Supplementary Material

In vitro antibacterial activities, DPPH radical scavenging, and molecular simulation of isolated compounds from the leaves of *Rhus ruspolii*

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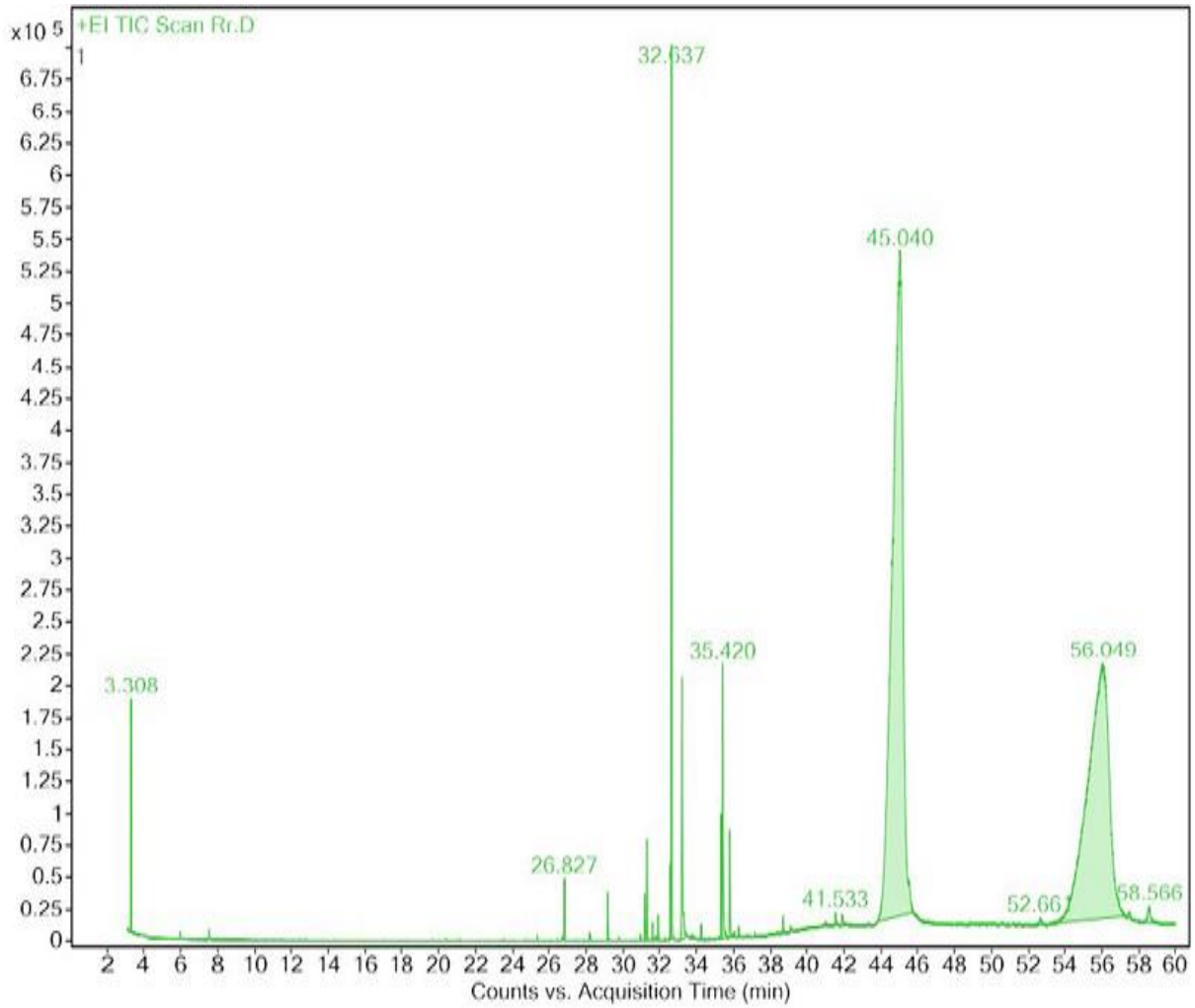


Figure S1. Total ion chromatogram (TIC) of combined fractions 6-10 of *R. ruspolii* leaves.

Table S-1. The ^{1}H-NMR (400.2 MHz) and ^{13}C-NMR (100.6 MHz) spectral data of compound **7** and NMR spectral data reported for palmitic acid.

C №	Compound **7**/ DMSO-d_6		Palmitic acid [38]
	δ^{1}H (*J* in Hz)	δ^{13}C	δ^{13}C/ $CDCl_3$
1	-	174.5	178.3
2	2.16 (t, *J* = 7.4, 2H)	33.7	33.0
3	1.45 (m, 2H)	24.5	24.6
4			
5			
6			
7			
8	1.23 (br. s, 24H)	28.5-29.0	29.0-29.5
9			
10			
11			
12			
13			
14		31.3	31.9
15		22.1	22.7
16	0.84 (t, *J* = 7.3, 3H)	13.9	14.1

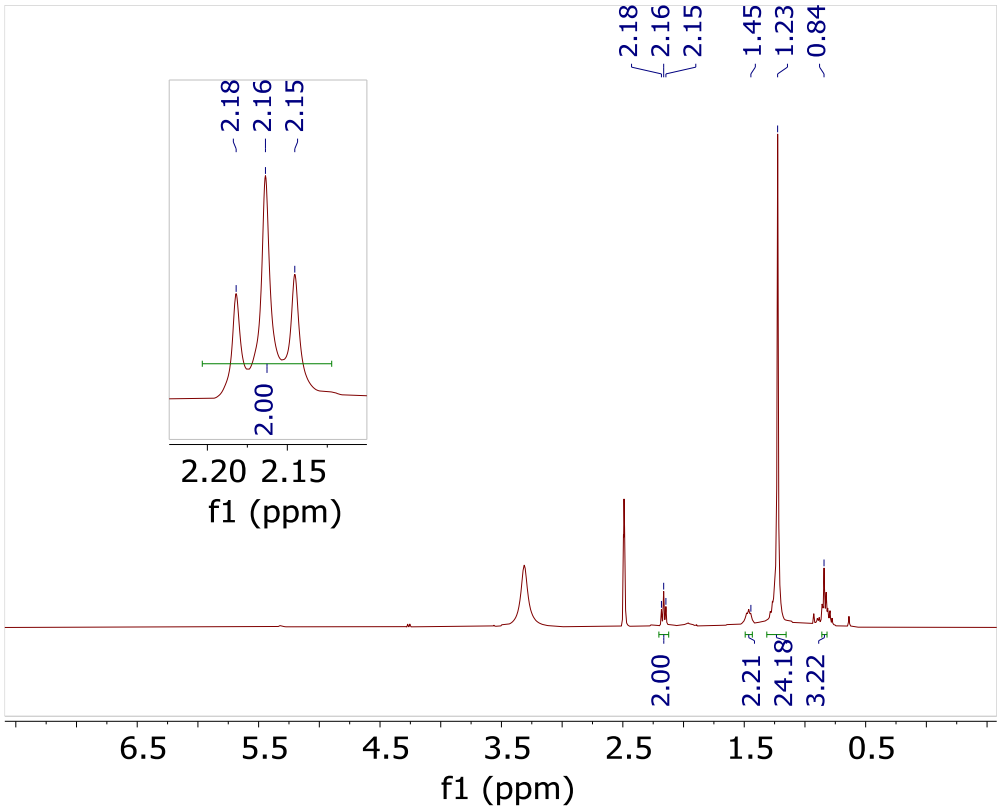


Figure S2. [1]H NMR spectrum of compound **7** with some expanded regions.

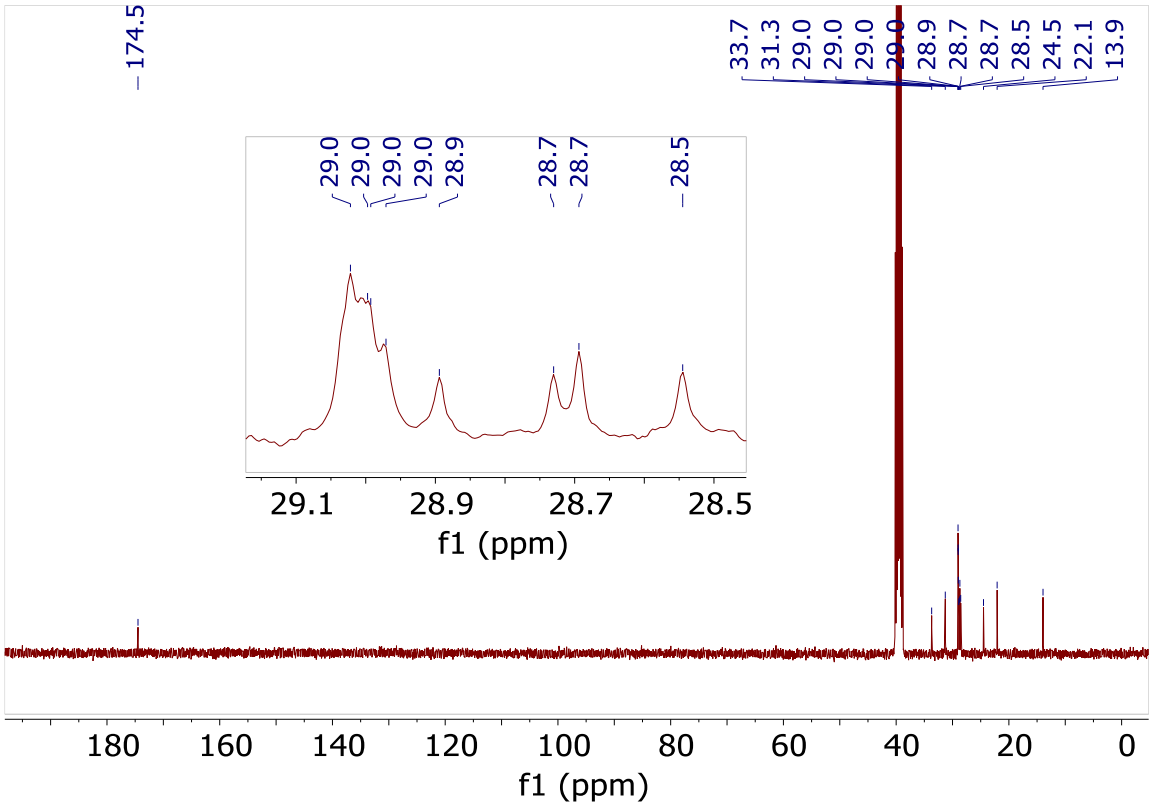


Figure S3. [13]C NMR spectrum of compound **7** with some expanded regions**.**

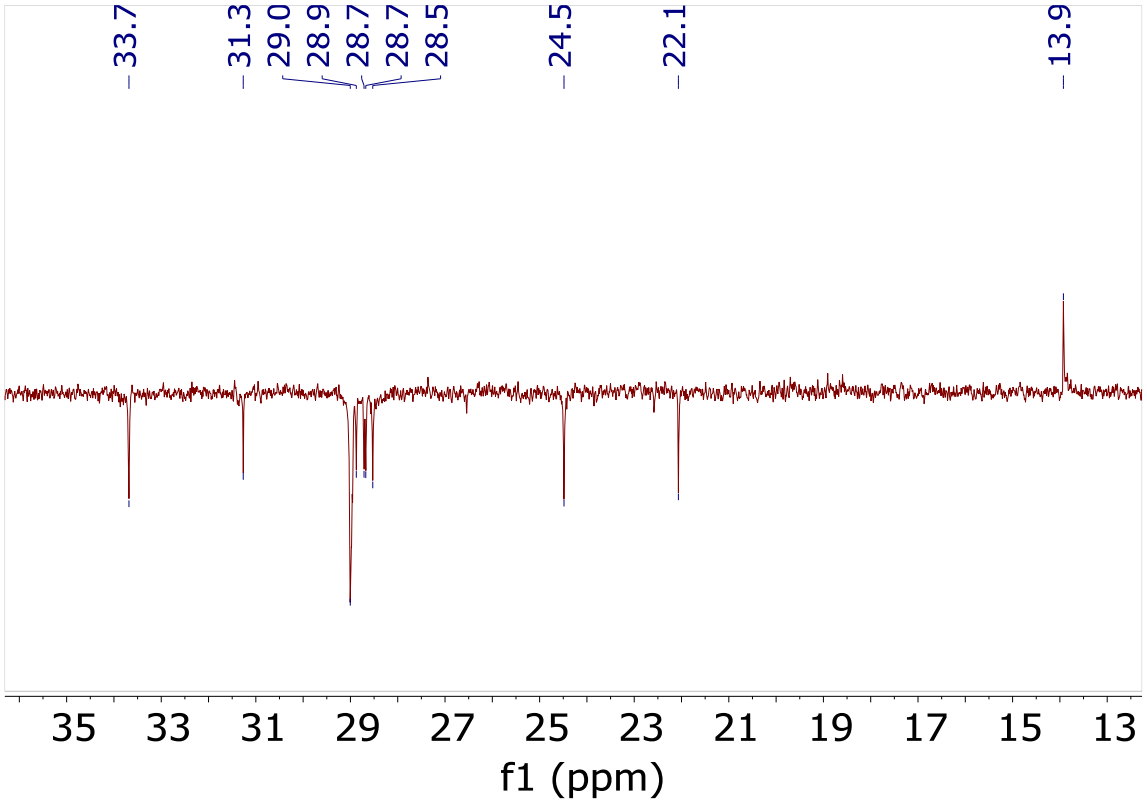


Figure S4. ^{13}C DEPT-135 NMR spectrum of compound **7**.

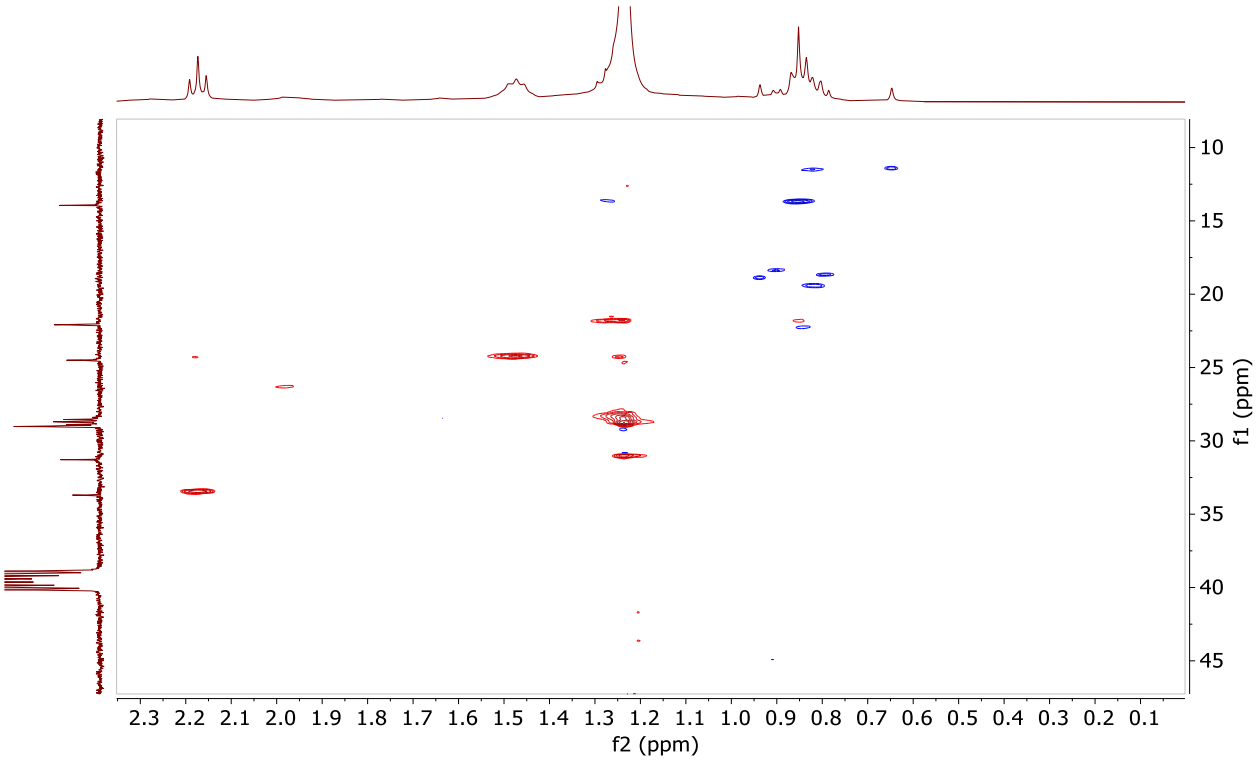


Figure S5. ^{1}H-^{13}C HSQC NMR spectrum of compound **7**.

