

***Pouteria lucuma* Pulp and Skin: In Depth Chemical Profile and Evaluation of Antioxidant Activity**

Milena Masullo¹, Antonietta Cerulli¹, Cosimo Pizza¹ and Sonia Piacente^{1,*}

¹ Dipartimento di Farmacia, Università degli Studi di Salerno, via Giovanni Paolo II n. 132, 84084 Fisciano (SA), Italy; piacente@unisa.it

* Correspondence: piacente@unisa.it; Tel.: +39089969763

Table S1. Molecular formula $[M-H]^-$, $[(M+HCOOH)-H]^-$, characteristic product ions (molecular formula and intensity) occurring in *P. lucuma* pulp *n*-BuOH extract and *P. lucuma* skin MeOH extract, identified by LCESI/LTQOrbitrap/MS/MS (negative ion mode).

Figure S1. Chromatogram of *P. lucuma* pulp extract on the C18 Synergi-Hydro-RP column

Figure S2. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 1

Figure S3. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 2

Figure S4. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 3

Figure S5. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 4

Figure S6. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 5

Figure S7. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 6

Figure S8. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 7

Figure S9. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 8

Figure S10. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 9

Figure S11. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 10

Figure S12. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 11

Figure S13. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 12

Figure S14. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 13

Figure S15. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **14**

Figure S16. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **15**

Figure S17. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **16**

Figure S18. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **17**

Figure S19. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **18**

Figure S20. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **19**

Figure S21. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **20**

Table S1. Molecular formula $[\text{M}-\text{H}]^-$, $[(\text{M}+\text{HCOOH})-\text{H}]^-$, characteristic product ions (molecular formula and intensity) occurring in *P. lucuma* pulp *n*-BuOH extract and *P. lucuma* skin MeOH extract, identified by LCESI/LTQOrbitrap/MS/MS (negative ion mode).

	compound	Molecular formula	$[(\text{M}+\text{HCOOH})-\text{H}]^-$	$[\text{M}-\text{H}]^-$	product ions (molecular formula, intensity)
1	galloyl 1- <i>O</i> - glucopyranoside	$\text{C}_{13}\text{H}_{16}\text{O}_{10}$		331.0664	169.03 ($\text{C}_7\text{H}_5\text{O}_5$, 99.6)
2	galocatechin	$\text{C}_{15}\text{H}_{14}\text{O}_7$		305.0656	287.16 ($\text{C}_{15}\text{H}_{11}\text{O}_6$, 33.2), 125.15 ($\text{C}_6\text{H}_5\text{O}_3$, 13.6)
3	<i>p</i> -coumaric acid	$\text{C}_9\text{H}_8\text{O}_3$	209.0451		119.08 ($\text{C}_8\text{H}_7\text{O}_0$, 26.6),
4	<i>p</i> -ferulic acid	$\text{C}_{10}\text{H}_{10}\text{O}_4$	239.0554		133.05 ($\text{C}_8\text{H}_5\text{O}_2$, 76.6),
5	epigallocatechin	$\text{C}_{15}\text{H}_{14}\text{O}_7$		305.0659	287.01 ($\text{C}_{15}\text{H}_{11}\text{O}_6$, 36.8), 125.11 ($\text{C}_6\text{H}_5\text{O}_3$, 16.3)
6	<i>p</i> -coumaroyl glucopyranoside	4- <i>O</i> - β -D- $\text{C}_{15}\text{H}_{18}\text{O}_8$		325.0928	163.12 ($\text{C}_6\text{H}_7\text{O}_3$, 21.5),
7	catechin	$\text{C}_{15}\text{H}_{14}\text{O}_6$		289.0713	179.05 ($\text{C}_9\text{H}_7\text{O}_4$, 17.47) 151.01($\text{C}_8\text{H}_7\text{O}_3$,0.75) 137.08 ($\text{C}_7\text{H}_5\text{O}_3$,3.69)
8	<i>p</i> -feruloyl-4- <i>O</i> - β -D- glucopyranoside	$\text{C}_{16}\text{H}_{20}\text{O}_9$		355.1025	193.18 ($\text{C}_{10}\text{H}_9\text{O}_4$, 36.8)
9	4-hydroxybenzoic acid glucopyranoside	4- <i>O</i> - β -D- $\text{C}_{13}\text{H}_{16}\text{O}_8$		299.0763	137.02 ($\text{C}_7\text{H}_6\text{O}_3$, 65.9)
10	epicatechin	$\text{C}_{15}\text{H}_{14}\text{O}_6$		289.0715	179.01 ($\text{C}_9\text{H}_7\text{O}_4$, 13.73) 151.02($\text{C}_8\text{H}_7\text{O}_3$, 0.93) 137.07 ($\text{C}_7\text{H}_5\text{O}_3$,3.68)
11	galocatechin-gallate	$\text{C}_{22}\text{H}_{18}\text{O}_{11}$		457.0769	287.11 ($\text{C}_{15}\text{H}_{11}\text{O}_6$, 32.21)

