Article

Prostaglandins Isolated from the Octocoral *Plexaura homomalla*: In Silico and In Vitro Studies Against Different Enzymes of Cancer

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Figure S1: ^{1}H NMR spectrum of Prostaglandin A_2-AcMe **(1)** in $CDCl_3$

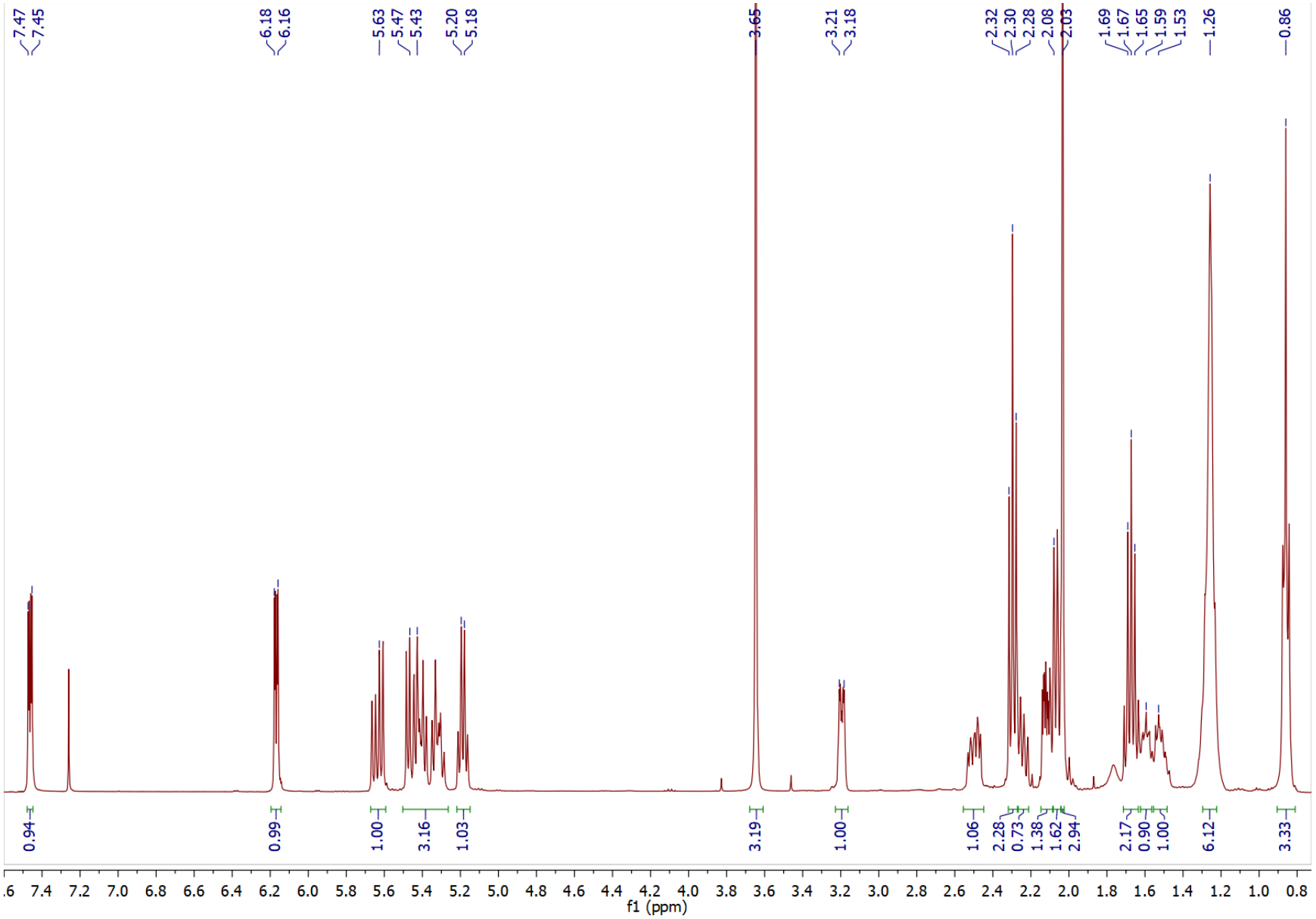

Figure S2: ^{13}C NMR spectrum of Prostaglandin A_2-AcMe **(1)** in $CDCl_3$