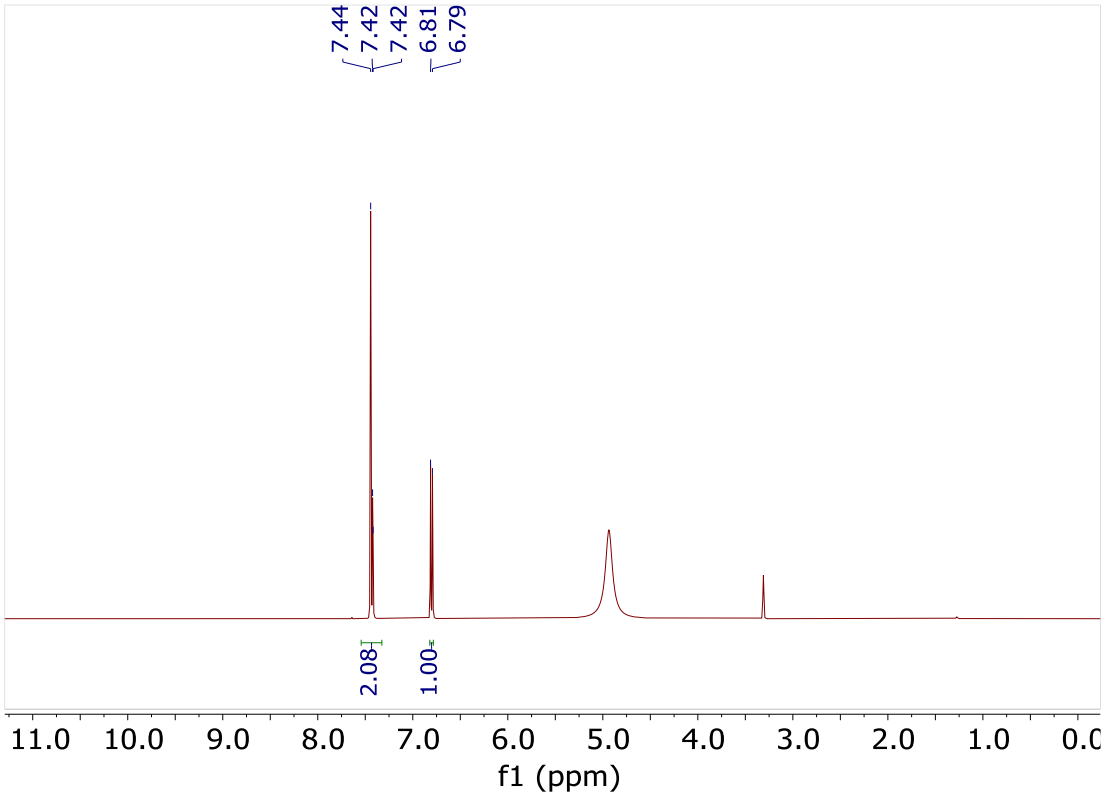


Figure S6. ^{1}H NMR spectrum of compound **17**.

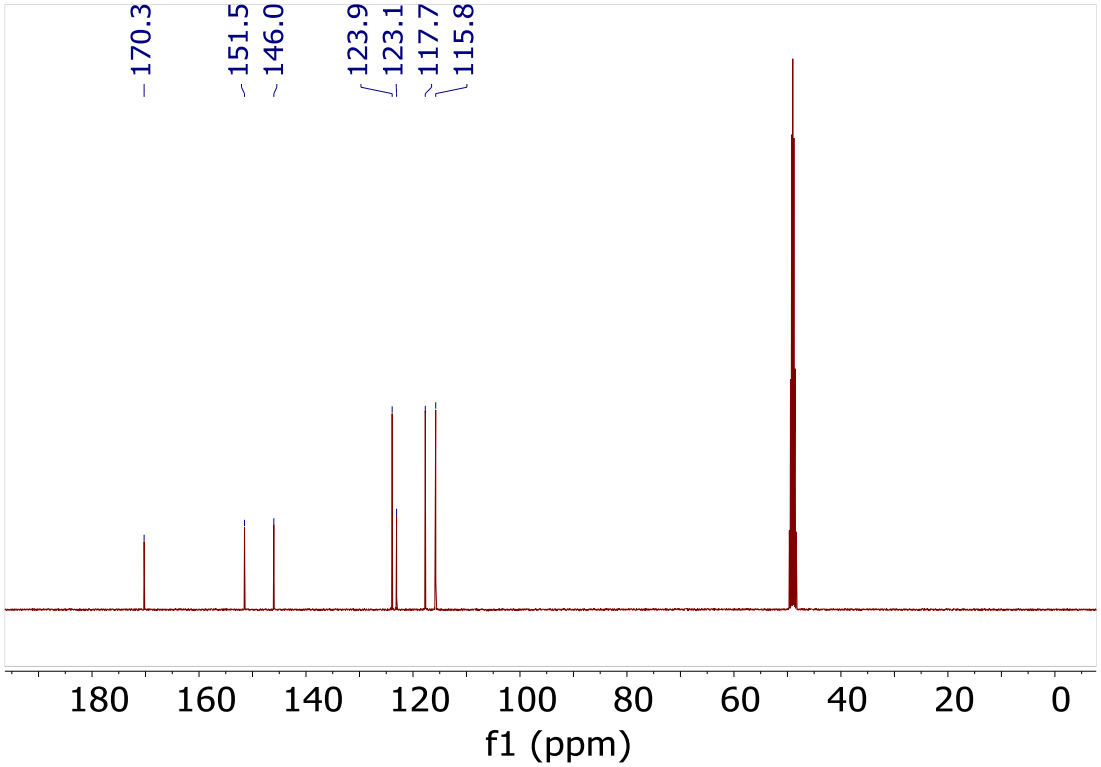


Figure S7. ^{13}C NMR spectrum of compound **17**.

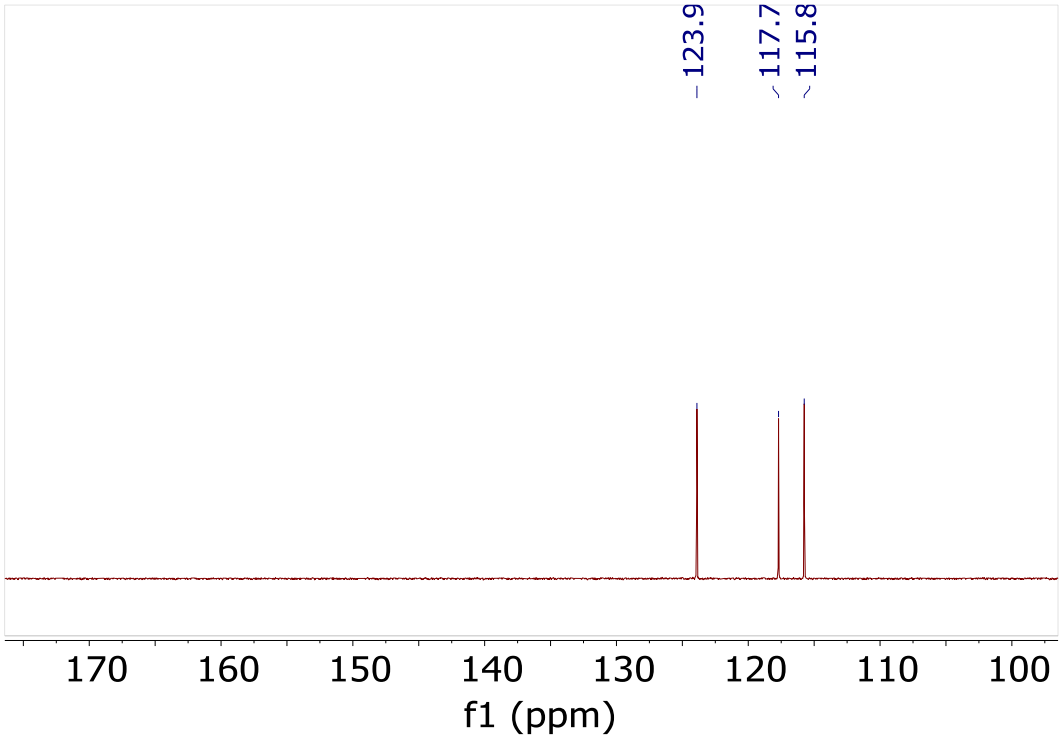


Figure S8. ^{13}C DEPT-135 NMR spectrum of compound **17**.

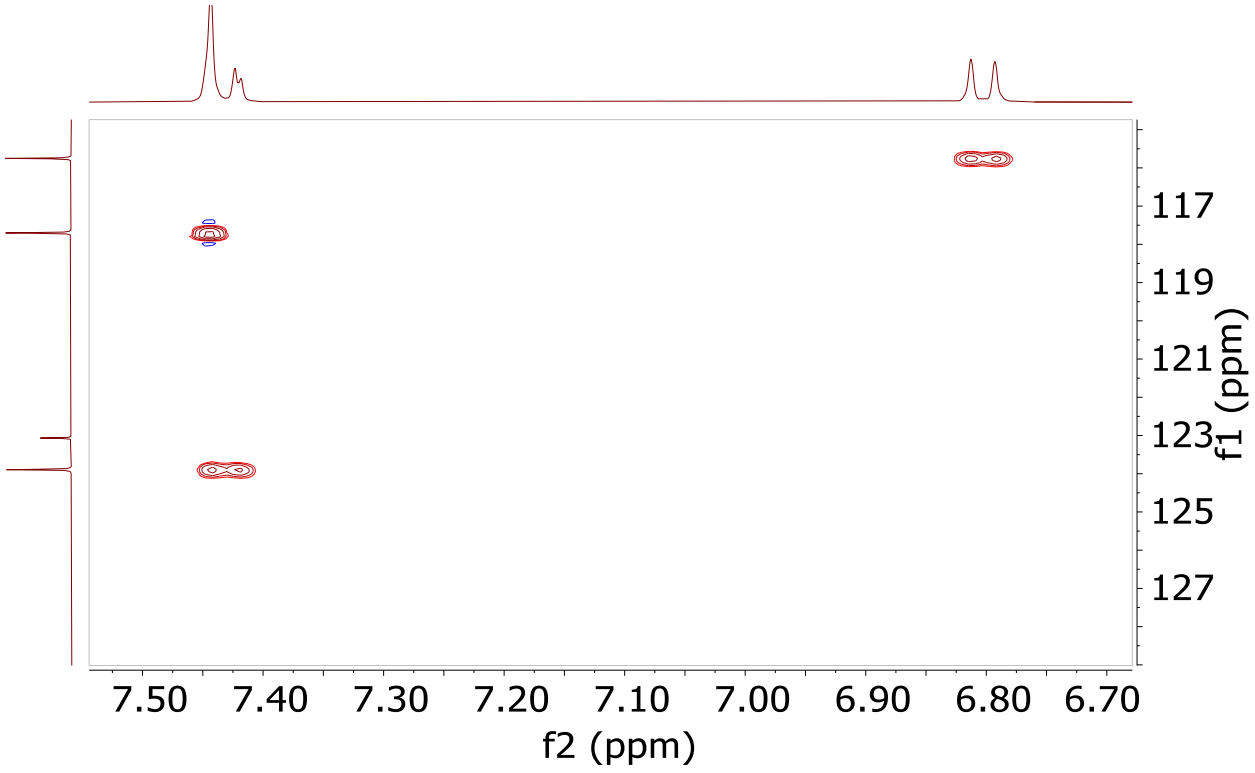


Figure S9. ^{1}H-^{13}C HSQC NMR spectrum with assignments of resonances of compound **17**.

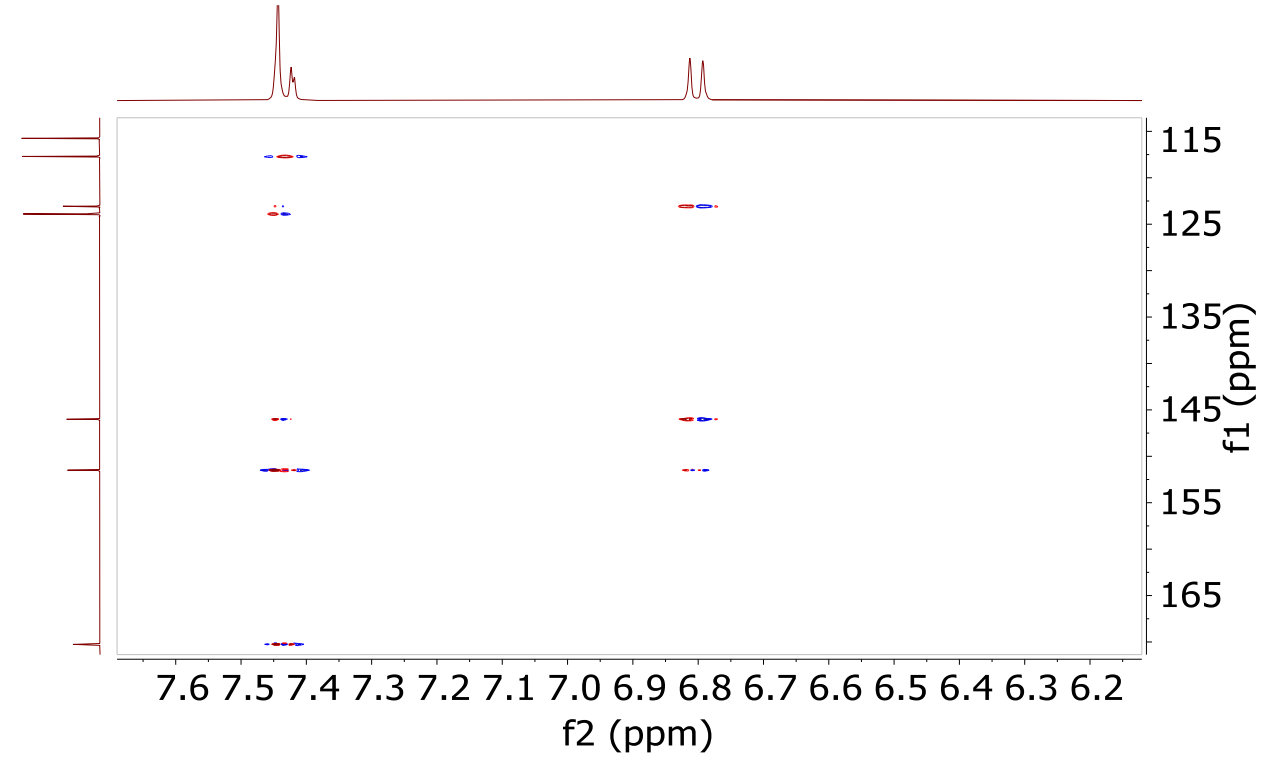


Figure S10. ^{1}H-^{13}C HMBC NMR spectrum of compound **17**.