					168.99 (C ₇ H ₅ O ₅ , 100.00)
12	ampelopsin		C ₁₅ H ₁₂ O ₈	319.0456	301.12 (C ₁₅ H ₉ O ₇ , 38.46)
13	myricetin	3-O- α -L-	C ₂₁ H ₂₀ O ₁₂	479.0824	317.10 (C ₁₅ H ₉ O ₈ , 58.95)
	rhamnopyranoside				
14	resveratrol-3-O- β -D-		C ₂₀ H ₂₂ O ₈	389.1232	227.15 (C ₁₄ H ₁₁ O ₃ , 99.85)
	glucopyranoside				
15	taxifolin		C ₁₅ H ₁₂ O ₇	303.0503	285.07 (C ₁₅ H ₉ O ₆ , 100.0), 176.96 (C ₉ H ₅ O ₄ , 10.87)
16	quercetin	3-O- β -D-	C ₂₁ H ₂₀ O ₁₁	447.0927	300.99 (C ₁₅ H ₉ O ₇ , 66.06)
	rhamnopyranoside				
17	eriodictyol		C ₁₅ H ₁₂ O ₆	287.0550	179.21 (C ₉ H ₇ O ₄ , 56.06) 153.07 (C ₇ H ₅ O ₄ , 32.03)
18	<i>p</i> -hydroxy benzoic acid		C ₇ H ₆ O ₃	137.0218	93.05 (C ₆ H ₅ O, 65.01)
19	quercetin		C ₁₅ H ₁₀ O ₇	301.0350	179.01 (C ₈ H ₃ O ₅ , 100.00) 151.01 (C ₈ H ₇ O ₃ , 71.98)
20	salicylic acid		C ₇ H ₆ O ₃	137.0218	93.03 (C ₆ H ₅ O, 75.03)
21	TriHoDe		C ₁₈ H ₃₂ O ₅	327.2171	229.05 (C ₁₂ H ₂₁ O ₄ , 100.00), 171.03 (C ₉ H ₁₅ O ₃ , 52.18)
22	TriHoMe		C ₁₈ H ₃₄ O ₅	329.2326	229.07 (C ₁₂ H ₂₁ O ₄ , 100.00), 171.08 (C ₉ H ₁₅ O ₃ , 55.15)
23	TriHoDe		C ₁₈ H ₂₈ O ₄	307.1909	171.03 (C ₉ H ₁₅ O ₃ , 55.26)
24	hydroxy-epoxy-octadecadienoic acid		C ₁₈ H ₃₀ O ₄	309.2065	201.21 (C ₁₀ H ₁₇ O ₄ , 52.99) 171.04 (C ₉ H ₁₅ O ₃ , 67.88)
25	hydroxy-epoxy-octadecadienoic acid isomer		C ₁₈ H ₃₀ O ₄	309.2065	201.26 (C ₁₀ H ₁₇ O ₄ , 56.83) 171.02 (C ₉ H ₁₅ O ₃ , 67.85)
26	DGMG (18:3)		C ₃₃ H ₅₆ O ₁₄	721.3634	415.26 (C ₁₅ H ₂₇ O ₁₃ , 3.35) 397.21 (C ₁₅ H ₂₅ O ₁₂ , 18.30) 235.15 (C ₉ H ₁₅ O ₇ , 0.43)
27	DGMG (18:3)		C ₃₃ H ₅₆ O ₁₄₆	721.3631	415.29 (C ₁₅ H ₂₇ O ₁₃ , 3.99) 397.24 (C ₁₅ H ₂₅ O ₁₂ , 15.78) 235.12 (C ₉ H ₁₅ O ₇ , 0.33)
28	DGMG (18:2)		C ₃₃ H ₅₈ O ₁₄	723.3796	415.00 (C ₁₅ H ₂₇ O ₁₃ , 3.56) 397.16 (C ₁₅ H ₂₅ O ₁₂ , 18.31)
29	DGMG (18:2)		C ₃₃ H ₅₈ O ₁₄	723.3795	415.26 (C ₁₅ H ₂₇ O ₁₃ , 0.99) 397.26 (C ₁₅ H ₂₅ O ₁₂ , 11.36)
30	DGMG (18:1)		C ₃₃ H ₆₀ O ₁₄	725.3937	415.52 (C ₁₅ H ₂₇ O ₁₃ , 1.18) 397.30 (C ₁₅ H ₂₅ O ₁₂ , 4.76)
31	DGMG (16:0)		C ₃₁ H ₅₈ O ₁₄	699.3788	415.03 (C ₁₅ H ₂₇ O ₁₃ , 0.58) 397.19 (C ₁₅ H ₂₅ O ₁₂ , 13.89) 235.14 (C ₉ H ₁₅ O ₇ , 0.62)
32	DGMG (18:1)		C ₃₃ H ₆₀ O ₁₄	725.3937	415.30 (C ₁₅ H ₂₇ O ₁₃ , 1.35) 397.49 (C ₁₅ H ₂₅ O ₁₂ , 0.68)
33	l-PC (16:0)		C ₂₄ H ₅₀ O ₇ NP	540.3296	255.37 (C ₁₆ H ₃₁ O ₂ , 100)