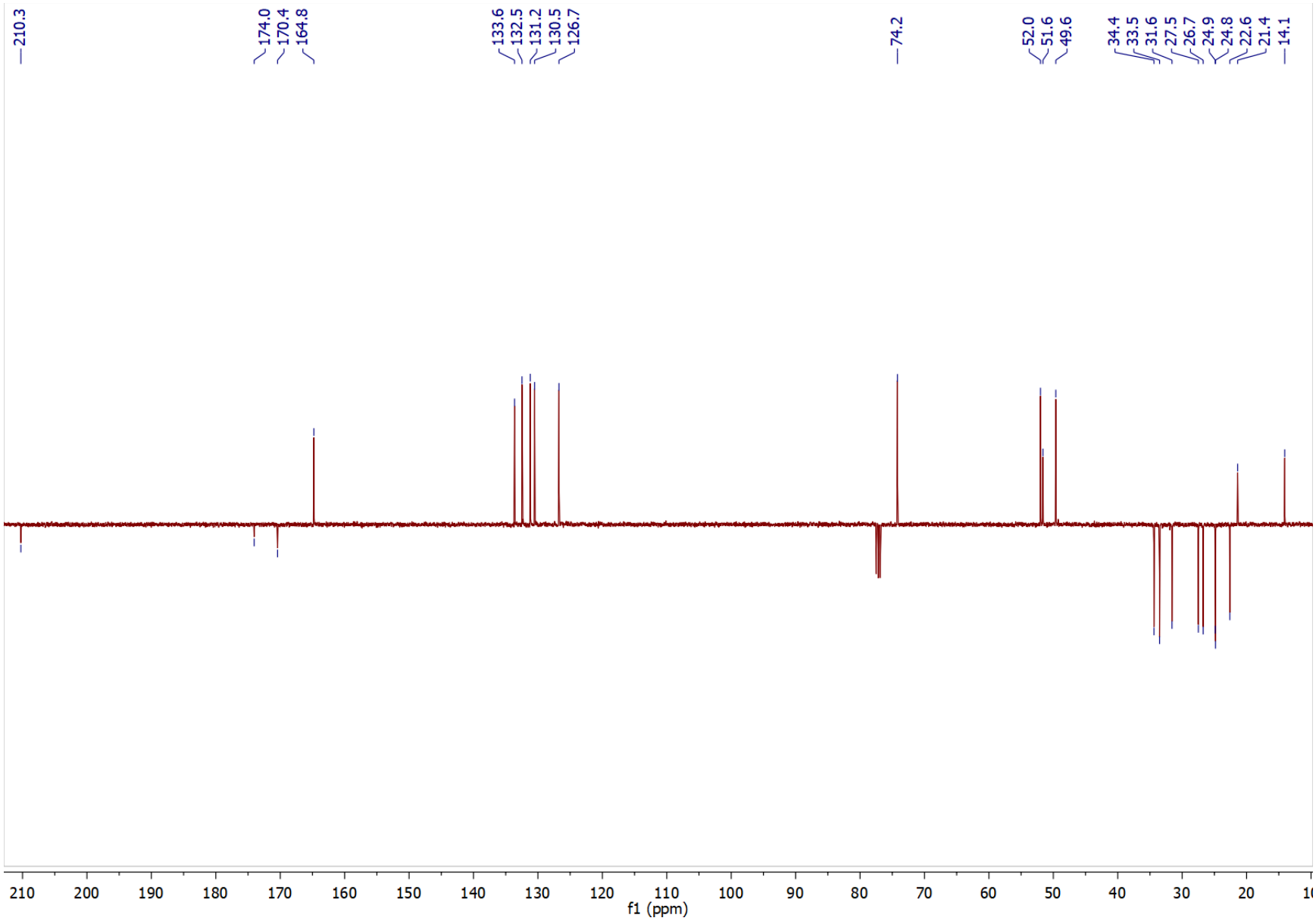

Figure S3: COSY NMR spectrum of Prostaglandin A_2-AcMe **(1)** in $CDCl_3$

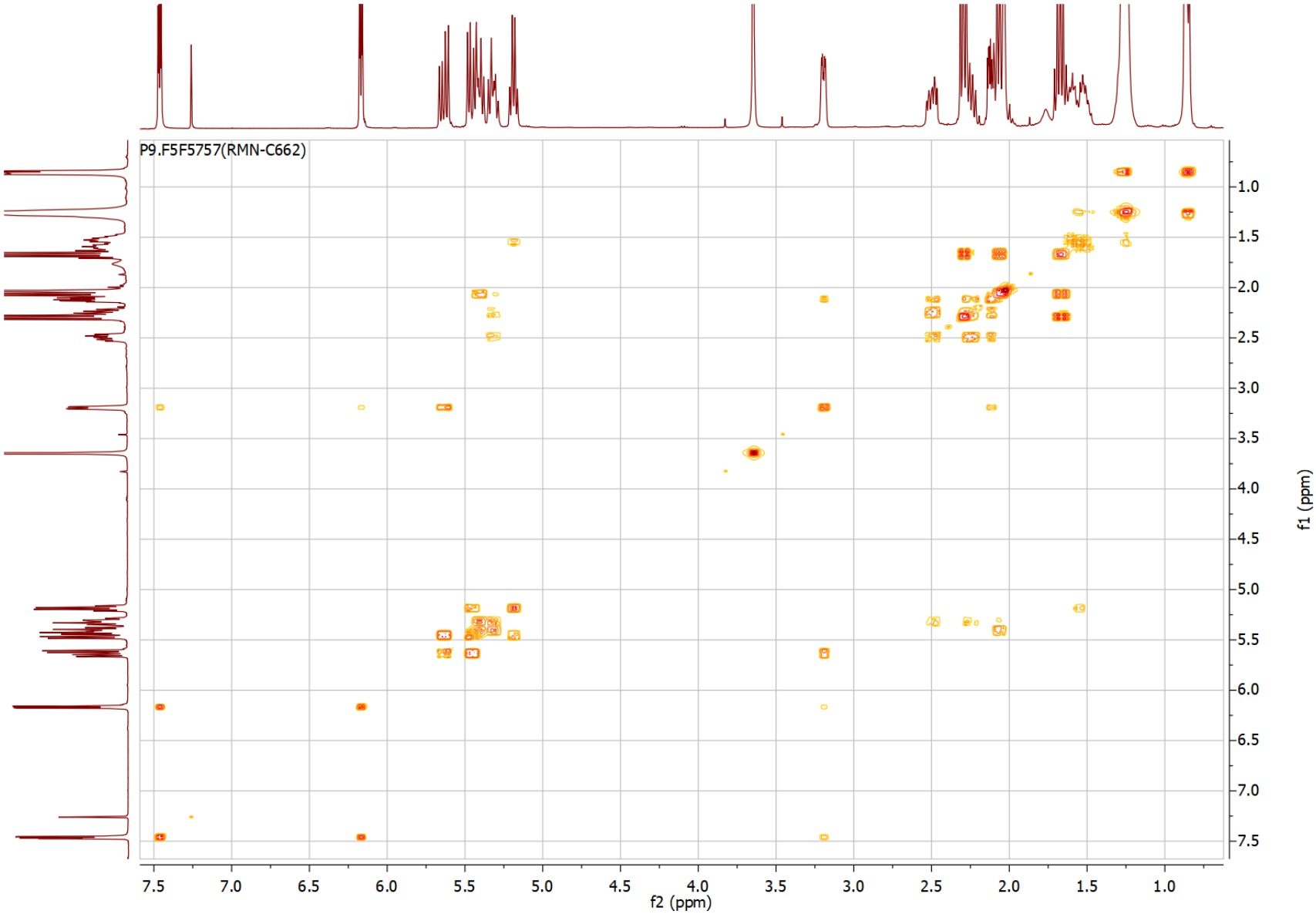

Figure S4: HSQC NMR spectrum of Prostaglandin A_2-AcMe **(1)** in $CDCl_3$

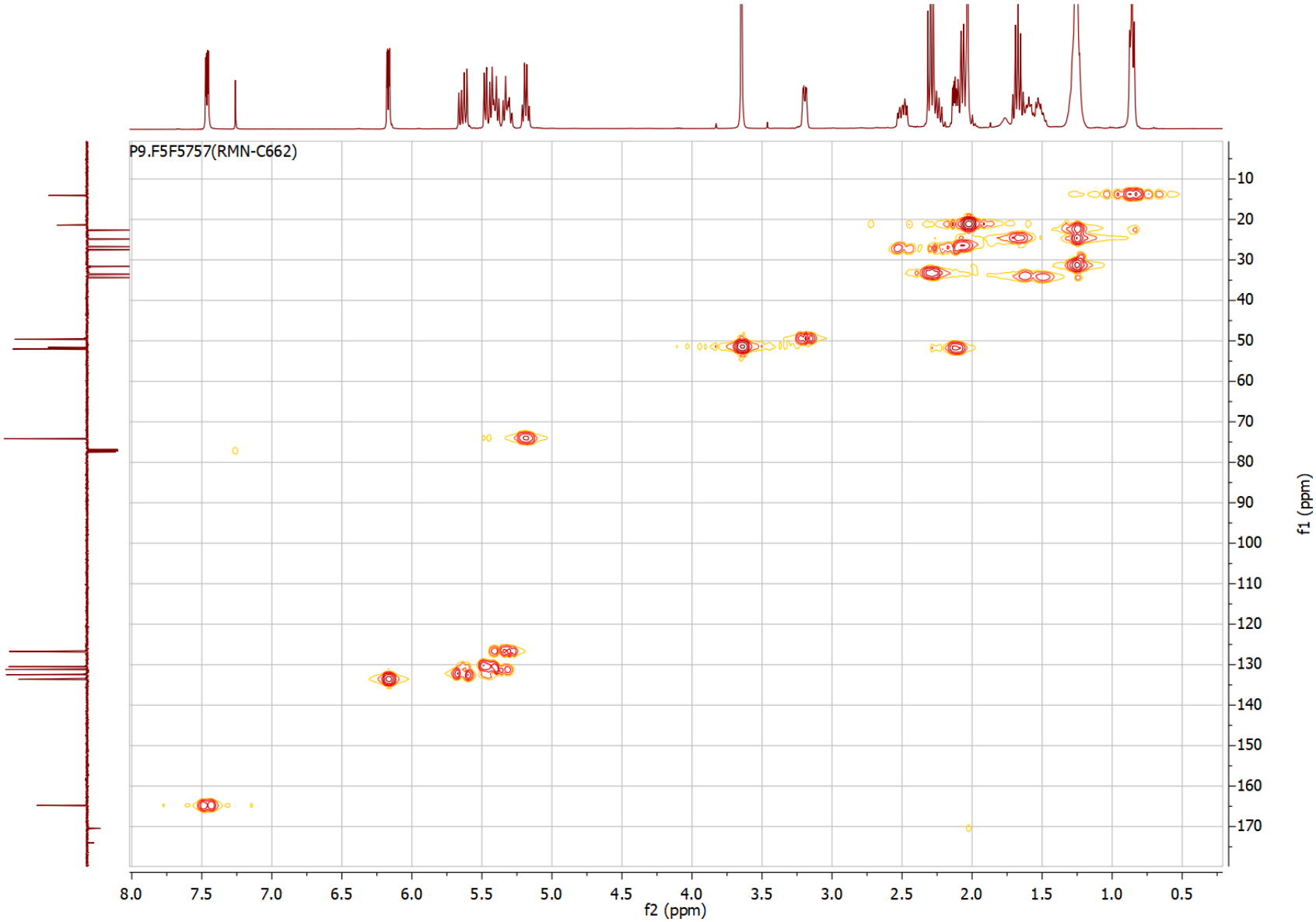

Figure S5: HMBC NMR spectrum of Prostaglandin A_2-AcMe **(1)** in $CDCl_3$