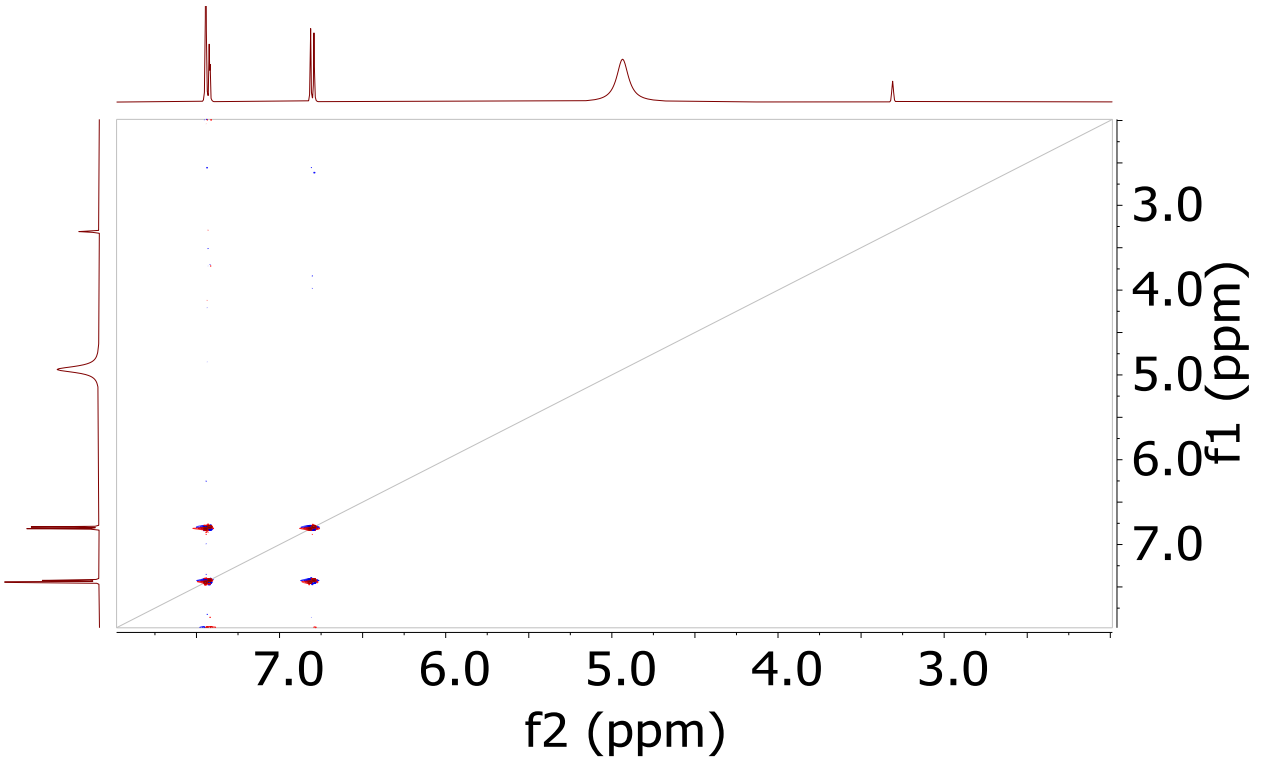


Figure S11. ^{1}H-^{1}H DQF-COSY NMR spectrum of compound **17**.

Table S-2. ^{1}H-NMR (400.2 MHz) and ^{13}C-NMR (100.6 MHz) spectral data of compound **19** and NMR data reported for amentoflavone.

	Compound **19**/ DMSO-d_6				δ^{13}C Amentoflavone [45, 46]	
C-No	δ^{1}H (*J* in Hz)	δ^{13}C	^{1}H-^{1}H COSY	^{1}H-^{13}C HMBC	Acetone-d_6 [46]	DMSO-d_6 [45]
2/2''	-	163.9/163.6			163.9/162.4	164.1/164.3
3/3''	6.83 (s, 1H)/ 6.78 (s, 1H)	102.9/102.6		C-2, 4, 10/2'',4'', 10''	103.0/102.8	103.2/102.8
4/4''	-	181.7/182.1			182.2/182.4	181.9/182.2
5/5''	-	161.4/160.5			164.1/163.8	161.6/160.8
6/6''	6.19 (d, *J*= 2.4, 1H)/ 6.37 (s, 1H)	98.8/98.9		C-5, 10/5'', 7'', 8'', 10''	98.8/99.9	98.8/99.1
7/7''	-	164.1/162.8 (weak)			164.6/161.1	163.9/161.9
8/8''	6.45 (d, *J*= 2.4,1H)/-	94.0/104.3		C-9, 10/-	93.9/104.4	94.2/104.1
9/9''	-	157.4/154.5			155.2/157.9	157.6/154.7
10/10''	-	103.7/103.5			104.1/104.0	104.0/104.0
1'/1'''	-	120.6/121.4			121.3/127.4	120.3/121.4
2'/2'''	8.03 (d, *J*= 2.4, 1H)/ 7.58 (dd, *J*= 8.8, 2.4, 1H)	131.4/128.2	-/H-3'''	C-2, 4', 8''/2'', 4''', 6'''	131.6/128.2	127.9/128.3
3'/3'''	-/6.70 (dd, *J*= 8.8, 2.4, 1H)	120.3/115.7	-/H-2'''	-/C-5'''	117.6/115.8	121.7/116.0
4'/4'''	-	160.1/161.0			160.9/163.9	159.6/161.1
5'/5'''	7.14 (d, *J*= 8.7, 1H)/ 6.70 (dd, *J*= 8.8, 2.4, 1H)	116.5/115.7	H-6'/6'''	C-1'/1'''	117.6/115.8	116.4/116.0
6'/6'''	7.99 (dd, *J*= 8.7, 2.4, 1H)/ 7.58 (dd, *J*= 8.8, 2.4, 1H)	127.7/128.2	H-5'/5'''	C-2'/2'''	127.4/128.2	131.6/128.3
OH-5/ OH-5''	12.98 (s, 1H)/ 13.11 (s, 1H)	-		C-5, 6, 10/5'', 6'',10''		-

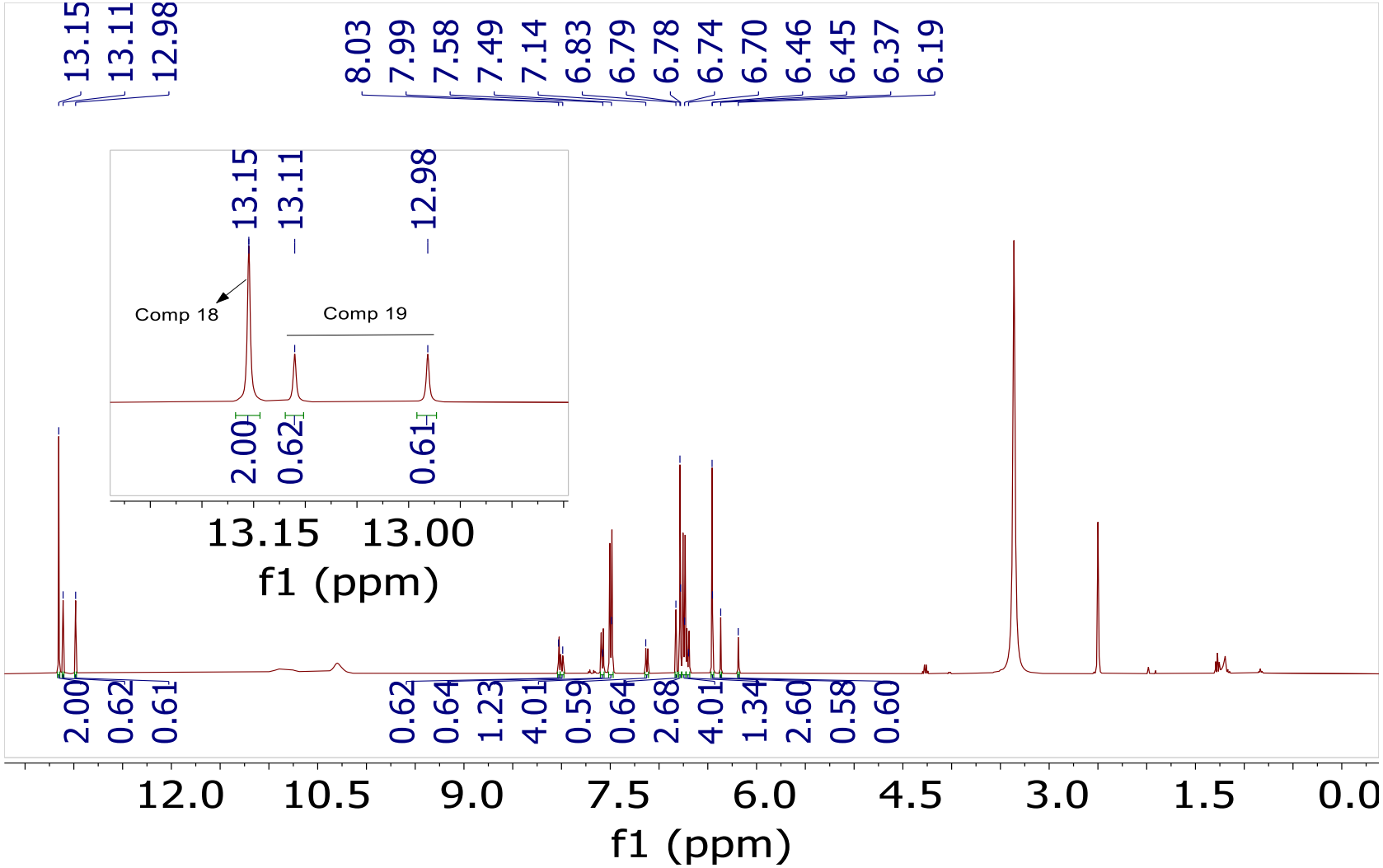


Figure S12. ^{1}H NMR spectra of compounds **18** and **19.**

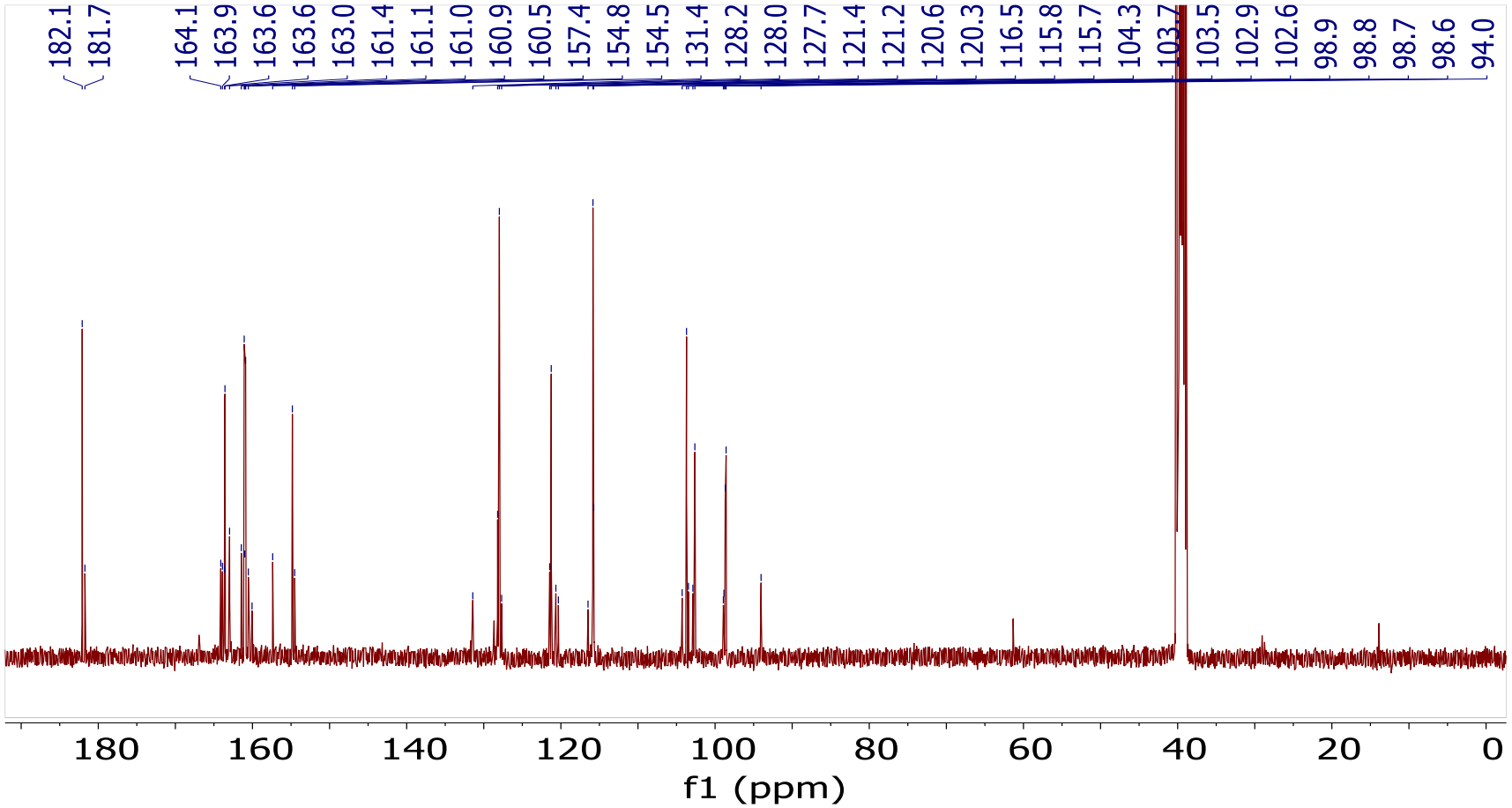


Figure S13. ^{13}C NMR spectrum of compounds **18** and **19.** .