34	MGMG (16:3)	C ₂₅ H ₄₂ O ₉		485.2744	235.14 (C ₉ H ₁₅ O ₇ , 0.35)
35	l-PC (18:1)	C ₂₆ H ₅₂ O ₇ NP	566.3451		281.25 (C ₁₈ H ₃₃ O ₂ , 46.23)
36	DGMG (18:0)	C ₃₃ H ₆₂ O ₁₄	727.4096		415.37 (C ₁₅ H ₂₇ O ₁₃ , 2.38)
					397.24 (C ₁₅ H ₂₅ O ₁₂ , 17.97)
					235.23 (C ₉ H ₁₅ O ₇ , 0.73)
1	galloyl 1-O- glucopyranoside	C ₁₃ H ₁₆ O ₁₀		331.0668	169.03 (C ₇ H ₅ O ₅ , 99.8)
15	taxifolin	C ₁₅ H ₁₂ O ₇		303.0503	285.08 (C ₁₅ H ₉ O ₆ , 100.0), 176.96 (C ₉ H ₅ O ₄ , 10.83)
17	eriodictyol	C ₁₅ H ₁₂ O ₆		287.0558	179.21 (C ₉ H ₇ O ₄ , 56.06) 153.07 (C ₇ H ₅ O ₄ , 32.03)
19	quercetin	C ₁₅ H ₁₀ O ₇		301.0346	179.01 (C ₈ H ₃ O ₅ , 100.00) 151.02 (C ₈ H ₇ O ₃ , 71.96)
21	TriHoDe	C ₁₈ H ₃₂ O ₅		327.2169	229.04 (C ₁₂ H ₂₁ O ₄ , 100.00), 171.03 (C ₉ H ₁₅ O ₃ , 52.16)
22	TriHOME	C ₁₈ H ₃₄ O ₅		329.2326	229.16 (C ₁₂ H ₂₁ O ₄ , 100.00), 170.96 (C ₉ H ₁₅ O ₃ , 77.24)
37	ellagic acid	C ₁₄ H ₆ O ₈		300.9983	257.04 (C ₁₃ H ₅ O ₆ , 76.37)
38	DGDG (18.3, 16:0)	C ₄₉ H ₈₆ O ₁₅		959.5934	415.26 (C ₁₅ H ₂₇ O ₁₃ , 3.35) 397.21 (C ₁₅ H ₂₅ O ₁₂ , 18.30) 235.15 (C ₉ H ₁₅ O ₇ , 0.43)