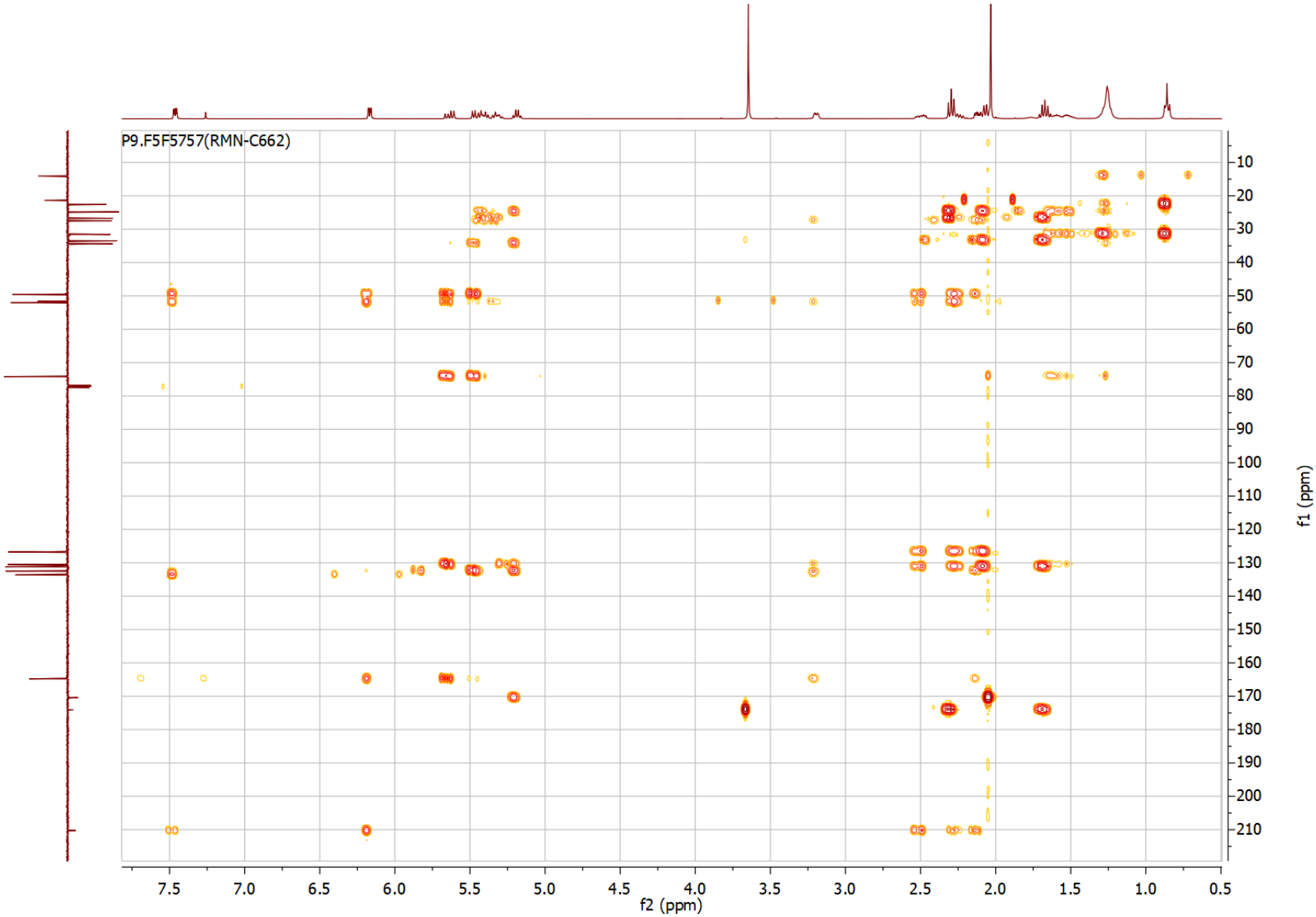

Figure S6: ^{1}H NMR spectrum of Prostaglandin A$_2$ **(2)** in CDCl$_3$

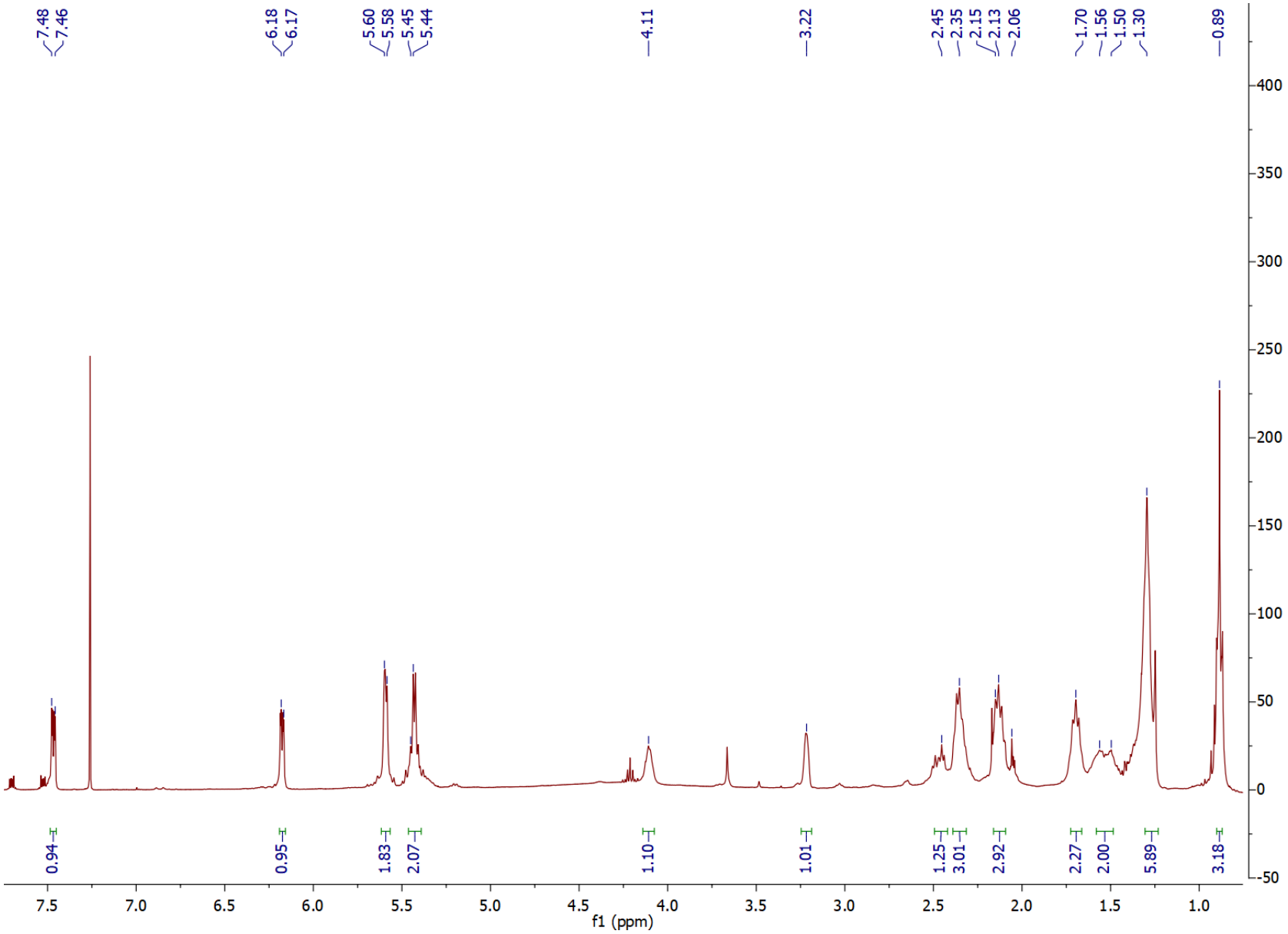

Figure S7: ^{13}C NMR spectrum of Prostaglandin A_2 **(2)** in $CDCl_3$

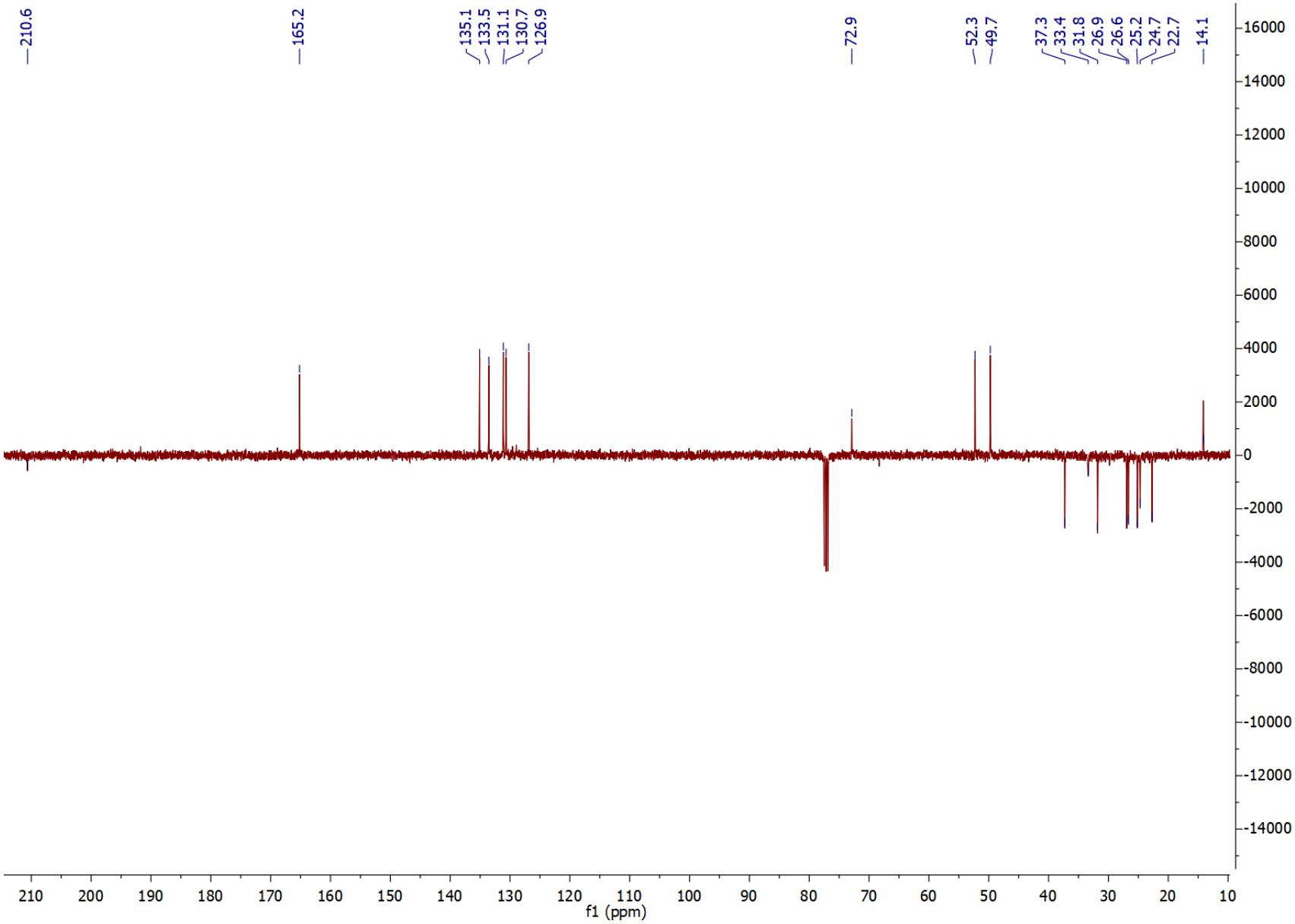

Figure S8: HMBC NMR spectrum of Prostaglandin A_2 **(2)** in $CDCl_3$