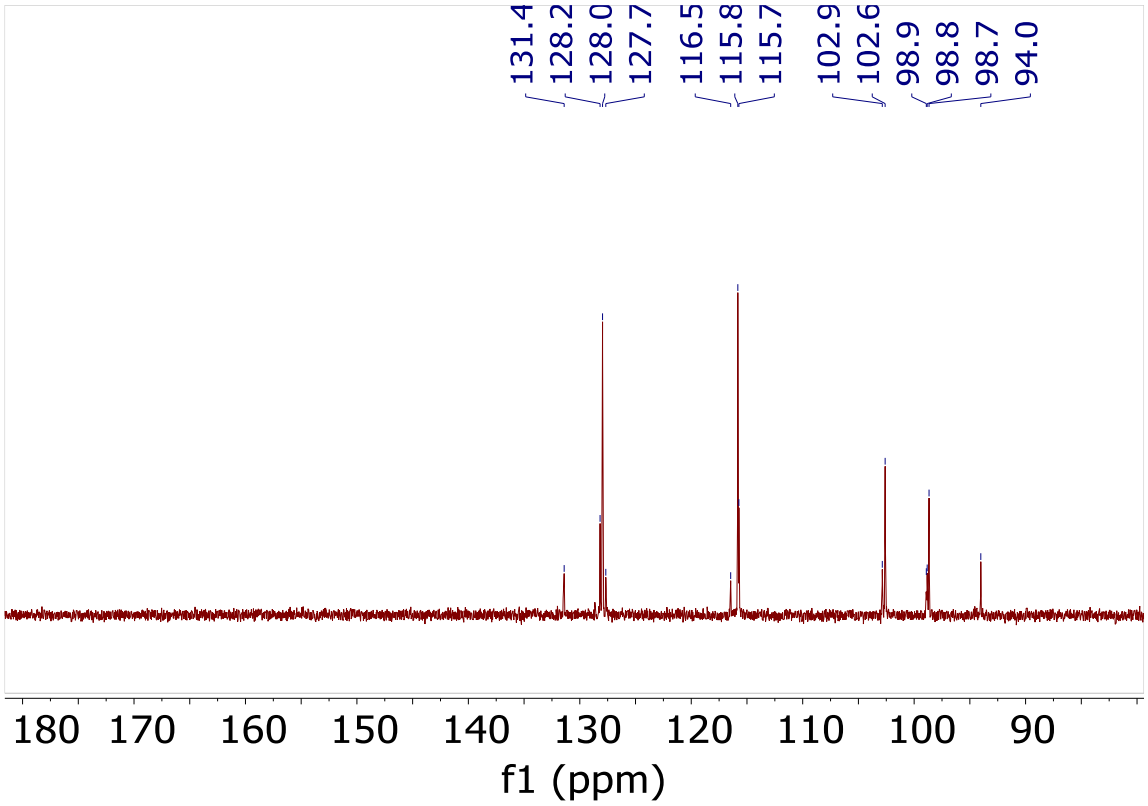


Figure S14. ^{13}C DEPT-135 NMR spectrum of compounds **18** and **19.**

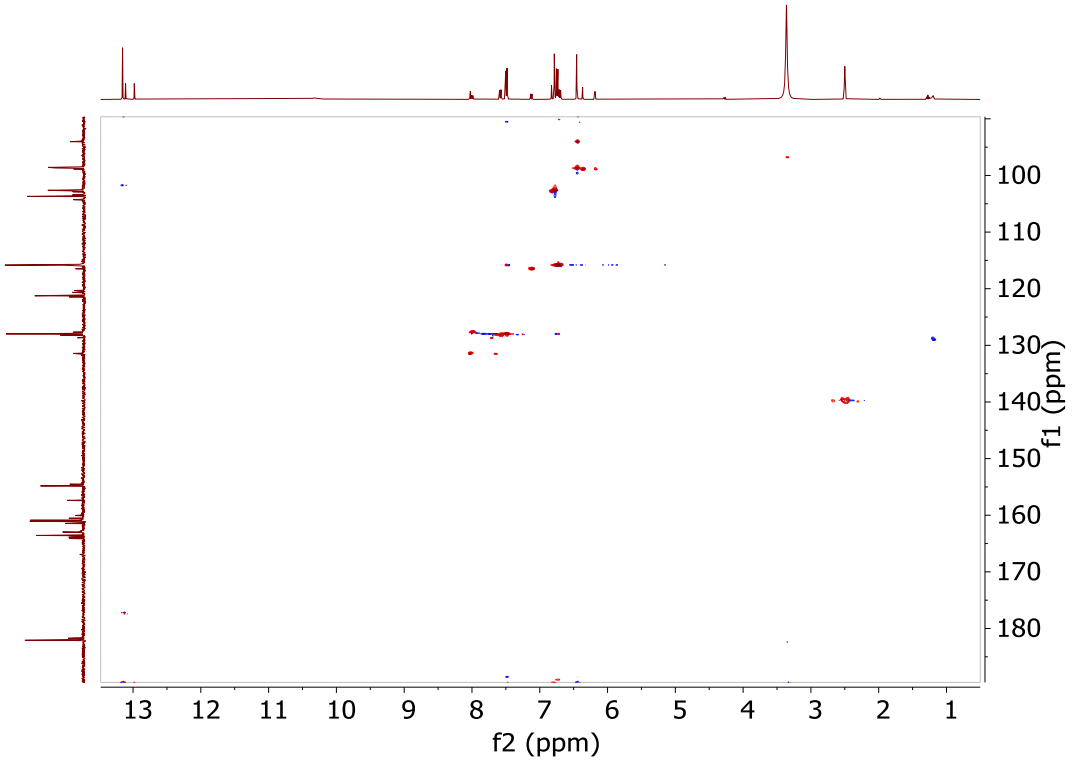


Figure S15. ^{1}H-^{13}C HSQC NMR spectrum of compounds **18** and **19.**

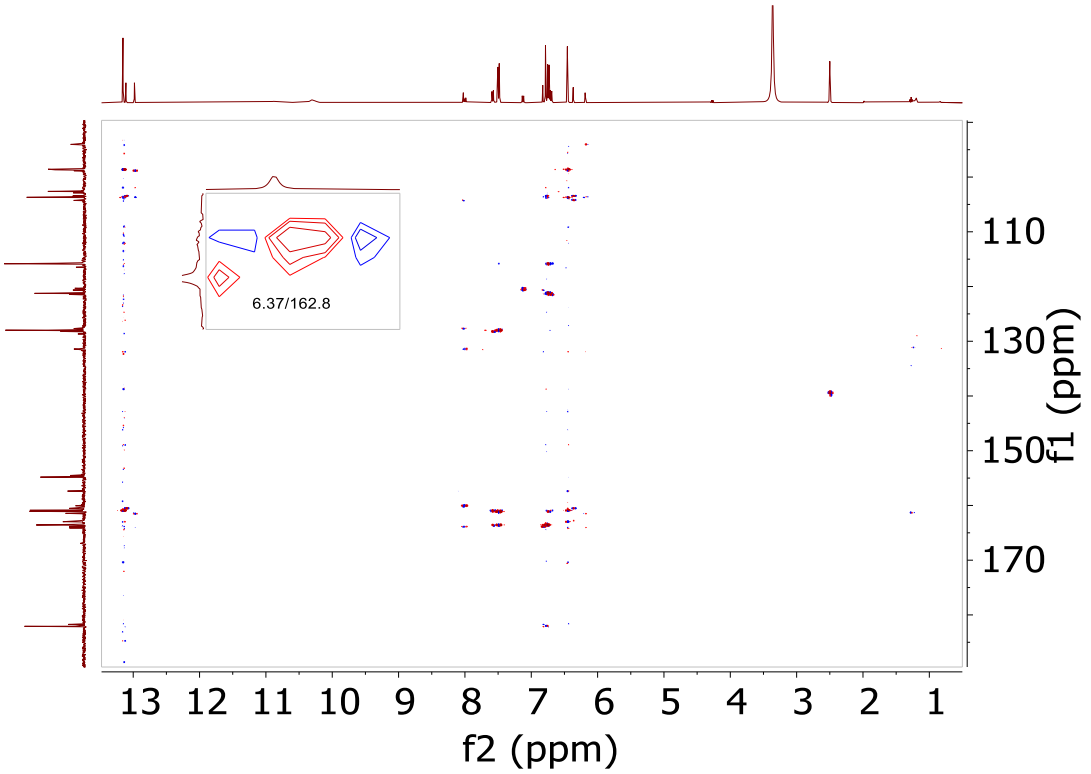


Figure S16. ^{1}H-^{13}C HMBC NMR spectrum of compounds **18** and **19** and the expanded region used to assign C-7'' of compound **19**.

