

Anti-inflammatory Activity of Tanshinone-related Diterpenes from *Perovskia artemisioides* Roots

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Supplementary materials

Table S1. Retention Times (R_t), $[M+H]^+$, $[M+Na]^+$, Molecular Formula, Δ ppm and MS/MS Values of Compounds **1-25** of *n*-Hexane Extract of *P. artemisioides* roots by LC-ESI/LTQOrbitrap/MS.

Figure S1. ESI/LTQOrbitrap spectrum of compound **2**, in positive ion mode.

Figure S2. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **2**.

Figure S3. ^{13}C Spectrum (150 MHz, CD_3OD) of compound **2**.

Figure S4. HSQC Spectrum (CD_3OD) of compound **2**.

Figure S5. HMBC Spectrum (CD_3OD) of compound **2**.

Figure S6. COSY Spectrum (CD_3OD) of compound **2**.

Figure S7. ROESY Spectrum (CD_3OD) of compound **2**.

Figure S8. ESI/LTQOrbitrap spectrum of compound **9**, in positive ion mode.

Figure S9. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **9**.

Figure S10. ^{13}C Spectrum (150 MHz, CD_3OD) of compound **9**.

Figure S11. HSQC Spectrum (CD_3OD) of compound **9**.

Figure S12. HMBC Spectrum (CD_3OD) of compound **9**.

Figure S13. COSY Spectrum (CD_3OD) of compound **9**.

Figure S14. ROESY Spectrum (CD_3OD) of compound **9**.

Figure S15. ESI/LTQOrbitrap spectrum of compound **10**, in positive ion mode.

Figure S16. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **10**.

Figure S17. ^{13}C Spectrum (150 MHz, CD_3OD) of compound **10**.

Figure S18. HSQC Spectrum (CD_3OD) of compound **10**.

Figure S19. HMBC Spectrum (CD_3OD) of compound **10**.

Figure S20. COSY Spectrum (CD_3OD) of compound **10**.

Figure S22. ESI/LTQOrbitrap spectrum of compound **11**, in negative ion mode.

Figure S23. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **11**.

Figure S24. ^{13}C Spectrum (150 MHz, CD_3OD) of compound **11**.

Figure S25. HSQC Spectrum (CD₃OD) of compound **11**.

Figure S26. HMBC Spectrum (CD₃OD) of compound **11**.

Figure S27. COSY Spectrum (CD₃OD) of compound **11**.

Figure S28. ROESY Spectrum (CD₃OD) of compound **11**.

Figure S29. ESI/LTQOrbitrap spectrum of compound **16**, in negative ion mode.

Figure S30. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **16**.

Figure S31. ¹³C Spectrum (150 MHz, CD₃OD) of compound **16**.

Figure S32. HSQC Spectrum (CD₃OD) of compound **16**.

Figure S33. HMBC Spectrum (CD₃OD) of compound **16**.

Figure S34. COSY Spectrum (CD₃OD) of compound **16**.

Figure S36. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **20**.

Figure S37. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **20**.

Figure S38. ¹³C Spectrum (150 MHz, CD₃OD) of compound **20**.

Figure S39. HSQC Spectrum (CD₃OD) of compound **20**.

Figure S40. HMBC Spectrum (CD₃OD) of compound **20**.

Figure S41. COSY Spectrum (CD₃OD) of compound **20**.

Table S1. Retention Times (R_t), $[M+H]^+$, $[M+Na]^+$, Molecular Formula, Δ ppm, and MS/MS Values of Compounds **1-25** of *n*-Hexane Extract of *P. artemisioides* roots by LC-ESI/LTQOrbitrap/MS.

	R_t	$[M+H]^+$	Mol Formula	Δ ppm	MS/MS	Name
1	3.52	327.1218	C ₁₉ H ₁₈ O ₅	-2.69	309, 283	castanol A
2	5.02	313.1423	C ₁₉ H ₂₀ O ₄	-3.72	269, 294, 252	1 β -hydroxy-isocryptotanshinone
3	7.73	311.1270	C ₁₉ H ₁₈ O ₄	-2.40	265, 283, 293	1-oxocryptotanshinone
4	10.41	329.1374	C ₁₉ H ₂₀ O ₅	-2.92	314, 267	15 hydroxy-anhydride-16R cryptotanshinone
5	10.74	311.1269	C ₁₉ H ₁₈ O ₄	-2.59	265, 281, 293	1 α -hydroxytanshinone
6	12.86	309.1112	C ₁₉ H ₁₆ O ₄	-2.90	281, 263, 235	1-oxotanshinone IIA
7	13.25	317.2104	C ₂₀ H ₂₈ O ₃	-2.21	299, 273, 213	1,14-dihydroxy-8,11,13-abietatrien-7-one
8	14.73	315.1579	C ₁₉ H ₂₂ O ₄	-3.57	297, 241	miltiorin D
9	15.03	331.1534	C ₁₉ H ₂₂ O ₅	-1.96		perovskin A
10	15.51	345.1685	C ₂₀ H ₂₄ O ₅	-3.45	327, 313, 179, 123	perovskin B
11	16.00	287.1332	C ₁₈ H ₂₂ O ₃	-0.96	269, 217	perovskin C
12	16.39	241.1584	C ₁₇ H ₂₀ O			12-hydroxy-16,17-bis-nor-simonellite
13	16.67	317.2102	C ₂₀ H ₂₉ O ₃	-2.78	299, 271, 199	demethylsalvican-11,12-dione
14	16.69	273.1844	C ₁₈ H ₂₄ O ₂	-1.89		przewalskin
15	17.52	313.1430	C ₁₉ H ₂₀ O ₄	-1.26	295, 267, 243	1 β -hydroxycryptotanshinone
16	18.07	271.1684	C ₁₈ H ₂₂ O ₂	-3.05	229, 201	perovskin D
17	19.32	303.1945	C ₂₀ H ₃₀ O ₂		203, 189, 161	pisiferol
18	20.02	297.1481	C ₁₉ H ₂₀ O ₃	-1.42	279, 251	cryptotanshinone
19	20.62	301.2154	C ₂₀ H ₂₈ O ₂	-2.71	259, 163, 173	11-hydroxyabieta-8,11,13-trien-7-one
20	22.11	329.1739	C ₂₀ H ₂₄ O ₄	-2.66	315, 297, 241	12- <i>O</i> -methyl-miltiorin D
21	23.26	287.1633	C ₁₈ H ₂₂ O ₃	-3.033	269	epicryptoacetalide
22	23.34	315.1945	C ₂₀ H ₂₇ O ₃	-2.92	205, 179	montbretol
23	24.97	317.2101	C ₂₀ H ₂₈ O ₃	-3.19	299, 27	6-deoxy-salviphomone
24	25.25	299.1630	C ₁₉ H ₂₃ O ₃	-3.71		miltiodiol
25	26.19	269.1528	C ₁₈ H ₂₁ O ₂	-0.78		salviolone

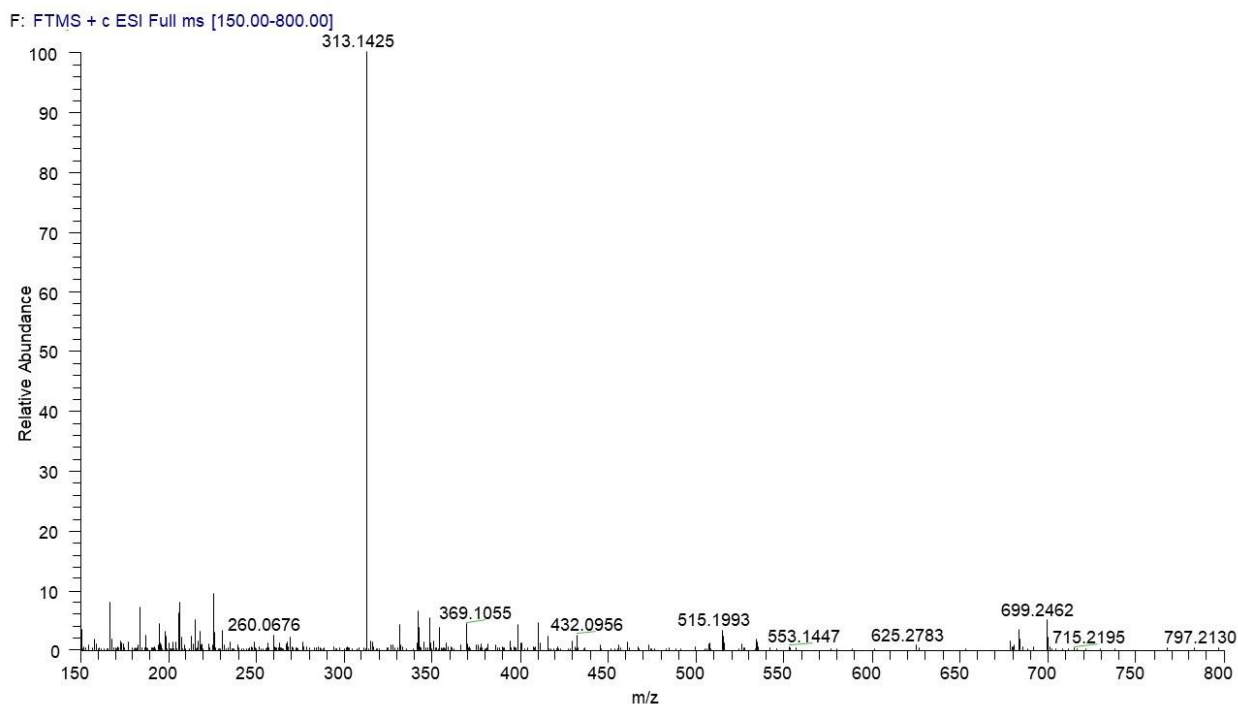


Figure S1. ESI/LTQOrbitrap spectrum of compound **2**, in positive ion mode.

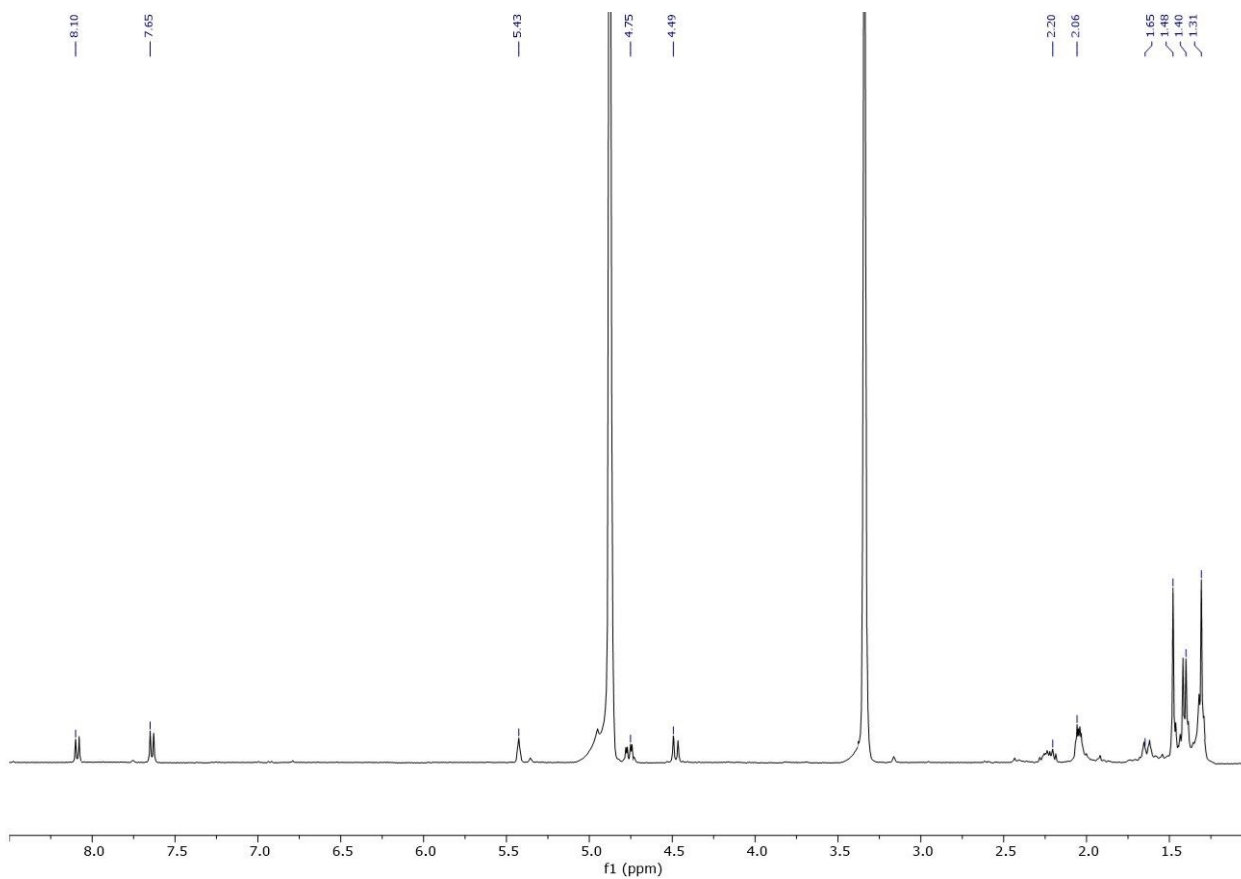


Figure S2. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **2**.

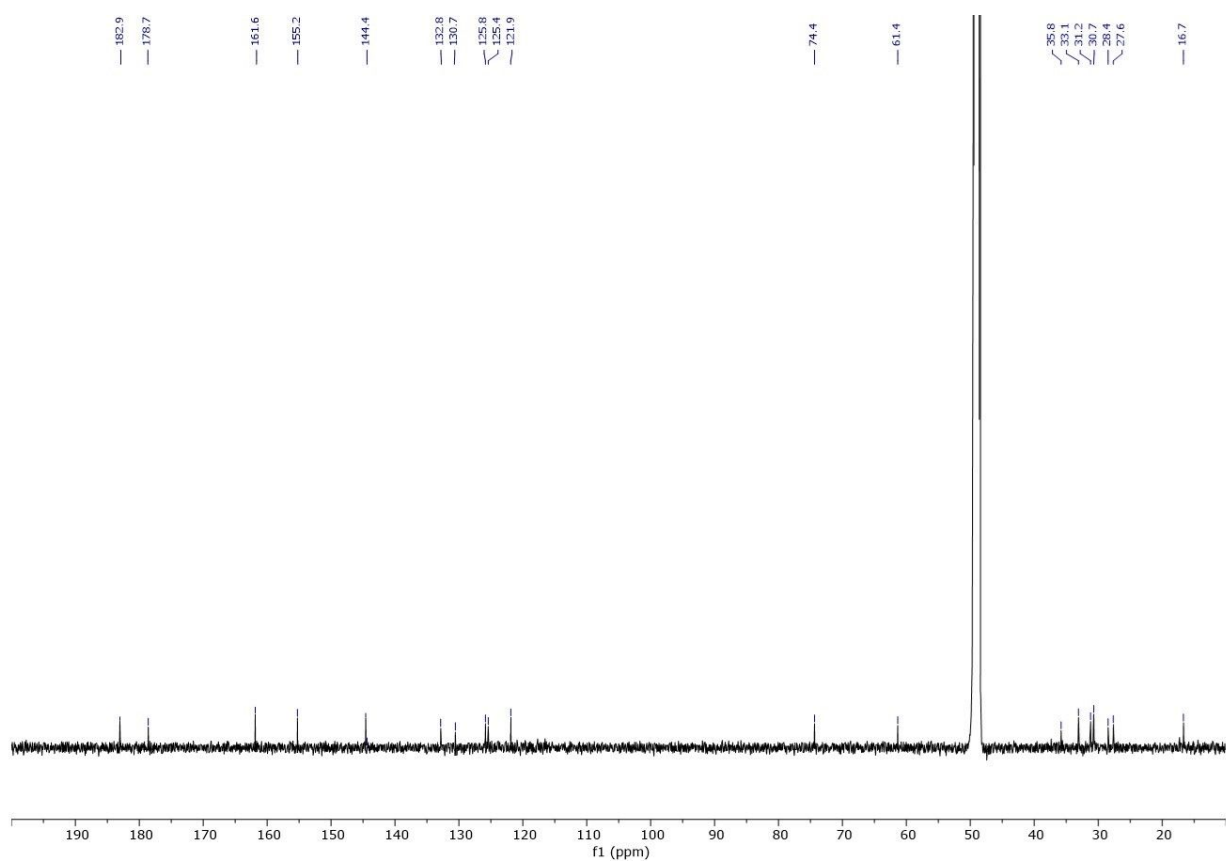


Figure S3. ^{13}C Spectrum (150 MHz, CD_3OD) of compound **2**.

