Supporting Information

Cyclohexadepsipeptides of the Isaridin Class from the Marine-Derived Fungus *Beauveria felina* EN-135

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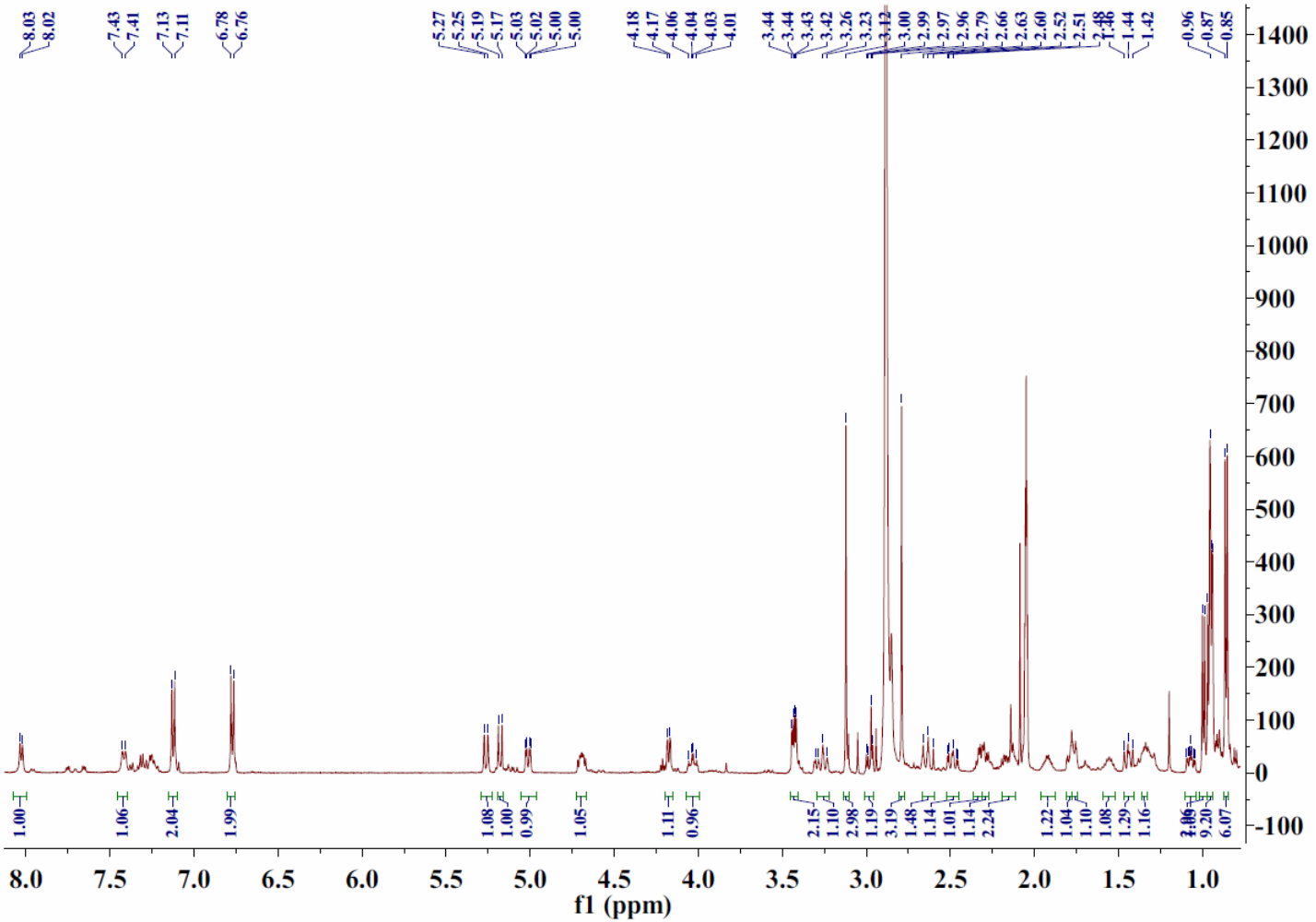
Table S1. Main torsion angels in the crystal structures of compounds **1–3**.

Residue		Torsion angel (°)		
		Isaridin G (**1**)	desmethylisaridin G (**2**)	desmethylisaridin C1 (**3**)
HMPA[1]	φ_1	-60.2	-109.4	-66.1
	ψ_1	147.7	142.1	-42.7
	ω_1	9	-9.8	176.9
Pro[2]	φ_2	-81.4	-66.5	-68.3
	ψ_2	-2	156.4	155.0
	ω_2	166.5	175.4	177.1
Tyr[3]/Tyr[3]/Phe[3]	φ_3	-64.3	-61.5	-97.2
	ψ_3	141.8	142.5	124.8
	ω_3	178.0	-2.6	2.8
N-Me-Val[4]	φ_4	-104.7	-111.9	-114.8
	ψ_4	103.0	52.6	68.1
	ω_4	6	-178.9	-170.5
N-Me-Leu[5]/Leu[5]/Leu[5]	φ_5	-124.5	-104.8	-115.3
	ψ_5	107.9	-24.2	-8.5
	ω_5	177.4	-170.4	-175.8
	ω_5'		-178.3	
β-Ala[6]	φ_6	-137.5	-162.4	83.2
	φ_6'		82.0	
	θ_6	-59.1	-56.7	71.2
	θ_6'		60.8	
	ψ_6	124.1	-82.4	-164.5
	ψ_6'		-168.0	
	ω_6	-170.0	175.9	177.7
	ω_6'		156.9	

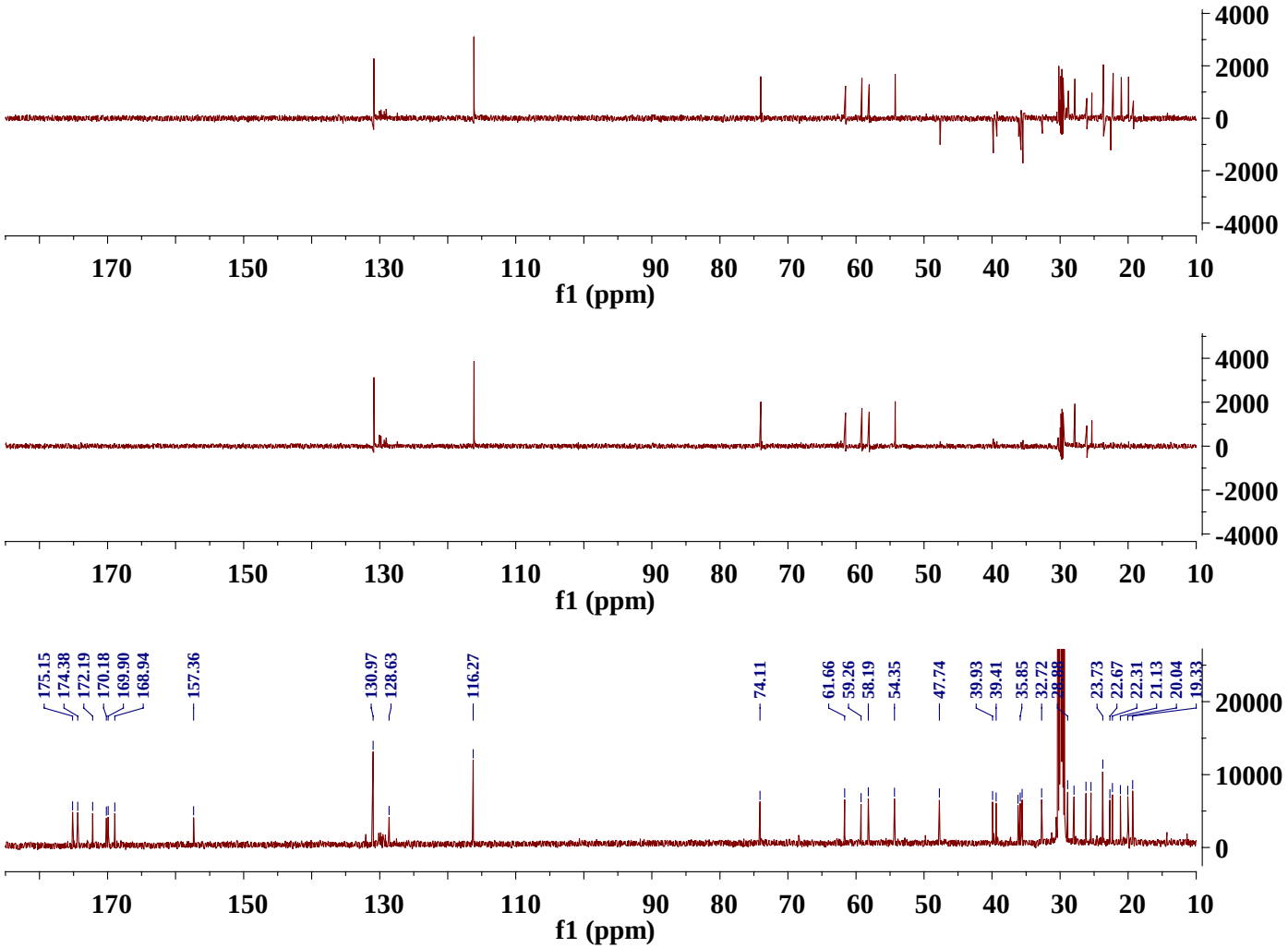
Table S2. H-bonds parameters for compounds **1–3**.