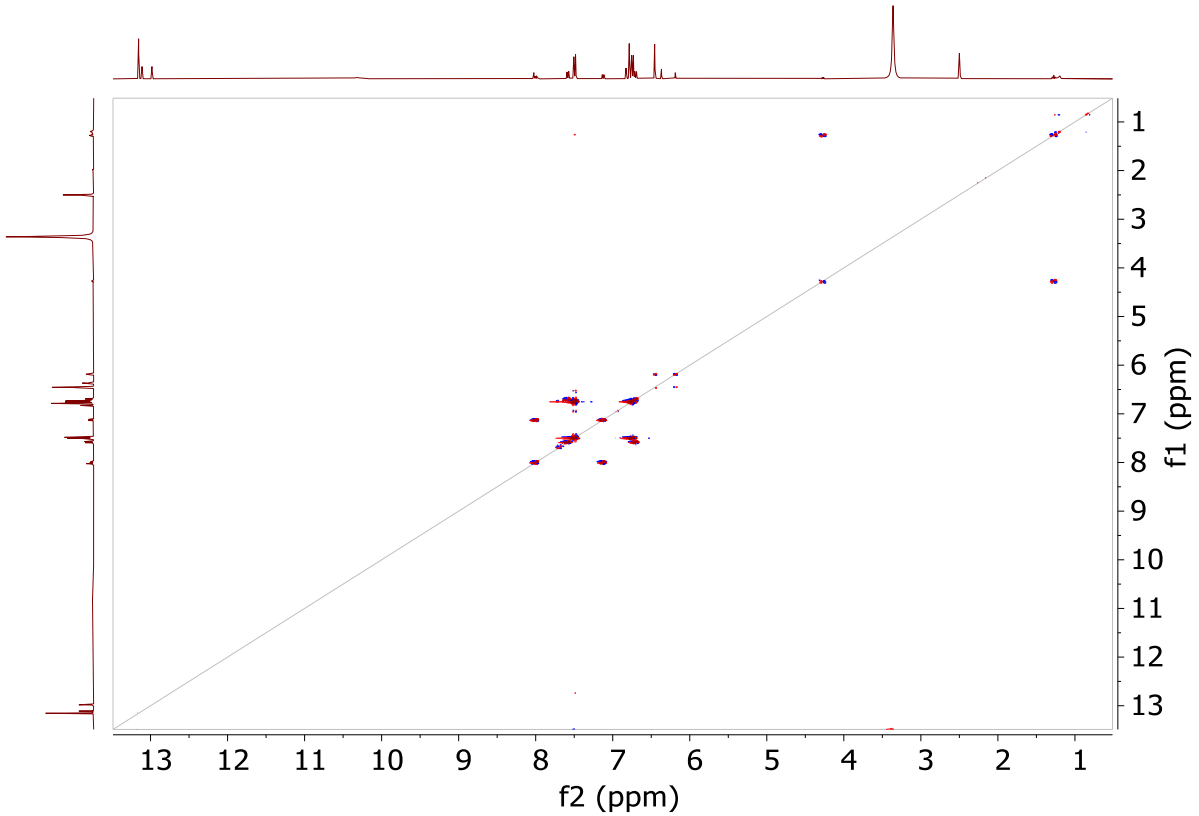


Figure S17. ^{1}H-^{1}H DQF-COSY NMR spectrum of compounds **18** and **19.**

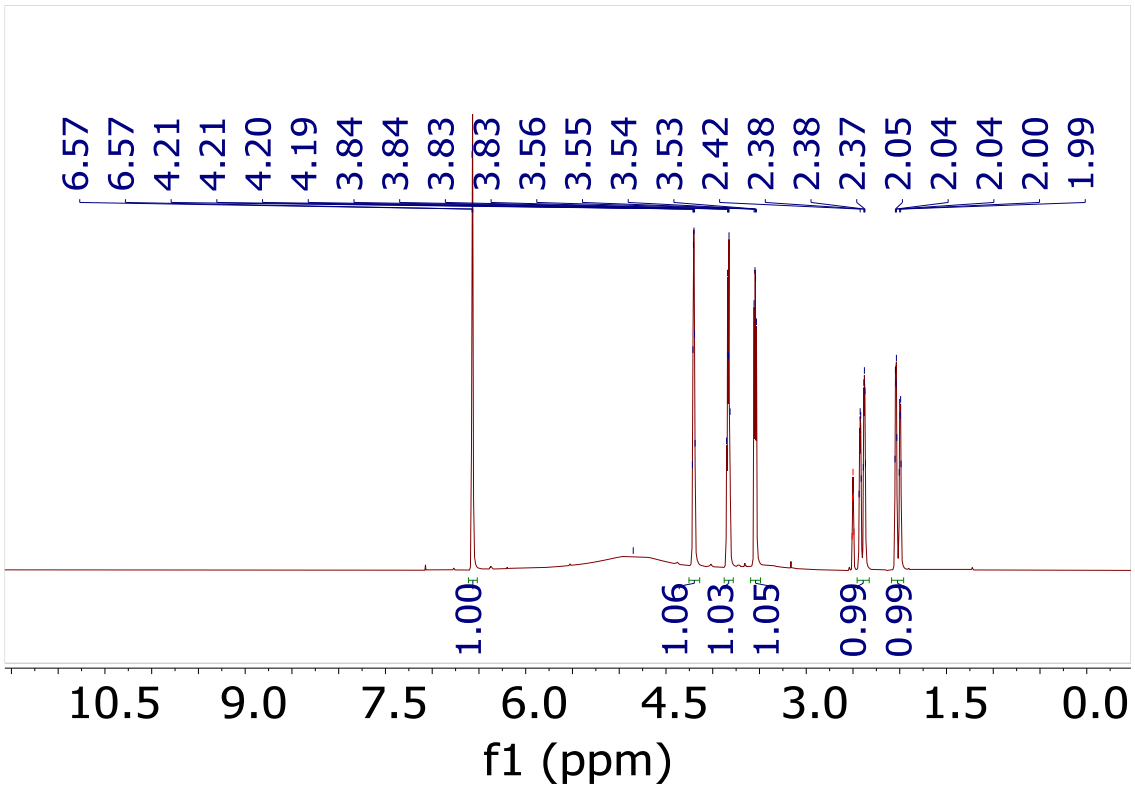


Figure S18. ^{1}H NMR spectrum of compound **20.**

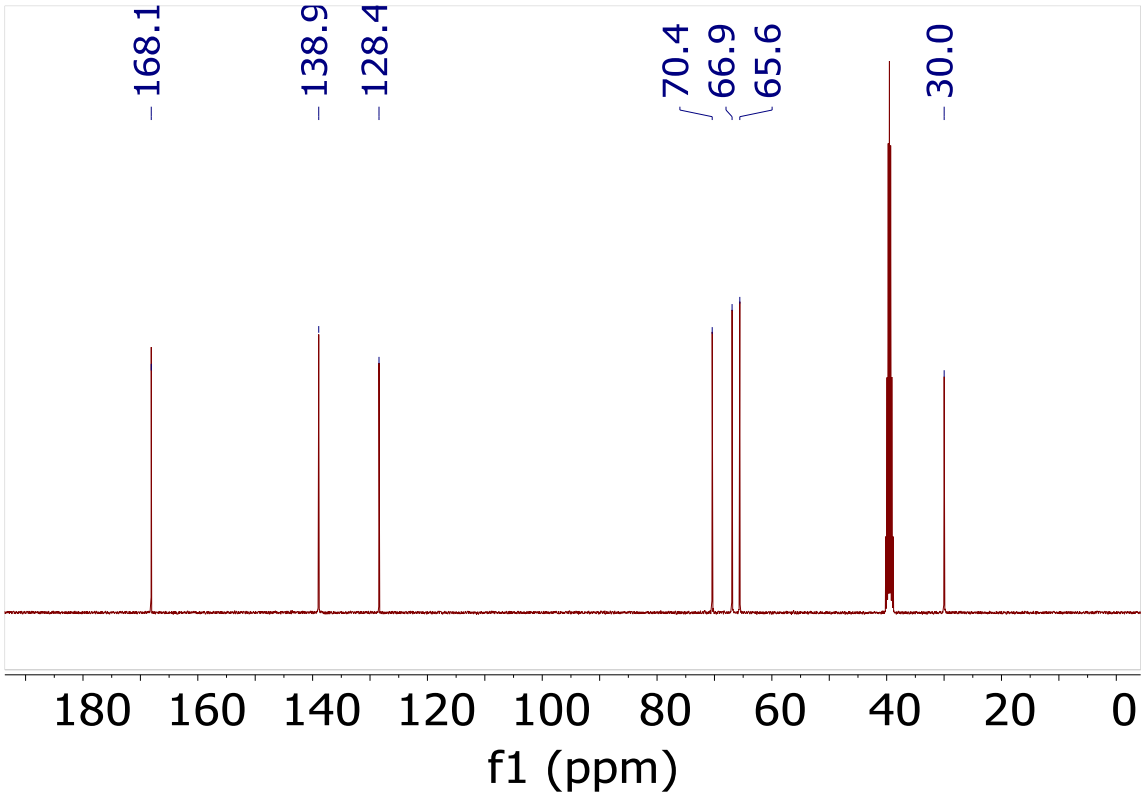


Figure S19. ^{13}C NMR spectrum of compound **20.**

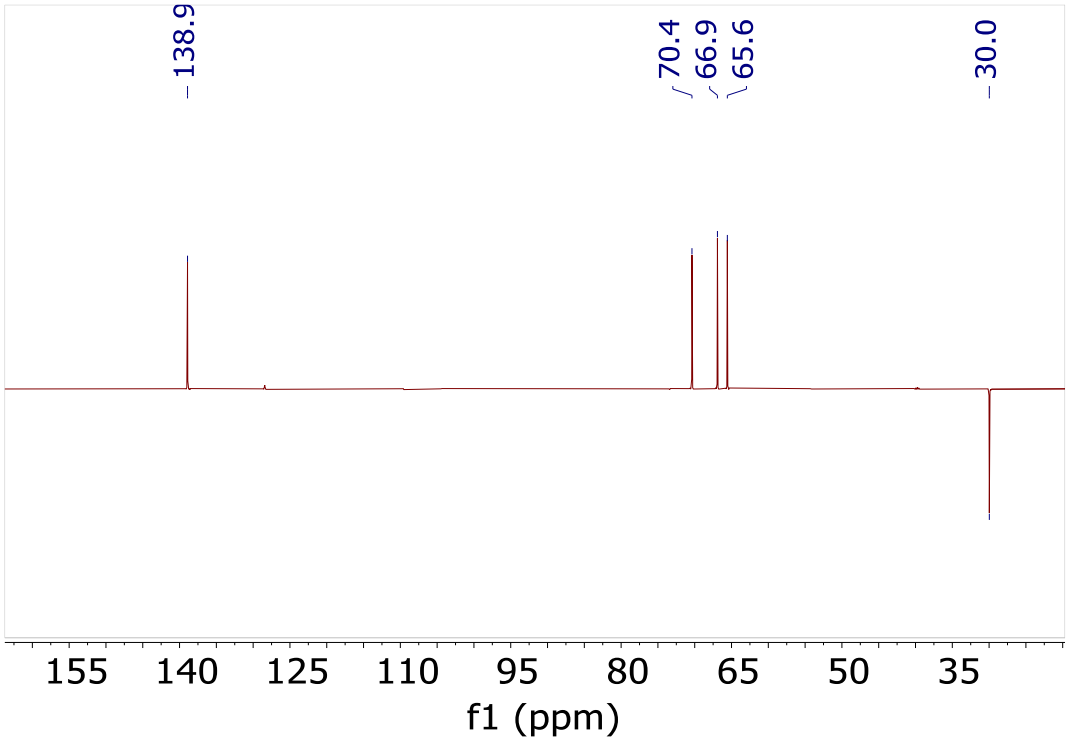


Figure S20. ^{13}C DEPT-135 NMR spectrum of compound **20.**

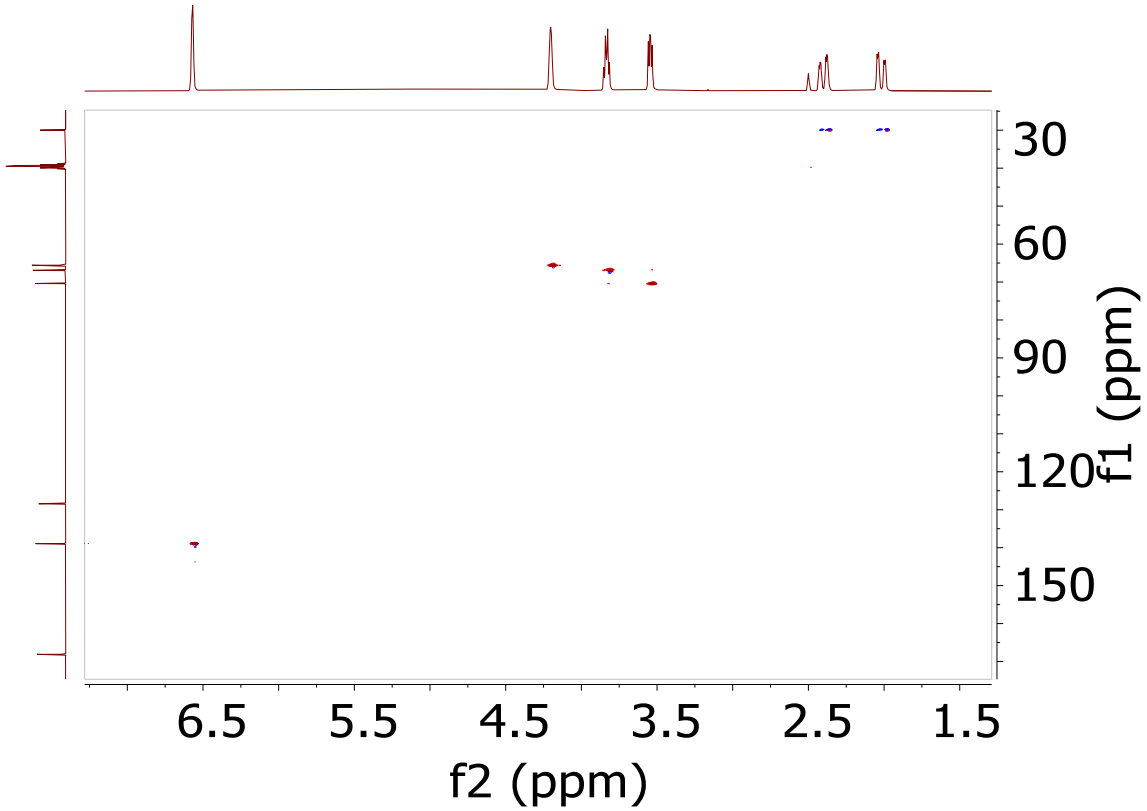


Figure S21. ^{1}H-^{13}C HSQC NMR spectrum of compound **20**.

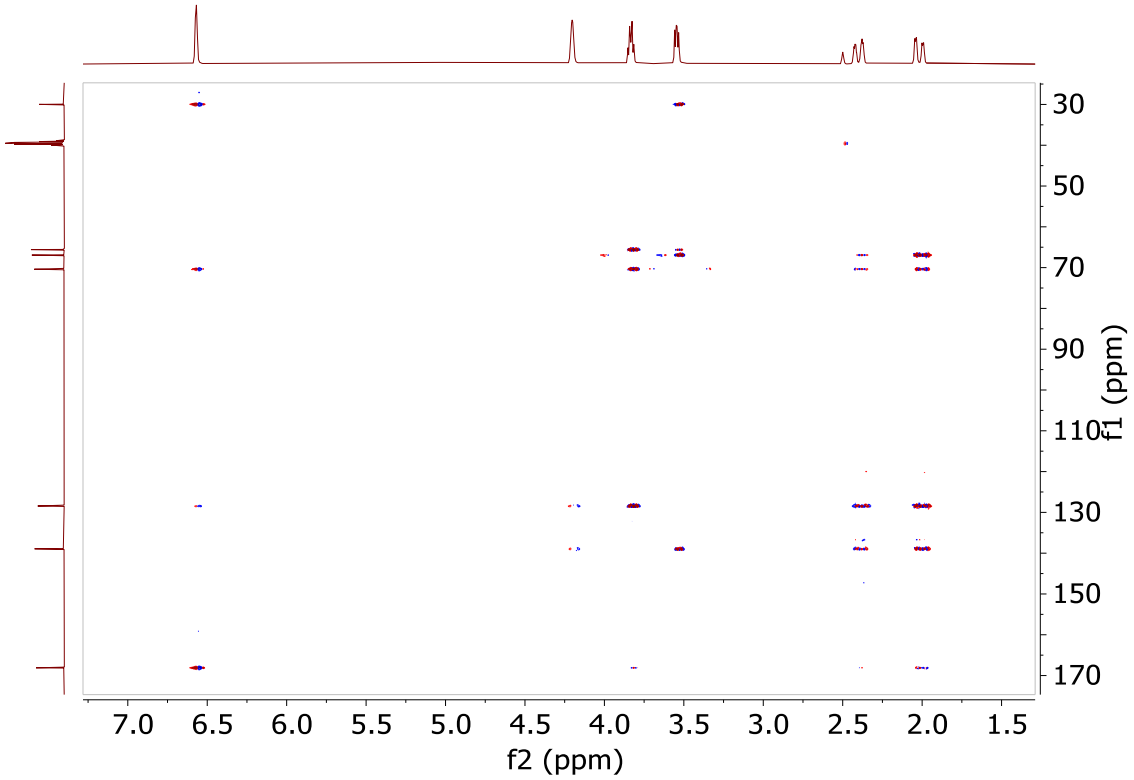


Figure S22. ^{1}H-^{13}C HMBC NMR spectrum of compound **20**.

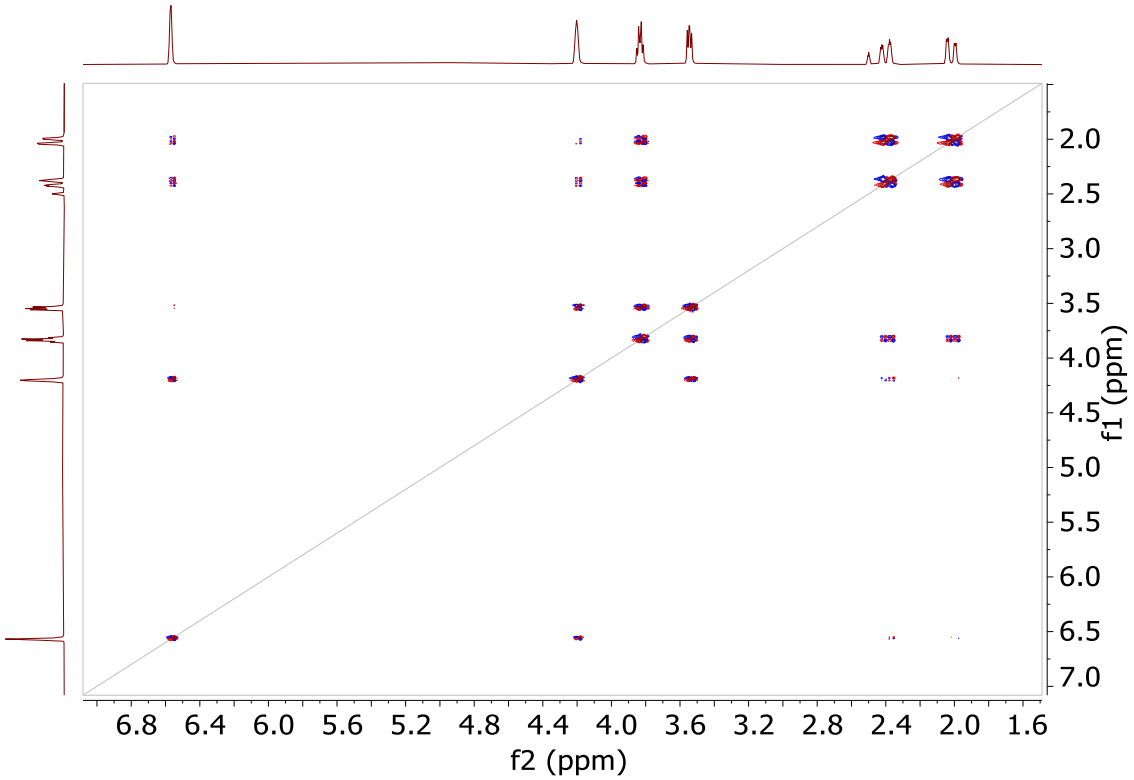


Figure S23. ^{1}H-^{1}H DQF-COSY NMR spectrum of compound **20**.

Table S-3. ^{1}H-NMR (400.2 MHz) and ^{13}C-NMR (100.6 MHz) spectral data of compound **22** and NMR data reported [61].

C-No	Compound **22**/CD_3OD				Myricetin-3-O-α-L-3′′-acetylarabinofuranoside [61]
	δ^{1}H (*J* in Hz)	δ^{13}C	^{1}H-^{1}H COSY	^{1}H-^{13}C HMBC	δ^{13}C/ acetone-d_6
2		159.9			158.3
3		134.9			134.9
4		179.7			179.4
5		163.1			163.1
6	6.21 (d, *J*= 1.7, 1H)	99.9		C-8, 10	99.8
7		166.2			165.6
8	6.39 (d, *J*= 1.7, 1H)	94.8		C-6, 10	95.1
9		158.6			158.2
10		105.6			105.6
1’		122.0			122.5
2’	7.10 (s, 1H)	109.6		C-2, 1’, 3’, 4’	110.1
3’	-	146.8			146.6
4’		137.9			136.7
5’	-	146.8			146.6
6’	7.10 (s, 1H)	109.6		C-2, 1’, 3’, 4’	110.1
1’’	5.41 (br. s, 1H)	109.6	H-2’’	C-3, 4’’	109.6
2’’	4.37 (m, 1H)	83.6	H-1’’		81.9
3’’	3.80 (m, 1H)	79.3	H-2’’		81.7
4’’	3.91 (1H)	84.2		C-2’’’	87.1
5’’	4.10 (1H) 3.93 (1H)	65.0		C-1’’’	63.1
1’’’	-	172.6			171.4
2’’’	1.96 (s, 3H)	20.6		C-1’’’	21.3