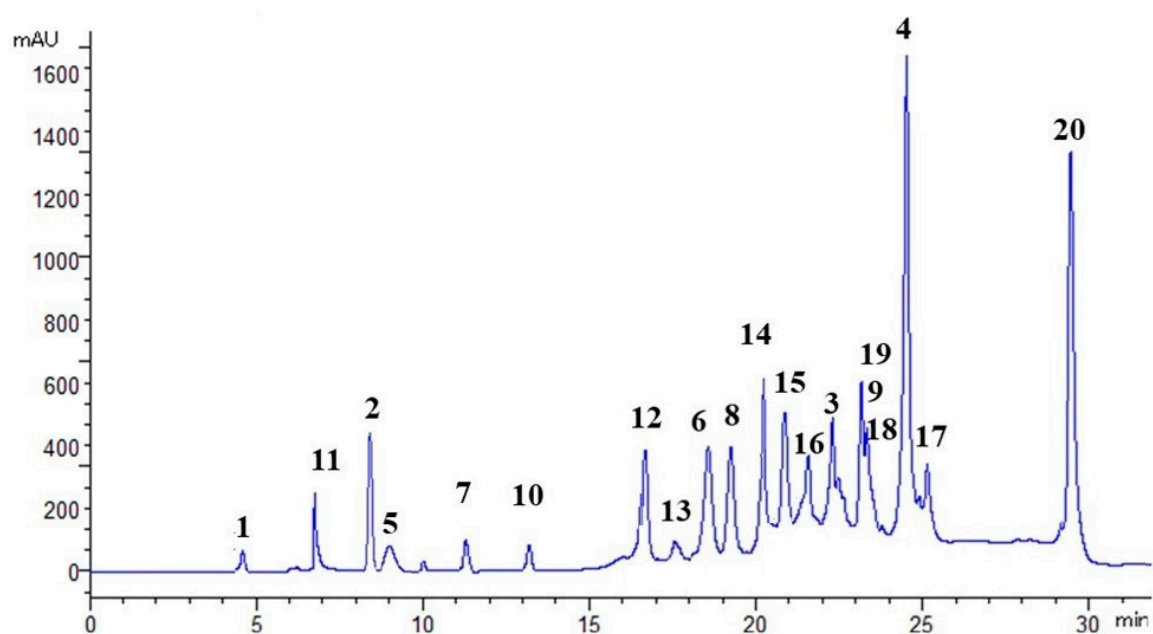


Figure S1. HPLC-UV Chromatogram of *P. lucuma* pulp extract at wavelength 310 nm.