Donor	Acceptor	*d*(D···A)[Å]	*d*(H···A)[Å]
isaridin G (**1**)			
NH (*β*-Ala[6])	CO (Tyr[3])	2.876	2.071
NH (Tyr[3])	CO (*β*-Ala[6])	3.080	2.542
desmethylisaridin G (**2**)			
NH (Leu[5])	CO (Pro[2])	2.938	2.104
NH (*β*-Ala[6])	CO (*β*-Ala[6])	2.940	2.319
NH′ (*β*-Ala[6])	HN (Leu[5])	2.714	2.293
desmethylisaridin C1 (**3**)			
NH (Leu[5])	CO (Pro[2])	2.820	1.986

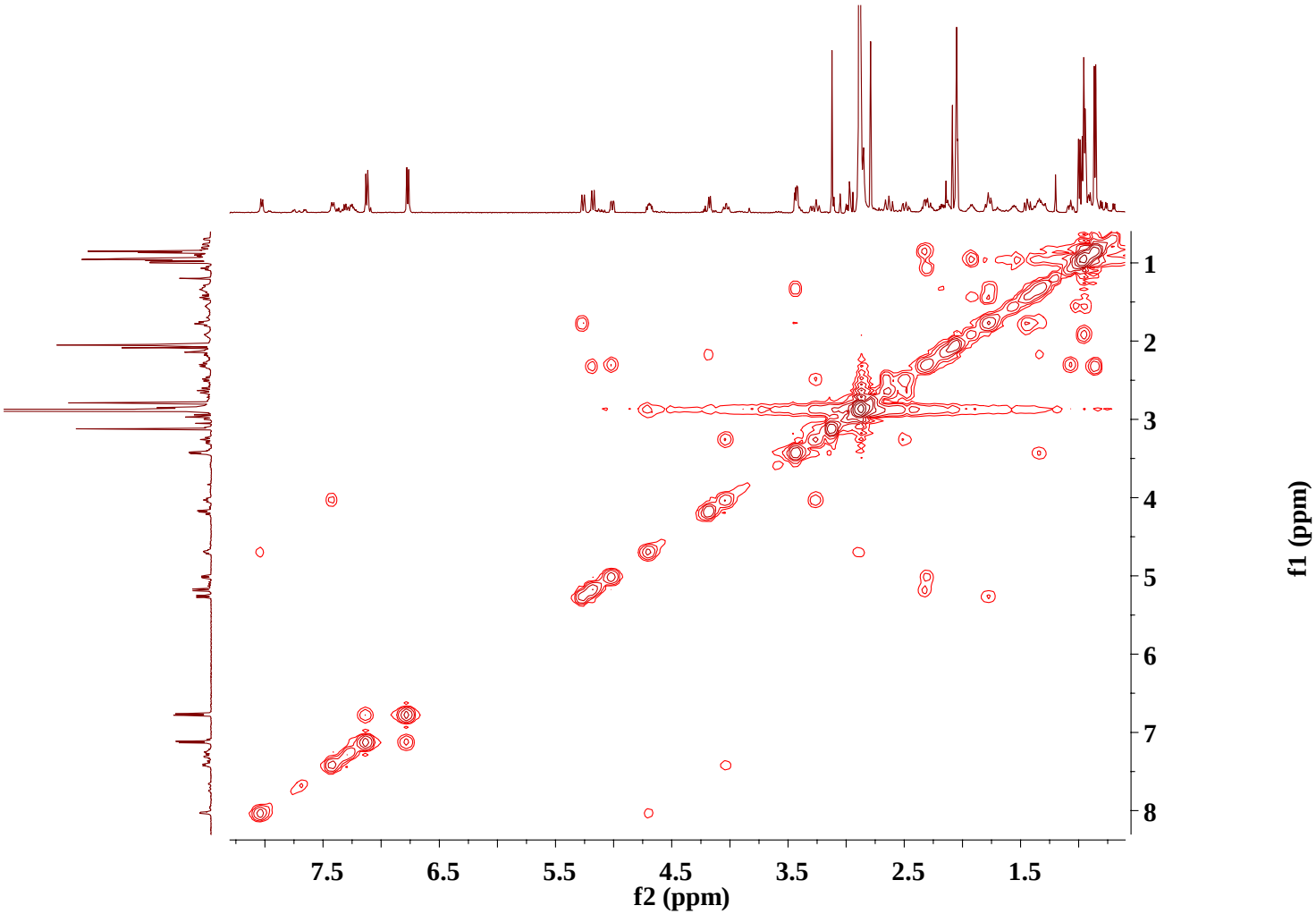
^{1}H NMR (500 MHz, Acetone-d_6) spectrum of compound **1**.



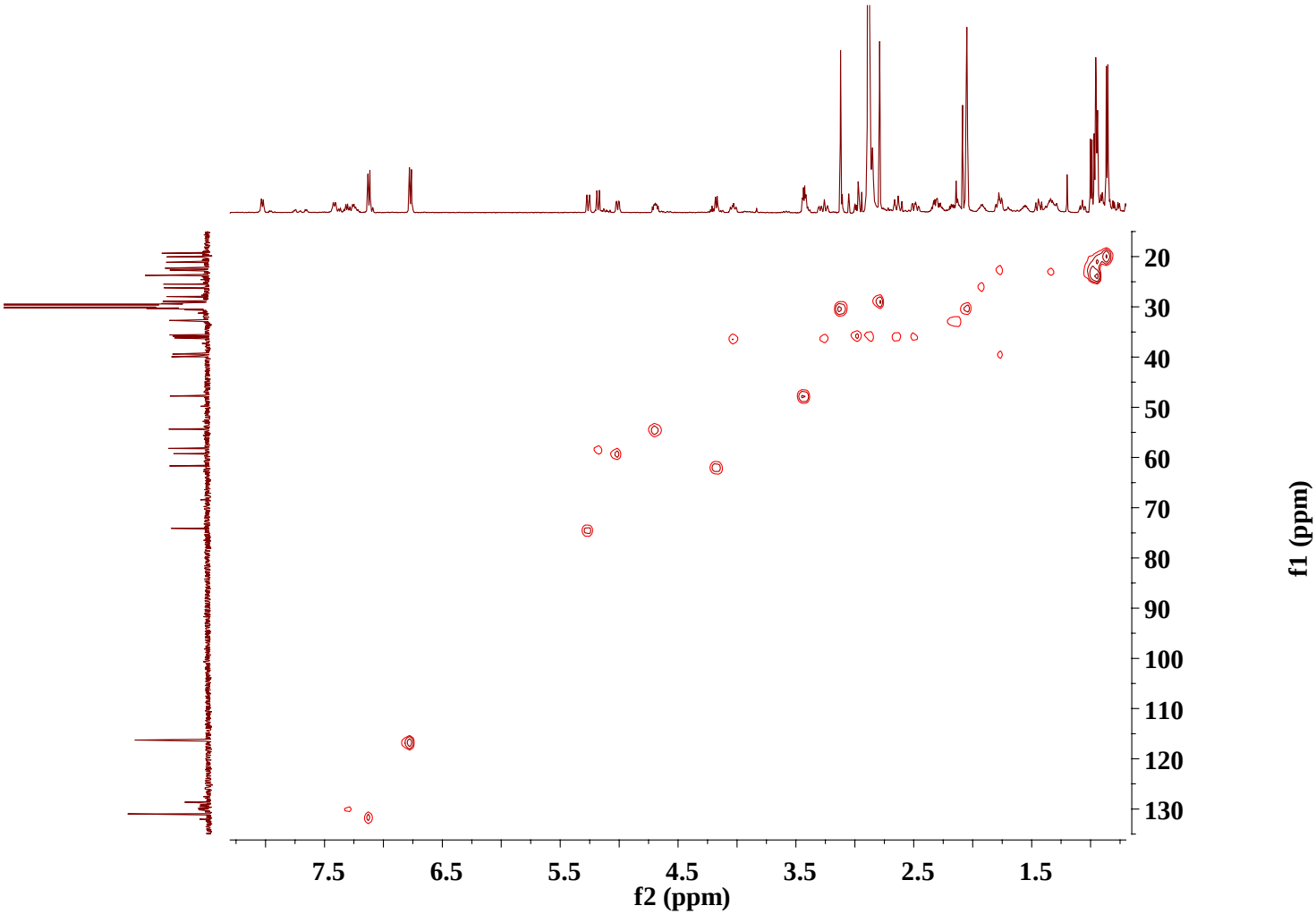
DEPT spectrum of compound **1**.