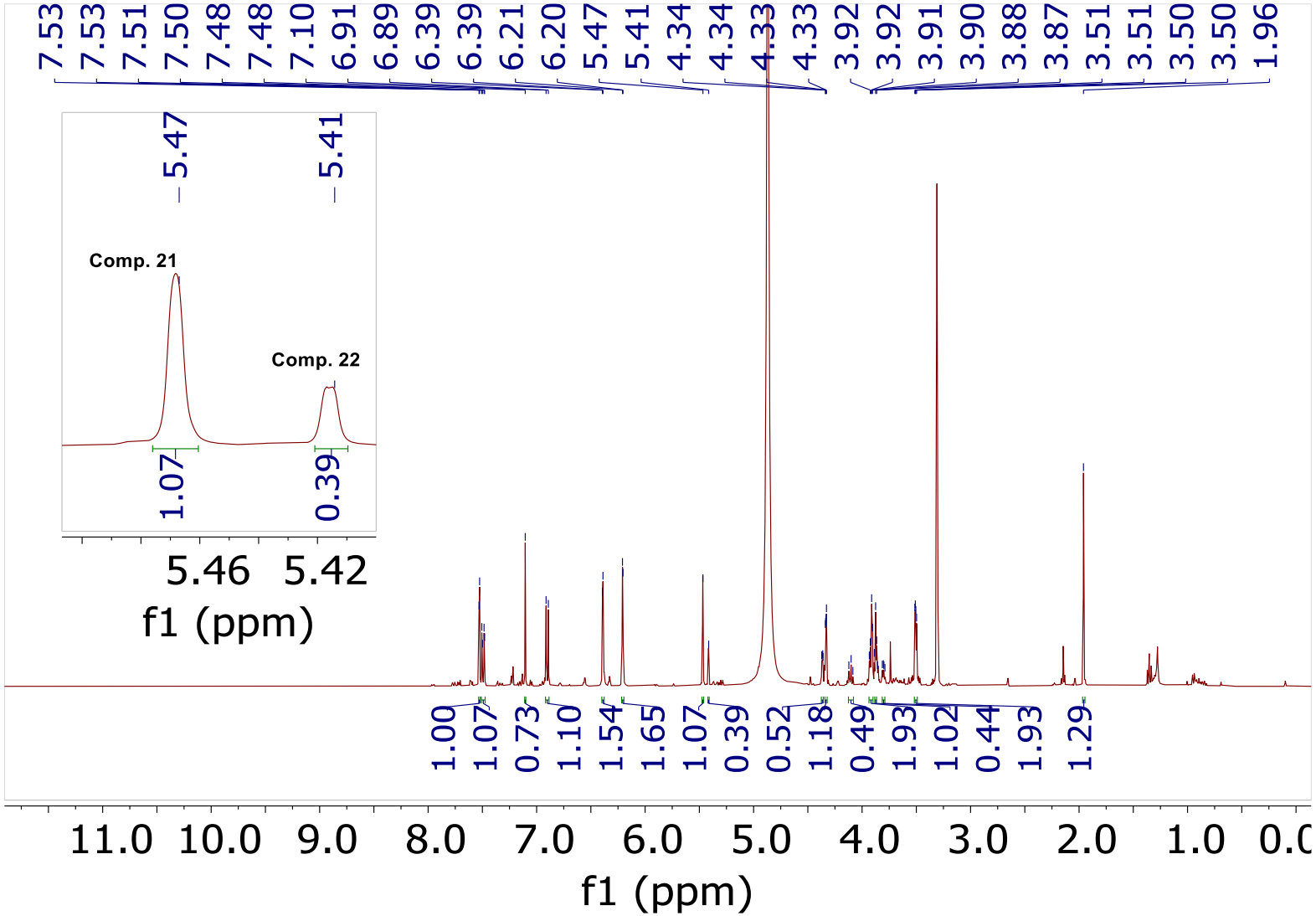


Figure S24. ^{1}H NMR spectrum of compounds **21** and **22** with an expanded region.

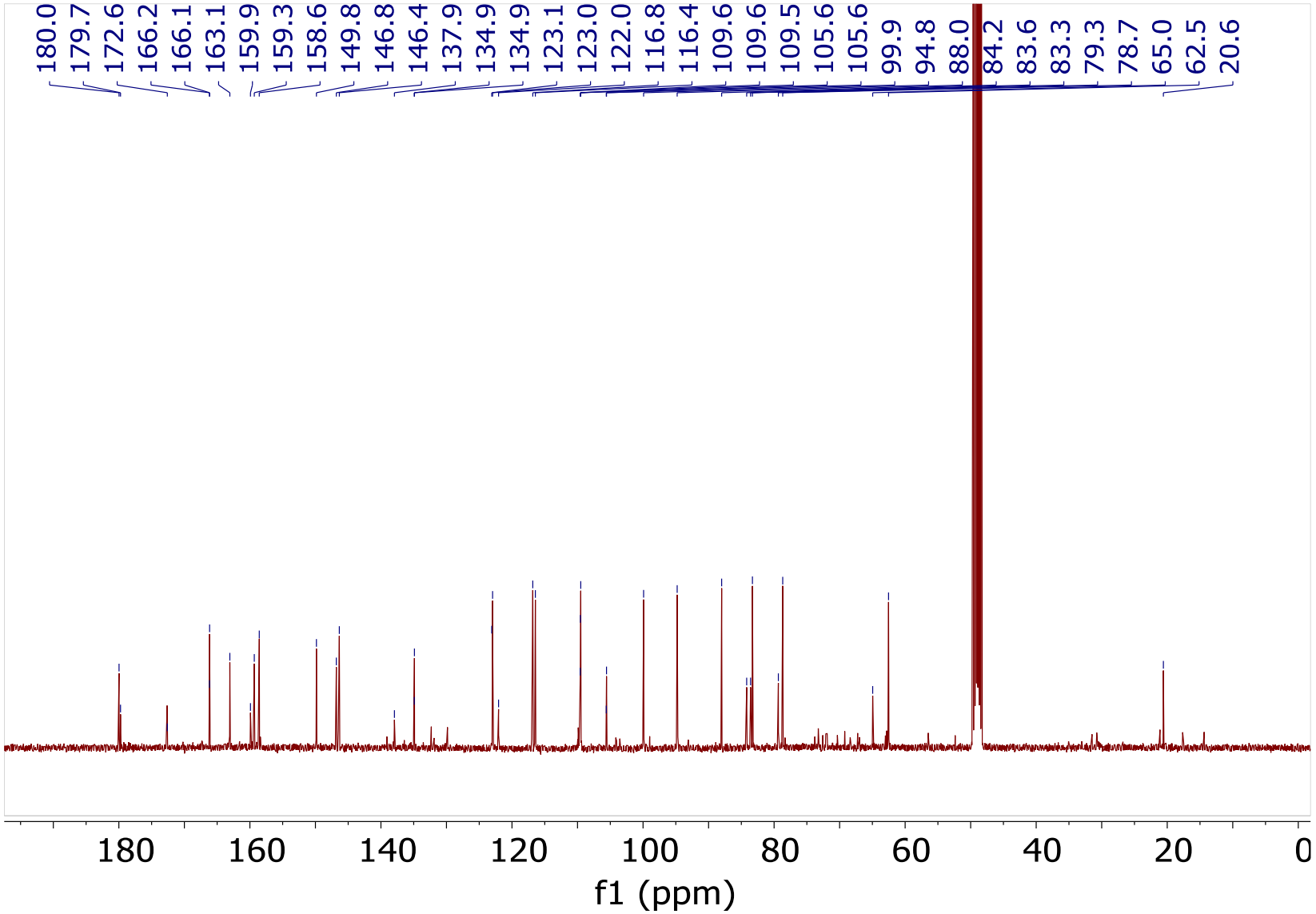


Figure S25. ^{13}C NMR spectrum of compounds **21** and **22**.

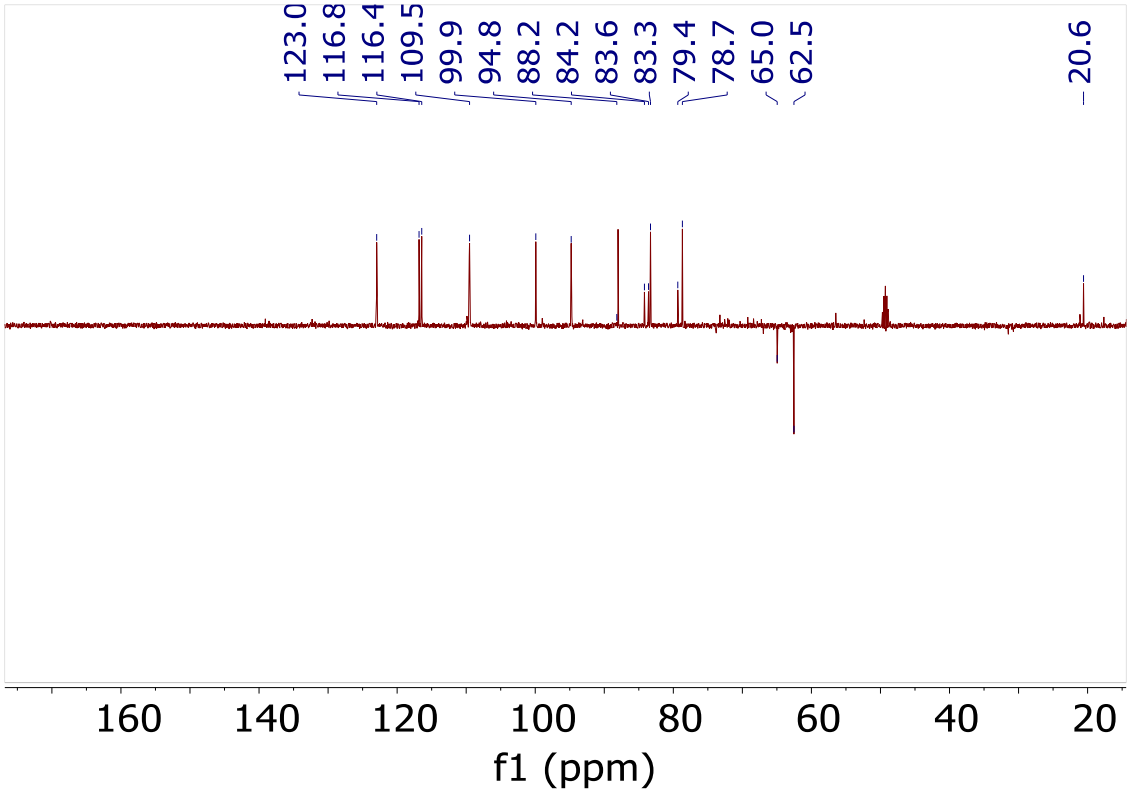


Figure S26. ^{13}C DEPT-135 NMR spectrum of compounds **21** and **22**.

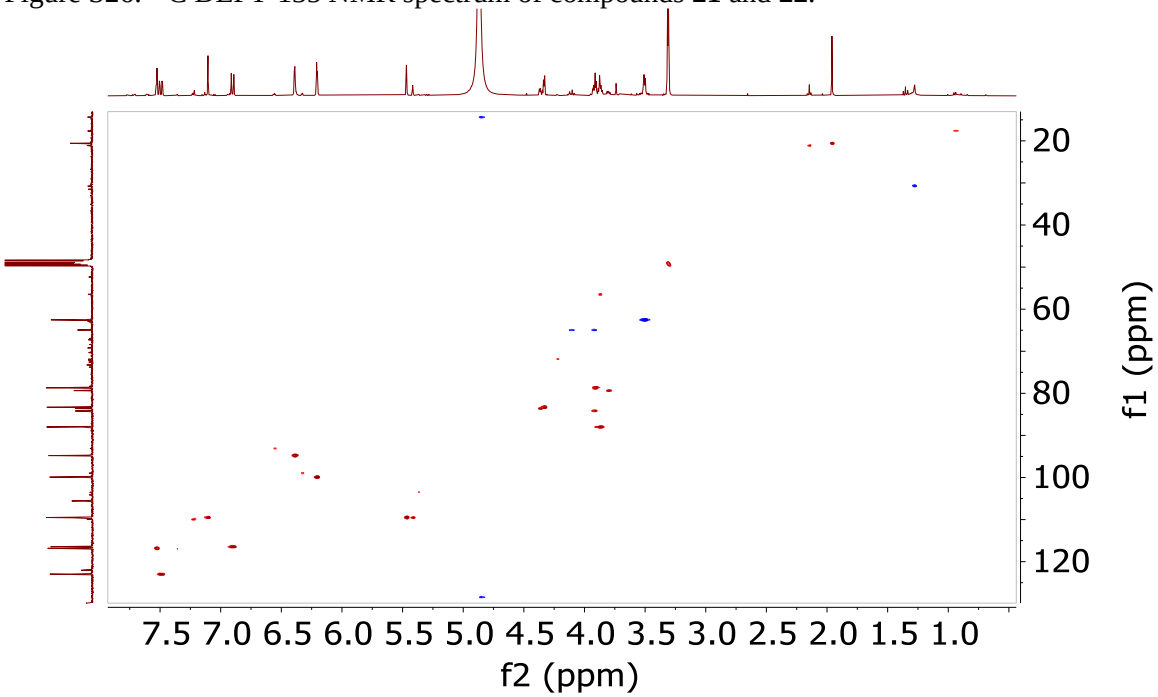


Figure S27. ^{1}H-^{13}C HSQC NMR spectrum of compounds **21** and **22**.

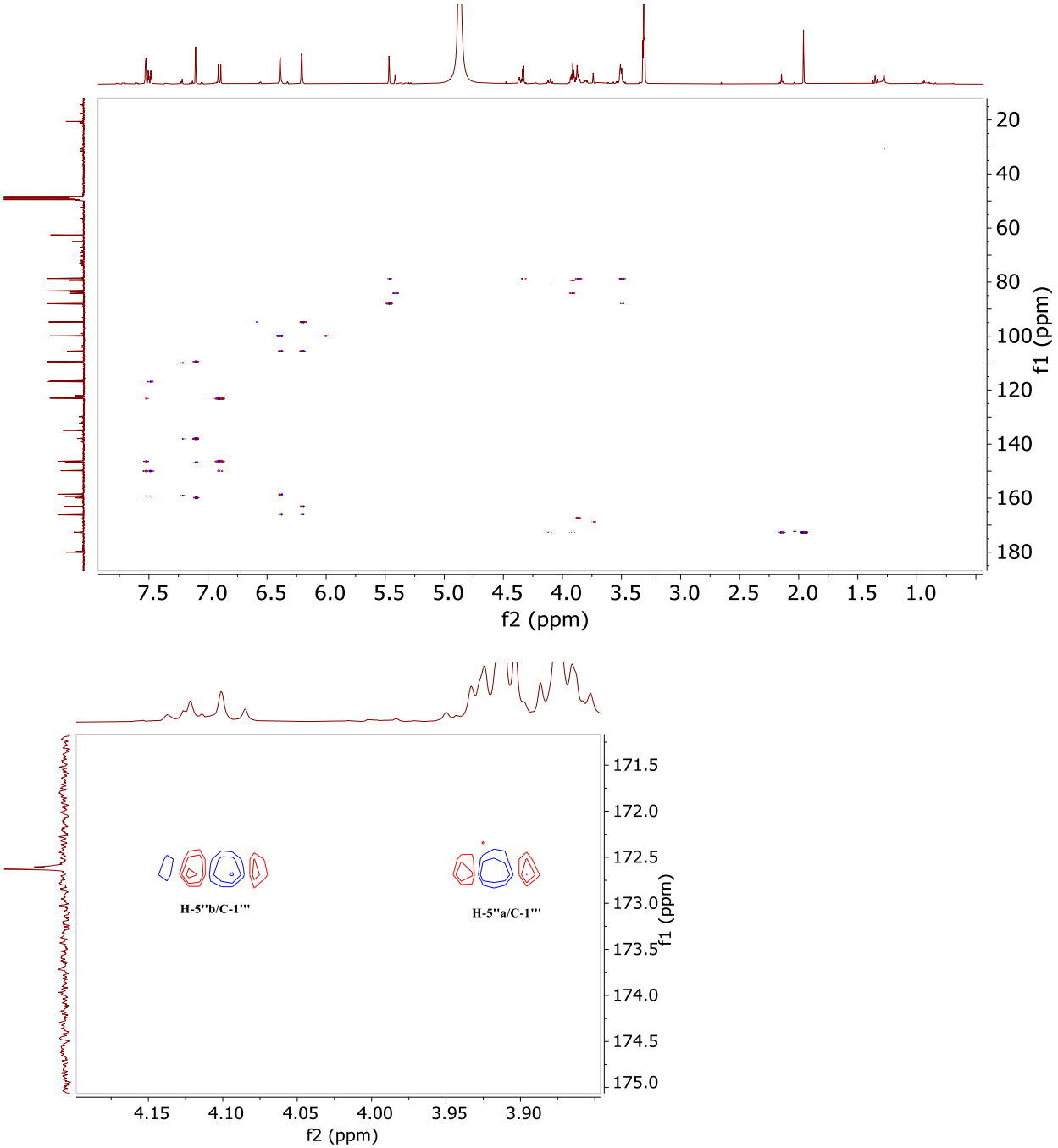


Figure S28. ^{1}H-^{13}C HMBC NMR spectrum of compounds **21** and **22** (top) and the expanded region (bottom) used to assign the position of the acetyl group of compound **22**.