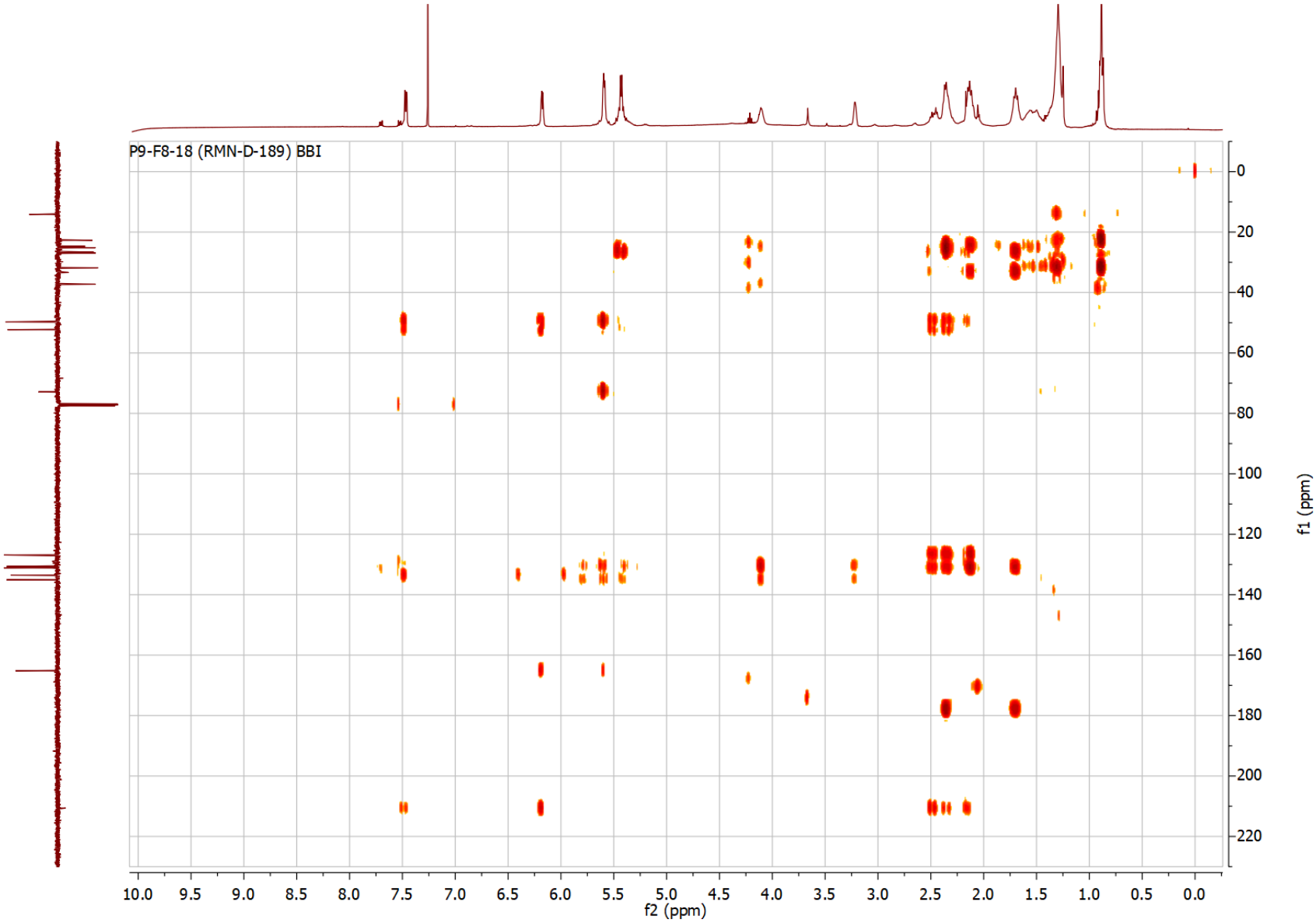

Figure S9: ^{1}H NMR spectrum of derivative **3** in $CDCl_3$

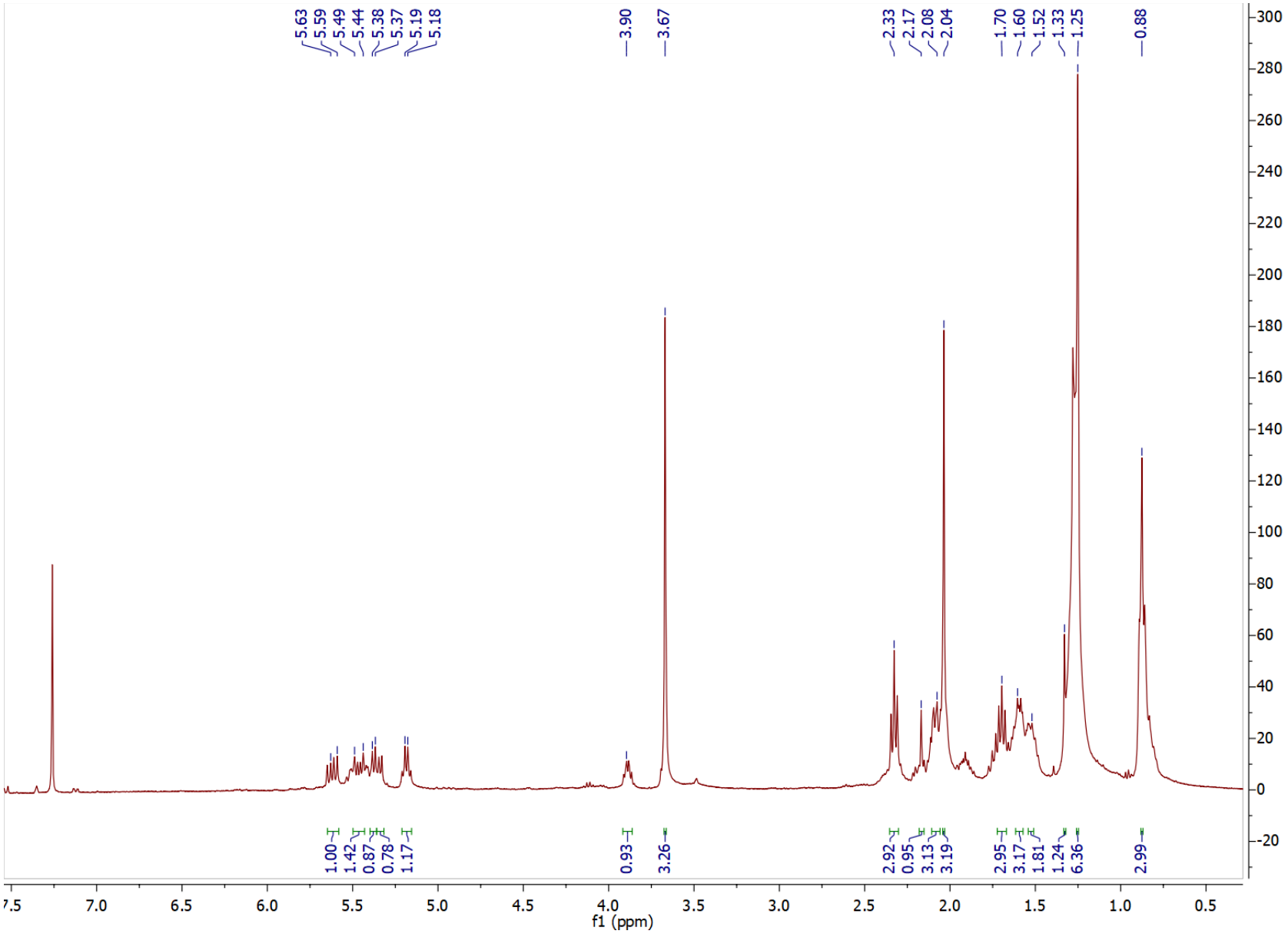

Figure S10: ^{13}C NMR spectrum of derivative **3** in $CDCl_3$

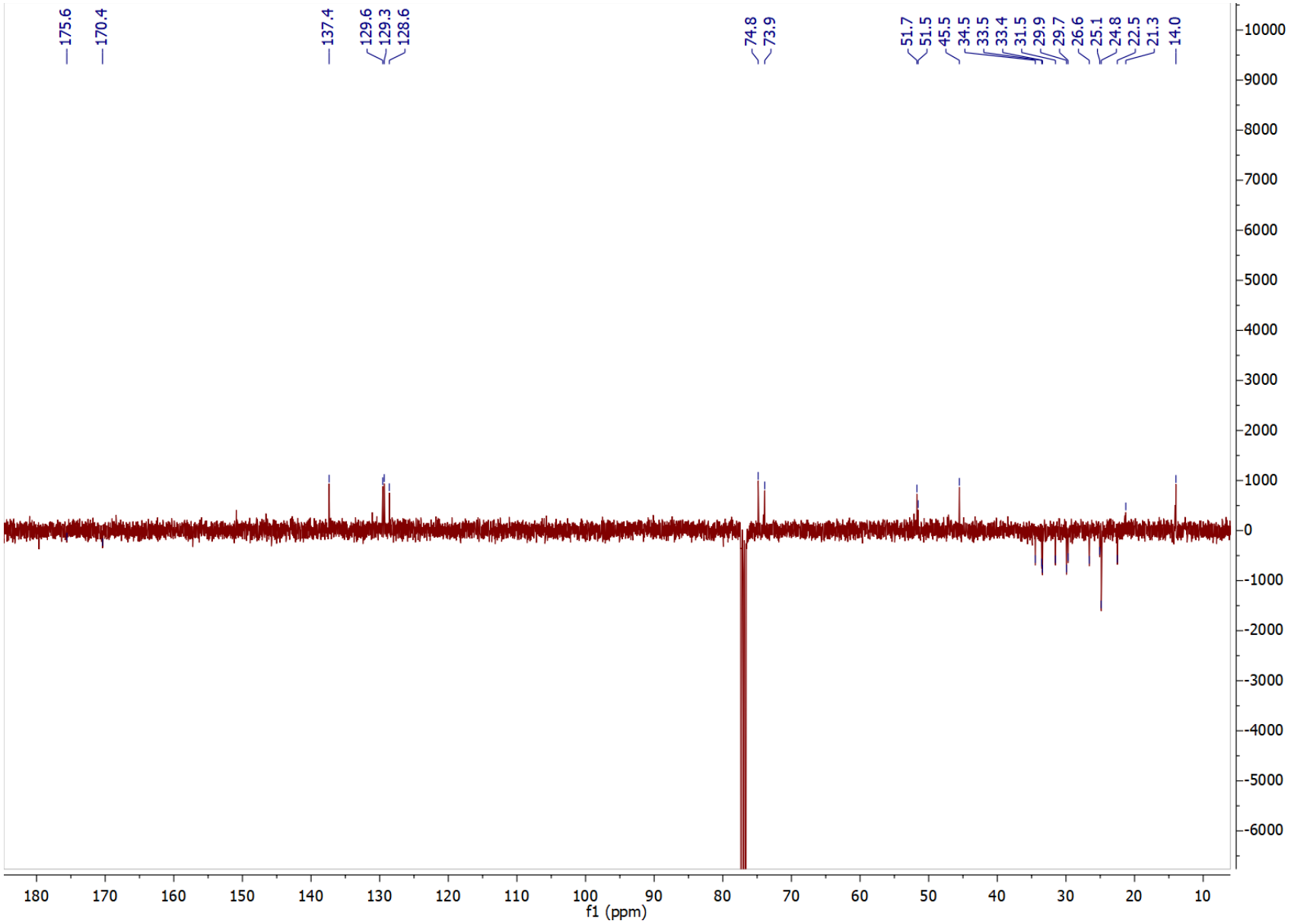

Figure S11: ^{1}H NMR spectrum of derivative **4** in $CDCl_3$

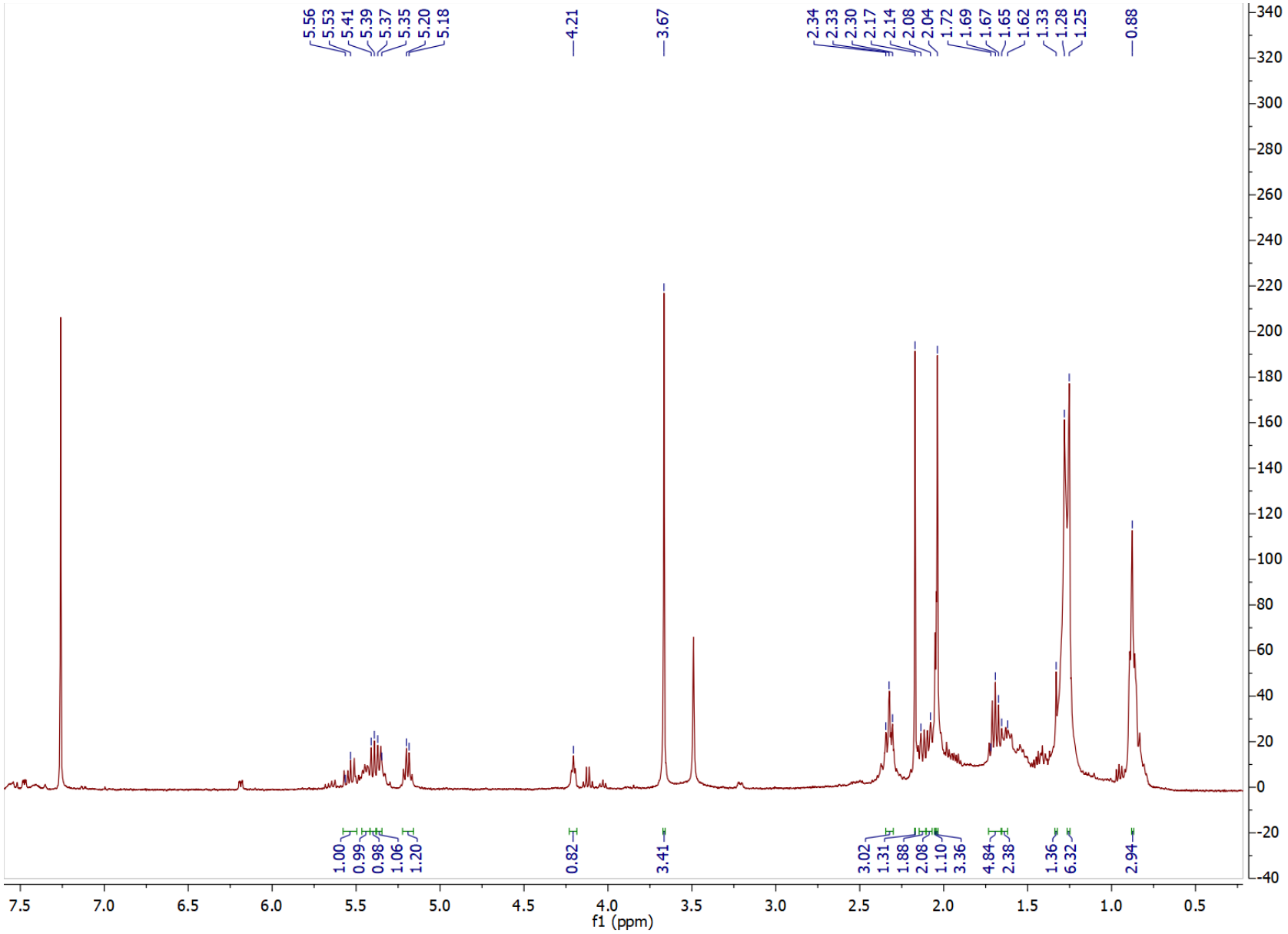