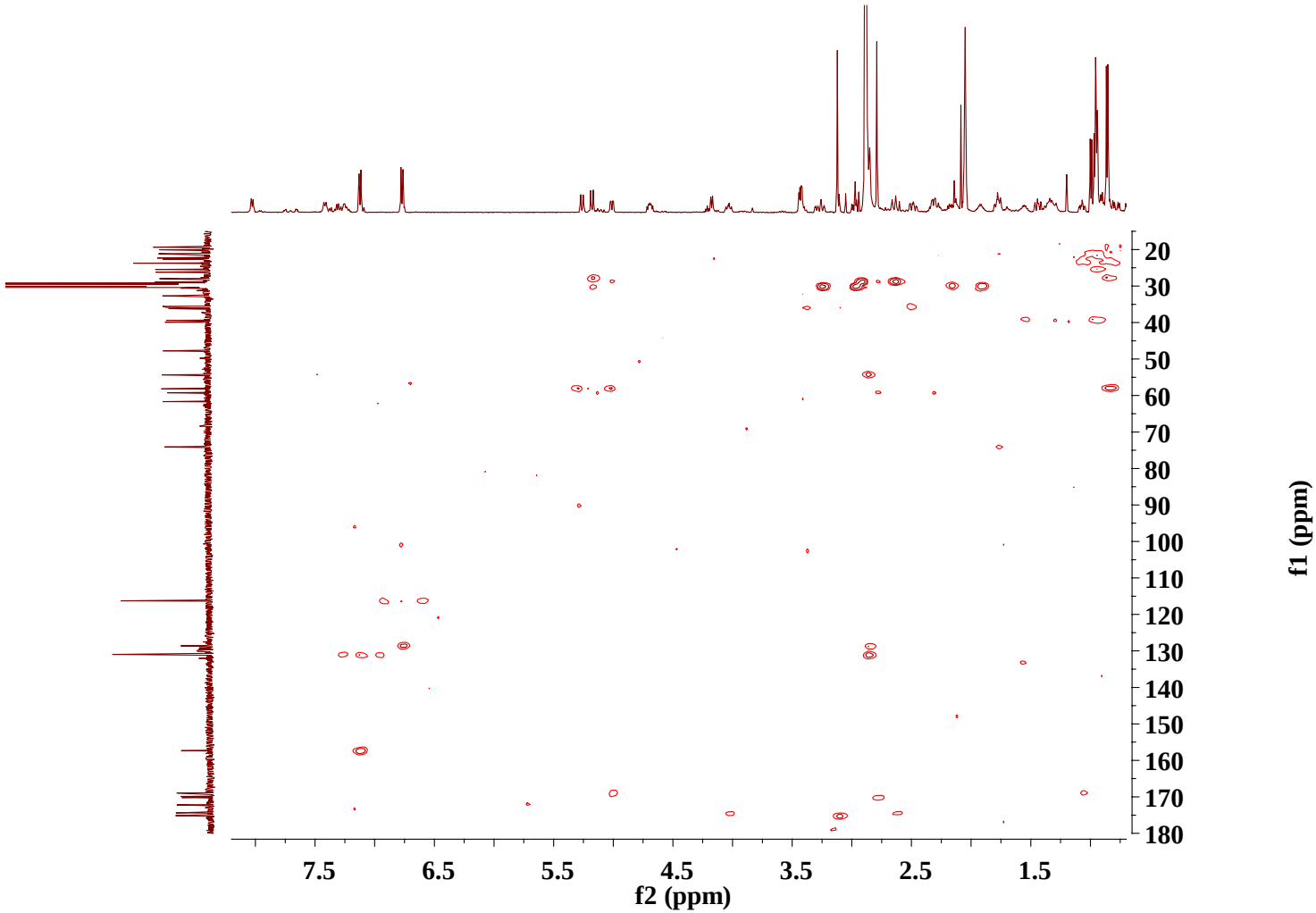
^{1}H-^{1}H COSY spectrum of compound **1**.



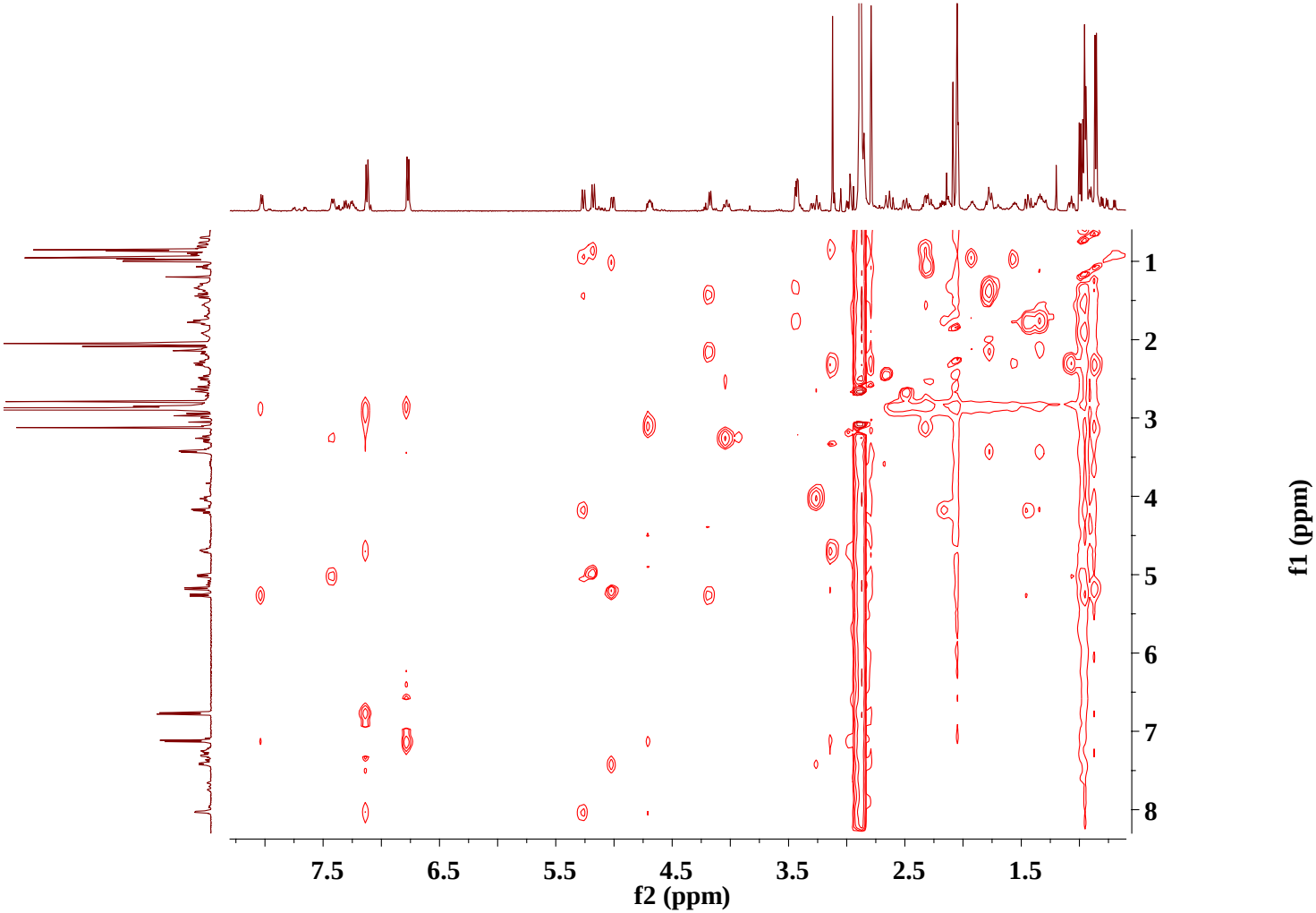
HSQC spectrum of compound **1**.



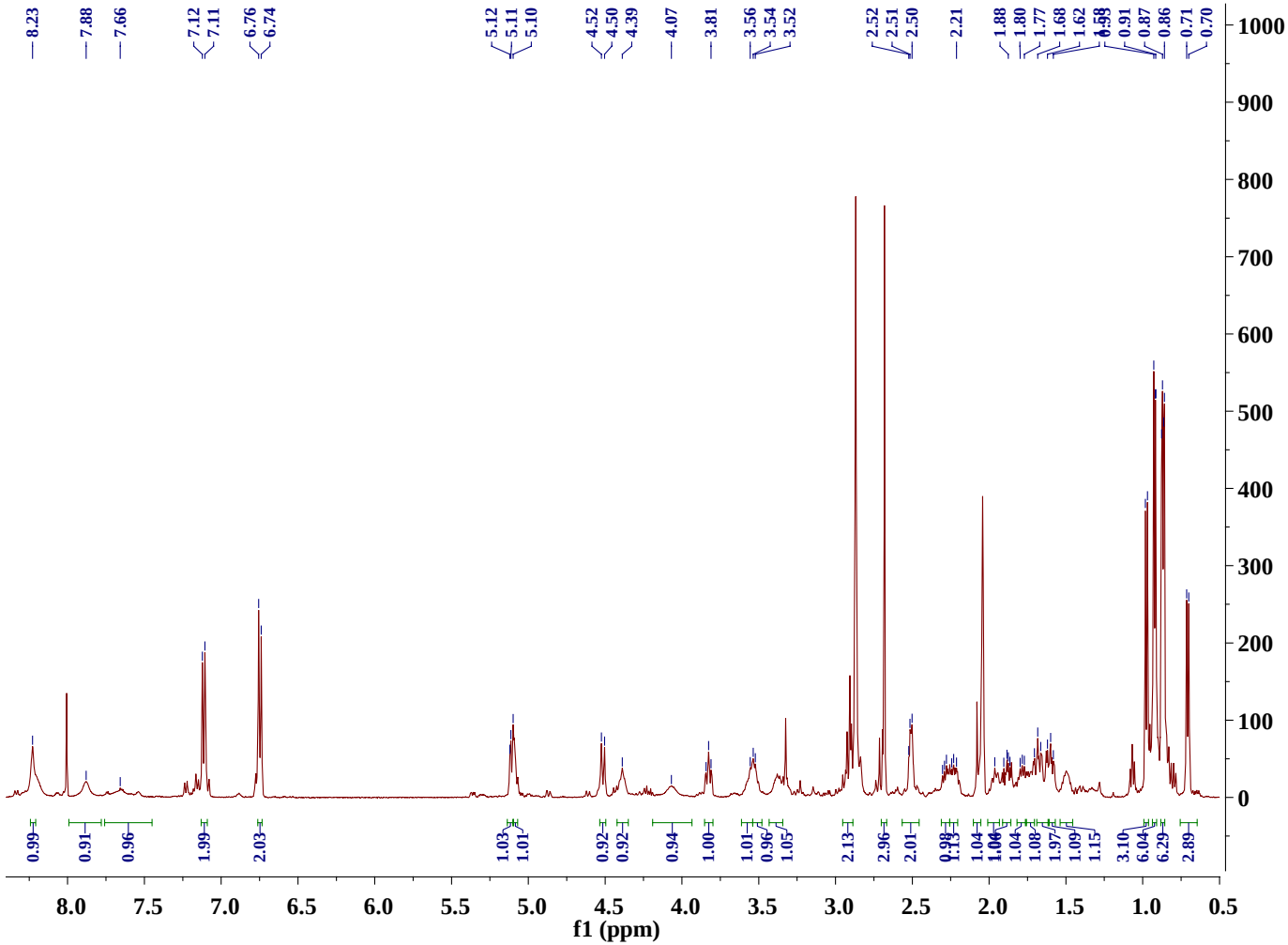
HMBC spectrum of compound **1**.