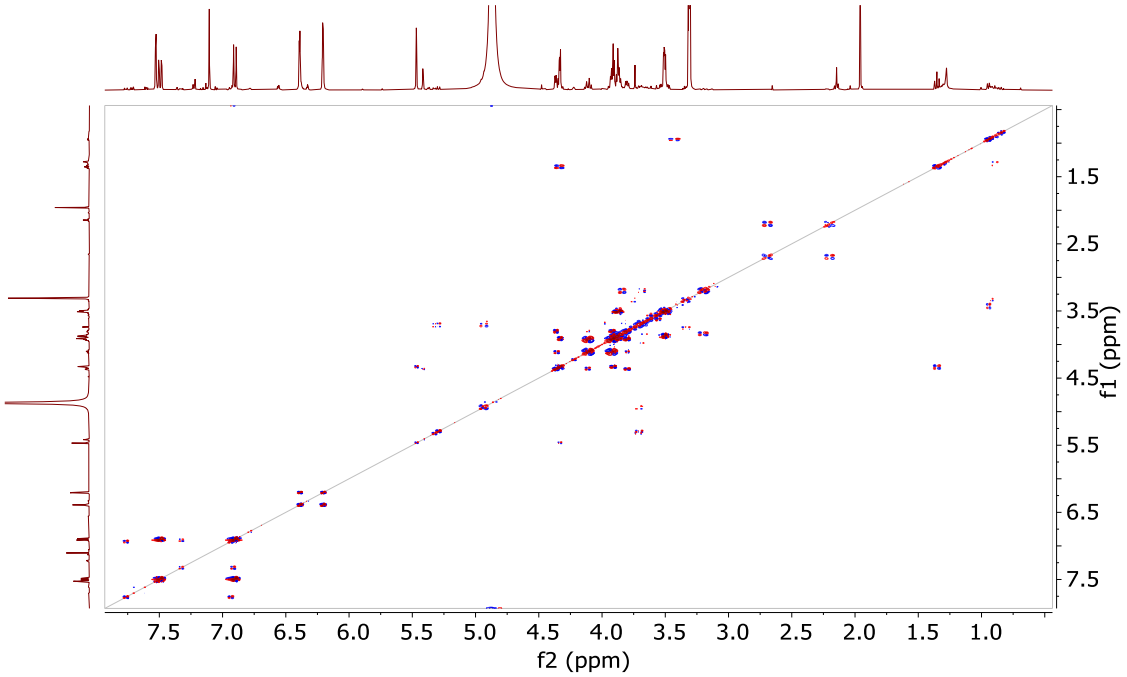


Figure S29. ^{1}H-^{1}H DQF-COSY NMR spectrum of compounds **21** and **22.**

Table S-4. Molecular docking results of isolated compounds against *E. coli* DNA Gyrase B and *Pseudomonas* quinolone signal A (PqsA).

Target	Ligand	Binding affinity (kcal/mol)	H-bonding	Hydrophobic and Electrostatic	Van der Waals
E. coli DNA gyrase B	17	-5.9	Val-167, 71	Amide pi-stacked: Asn-46; Pi-alkyl: Ile-78, Val-120	Ile-94, Asp-73, Thr-165, Ala-47, Met-166, Val-43
	18	-10.3	Glu-50, Arg-76, Gly-77, Val-43	Pi-anion: Glu-50; Pi-sigma: Thr-165, Asp-49; Pi-alkyl: Ala-53, Ile-78, 94	Leu-52, Pro-79, Arg-136, Asp-73, Ala-47, Val-167, 71, 120, Gly-119, Asn-46
	19	-11.1	Glu-50, Arg-76, Gly-77, Val-97	Pi-anion: Glu-50; Pi-sigma: Ile-94; Amide pi-stacked: Asn-46; Pi-alkyl: Ile-78, 94, Val-120	Asp-49, 73, Pro-79, Arg-136, Thr-165, Val-43, 167, 93, His-83
	20	-5.5	Thr-165, Gly-77	Carbon hydrogen bond: Pro-79	Arg-136, 76, Glu-50, Gly-75, 164. Asp-73, Ile-78, 94
	21	-8.0	GLY-77	Pi-cation and anion: Arg-76, Glu-50; Pi-alkyl: Pro-79, Ile-78	Arg-136, Ala-47, Asp-73, Val-71, 43, 167, 120, Thr-165, Asn-46, Ile-94, Gly-119, Asp-49
	22	-7.6	Arg-76, Gly-77, Thr-165, Asp-73	Pi-anion: Glu-50; Amide pi-stacked: Asn-46; Pi-alkyl: Pro-79, Ile-78	Ile-94, Asp-49, Ala-53, Gly-75, 164
	Ciprofloxacin	-7.4	Arg-76	Carbon hydrogen bond: Asp-73; Halogen: Asp-73; Amide pi-stacked: Gly-77; Alkyl and pi-alkyl:Pro-79, Ile-94, 78	Arg-136, Glu-50, Thr-165, Val-120, 167, 43, Asn-46, Ala-47
PqsA	17	-7.3	Gly-279, 302, 307, Thr-307	Pi-pi stacked, Pi-pi T-shaped, and Amide pi-stacked: His-308, Tyr-211, Gly-2010	Ile-301, Val-309, Ala-303, 278
	18	-9.1	Arg-372, Thr-380, 304	Pi-cation and anion: Asp-382, Arg-397; Pi-donor hydrogen bond: Thr-164; Pi-sigma: Ile-301; Amide pi-stacked: Gly-279; Pi-alkyl: Ala-303	Gly-102, 210, Ser-280, Pro-281, Tyr-378, 163, Phe-209

Table S-4 Contn'd.

Target	Ligand	Binding affinity (kcal/mol)	H-bonding	Hydrophobic and Electrostatic	Van der Waals
PqsA	19	-10.3	Thr-164, 304, 323, Glu-305, Gly-279, 300, Asp-299	Carbon hydrogen bond: 301; Pi-anion: Asp-382; Pi-sigma: Ile-301; Pi-pi T shaped and Amide pi-stacked: Ser-280, His-394, Gly-279; Pi-alkyl: Pro-281, Ala-303, Ile-301	Phe-209, Tyr-378, 380, Gly-302, Ala-278, Arg-397
	20	-6.1	Thr-304, Gly-307, 279, 302	Carbon hydrogen bond and Pi-donor hydrogen bond: His-308	Ala-303, 278, Gly-210, Tyr-211, Val-309, Ile-301
	21	-8.9	Thr-380, 304, Arg-397, Tyr-378, Glu-305	Carbon hydrogen bond and Pi-donor hydrogen bond: Tyr-211, Gly-279; Amide pi stacked: Gly-302; Pi-alkyl: Ala-278	Val-309, His-308, Gly-210, Ala-303, Thr-164, Asp-382
	22	-9.0	Arg-372, 397, Tyr-378, Glu-305, Thr-164, Asp-382, Thr-304	Carbon hydrogen bond and Pi-donor hydrogen bond: Gly-279, Tyr-211; Pi-alkyl: Ala-278	Lys-172, Ala-303, Gly-210, 302, Val-309, His-394
	Ciprofloxacin	-7.1	Arg-397, Gly-302, Asp-299	Carbon hydrogen bond: Gly-300, Thr-323; Halogen: Gly-302; Pi-cation and anion:Arg-397, Asp-382; Amide pi-stacked: Gly-279; Alkyl and Pi-alkyl: Ile-301, His-394, Arg-397	Ala-278, Leu-282, Phe-384, Pro-281, Ser-280

Table S-5. Molecular docking results of isolated compounds against Pyruvate kinase M2 (PKM2) and human topoisomerase II*β*.

Target	Ligand	Binding affinity (kcal/mol)	H-bonding	Hydrophobic and Electrostatic	Van der Waals
PKM2	17	-6.2	Tyr-390, Glu-397	Pi-sigma: Leu-394; Pi-pi stacked: Phe-26	Gln-393, Phe-26, Leu-27, 353, Ile-389
	18	-14.7	Tyr-390, Ala-388, Asp-354, 354, Lys-311	Pi-sigma: Leu-353; Pi-pi T-shaped: Phe-26, 26; Pi-alkyl: Leu-394, Met-30, Leu-353. 353	Ile-389, 383, His-29, Leu-33, 27, 27, 394, Lys-311, Met-30
	19	-13.6	Ala-388, Lys-311, Asp-354, Tyr-390, 390	Carbon hydrogen bond: Ile-389, 389; Pi-sigma: Leu-353; Pi-pi T-shaped: Phe-26, 26; Pi-alkyl: Leu-394, 394, Met-30	Leu-33, 27, 353, His-29, 391, Met-30, Gln-393, Glu-397, Lys-311, Asn-350, Asp-354
	20	-6.2	Tyr-390, Leu-394	-	Gln-393, Glu-397, Met-90, Leu-27, 353, Phe-26, 26, Asn-318, Ile-389
	21	-10.2	Asn-350, 350, Lys-311, Glu-397	Carbon hydrogen bond: Leu-27, Asp-354; Pi-sigma: Leu-353; Pi-pi T-shaped: Phe-26; Pi-alkyl: Leu-394	Phe-26, Met-30, Leu-353, 33, Lys-311, His-29, Ala-388, Ile-389, Tyr-390, Gln-393
	22	10.4	Lys-311, 311, His-29, Tyr-390, Ala-388, Glu-397, Met-30	Carbon hydrogen and pi-donor hydrogen bond: Asp-354, Leu-394, Phe-26; Pi-sigma: Leu-353; Pi-pi T-shaped: Phe-26; Pi-alkyl: Leu-394	Met-30, Asp-354, Asn-350, Leu-33, 27, 353, Ile-389, Gln-393
	PKM2-IN-1	-9.6	Lys-311	Pi-sigma: Leu-353; Pi-sulfur: Phe-26; Pi-pi T-shaped: Phe-26; Alkyl and Pi-alkyl: Leu-353, 353, Phe-26	Asp-354, 354, Lys-311, Tyr-390, 390, Ala-388, 388, Ile-389, 389, Met-30, His-29
Human topoisomerase II*β*	17	-3.2	Arg-503	Pi-sigma-Arg-503	-
	18	-6.9	Gln-778	Pi-donor hydrogen bond: Gln-778; Pi-alkyl: Arg-503	Gly-504, Asp-479
	19	-6.7	Gln-778	Carbon hydrogen bond: Gly-504; Pi-alkyl:Arg-503, Lys-505	Met-782
	20	-3.2	Arg-503	Carbon hydrogen bond: Arg-503	-
	21	-4.9	Lys-505, Gln-778, Gly, 776	-	Arg-503, Gly-504, His-775, Ala-779
	22	-5.0	Arg-503, Lys-505	Carbon hydrogen bond: Arg-503; Pi-sulfur: Mrt-782	Glu-522, Gly-504, Gln-778
	Etoposide	-5,3	Arg-503, Gln-778	Alkyl and Pi-alkyl: Ala-779	Gly-776

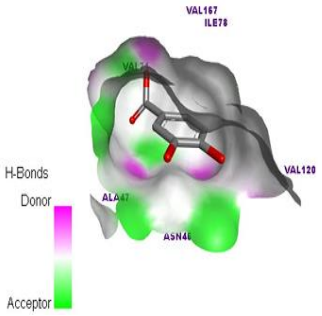
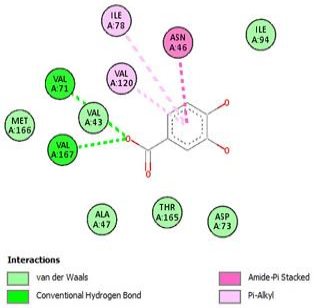
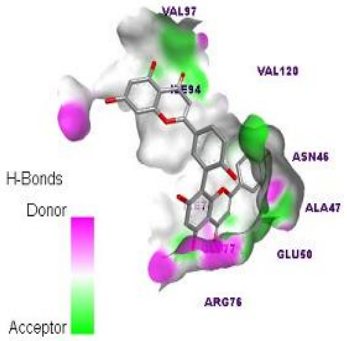
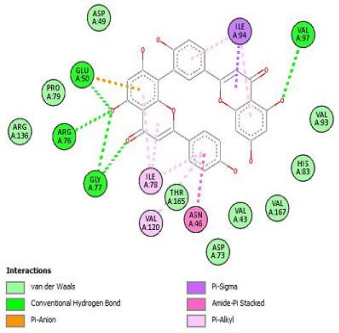
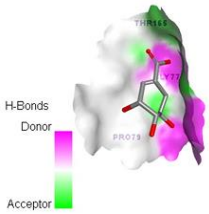
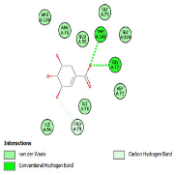
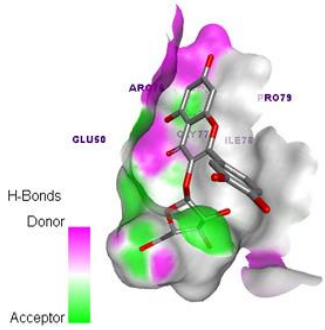
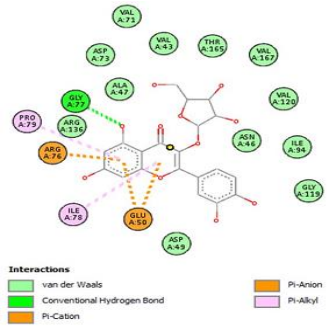
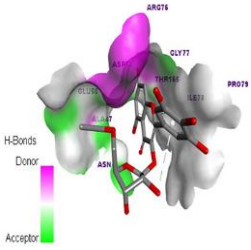
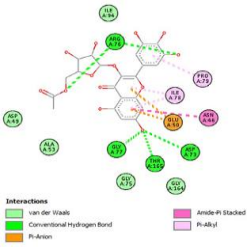
Target	Comp	3D	2D
E. coli DNA gyrase B	17		
	19		
	20		
	21		
	22		

Figure S30. The 3D and 2D binding interactions of compounds **17, 19,** and **20-22** against *E. coli* DNA Gyrase B.