Figure S12: ^{13}C NMR spectrum of derivative **4** in $CDCl_3$

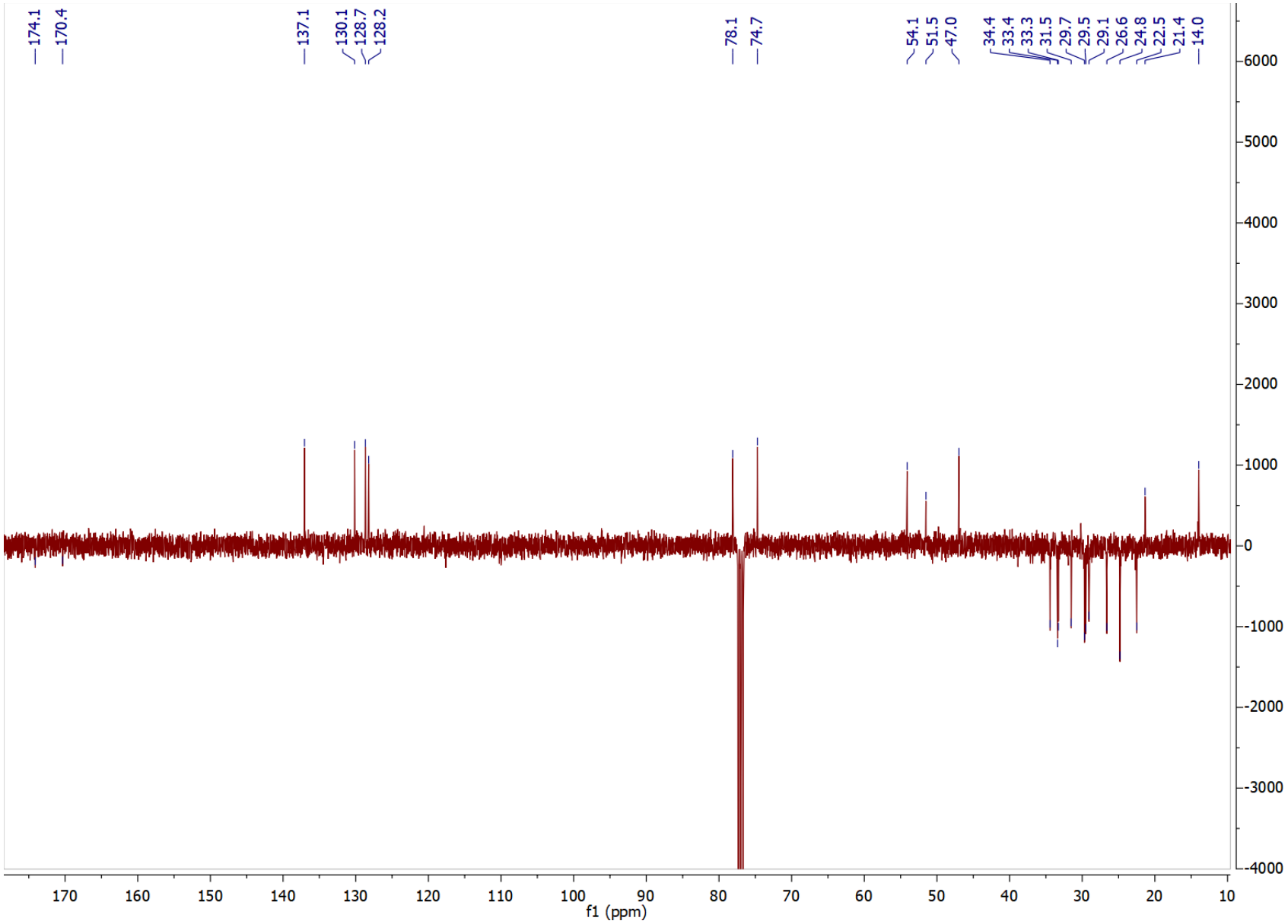

Figure S13: ^{1}H NMR spectrum of derivative **5** in $CDCl_3$

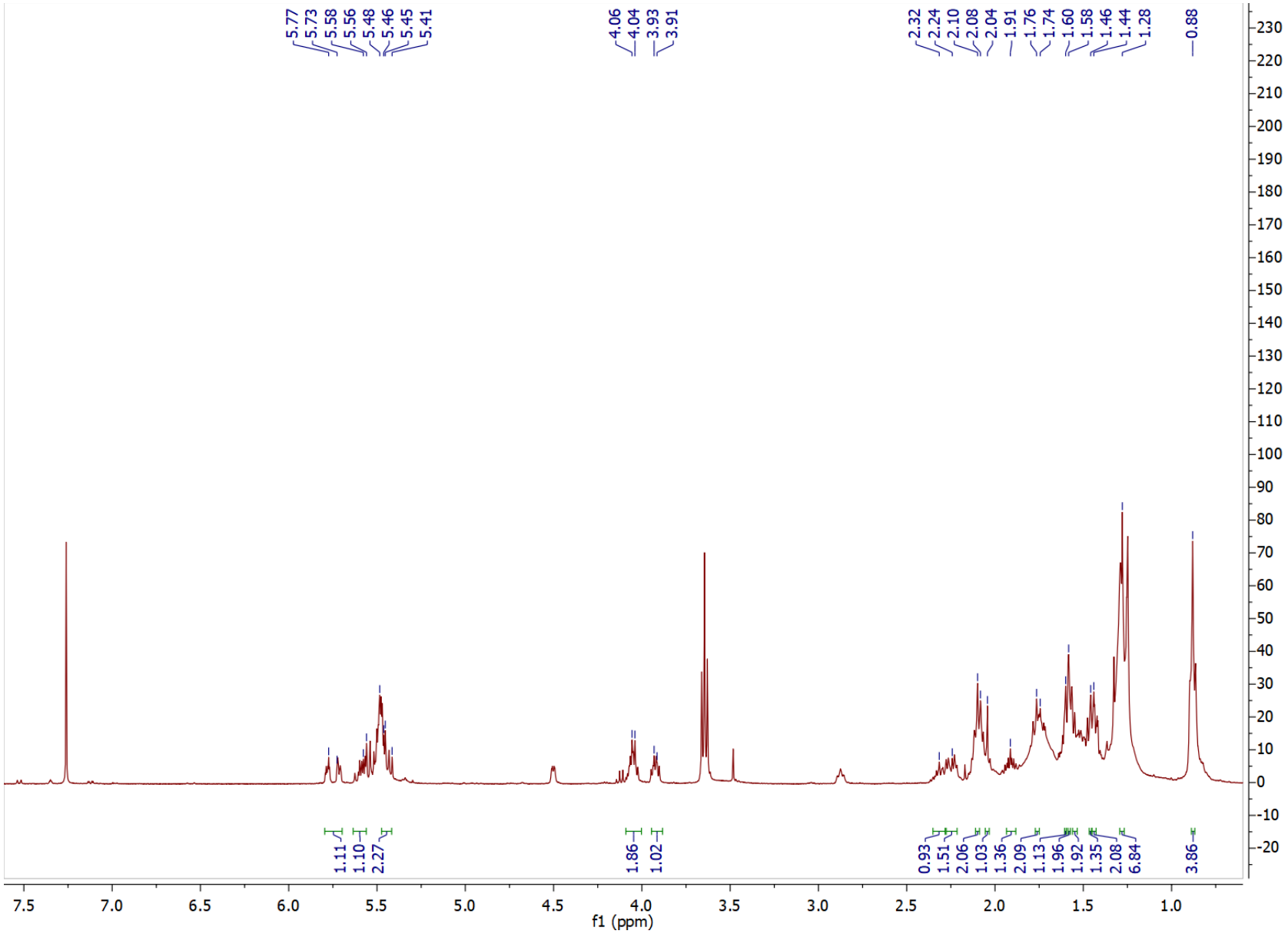

Figure S14: ^{13}C NMR spectrum of derivative **5** in $CDCl_3$

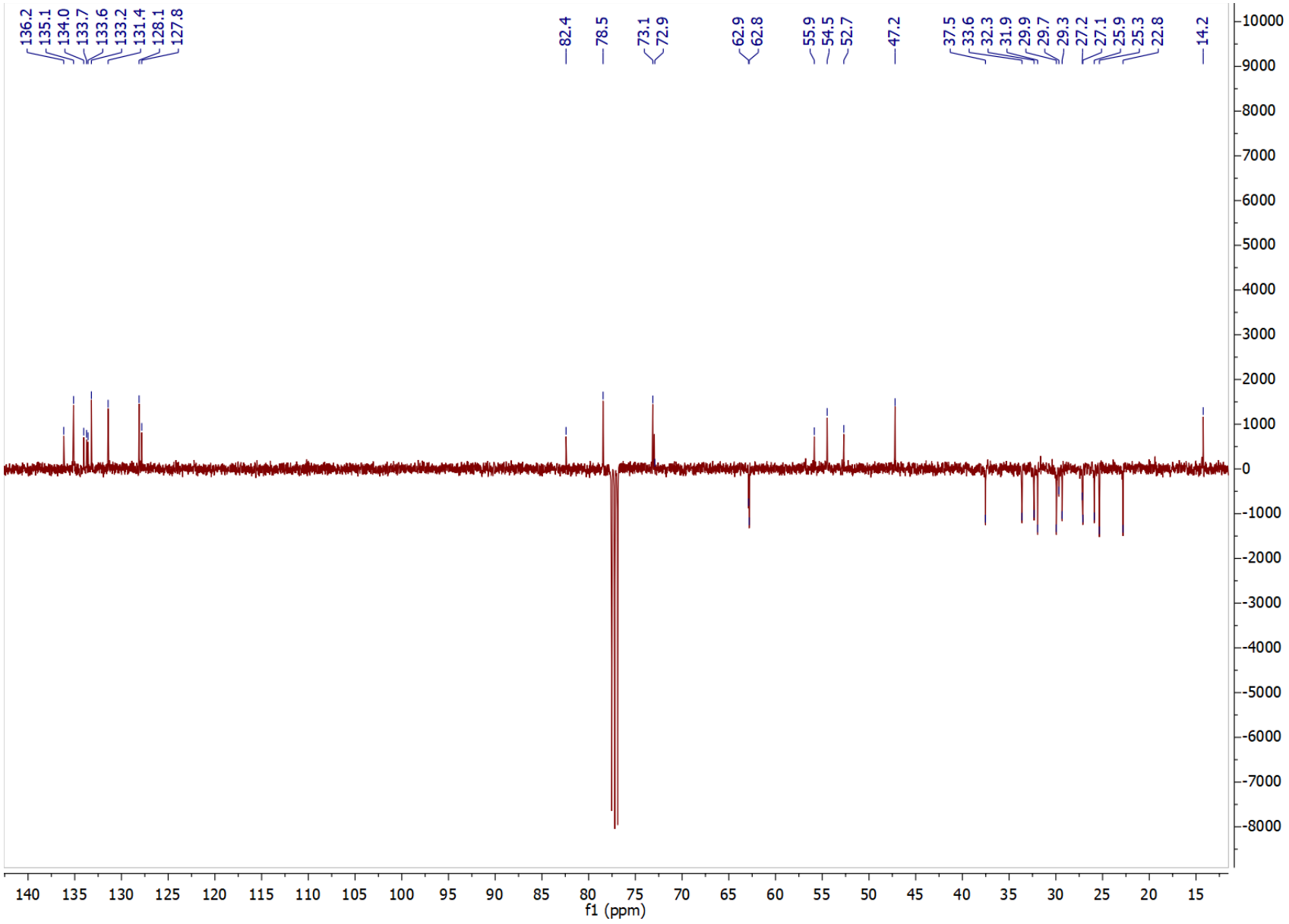