NOESY spectrum of compound **1**.

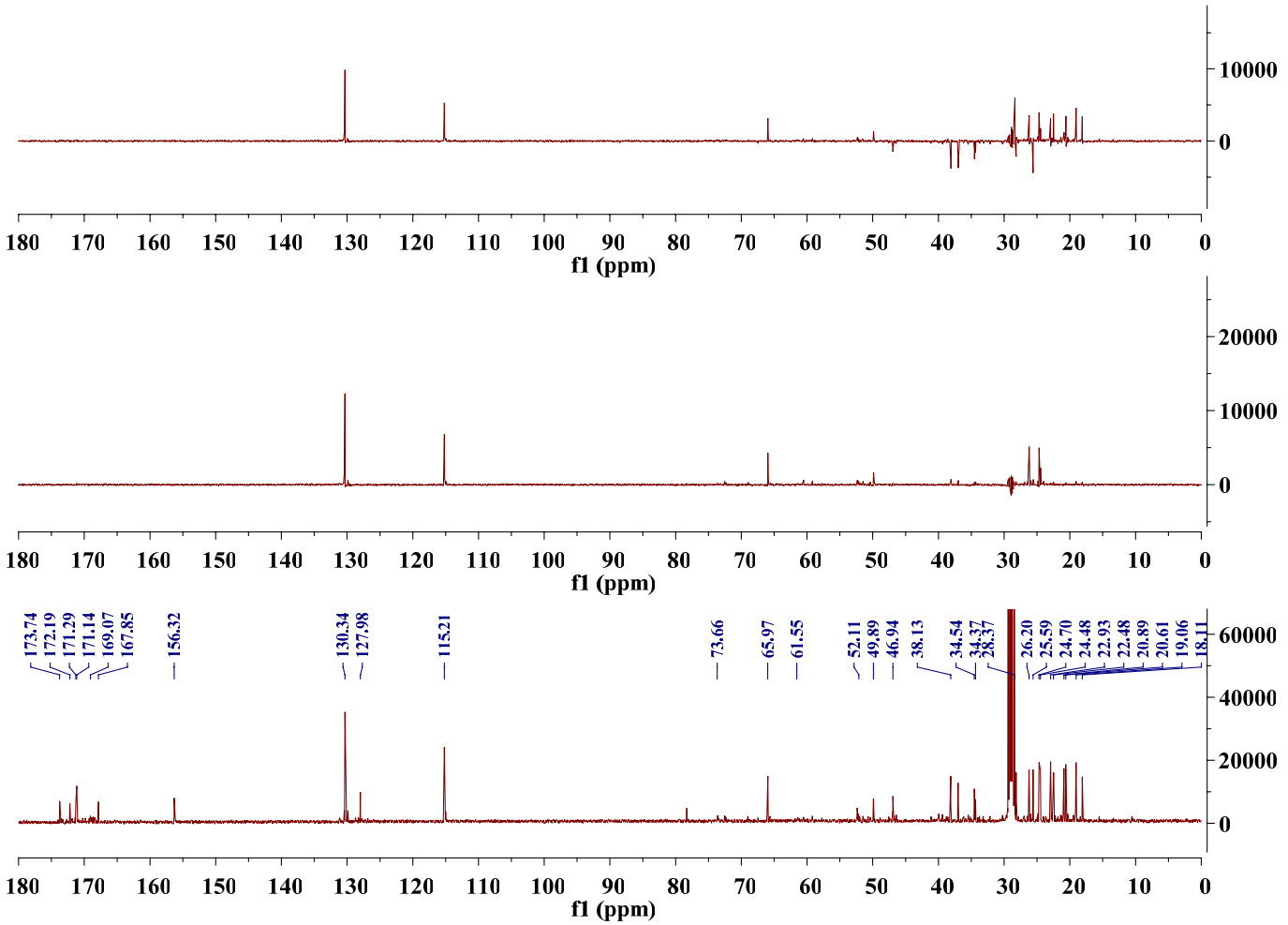


^{1}H NMR (500 MHz, Acetone-d_6) spectrum of compound **2**.

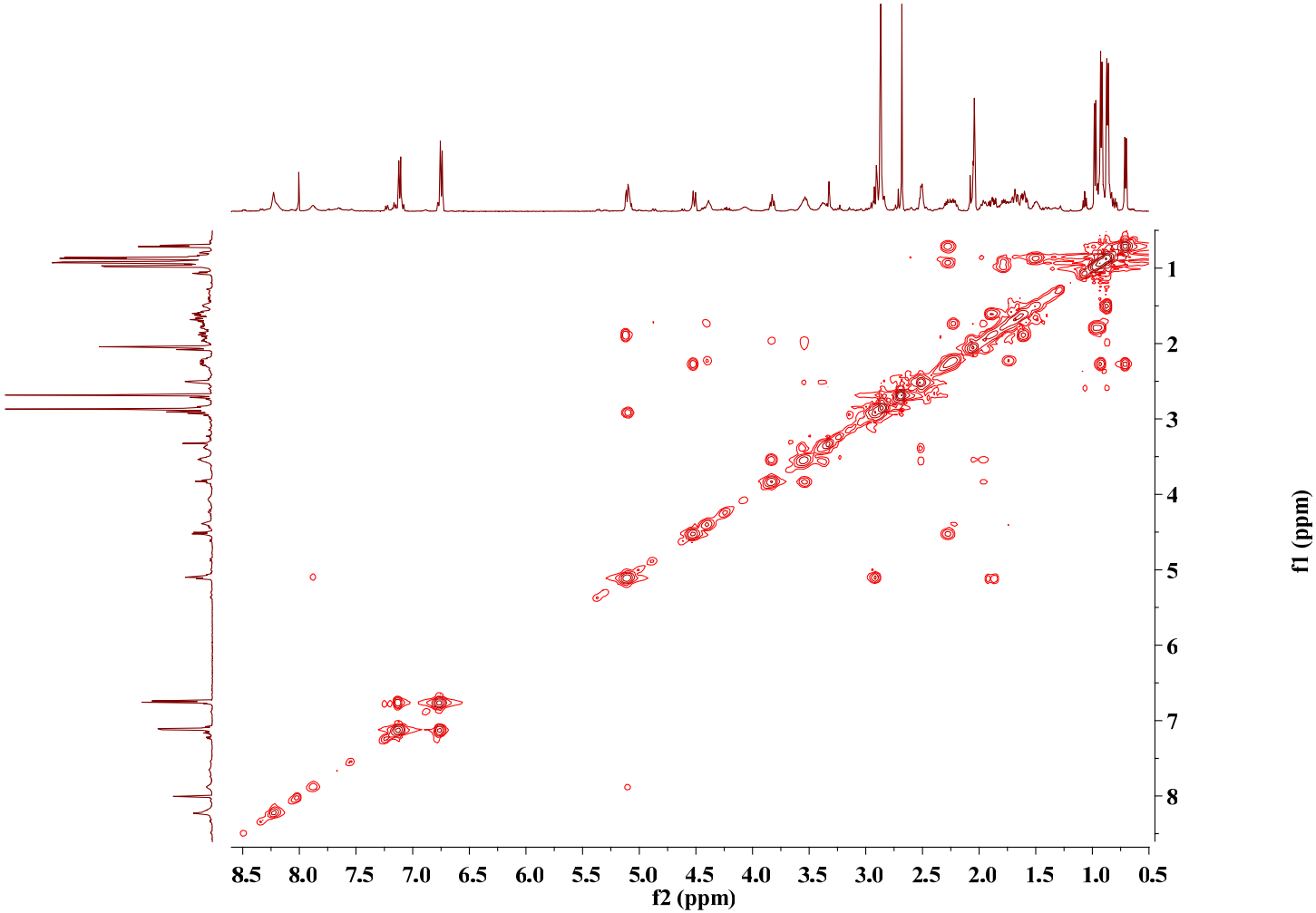


DEPT spectrum of compound **2**.