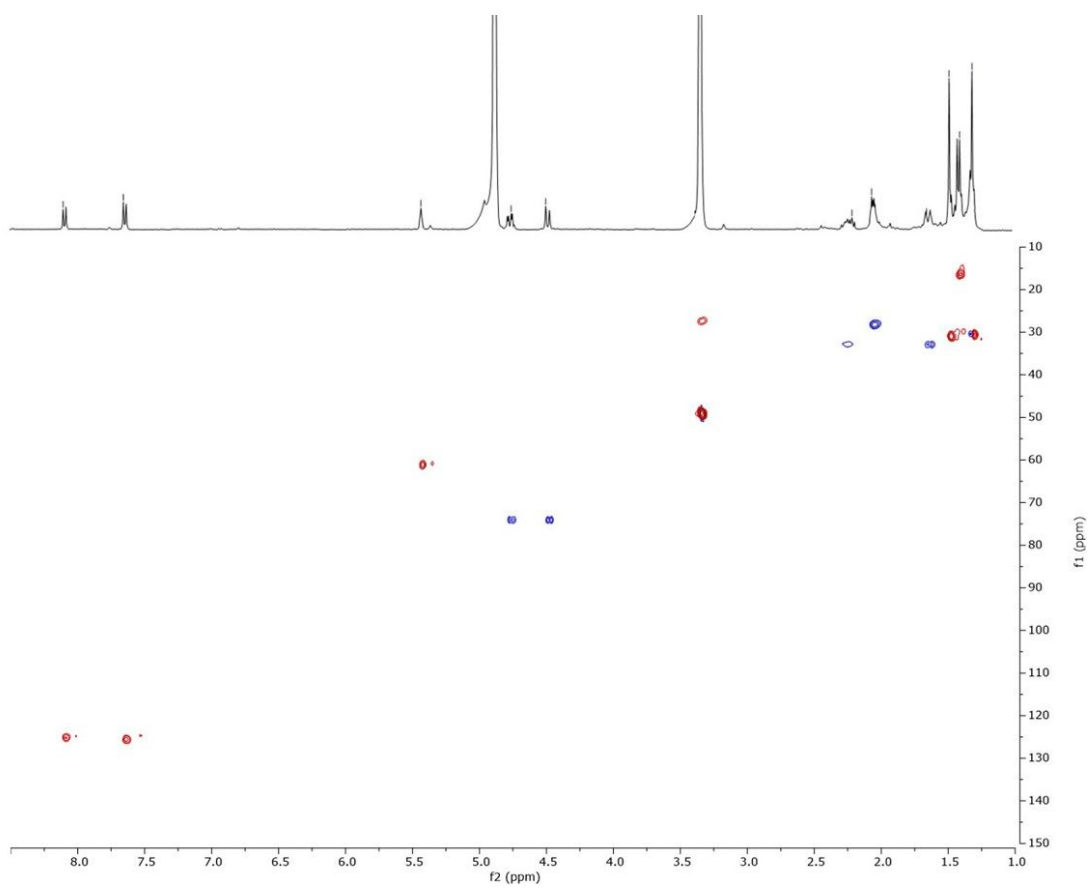


Figure S4. HSQC Spectrum (CD₃OD) of compound **2**.

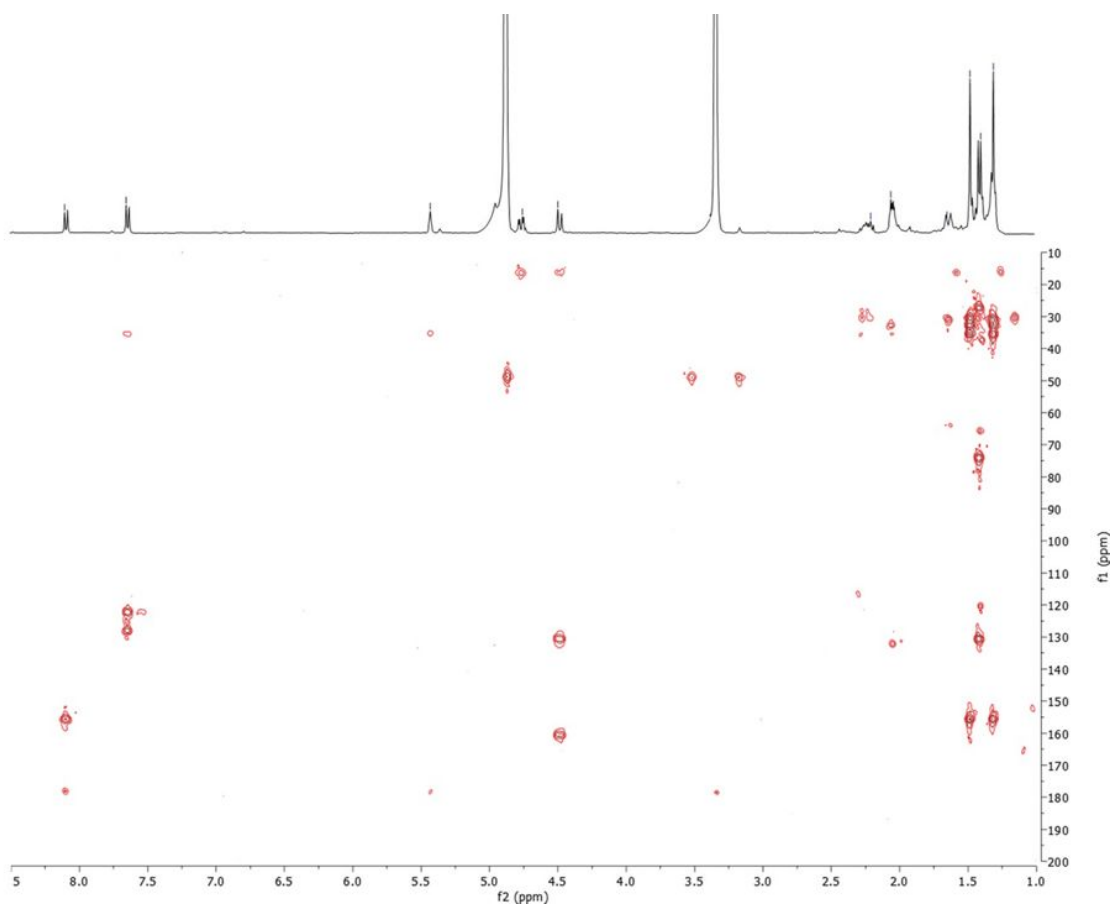


Figure S5. HMBC Spectrum (CD₃OD) of compound **2**.

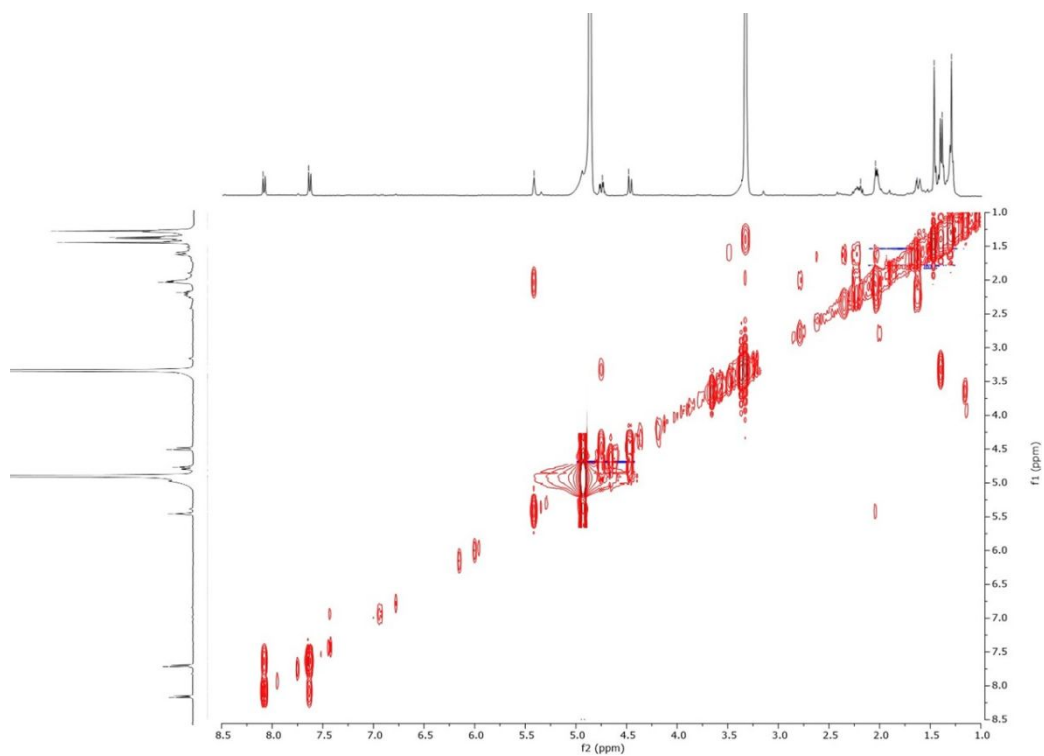


Figure S6. COSY Spectrum (CD₃OD) of compound **2**.

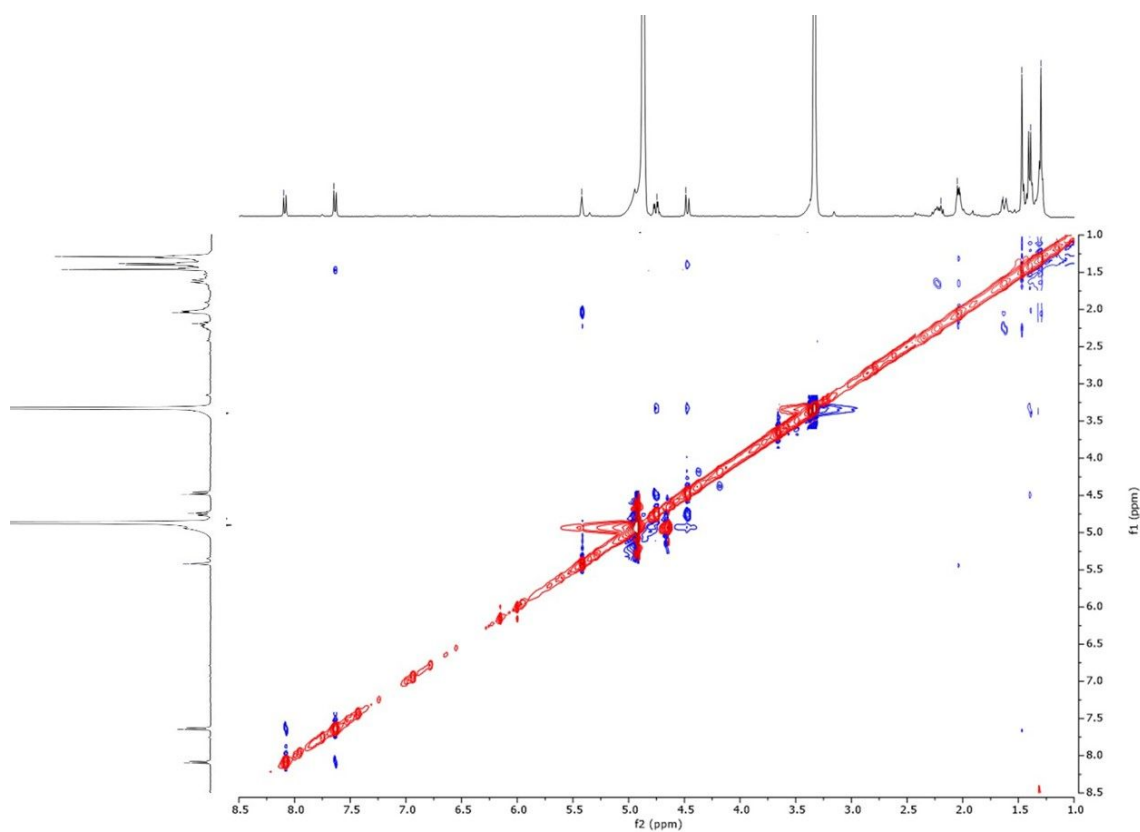


Figure S7. ROESY Spectrum (CD_3OD) of compound **2**.

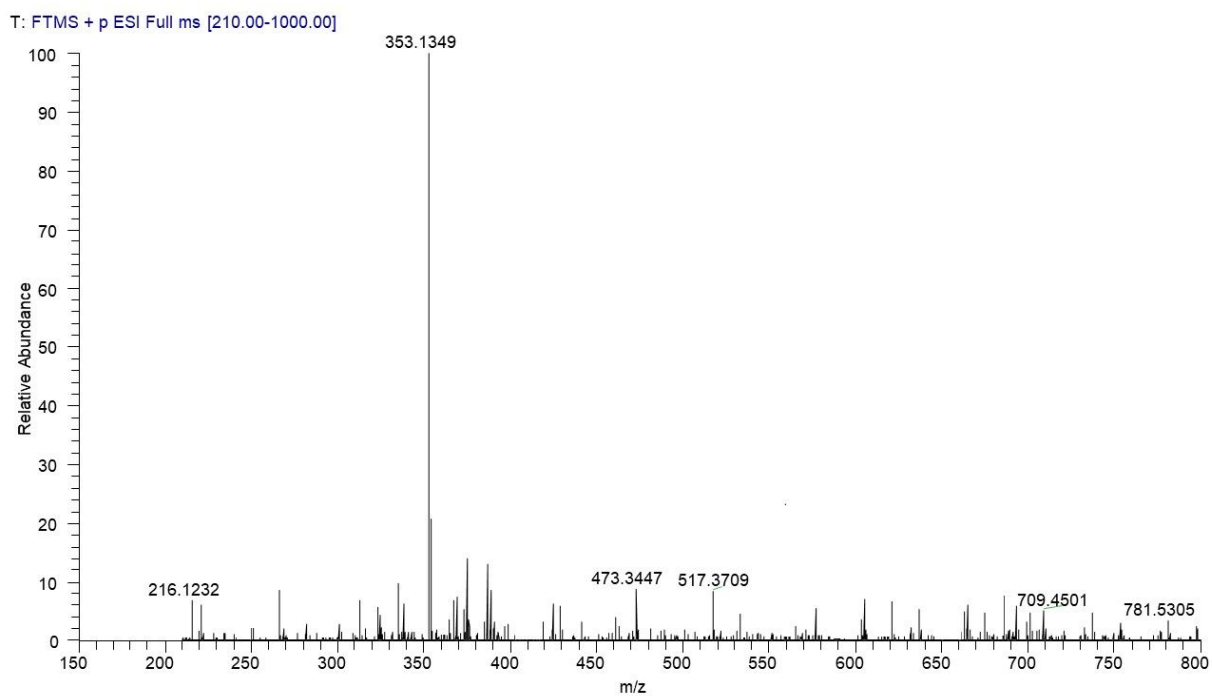


Figure S8. ESI/LTQOrbitrap spectrum of compound **9**, in positive ion mode.