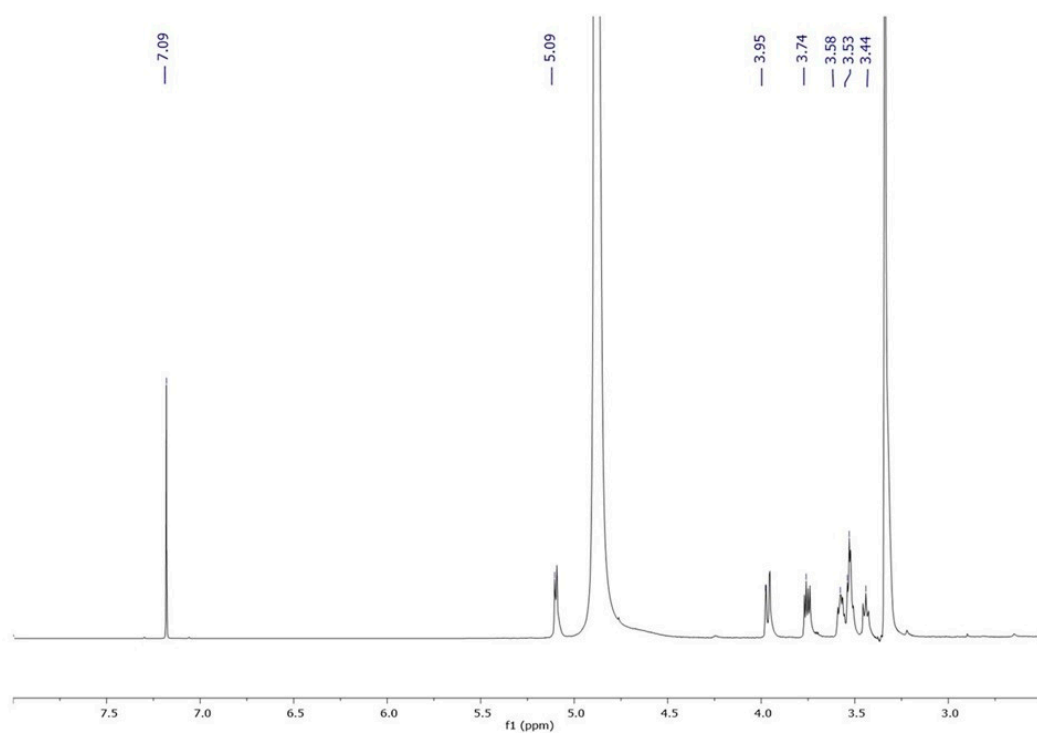


Figure S2. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 1

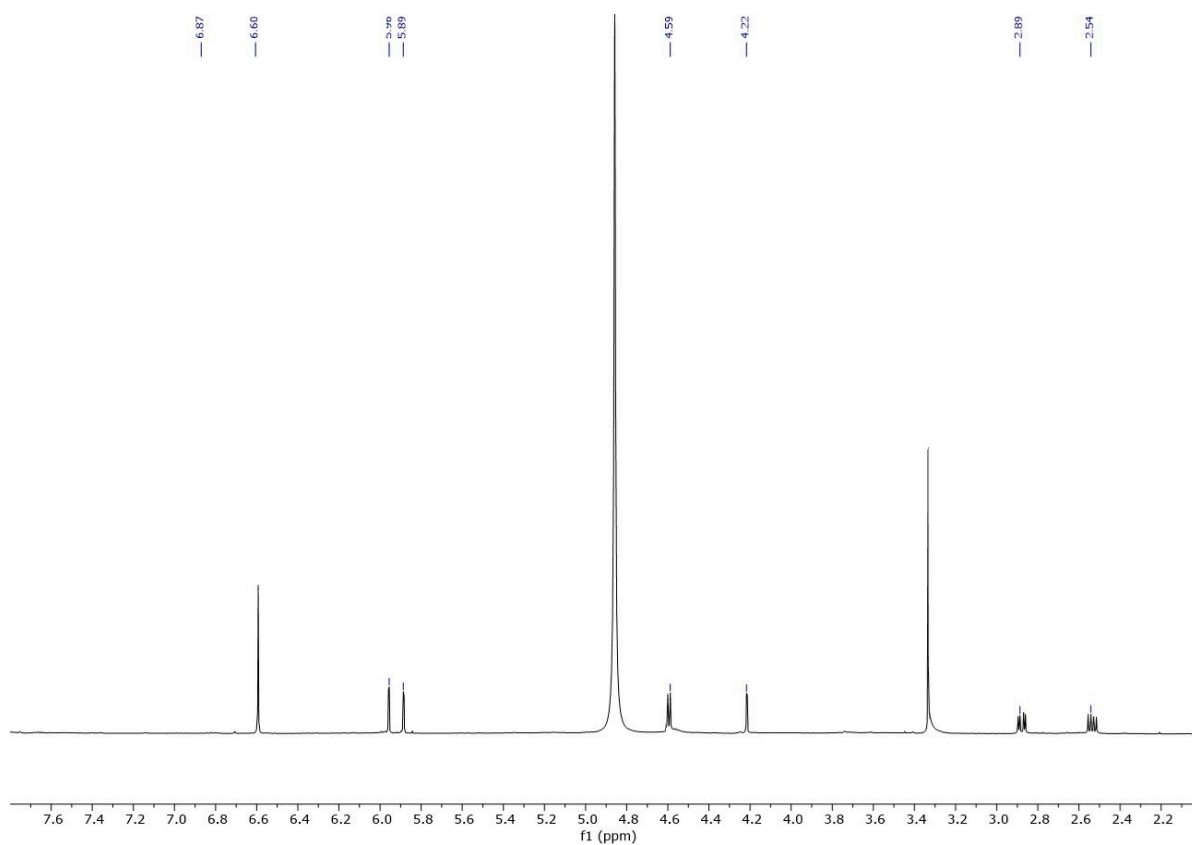


