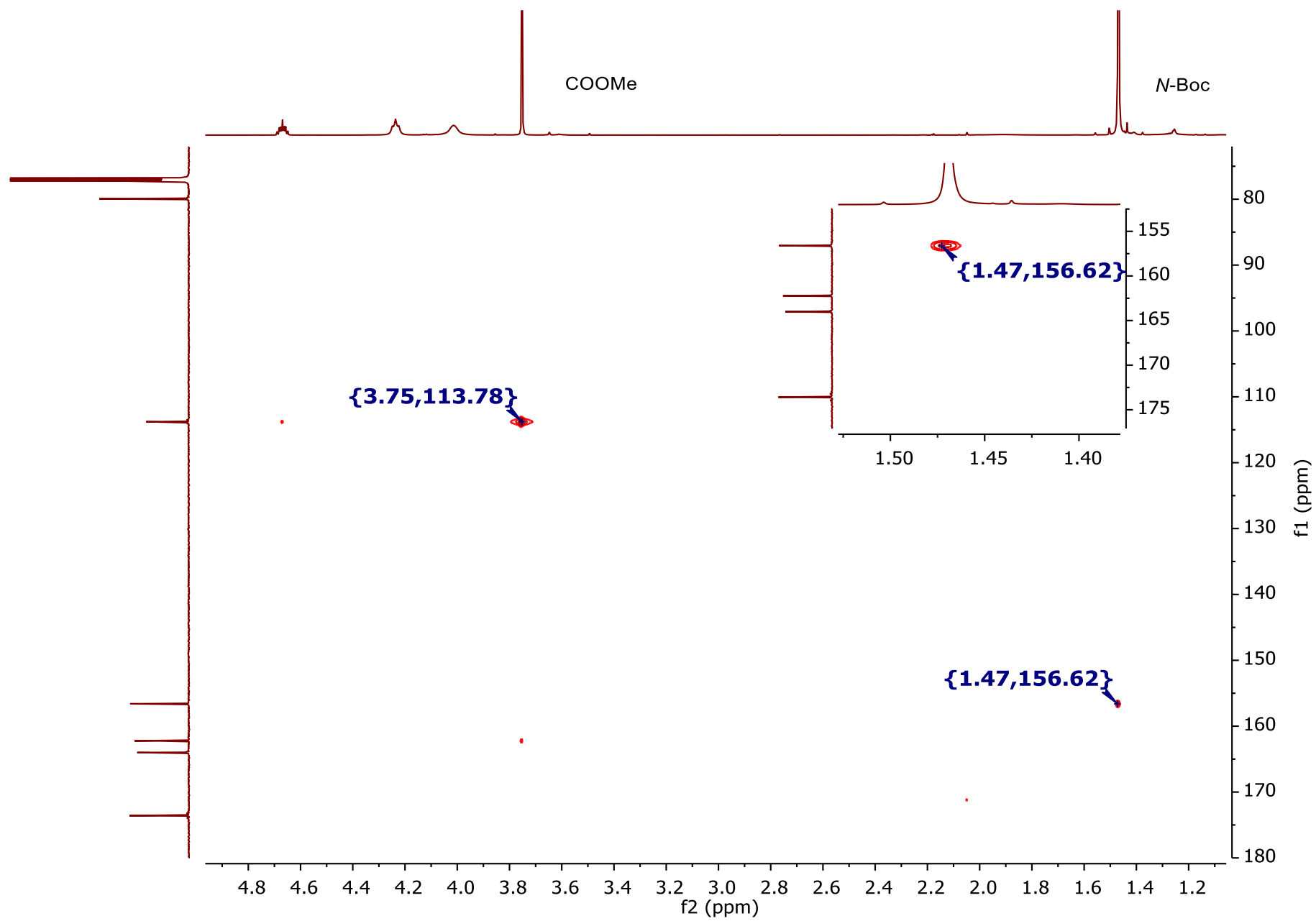


Figure S7. ^1H - ^{13}C 2 Hz LR-HSQC NMR spectra of compound 4.