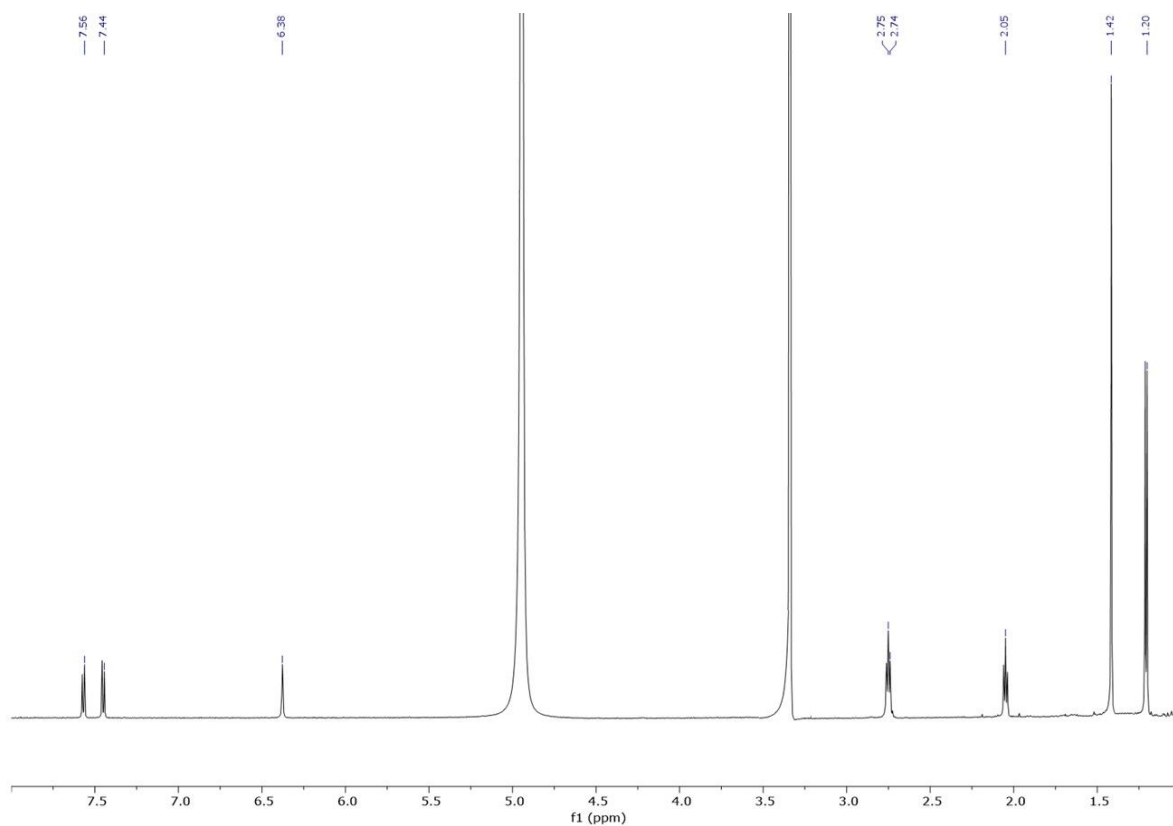


Figure S9. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **9**.

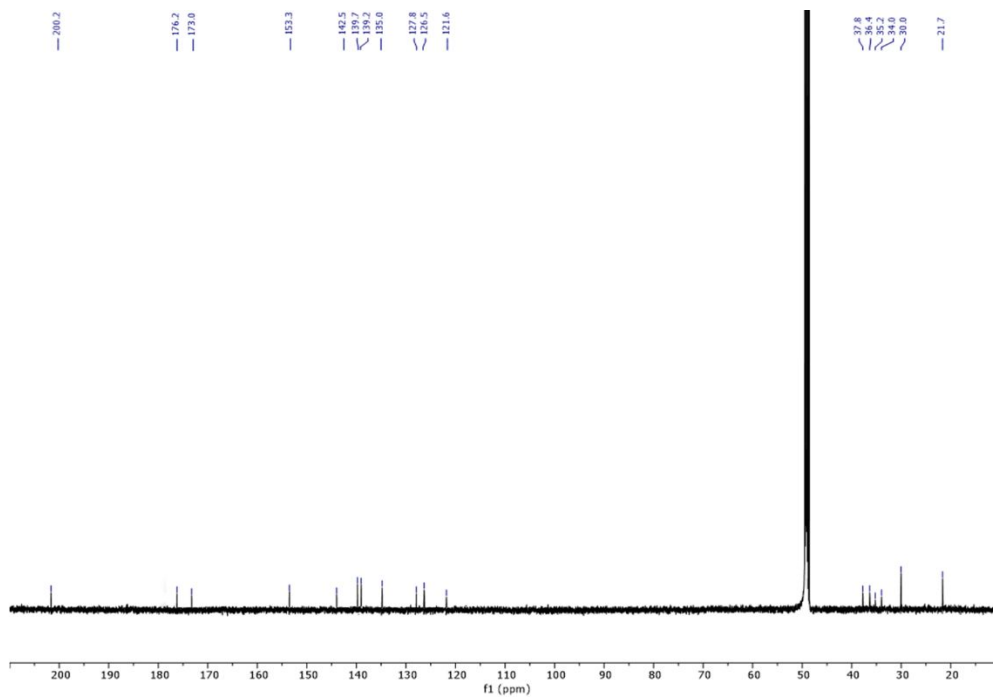


Figure S10. ^{13}C Spectrum (150 MHz, CD_3OD) of compound **9**.

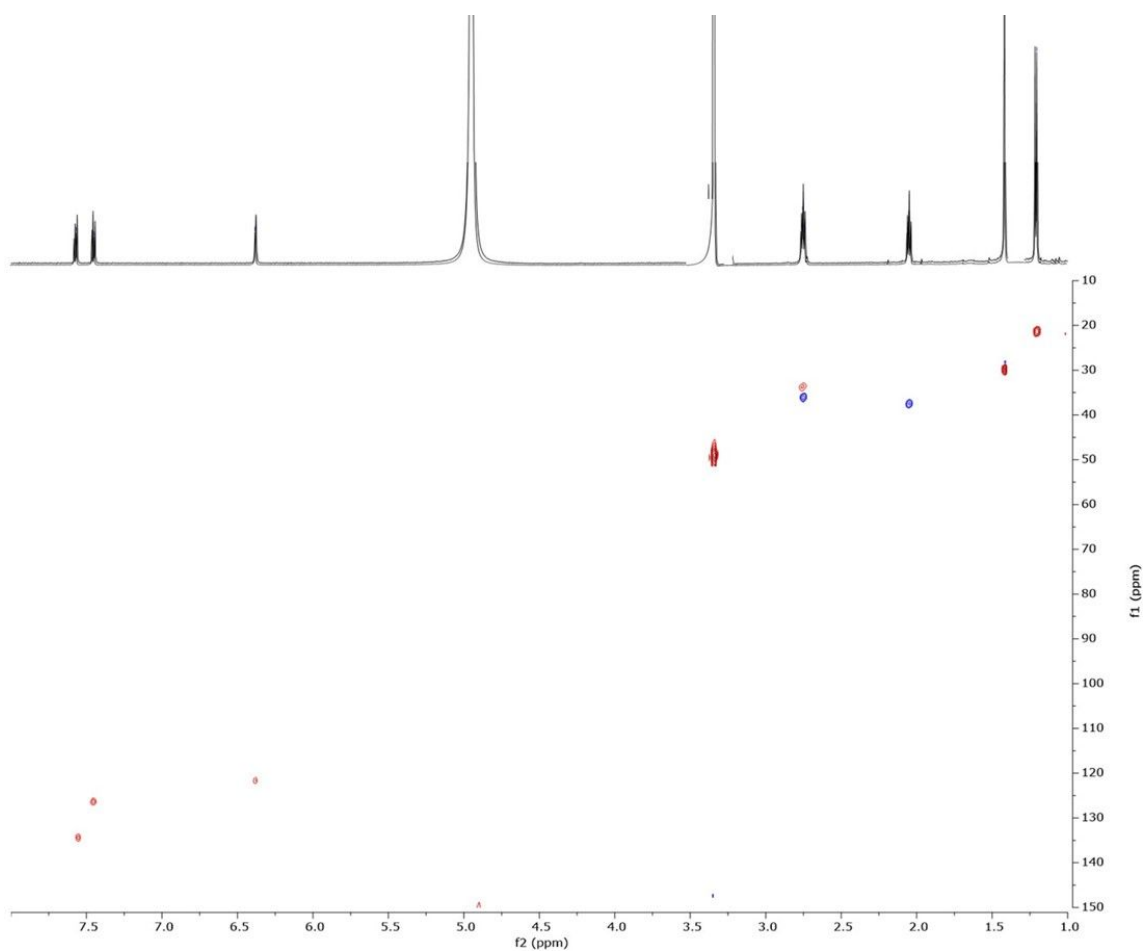


Figure S11. HSQC Spectrum (CD₃OD) of compound **9**.

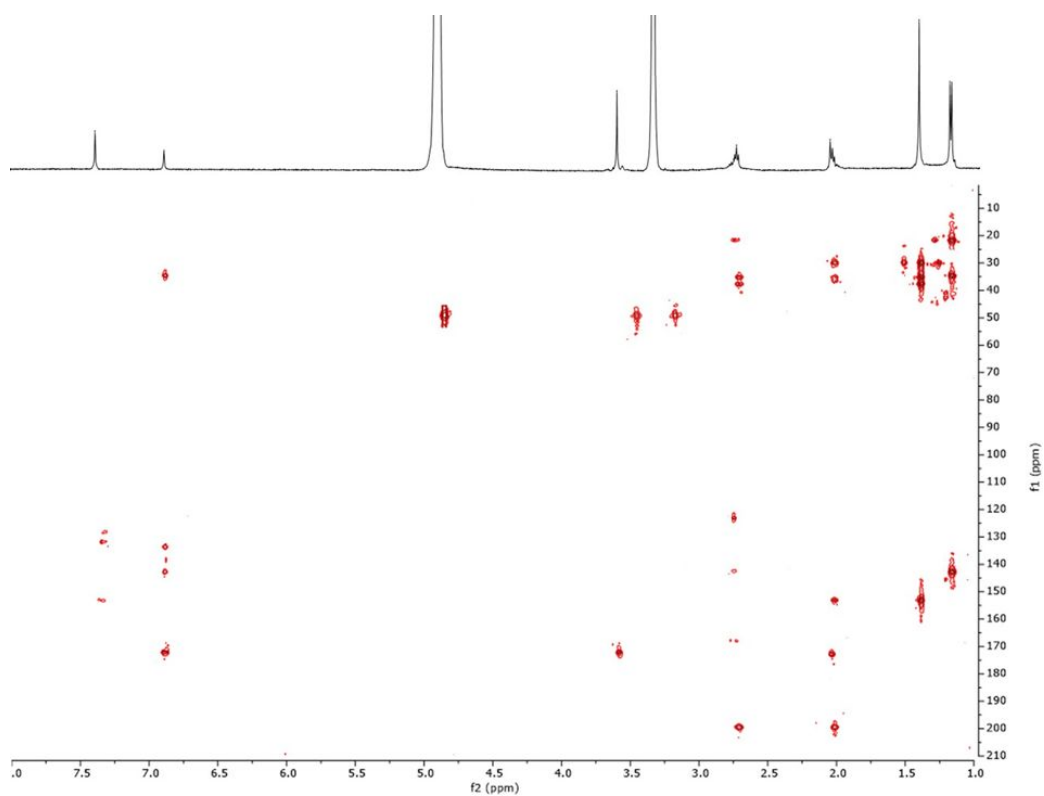


Figure S12. HMBC Spectrum (CD₃OD) of compound **9**.

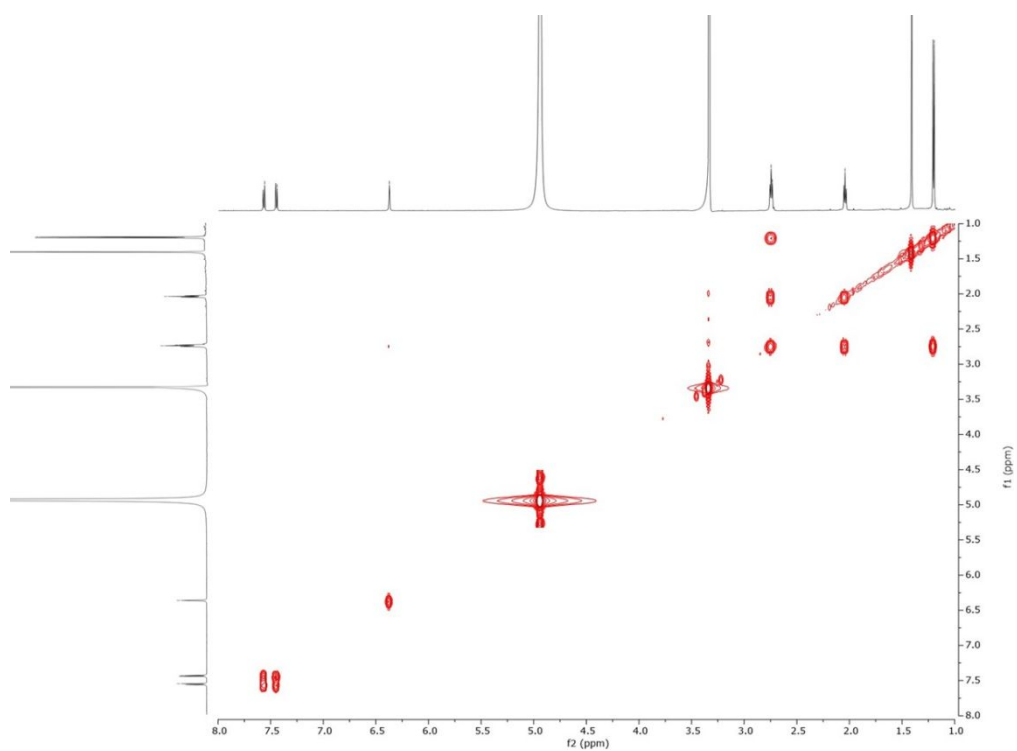


Figure S13. COSY Spectrum (CD_3OD) of compound **9**.