Figure S3. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound 2

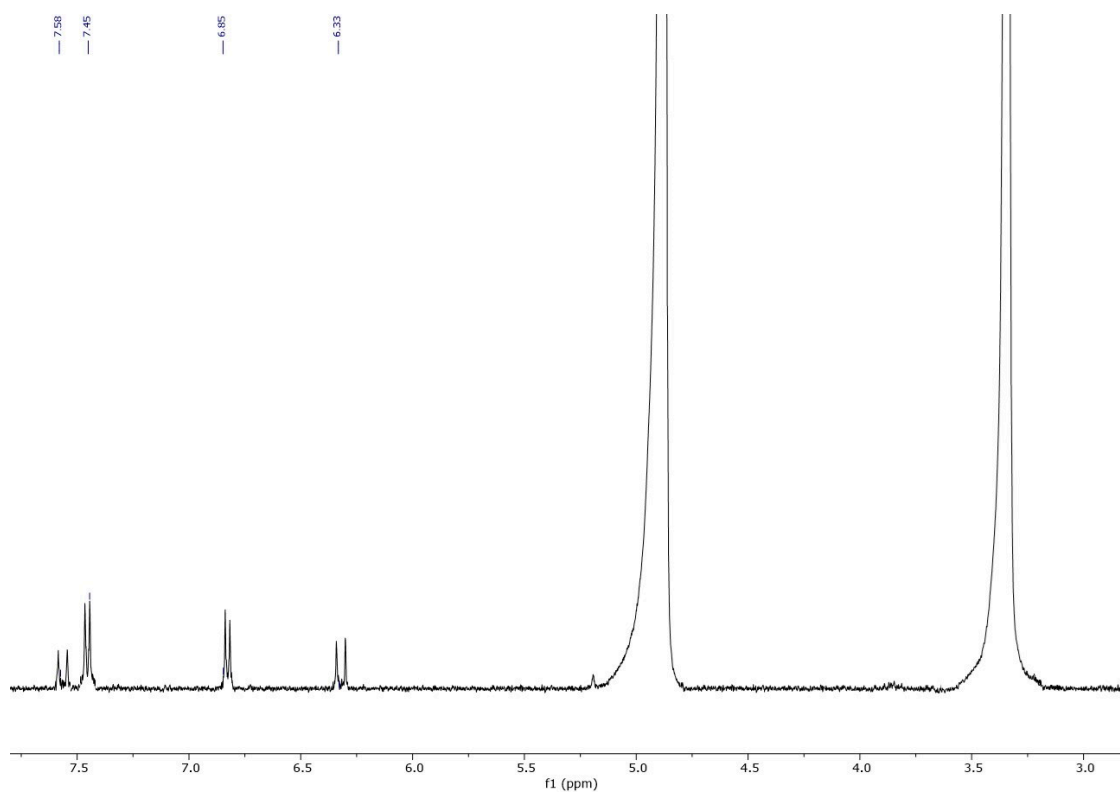


Figure S4. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **3**.