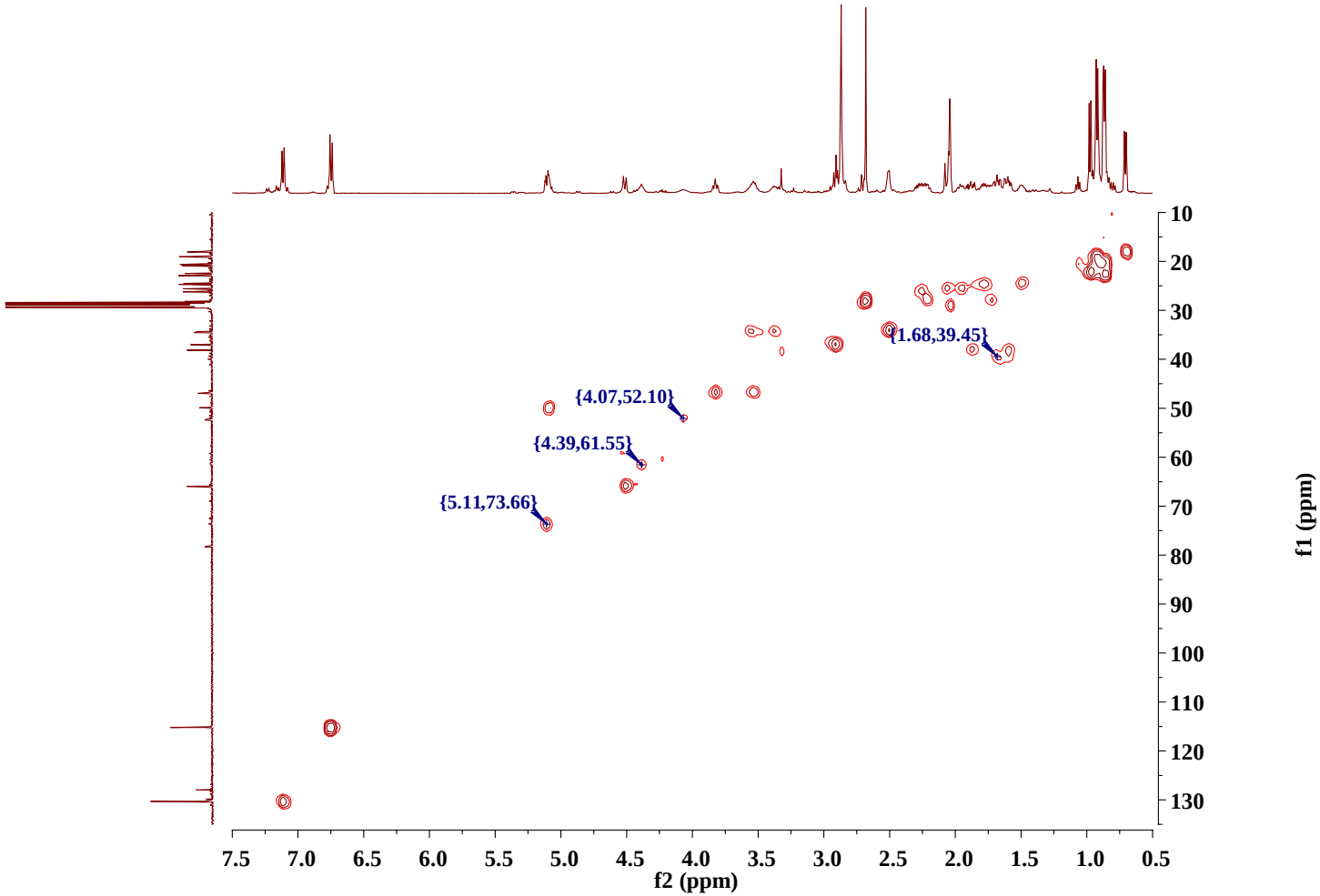
(Note: the weak signals were further confirmed by the following HSQC spectrum)



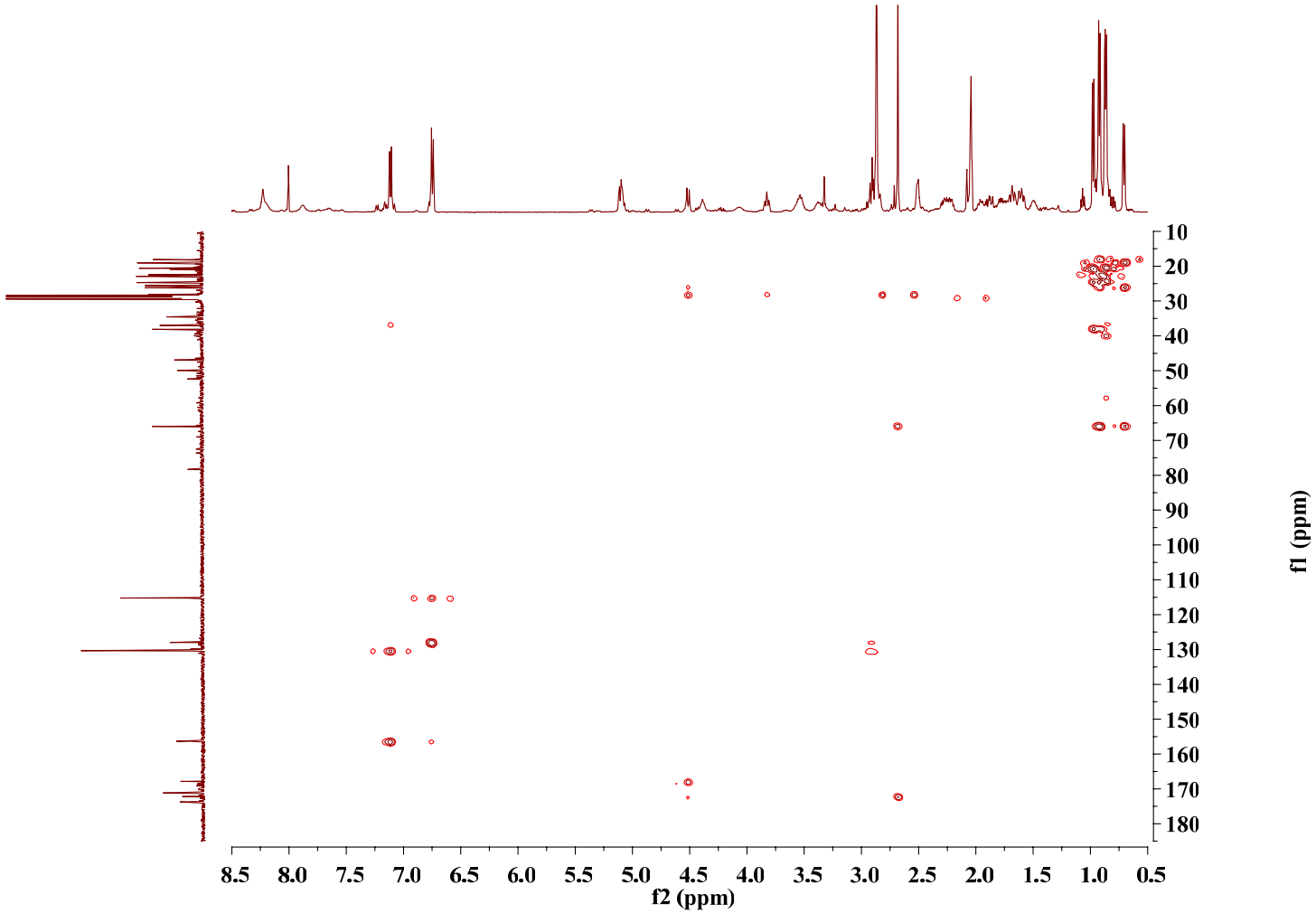
^{1}H-^{1}H COSY spectrum of compound **2**.