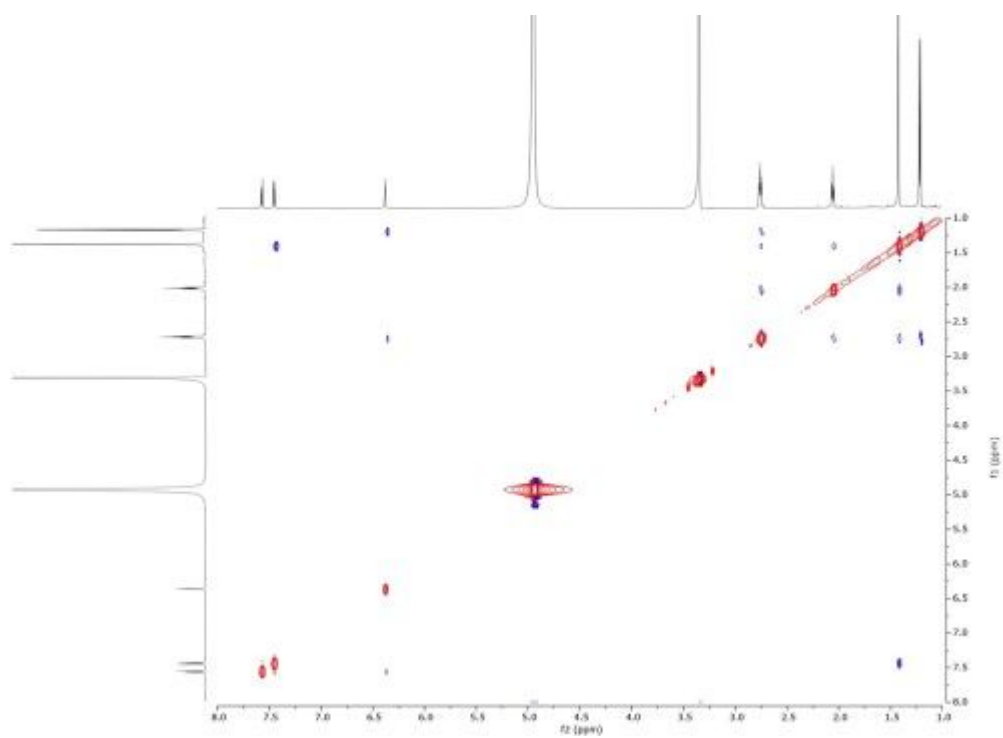


Figure S14. ROESY Spectrum (CD_3OD) of compound **9**

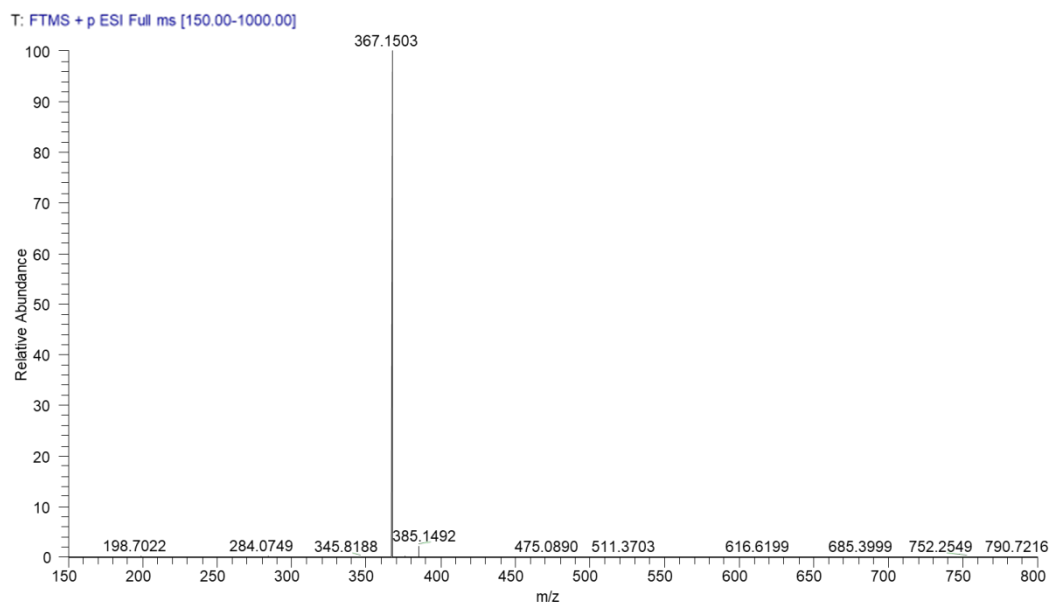


Figure S15. ESI/LTQOrbitrap spectrum of compound **10**, in positive ion mode.

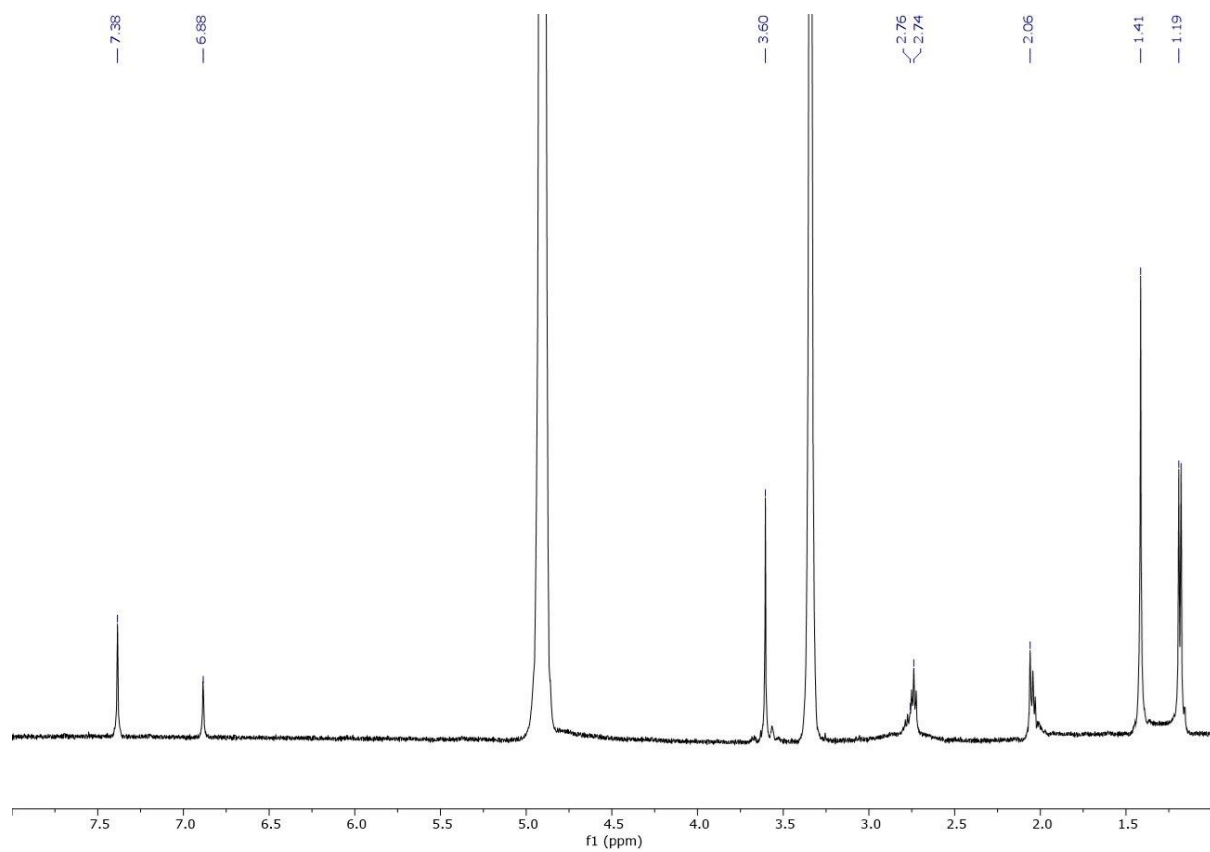


Figure S16. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **10**.

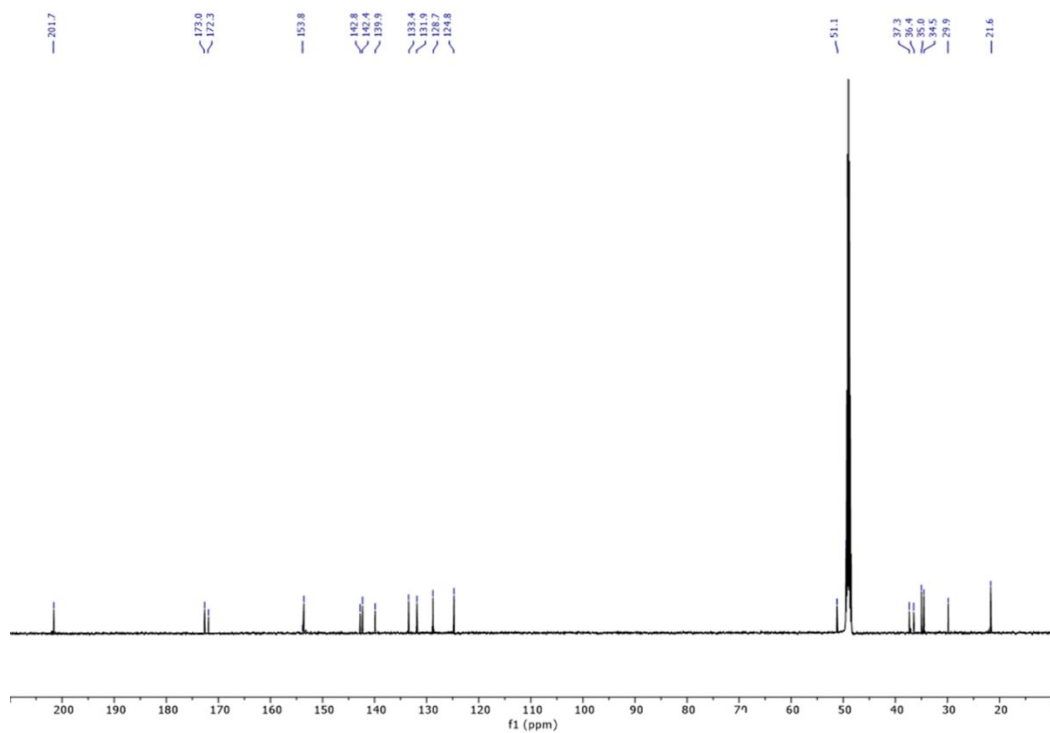


Figure S17. ^{13}C Spectrum (150 MHz, CD_3OD) of compound **10**.

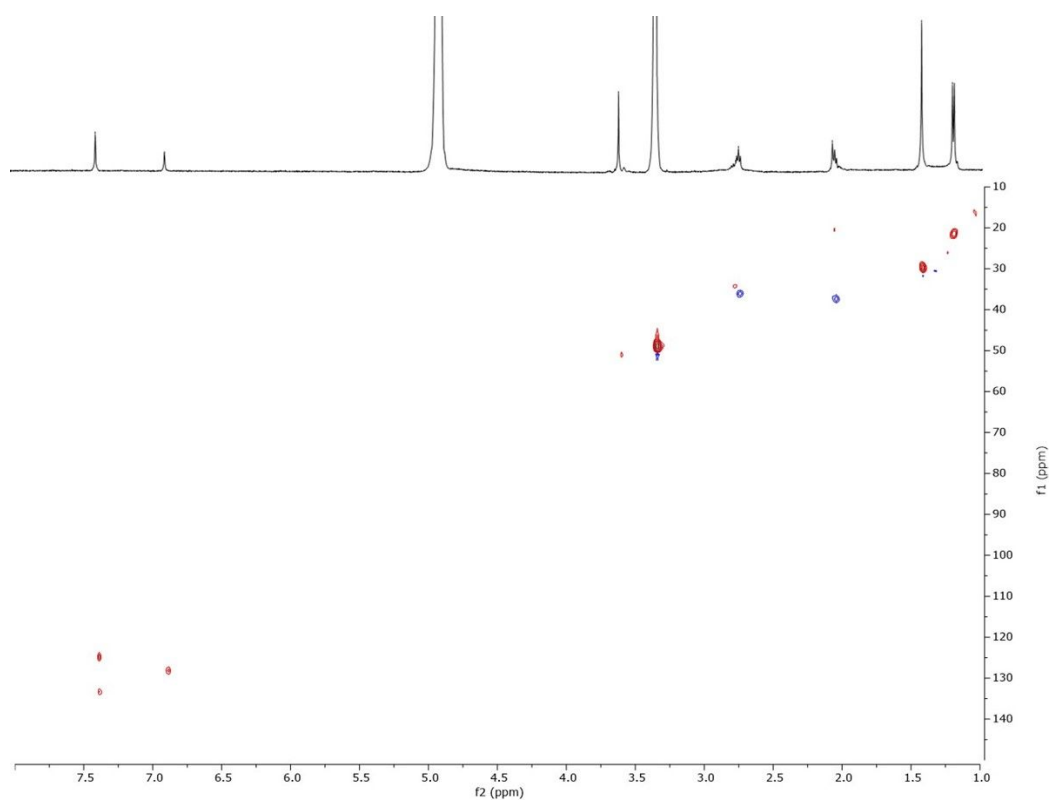


Figure S18. HSQC Spectrum (CD_3OD) of compound **10**.

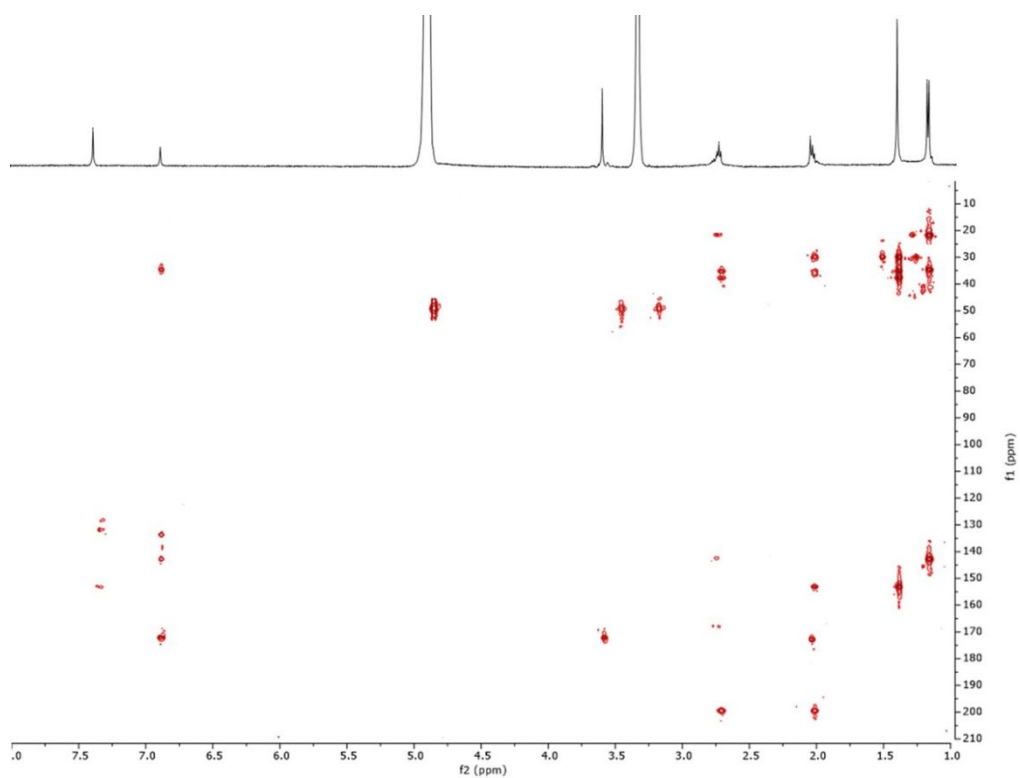


Figure S19. HMBC Spectrum (CD_3OD) of compound **10**.