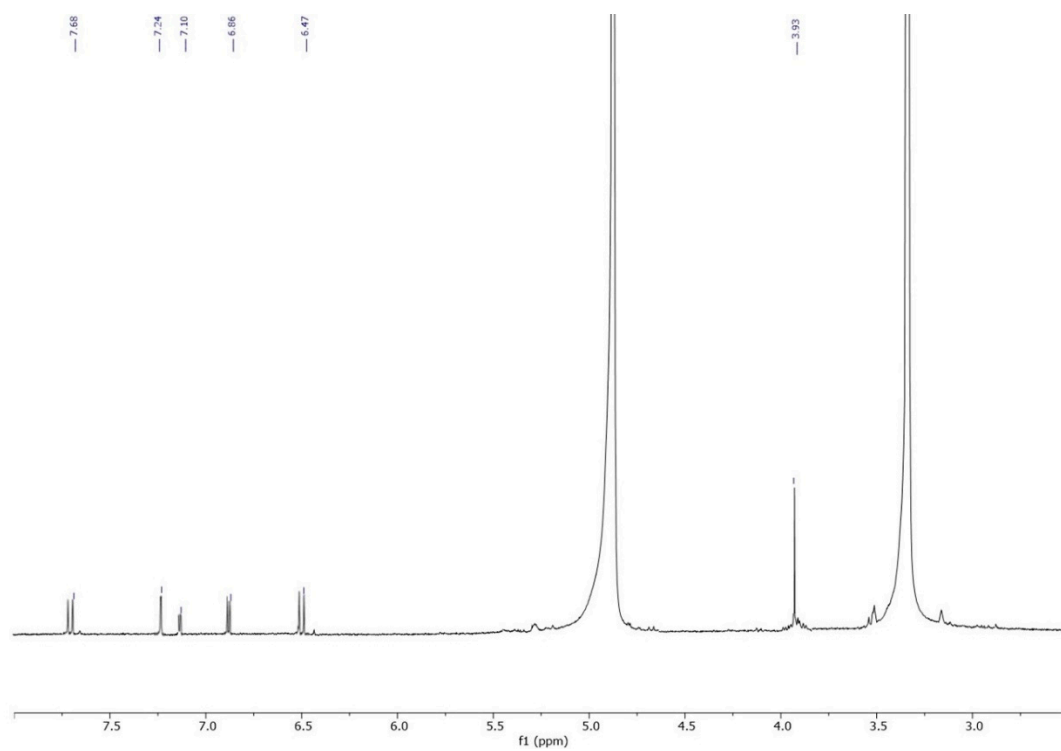


Figure S5. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **4**.