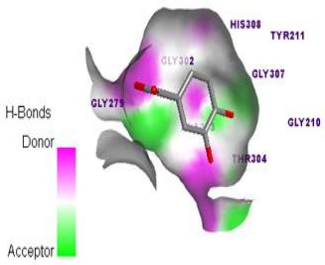
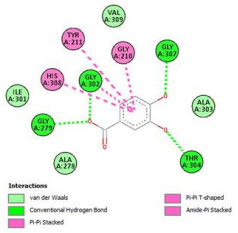
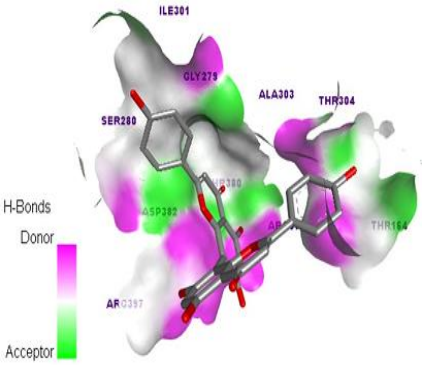
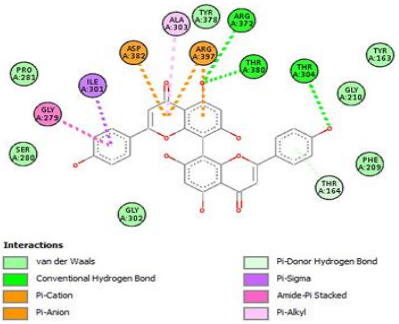
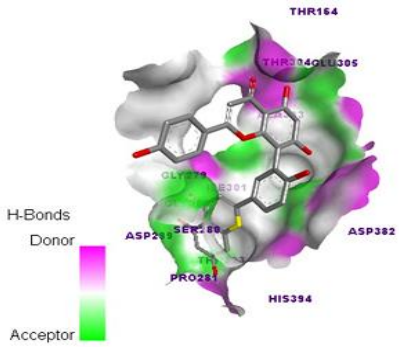
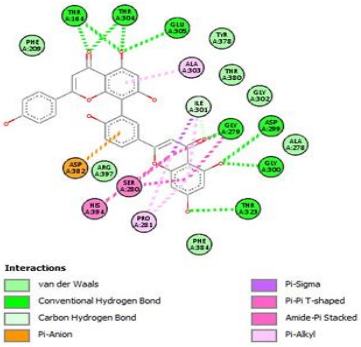
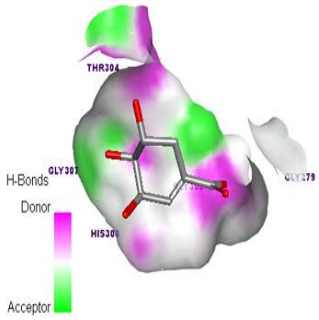
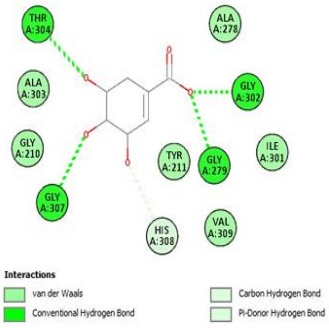
Target	Comp	3D	2D
PqsA	17		
	18		
	19		
	20		

Figure S31. The 3D and 2D binding interactions of compounds **17-22** and ciprofloxacin against PqsA.

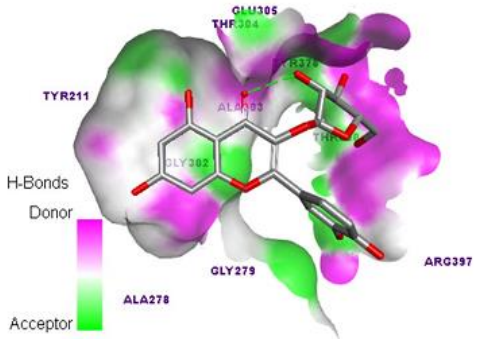
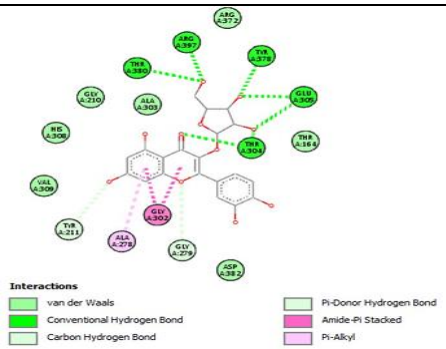
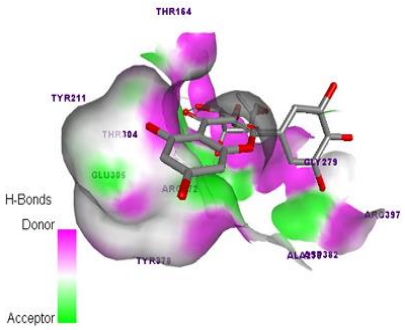
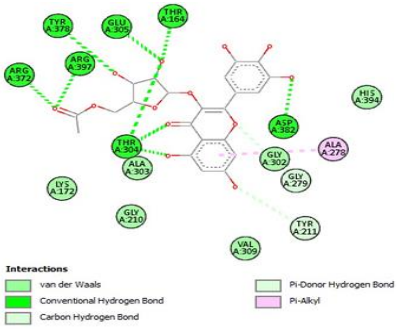
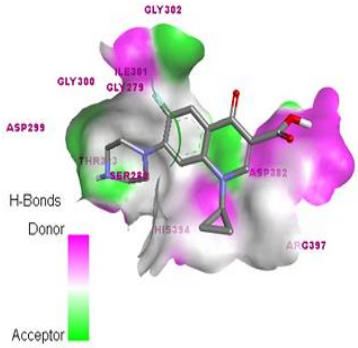
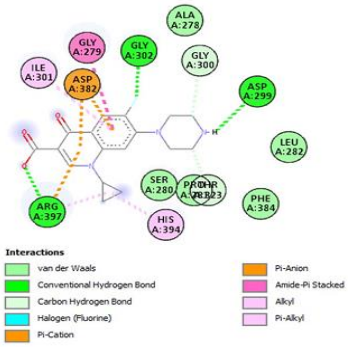
Target	Comp	3D	2D
PqsA	21		
	22		
	Ciprofloxacin		

Figure S31. Contn'd.

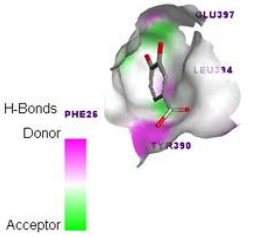
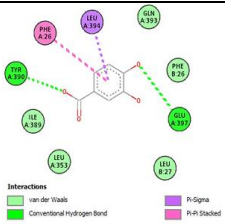
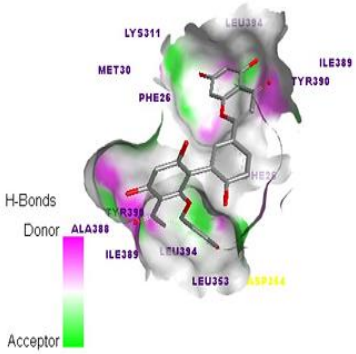
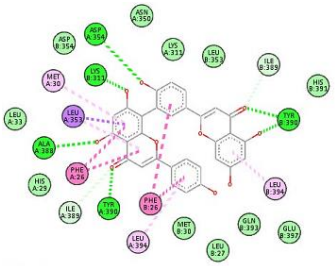
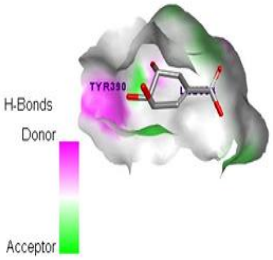
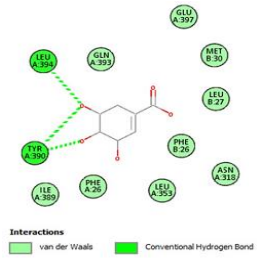
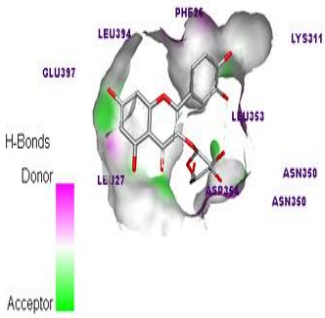
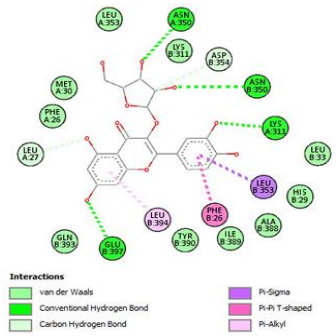
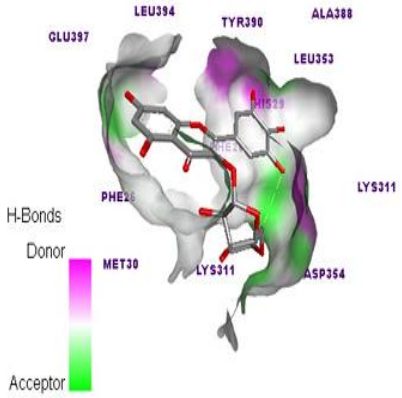
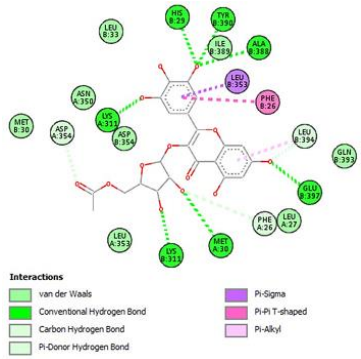
Target	Comp	3D	2D
PKM2	17		
	19		
	20		
	21		
	22		

Figure S32. The 3D and 2D binding interactions of compounds **17** and **19-22** with PKM2.

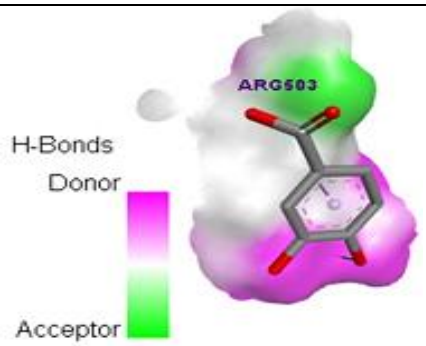
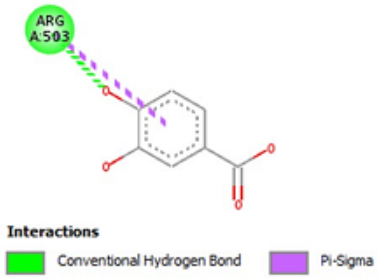
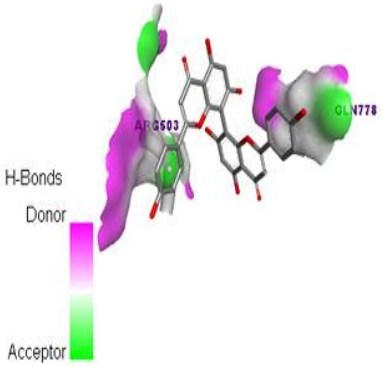
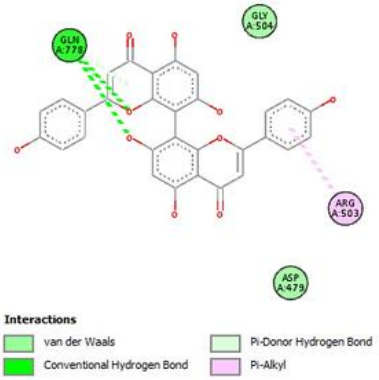
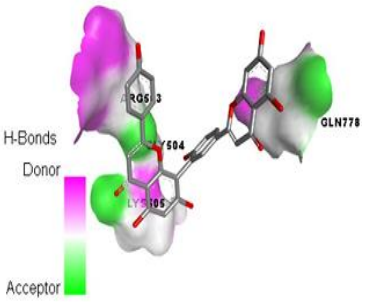
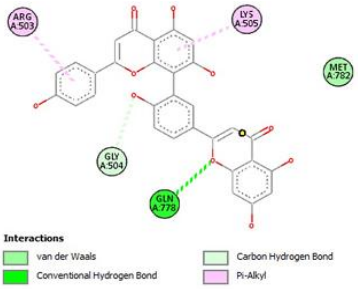
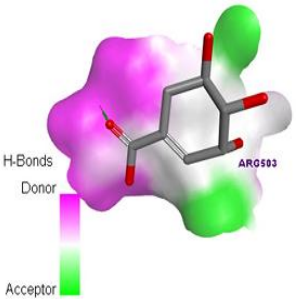
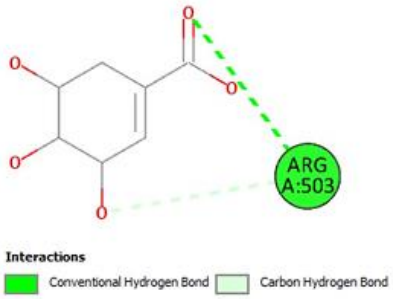
Target	Comp	3D	2D
Human topoisomerase IIβ	17		
	18		
	19		
	20		

Figure S33. The 3D and 2D binding interactions of compounds **17-22** and etoposide with human topoisomerase IIβ.

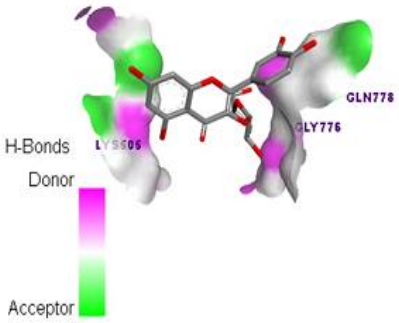
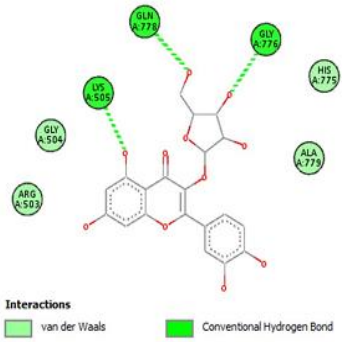
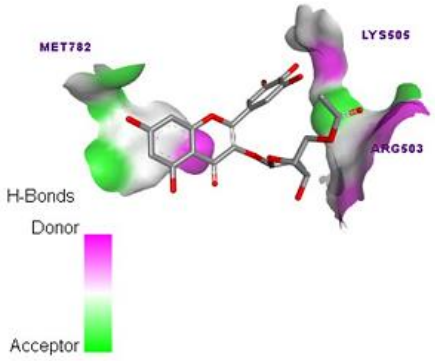
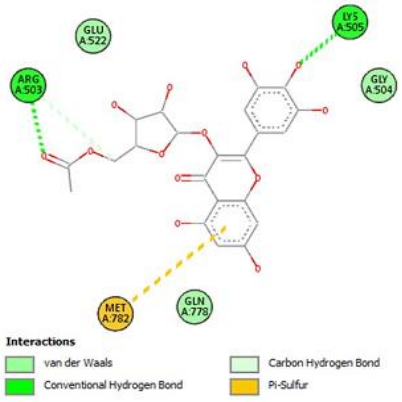
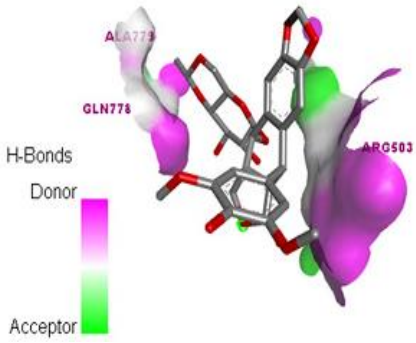
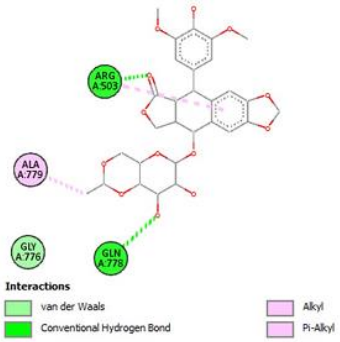
Target	Comp	3D	2D
human topoisomerase IIβ	21		
	22		
	Etoposide		

Figure S33**.** Contn'd.