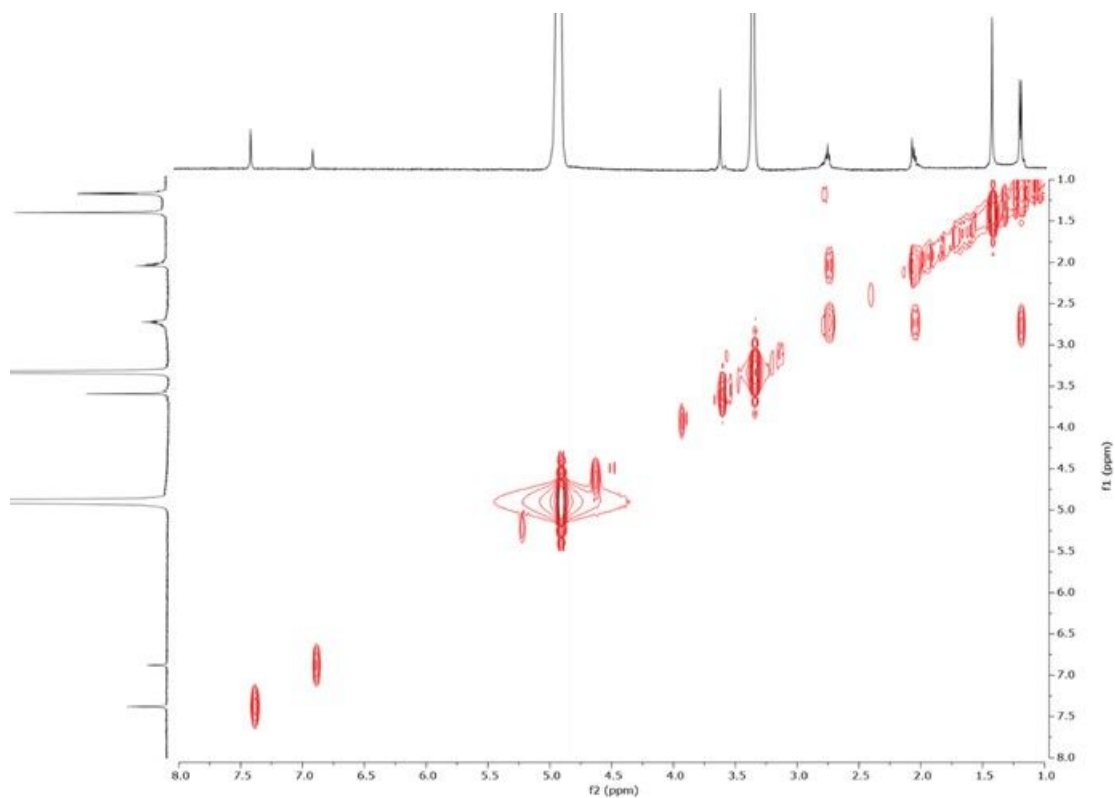


Figure S20. COSY Spectrum (CD_3OD) of compound **10**.

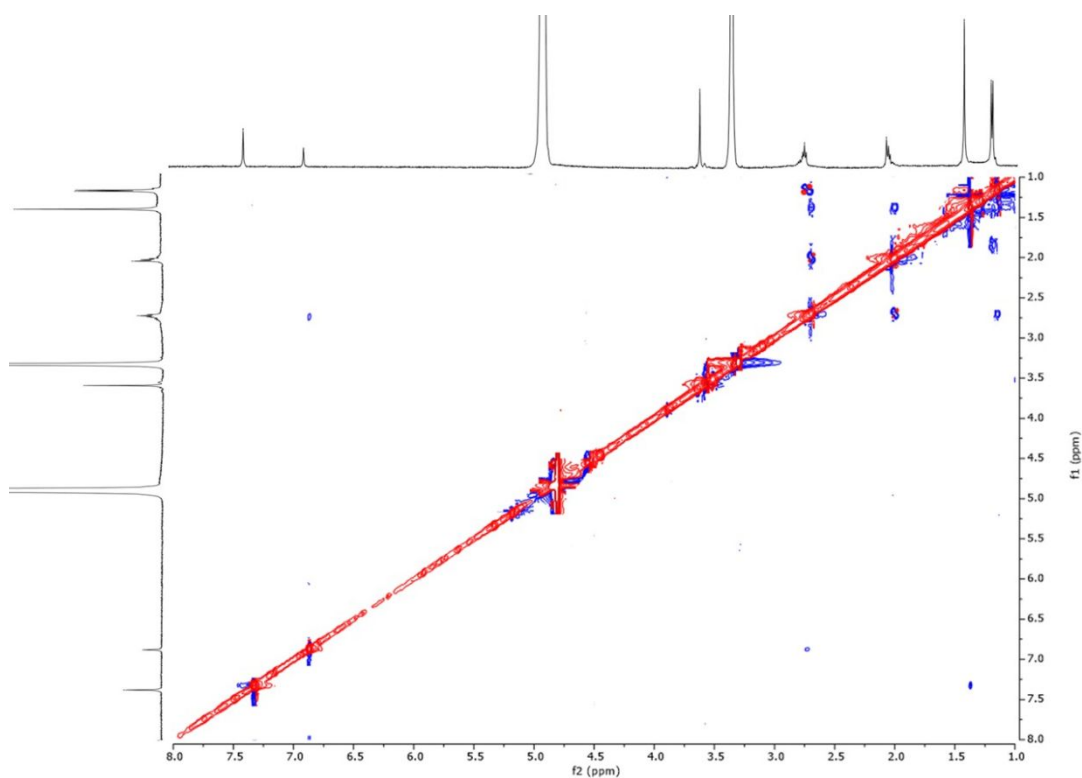


Figure S21. ROESY Spectrum (CD_3OD) of compound **10**.

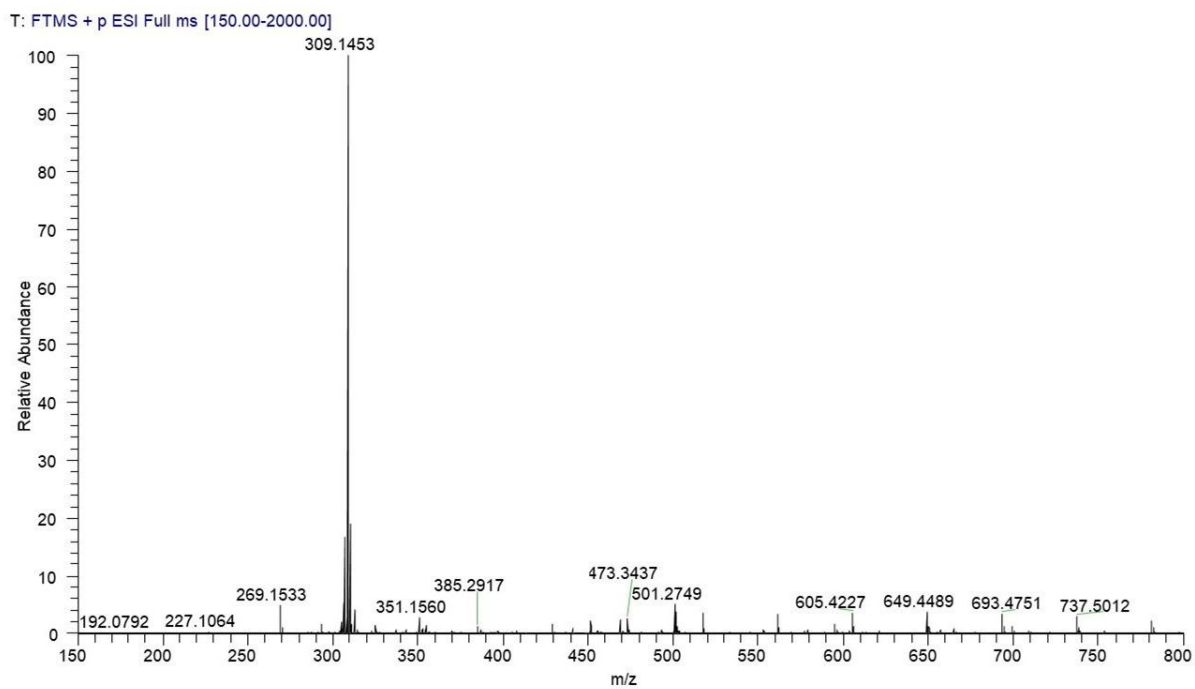


Figure S22. ESI/LTQ Orbitrap spectrum of compound **11**, in negative ion mode.

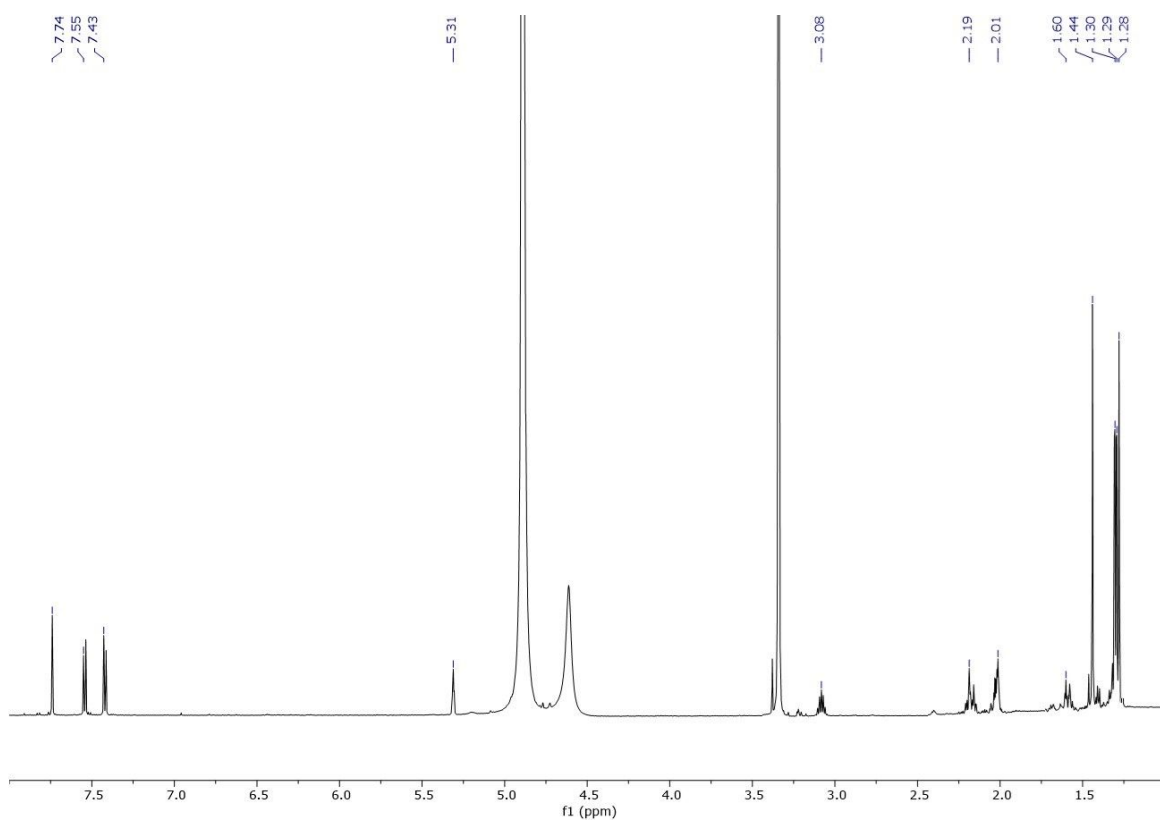


Figure S23. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **11**.

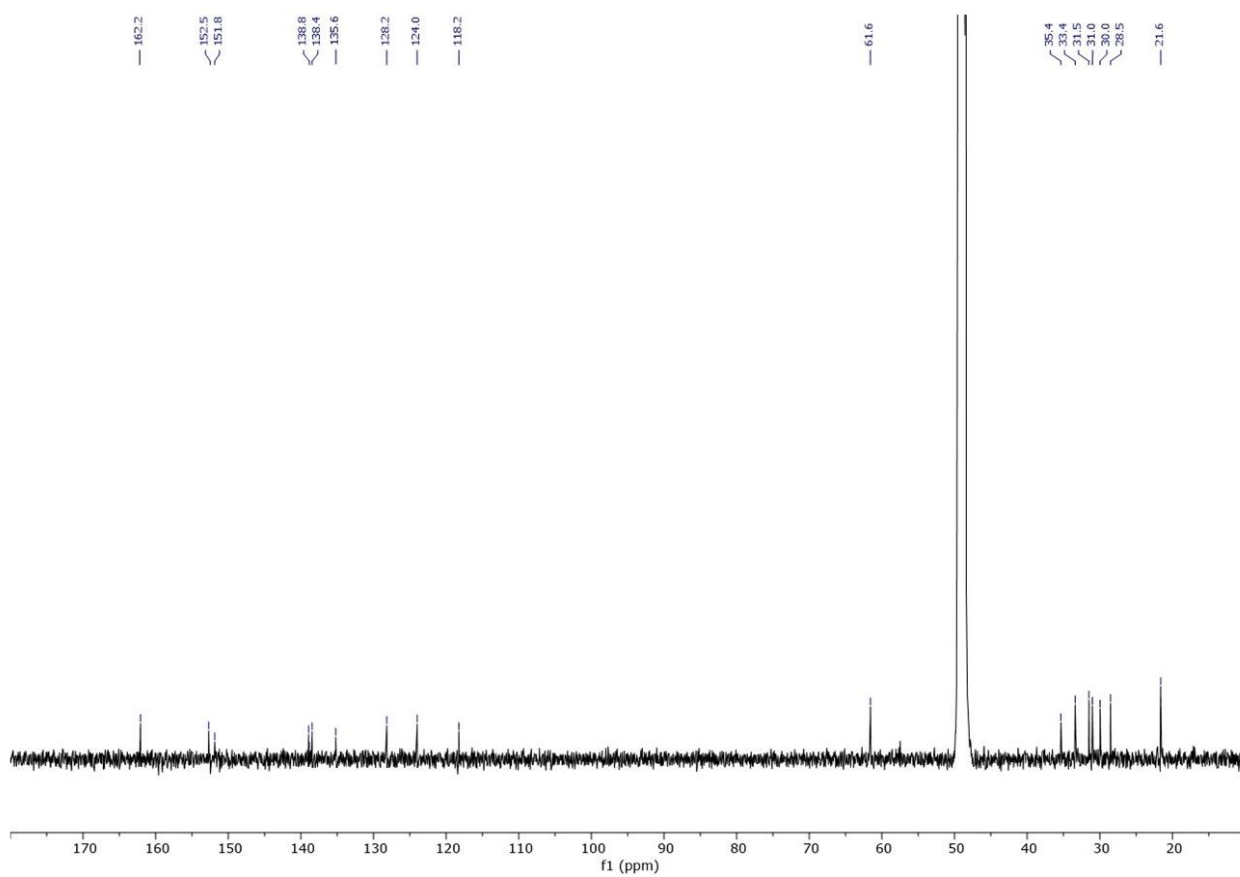


Figure S24. ^{13}C NMR Spectrum (150 MHz, CD_3OD) of compound **11**.

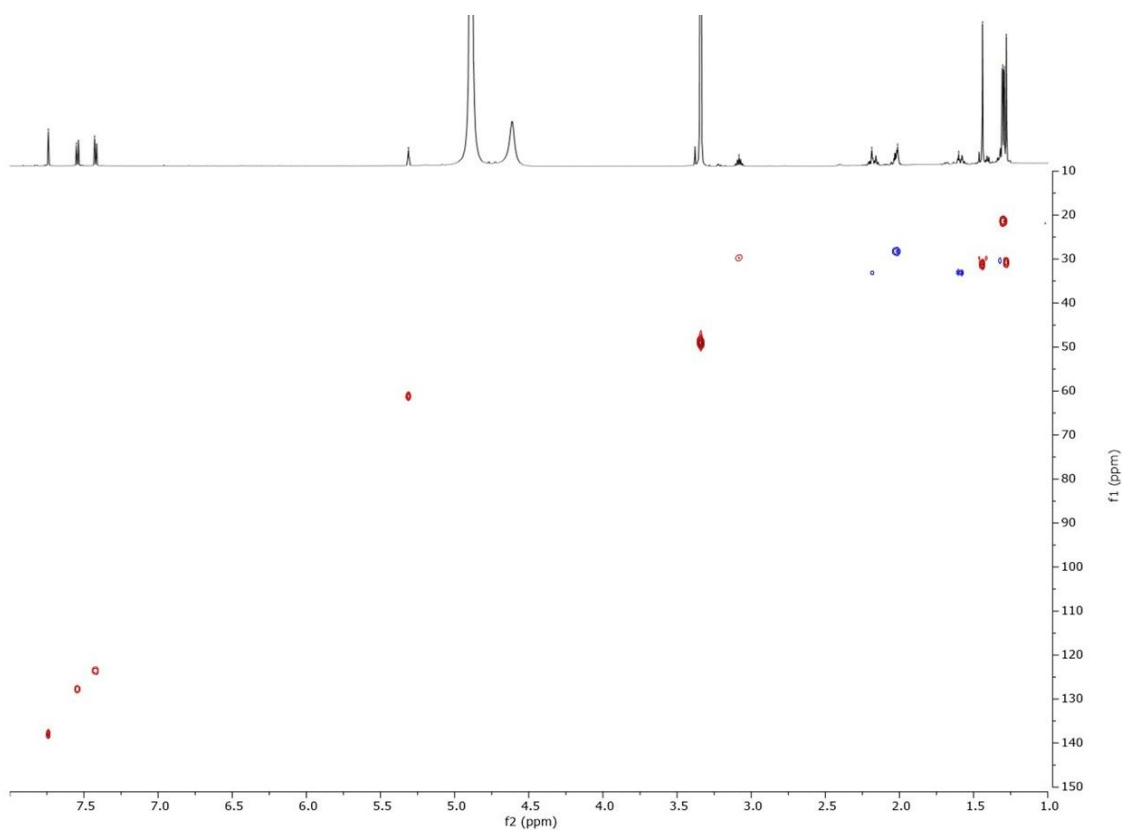


Figure S25. HSQC Spectrum (CD_3OD) of compound **11**.