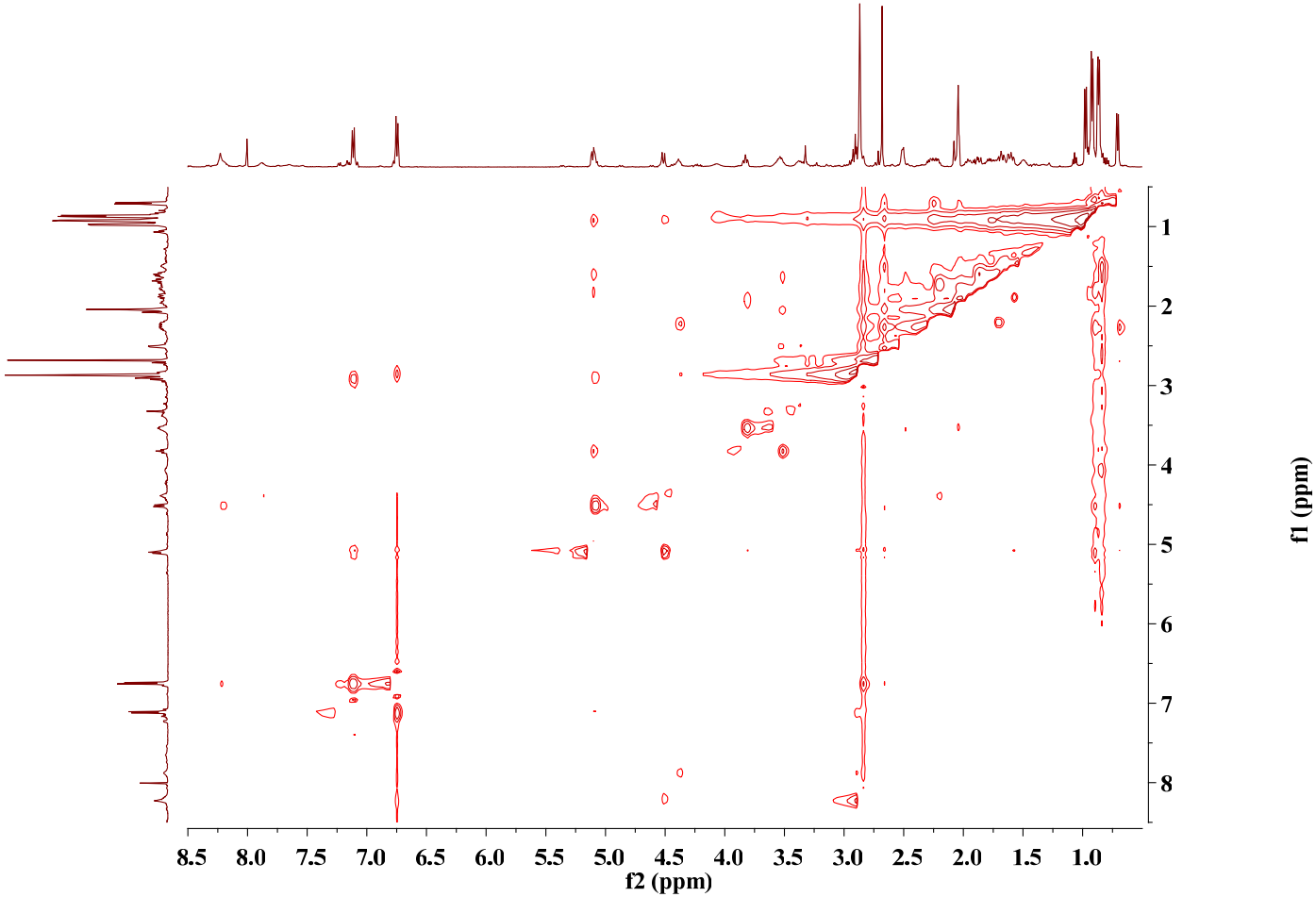
HSQC spectrum of compound **2**.



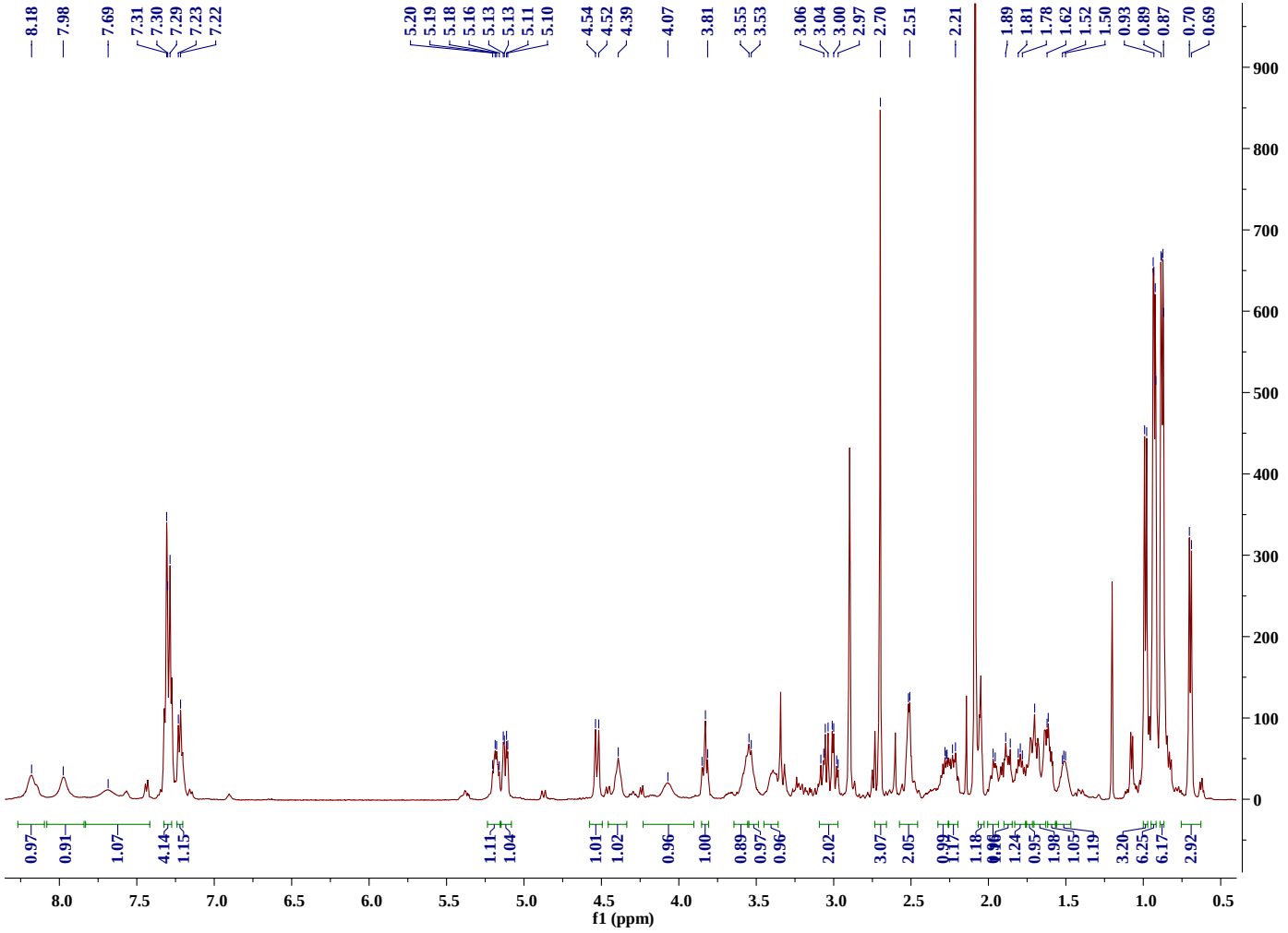
HMBC spectrum of compound **2**.



NOESY spectrum of compound **2**.

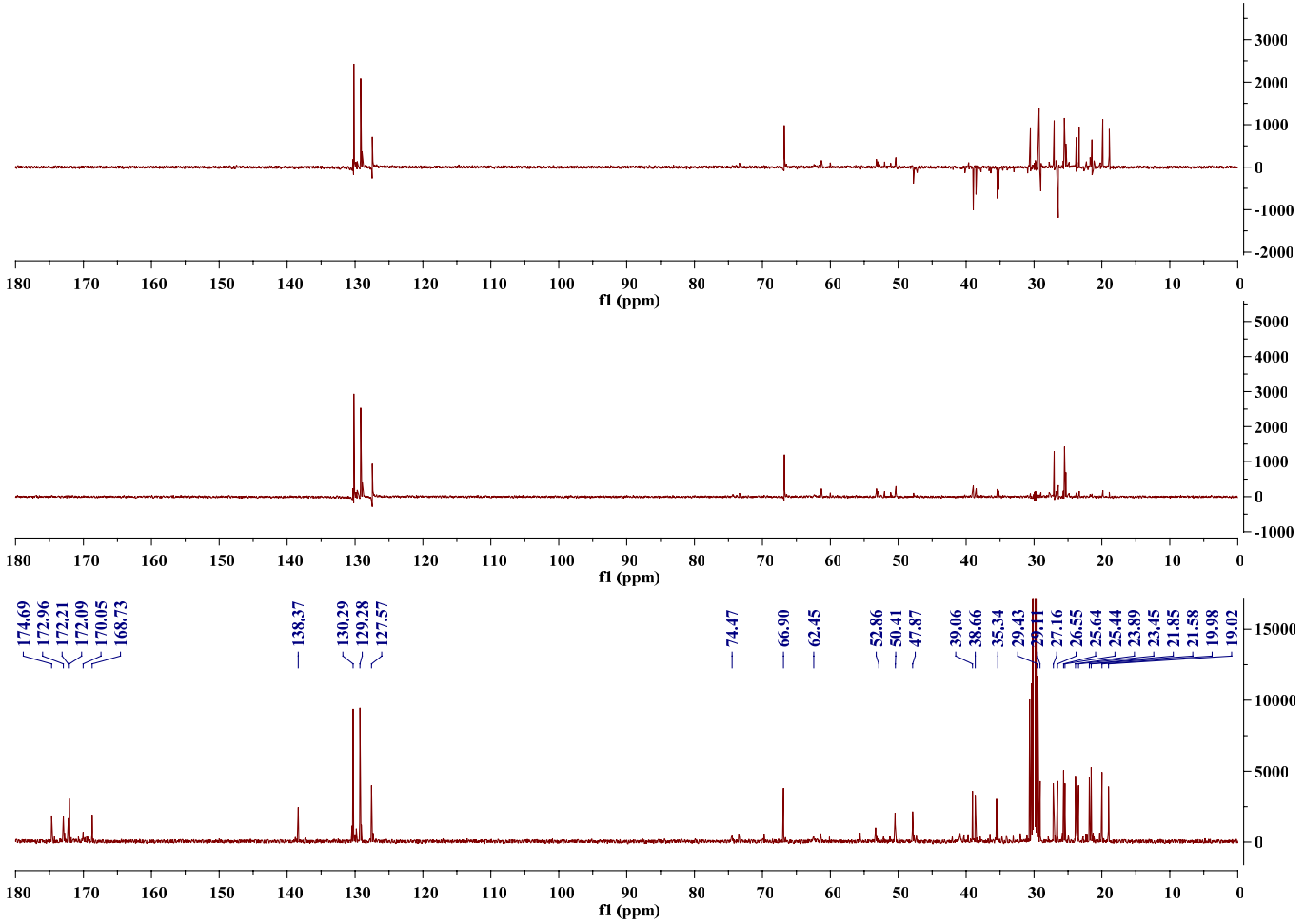


^{1}H NMR (500 MHz, Acetone-d_6) spectrum of compound **3**.