Figure S15: 3D interaction models of test compounds within the active site of p38α-kinase enzyme (PDB ID: 4FA2). a) **1** (blue sticks); b) **2** (light pink sticks); c) **3** (violet sticks); d) **4** (light green sticks); and e) **5** (white sticks). Hydrogen bonds and enzyme residues in dark green lines and light brown sticks, respectively.

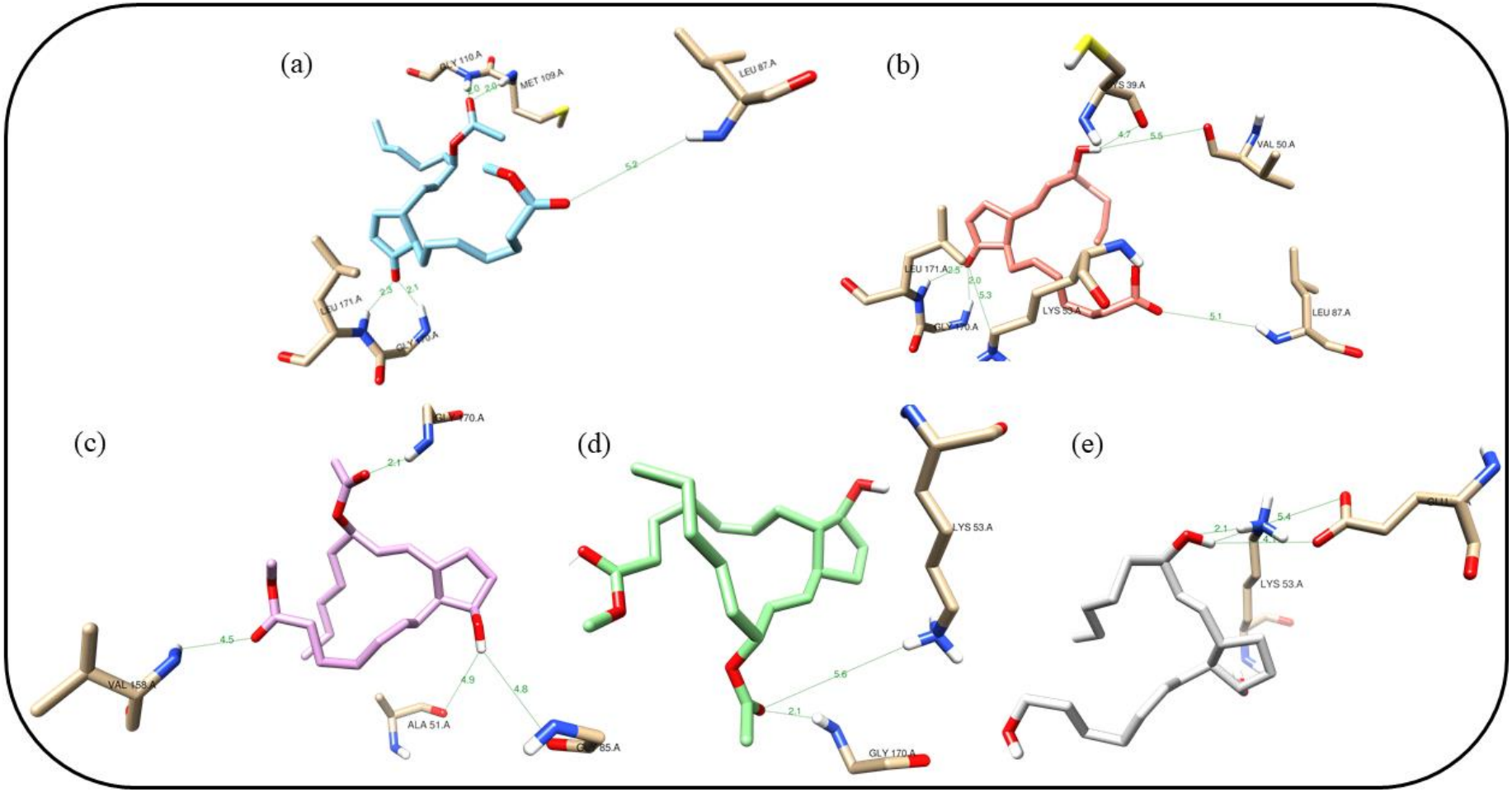

Figure S16: 3D interaction models of test compounds within active site of topoisomerase IIα enzyme (PDB ID: 1ZXM). a) **1** (blue sticks); b) **2** (light pink sticks); c) **3** (violet sticks); d) **4** (light green sticks); and e) **5** (white sticks). Hydrogen bonds and enzyme residues in dark green lines and light brown sticks, respectively.