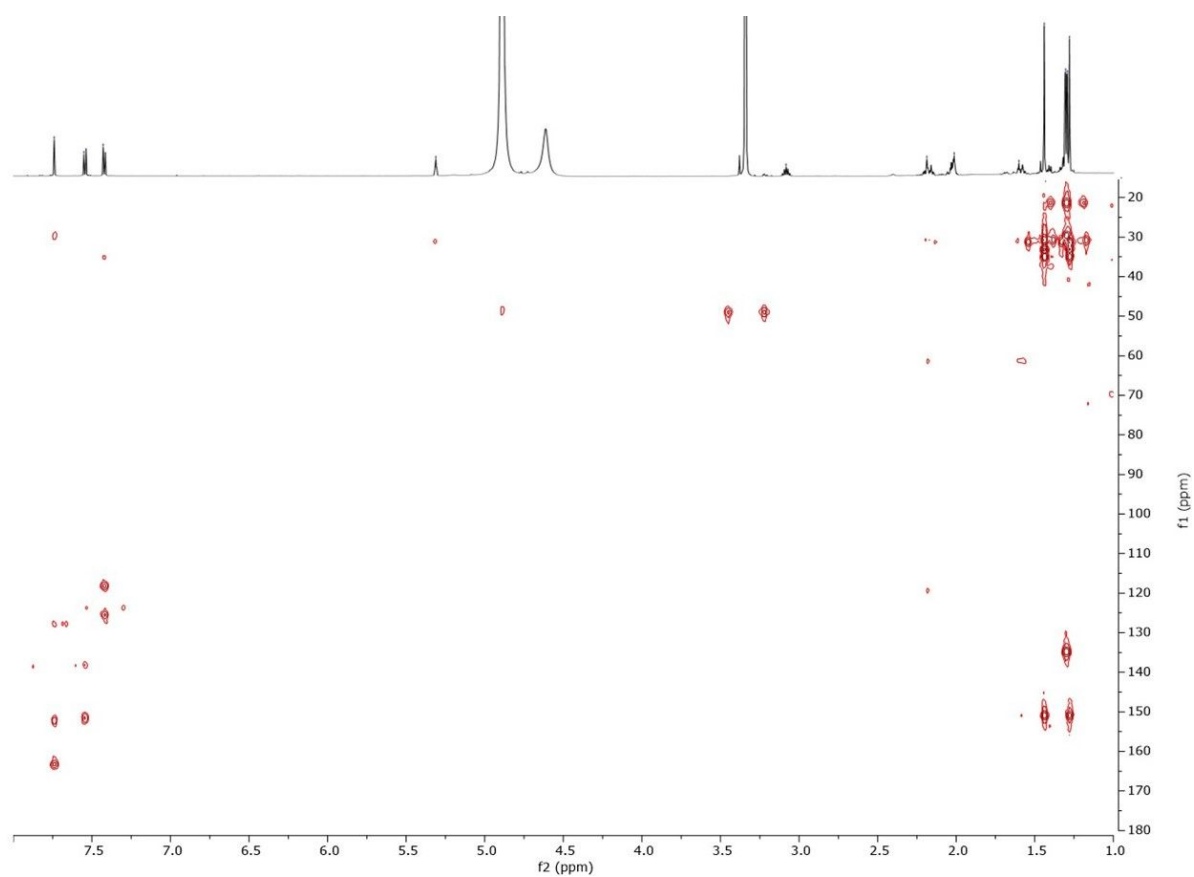


Figure S26. HMBC Spectrum (CD_3OD) of compound **11**.

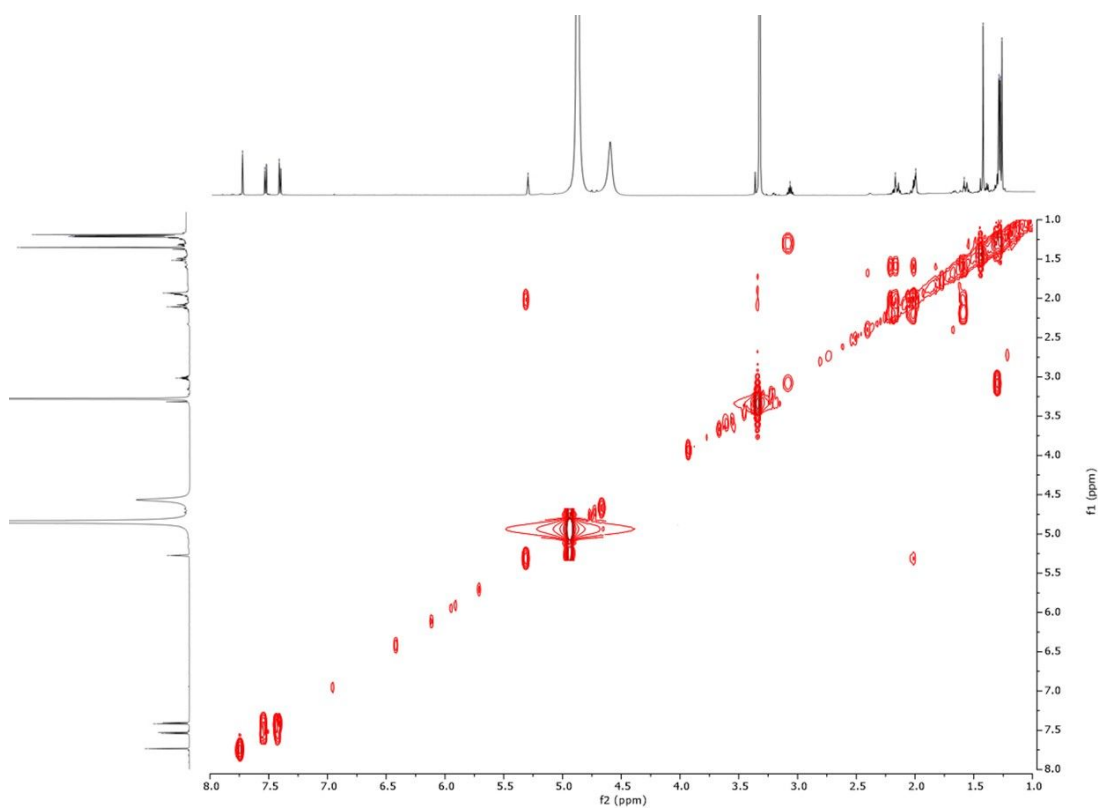


Figure S27. COSY Spectrum (CD_3OD) of compound **11**.

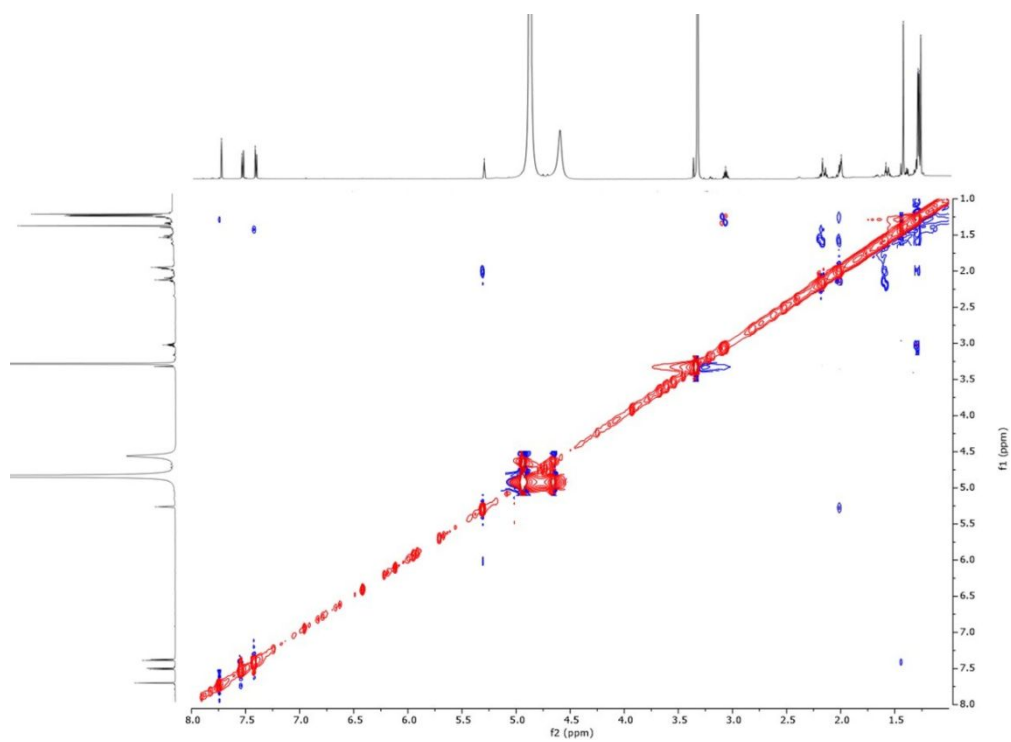


Figure S28. ROESY Spectrum (CD_3OD) of compound **11**.

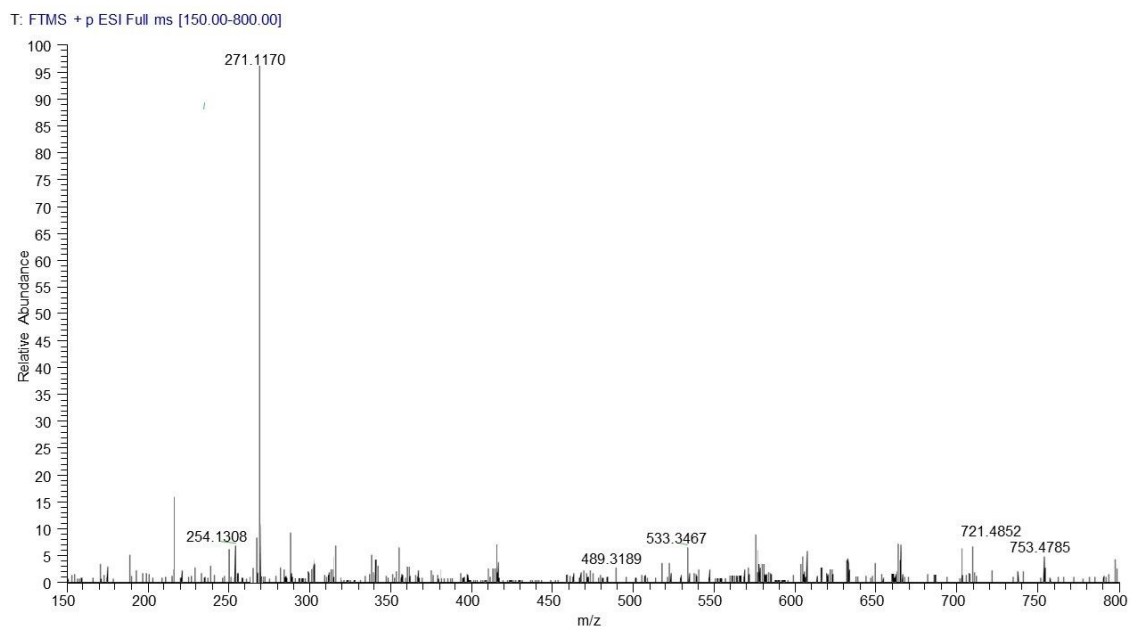


Figure S29. ESI/LTQ Orbitrap spectrum of compound **16**, in negative ion mode.

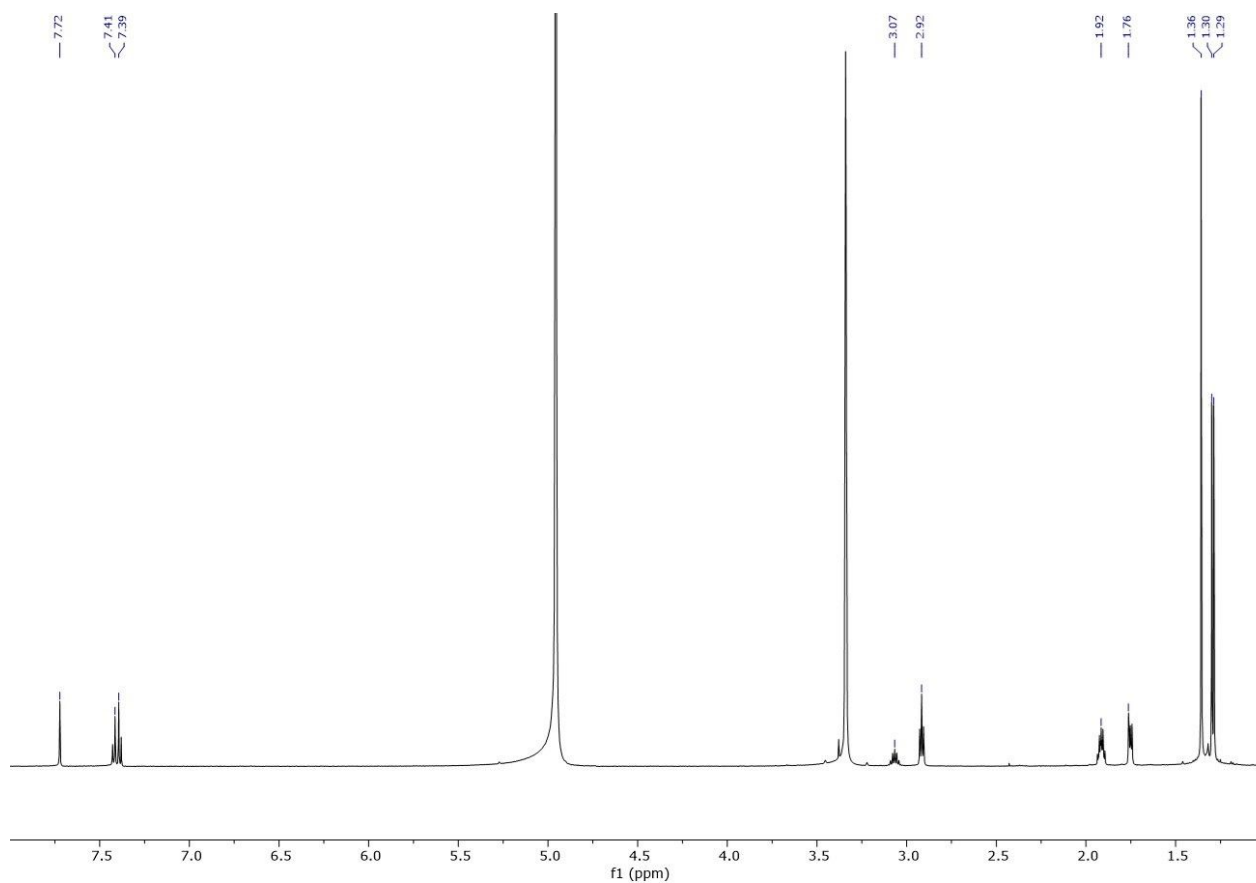


Figure S30. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **16**.