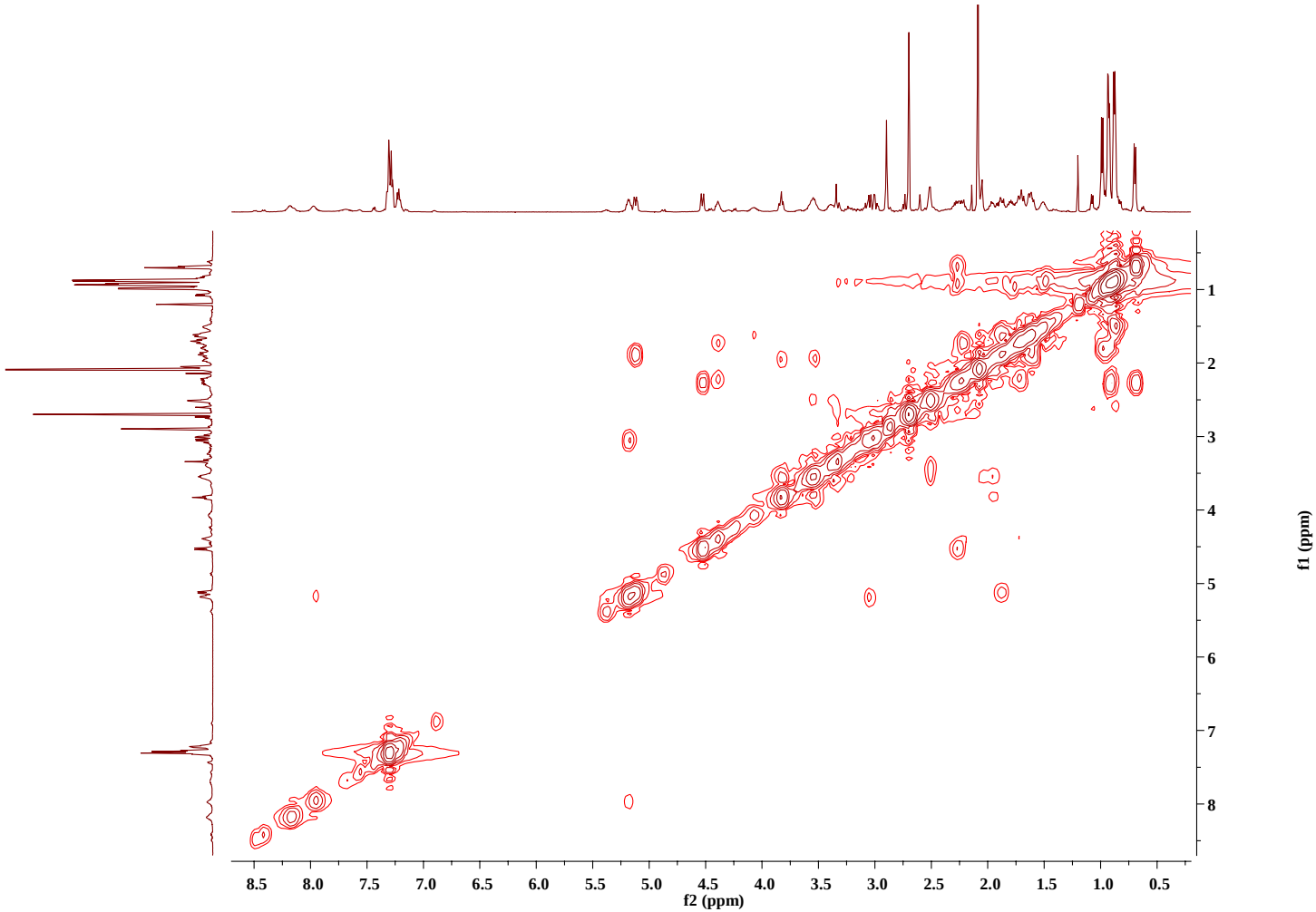


DEPT spectrum of compound **3**.

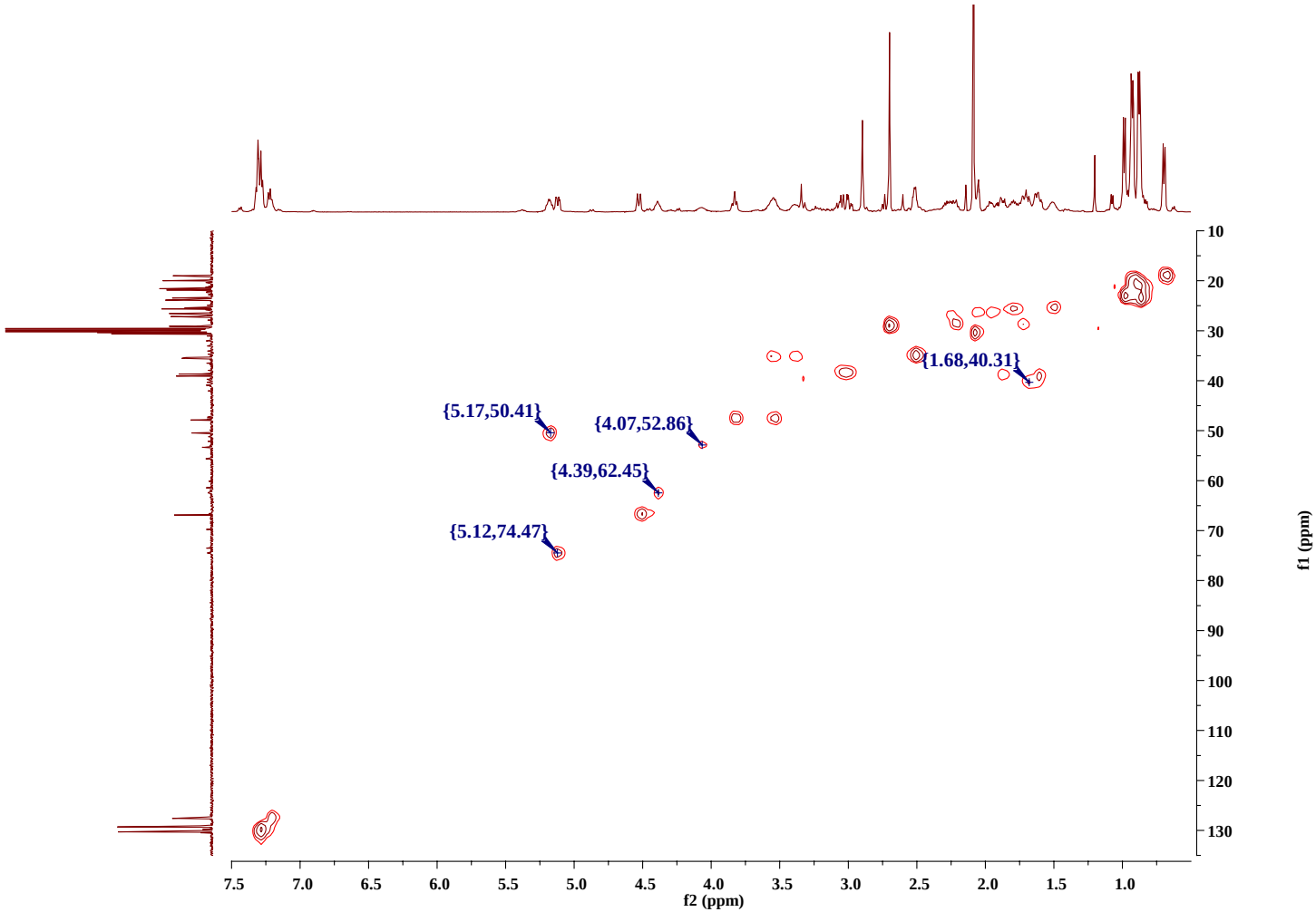
(Note: the weak signals were further confirmed by the following HSQC and HMBC spectra)