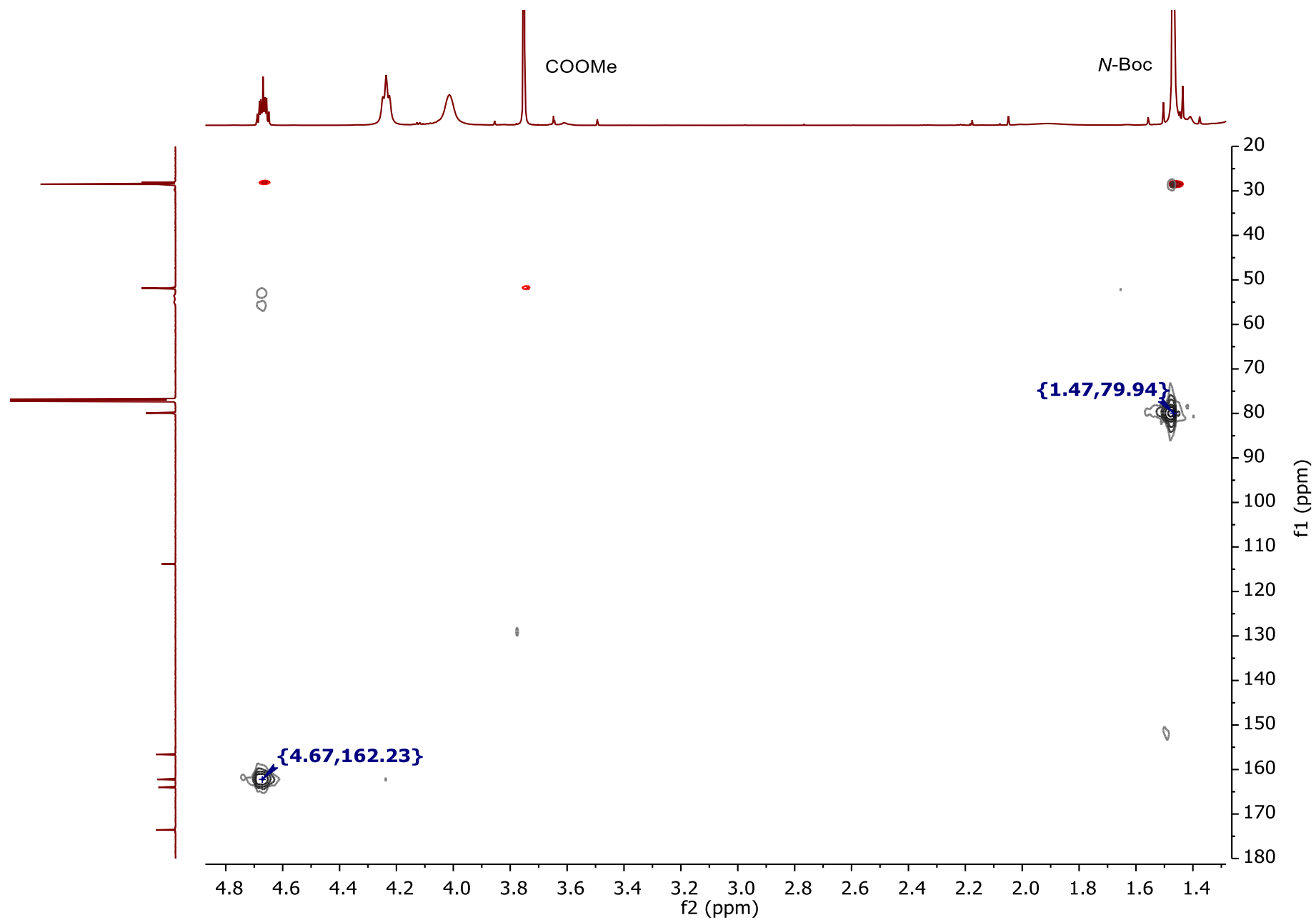


Figure S8. The overlaid ^1H - ^{13}C gs-HSQC (red) and 60 Hz 1,1-ADEQUATE (black) NMR spectra of compound 4.