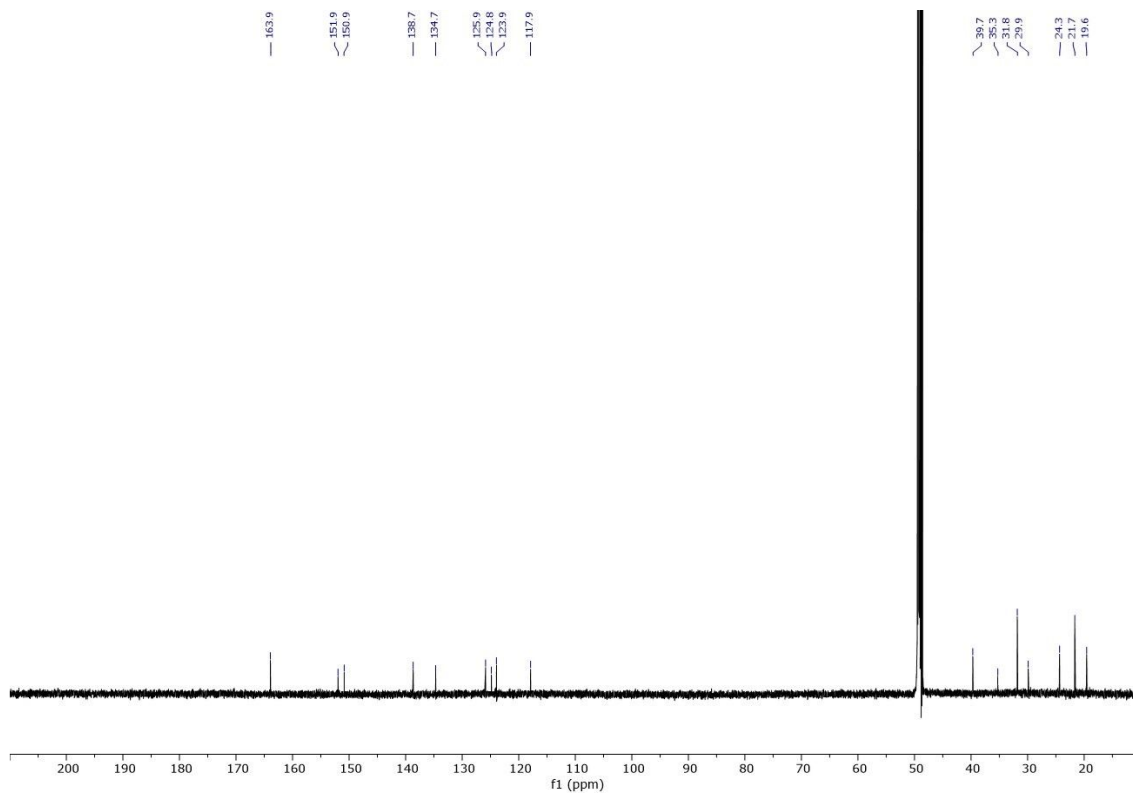


Figure S31. ^{13}C Spectrum (150 MHz, CD_3OD) of compound **16**.

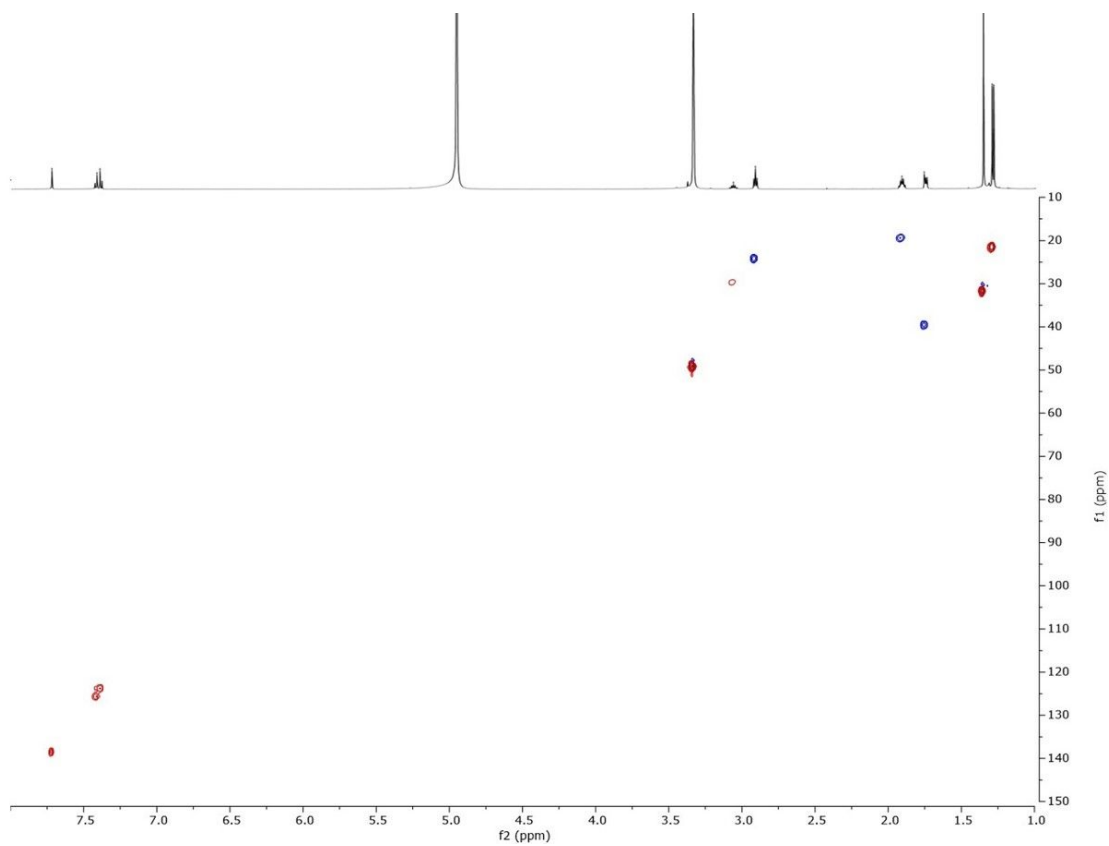


Figure S32. HSQC Spectrum (CD_3OD) of compound **16**.

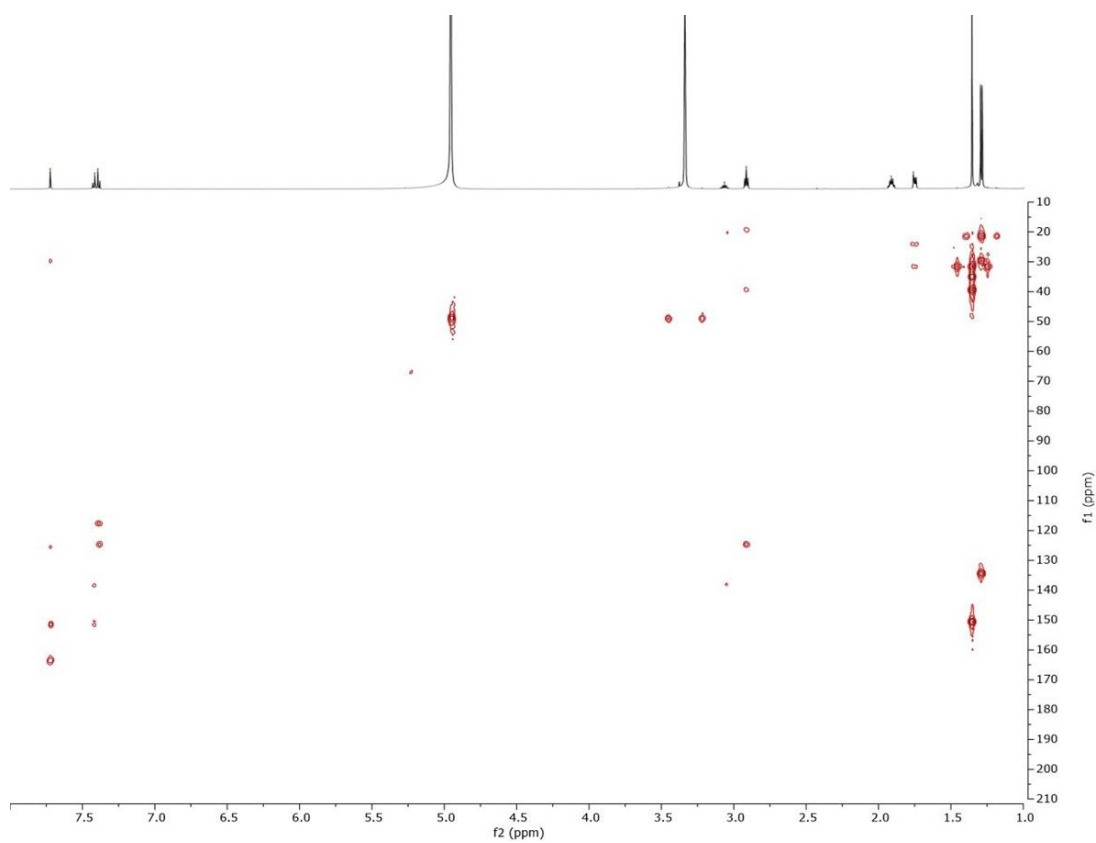


Figure S33. HMBC Spectrum (CD_3OD) of compound **16**.

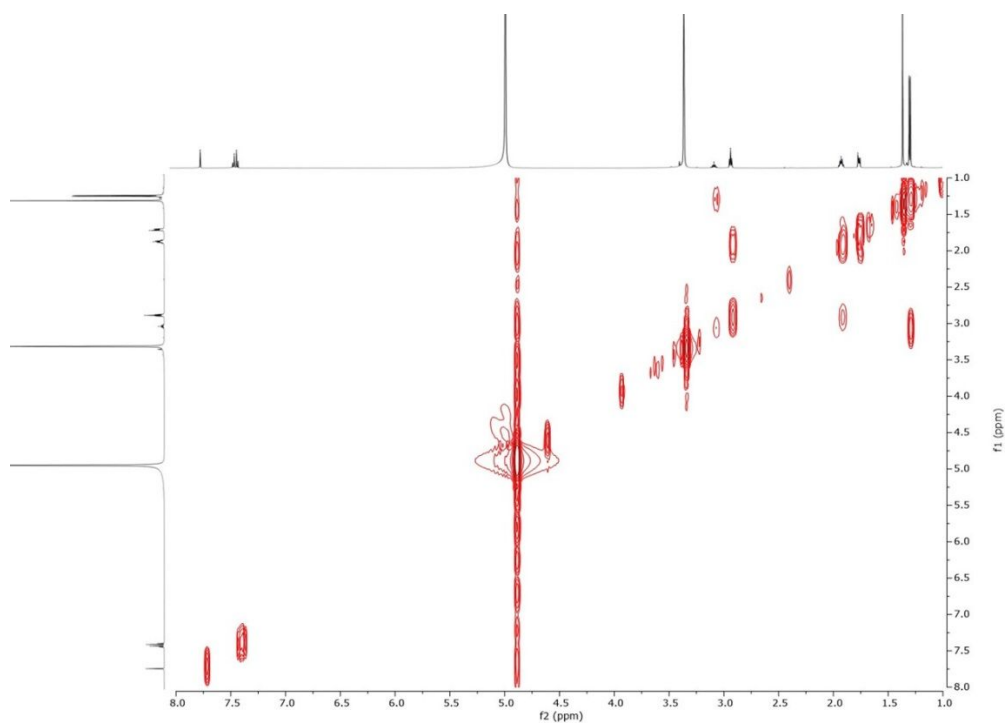


Figure S34. COSY Spectrum (CD_3OD) of compound **16**.

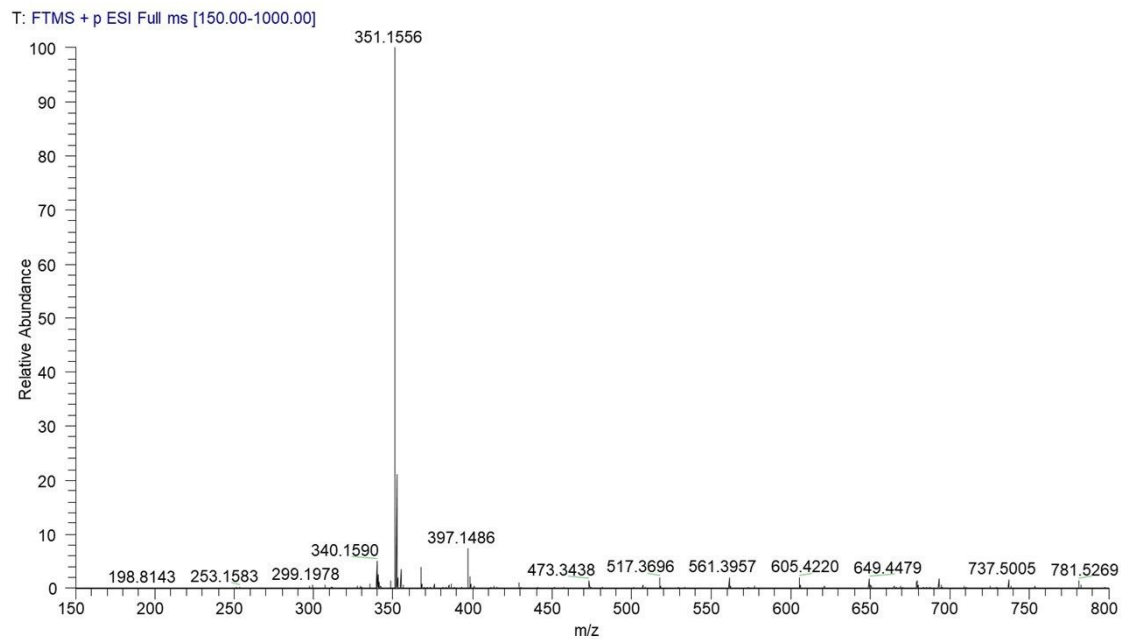


Figure S36. ESI/LTQOrbitrap spectrum of compound **20**, in negative ion mode.