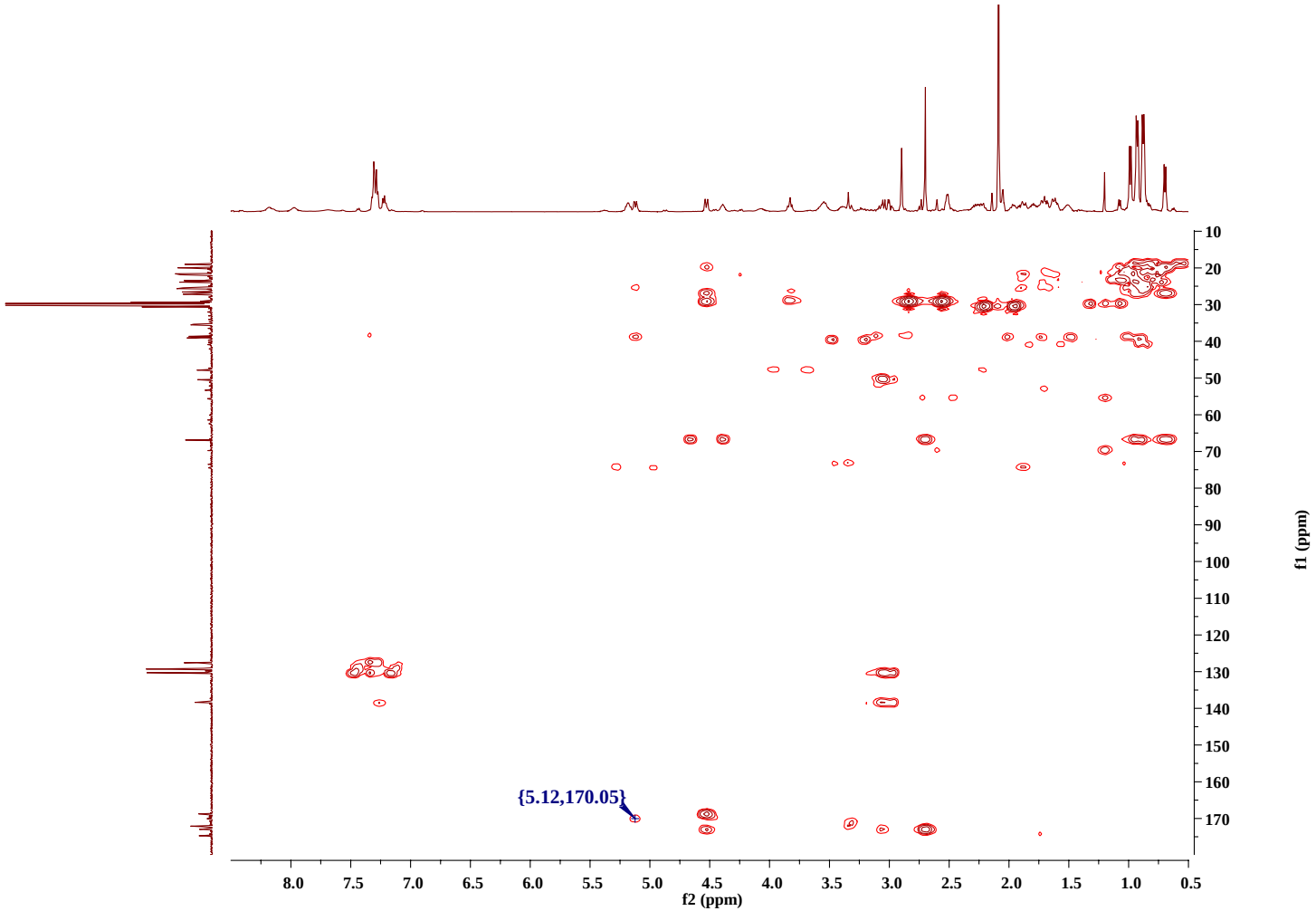
^{1}H-^{1}H COSY spectrum of compound **3**.



HSQC spectrum of compound **3**.



HMBC spectrum of compound **3**.



NOESY spectrum of compound **3**.

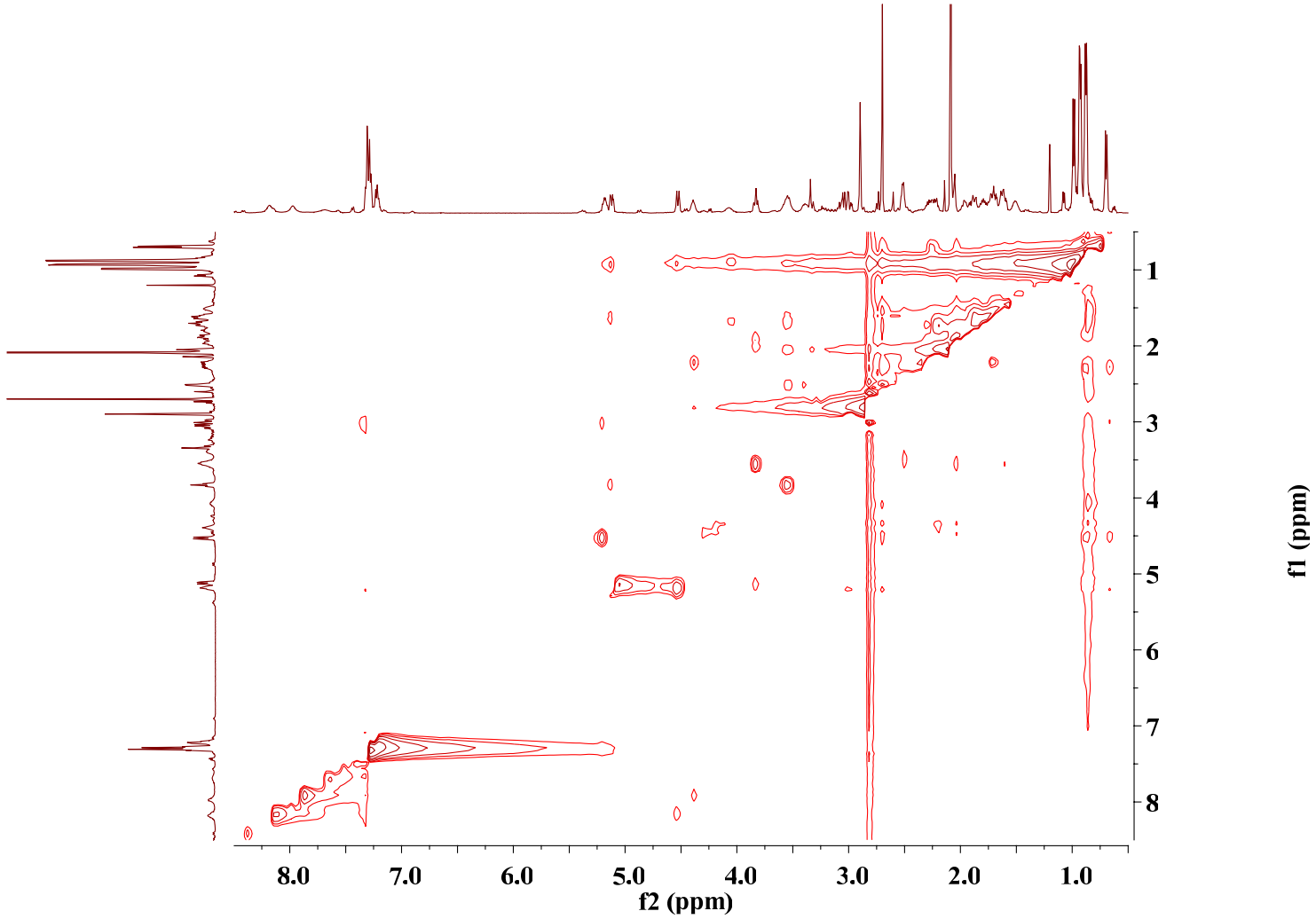


Table S3. 1D NMR data in acetone-d_6 for compound **5**[a].

position	δ_C (type)	δ_H (mult., J in Hz)
	HMPA[1]	
CO	170.1, C	
α	73.9, CH	5.17, dd (11.7, 2.5)
β	39.7, CH_2	1.75, dd (14.4, 2.6)
		1.26, dd (13.3, 11.0)
γ	25.2, CH	1.71, m
δ	23.8, CH_3	0.95, d (6.6)
δ'	20.8, CH_3	0.86, d (6.6)
	***β*-Me-Pro**[2]	
CO	171.9, C	
α	68.5, CH	3.65, d (2.4)
β	40.7, CH	2.44, m
γ	29.8, CH_2	1.50, m; 1.44, m
δ	45.8, CH_2	3.68, m; 3.26, m
β-Me	19.2, CH_3	1.06, d (7.0)
	Phe[3]	
CO	174.8, C	
α	54.1, CH	4.70, ddd (10.4, 7.6, 5.5)
β	36.3, CH_2	3.05, m
		2.97, m
γ	138.2, C	
δ, δ'	130.0, CH	7.32, m
ε, ε'	129.4, CH	7.30, m
θ	127.6, CH	7.26, m
NH		8.00, d (7.7)
	***N*-Me-Val**[4]	
CO	170.2, C	
α	58.1, CH	5.11, d (10.7)
β	27.9, CH	2.26, m
γ	19.7, CH_3	0.68, d (6.5)
γ'	19.3, CH_3	0.81, d (6.5)
N-Me	30.3, CH_3	3.08, s
	***N*-Me-Phe**[5]	
CO	168.6, C	
α	62.8, CH	5.14, m
β	37.2, CH_2	3.59, dd (13.3, 9.5)
		2.69, dd (13.4, 4.7)
γ	138.8, C	
δ, δ'	130.0, CH	7.32, m
ε, ε'	129.5, CH	7.30, m
θ	127.7, CH	7.26, m
N-Me	29.2, CH_3	2.95, s
	***β*-Ala**[6]	
CO	174.3, C	
α	35.7, CH_2	2.57, dt (14.8, 2.8)
		2.29, m
β	36.3, CH_2	3.92, m; 3.31, m
NH		7.39, br. s

[a]Recorded at 500 and 125 MHz for ^1H and ^{13}C, respectively.