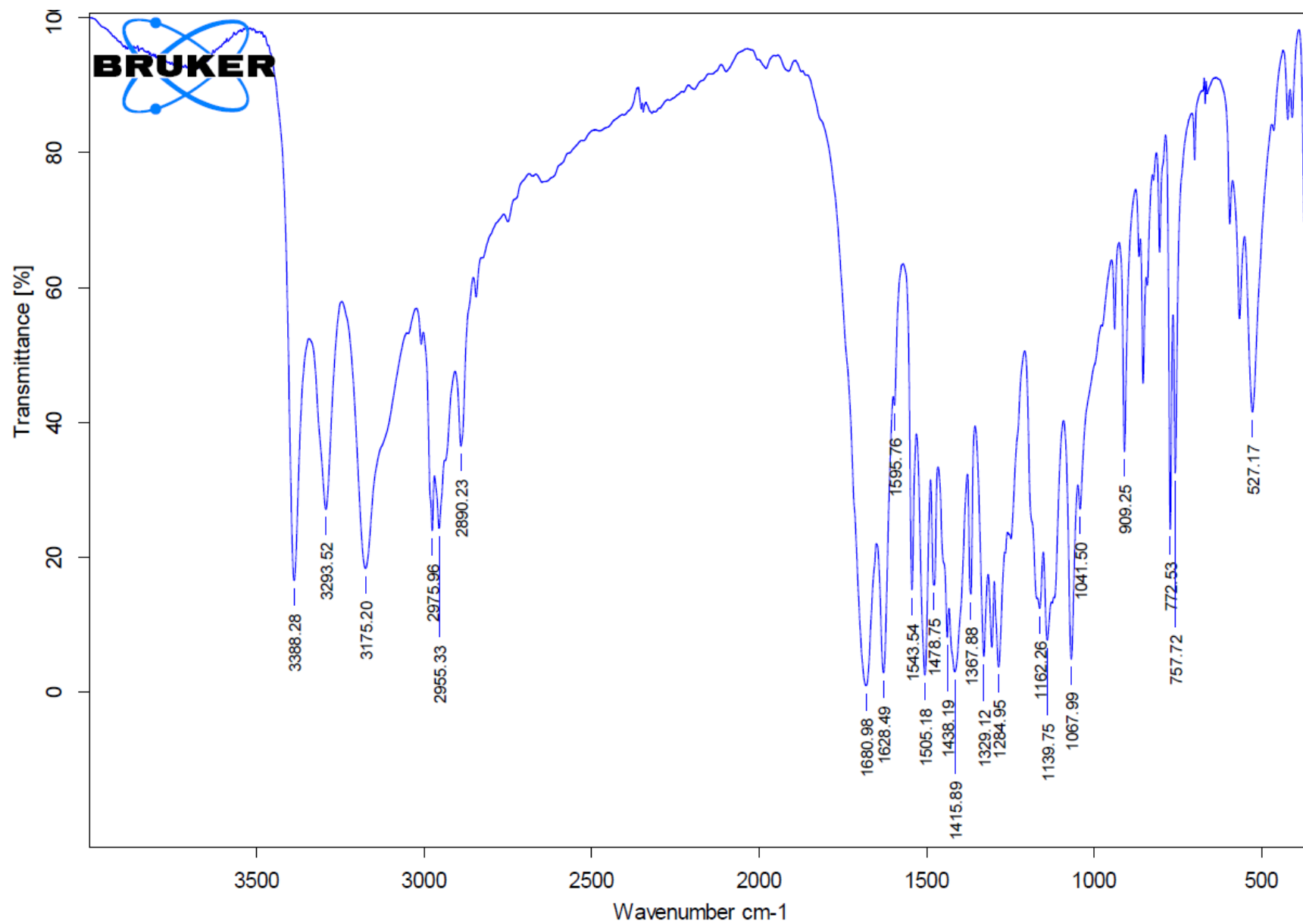


Figure S9. IR spectrum of Compound 4.

Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\KDP-063.d
Method DirectInfusion_TuneLow_pos.m
Sample Name KDP-063
Comment AB

Acquisition Date 9/23/2020 5:49:47 PM

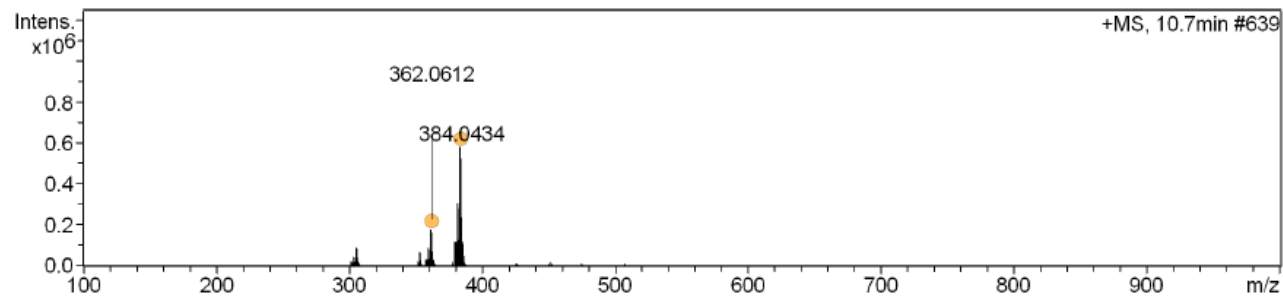
Operator hplc
Instrument micrOTOF-Q III 8228888.20448

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.	10.7	n.a.	Single spectrum	n.a.	n.a.	n.a.	384.0434	n.a.

+MS, 10.7min #639



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
362.0612	1	C ₁₃ H ₂₀ N ₃ O ₄ Se	362.0614	-0.5	8.6	1	100.00	5.5	even	ok
384.0434	1	C ₁₃ H ₁₉ N ₃ NaO ₄ Se	384.0434	0.0	14.5	3	100.00	5.5	even	ok

Figure S10. HRMS spectrum of Compound 4.