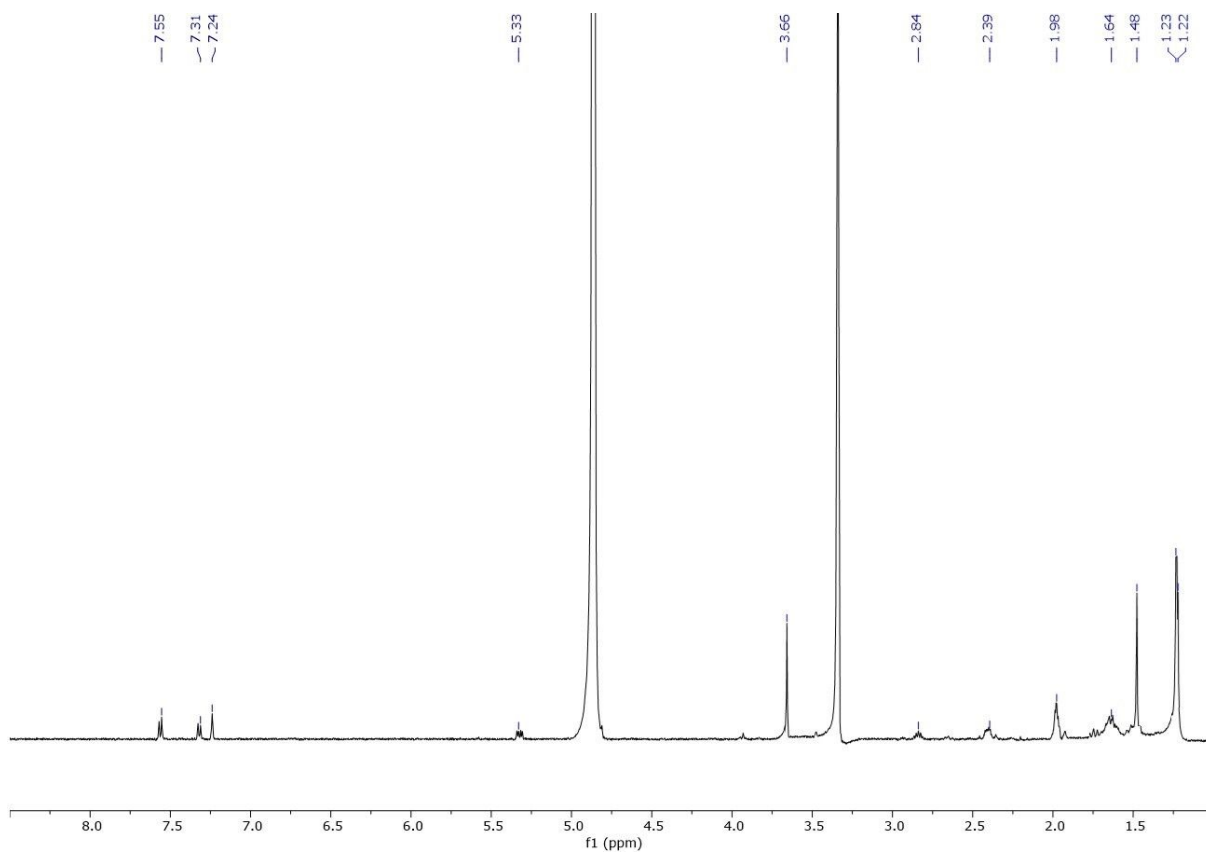


Figure S37. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **20**.

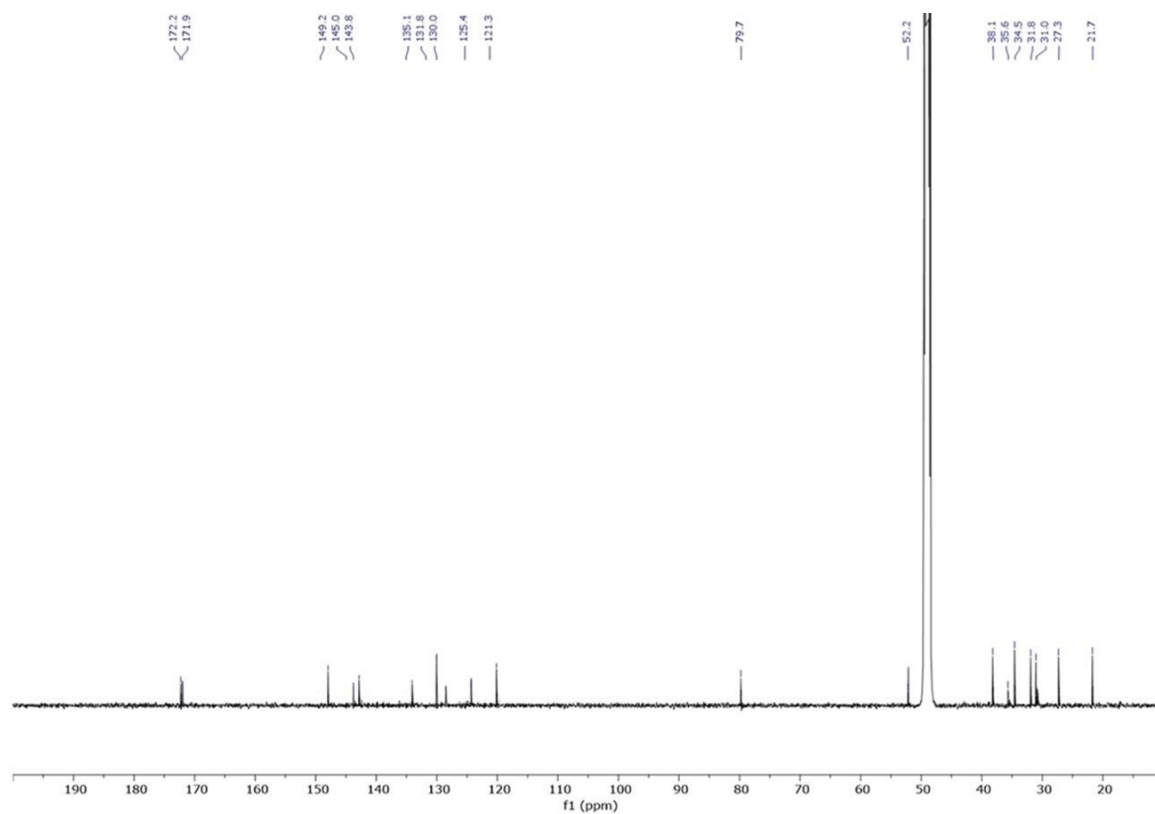


Figure S38. ^{13}C Spectrum (150 MHz, CD_3OD) of compound **20**.

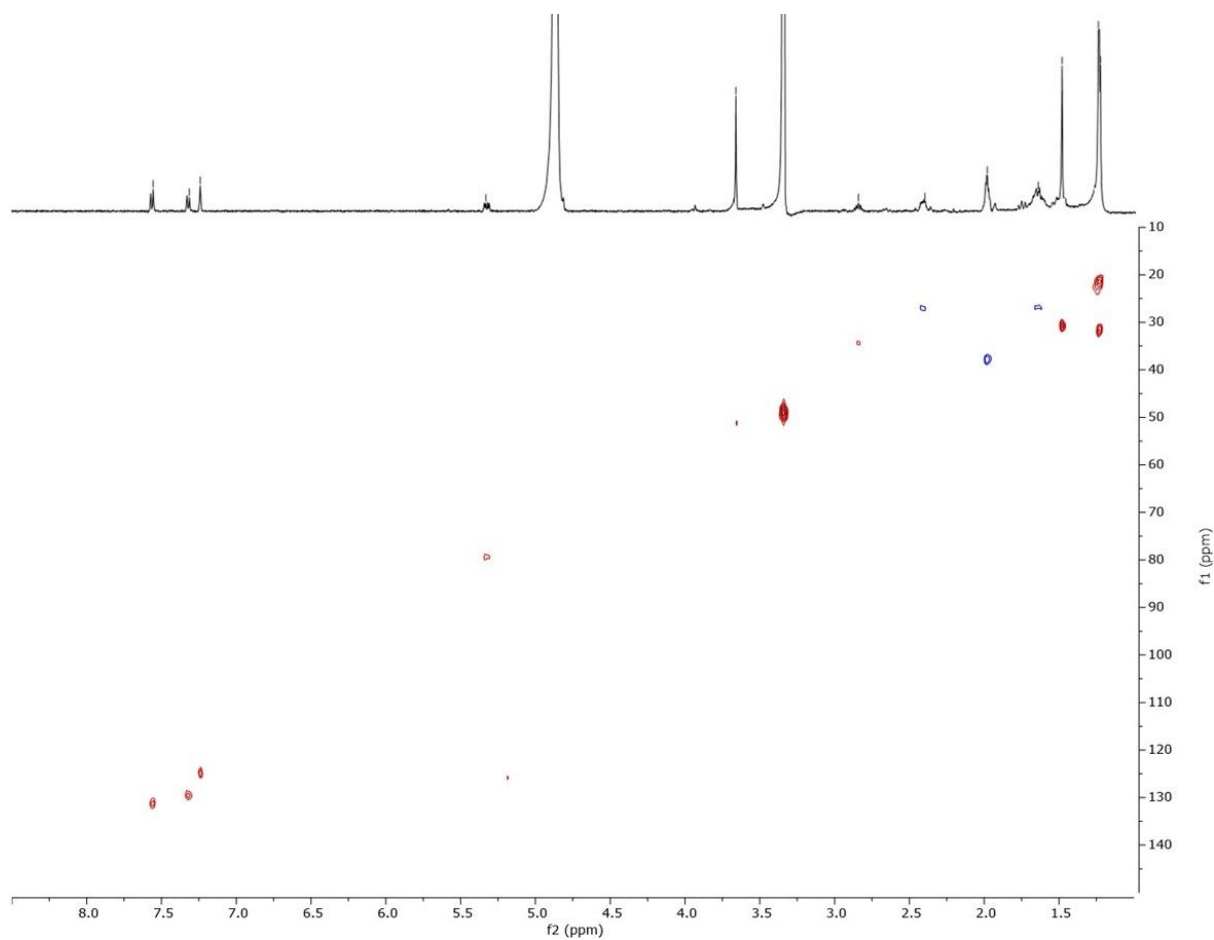


Figure S39. HSQC Spectrum (CD_3OD) of compound **20**.

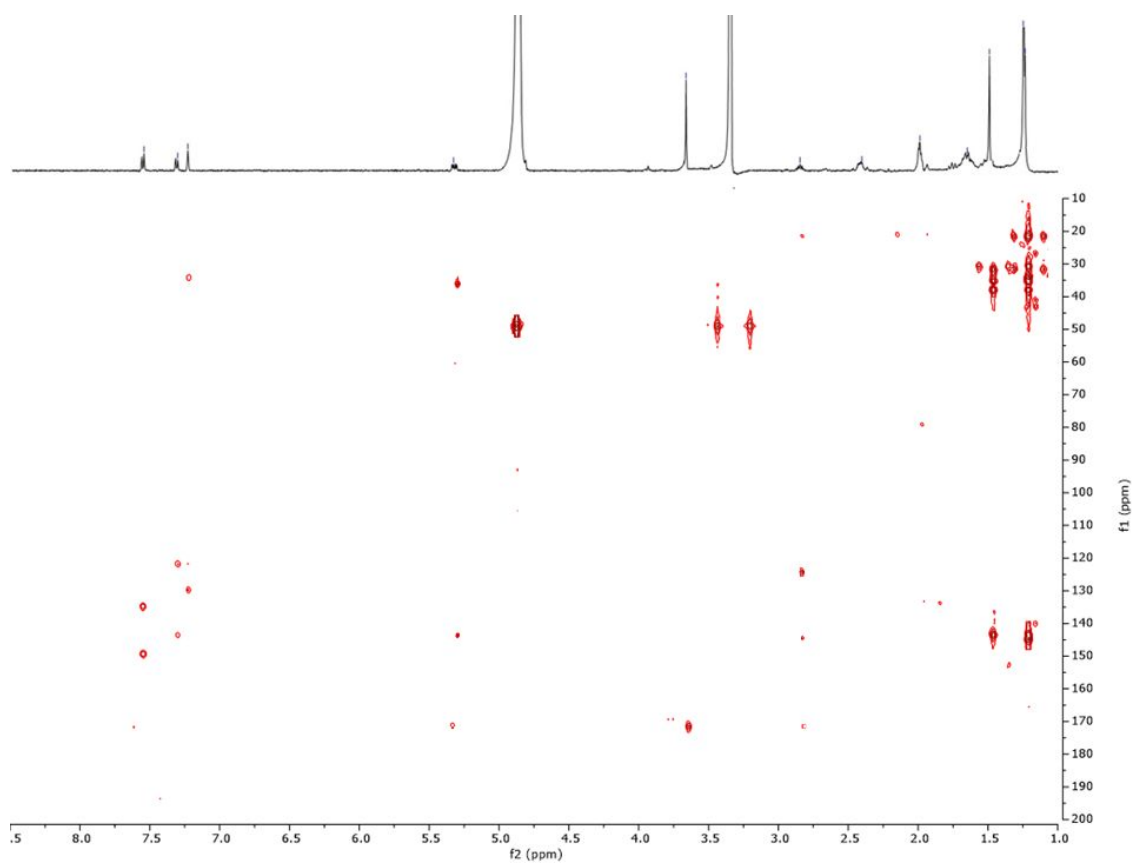


Figure S40. HMBC Spectrum (CD₃OD) of compound **20**.

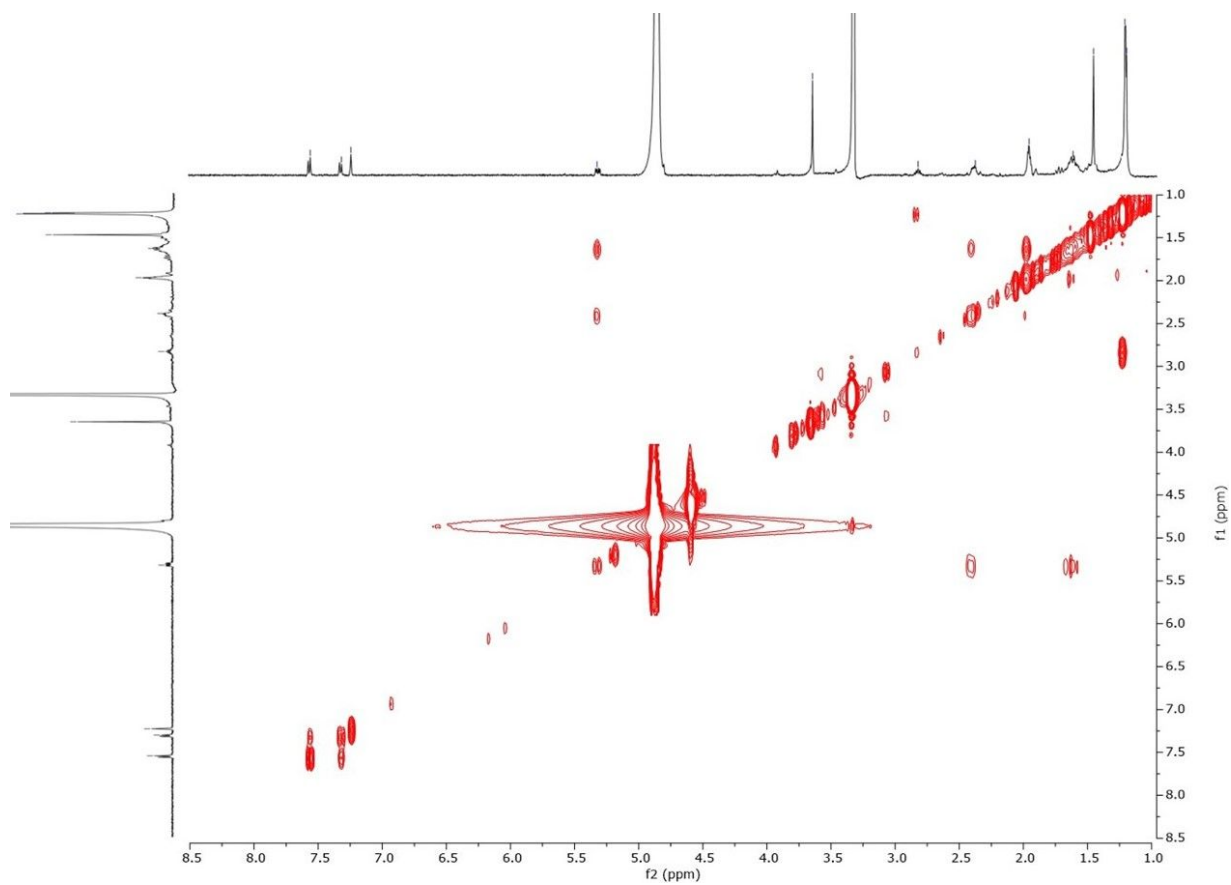


Figure S41. COSY Spectrum (CD₃OD) of compound **20**.