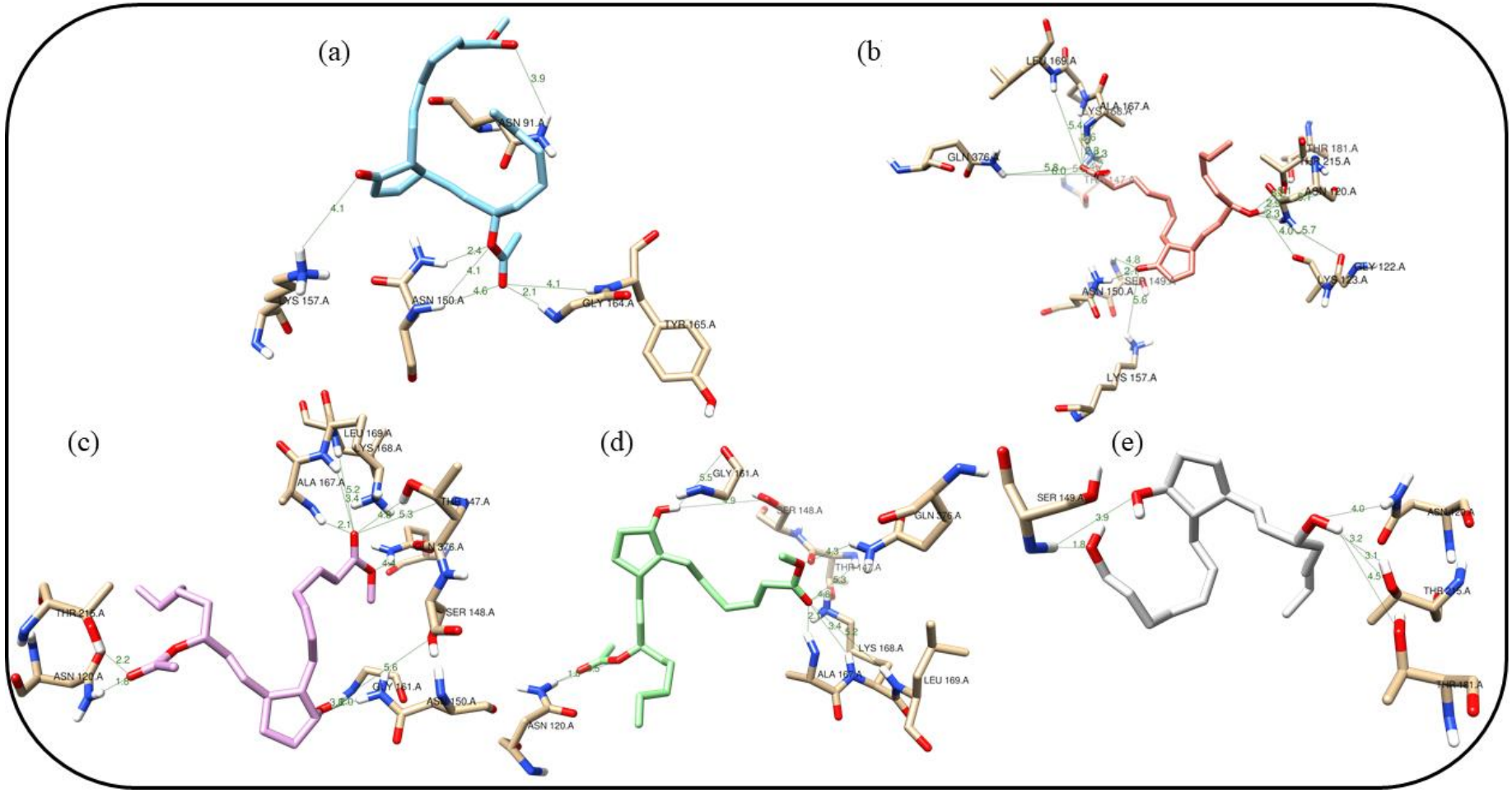

Figure S17: 3D interaction models of test compounds within the active site of Src-kinase enzyme (PDB ID: 2BDF). a) **1** (blue sticks); b) **2** (light pink sticks); c) **3** (violet sticks); d) **4** (light green sticks); and e) **5** (white sticks). Hydrogen bonds and enzyme residues in dark green lines and light brown sticks, respectively.

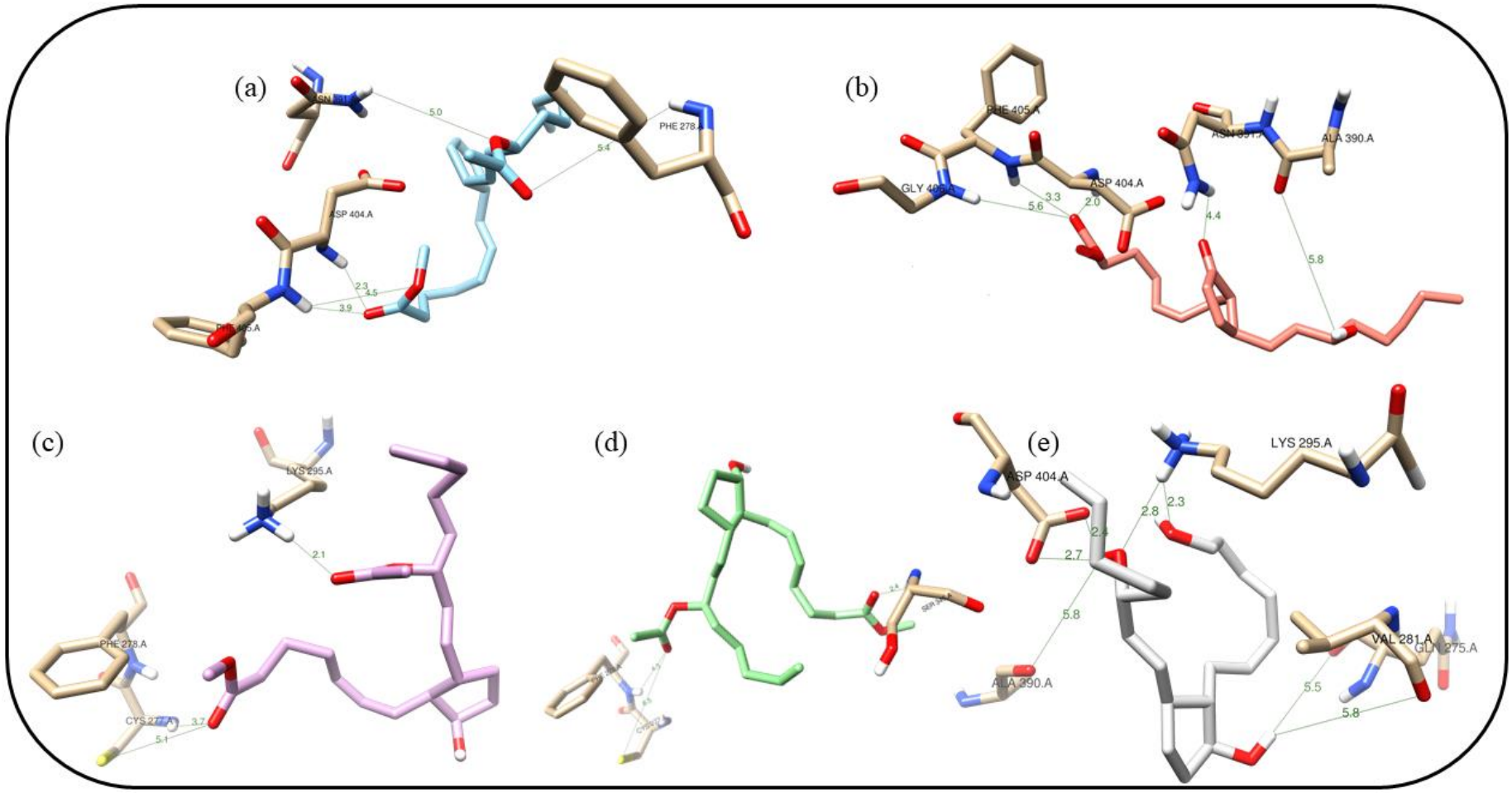

Table S1: Vina scores and binding features for the best pose of each test compound within the active site of p38α-kinase (PDB ID: 4FA2)

Compound	Vina Scores (kcal/mol)	Binding features		
		Residue	Type	Length (Å)
1	-8,3	[1]Gly110	*H*-Bond	2.0
		[1]Met109	*H*-Bond	2.0
		[1]Gly170	*H*-Bond	2.1
		[1]Leu171	*H*-Bond	2.3
2	-8,0	[1]Gly170	*H*-Bond	2.0
		[1]Leu171	*H*-Bond	2.5
3	-8,1	[1]Gly170	*H*-Bond	2.1
4	-8,1	[1]Gly170	*H*-Bond	2.1
5	-8,5	[3]Lys53	*H*-Bond	2.1

[1]Bonding to amide NH group; [2]Bonding to amide carbonyl group; [3]Bonding to side chain R

Table S2: Vina scores and binding features for the best pose of each test compound within the active site of topoisomerase IIα (PDB ID: 1ZXM)

Compound	Vina Scores (kcal/mol)	Binding features		
		Residue	Type	Length (Å)
1	-8,2	[1]Gly$_{164}$	*H*-Bond	2.1
		[3]Asn$_{150}$	*H*-Bond	2.4
2	-8,7	[3]Asn$_{150}$	*H*-Bond	2.1
		[3]Asn$_{120}$	*H*-Bond	2.3
		[1]Ala$_{167}$	*H*-Bond	2.3
		[1]Ala$_{167}$	*H*-Bond	2.3
3	-8,5	[3]Asn$_{120}$	*H*-Bond	1.8
		[3]Asn$_{150}$	*H*-Bond	2.0
		[1]Ala$_{167}$	*H*-Bond	2.1
		[3]Thr$_{215}$	*H*-Bond	2.2
4	-8,6	[3]Asn$_{120}$	*H*-Bond	1.8
		[1]Ala$_{167}$	*H*-Bond	2.1
5	-8,0	[1]Ser$_{149}$	*H*-Bond	1.8

[1]Bonding to amide NH group; [2]Bonding to amide carbonyl group; [3]Bonding to side chain R

Table S3: Vina scores and binding features for the best pose of each test compound within the active site of Src-kinase (PDB ID: 2BDF)

Compound	Vina scores (kcal/mol)	Binding features		
		Residue	Type	Length (Å)
1	-8,3	[1]Asp404	*H*-Bond	2.3
2	-8,9	[1]Asp404	*H*-Bond	2.0
		[3]Glu310	*H*-Bond	2.2
3	-7,9	[3]Lys295	*H*-Bond	2.1
4	-8,1	[1]Ser345	*H*-Bond	2.4
5	-8,1	[3]Lys295	*H*-Bond	2.3
		[2]Asp404	*H*-Bond	2.4
		[3]Asp404	*H*-Bond	2.7

[1]Bonding to amide NH group; [2]Bonding to amide carbonyl group; [3]Bonding to side chain R