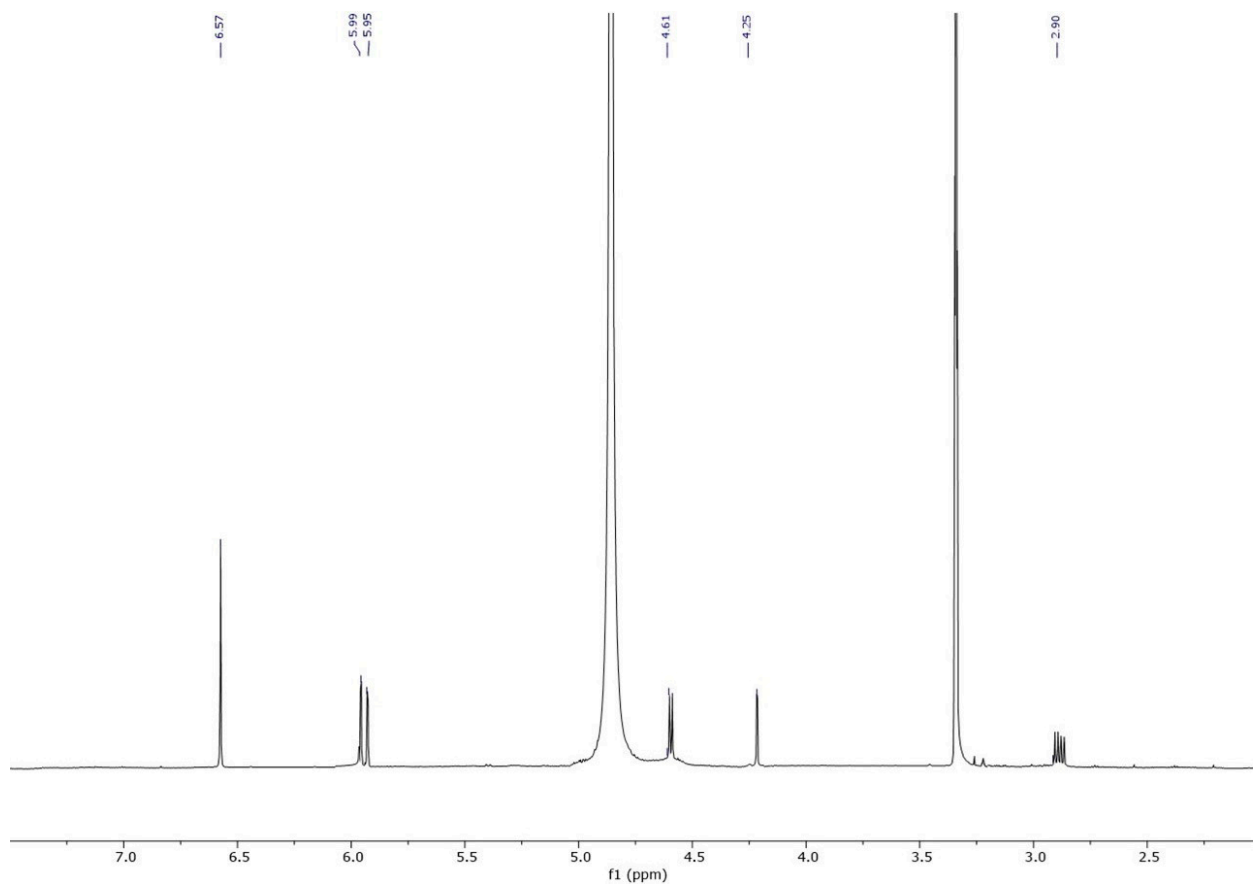


Figure S6. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **5**.

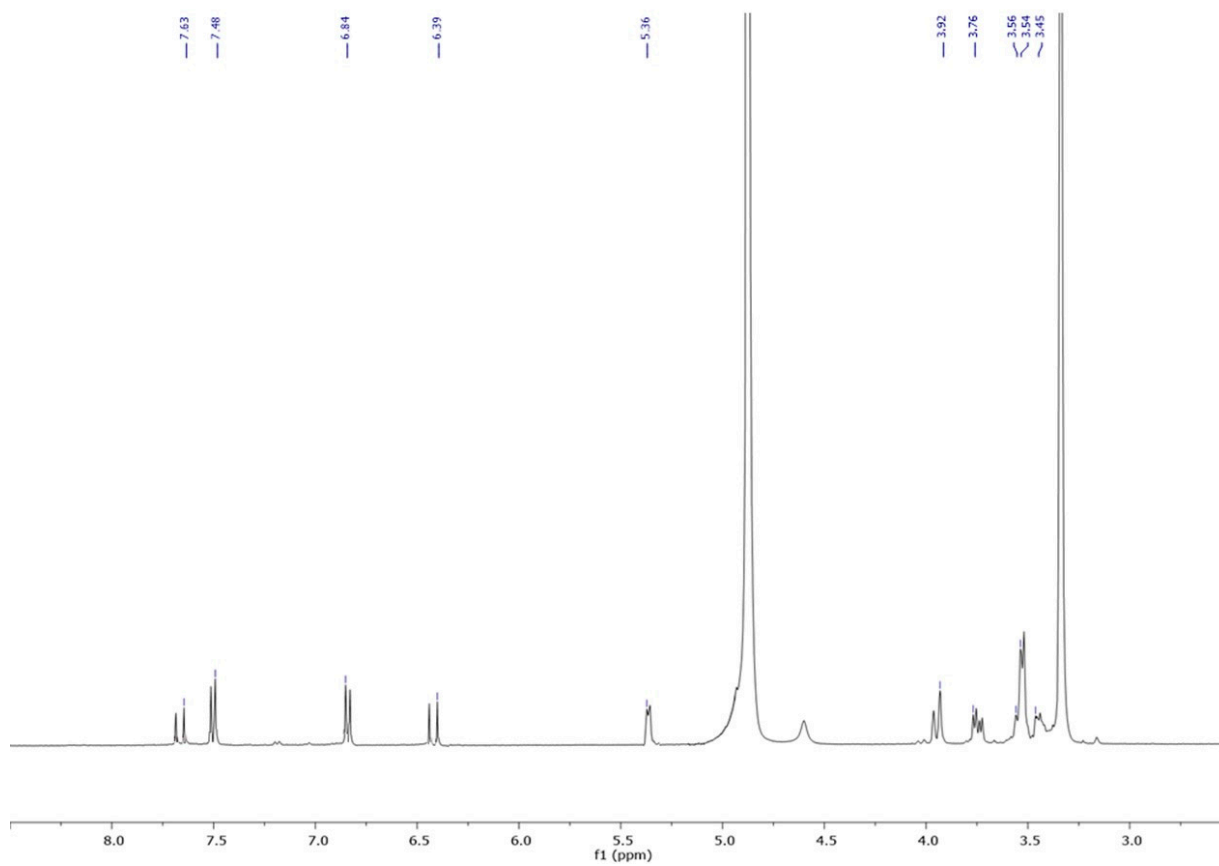


Figure S7. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **6**.

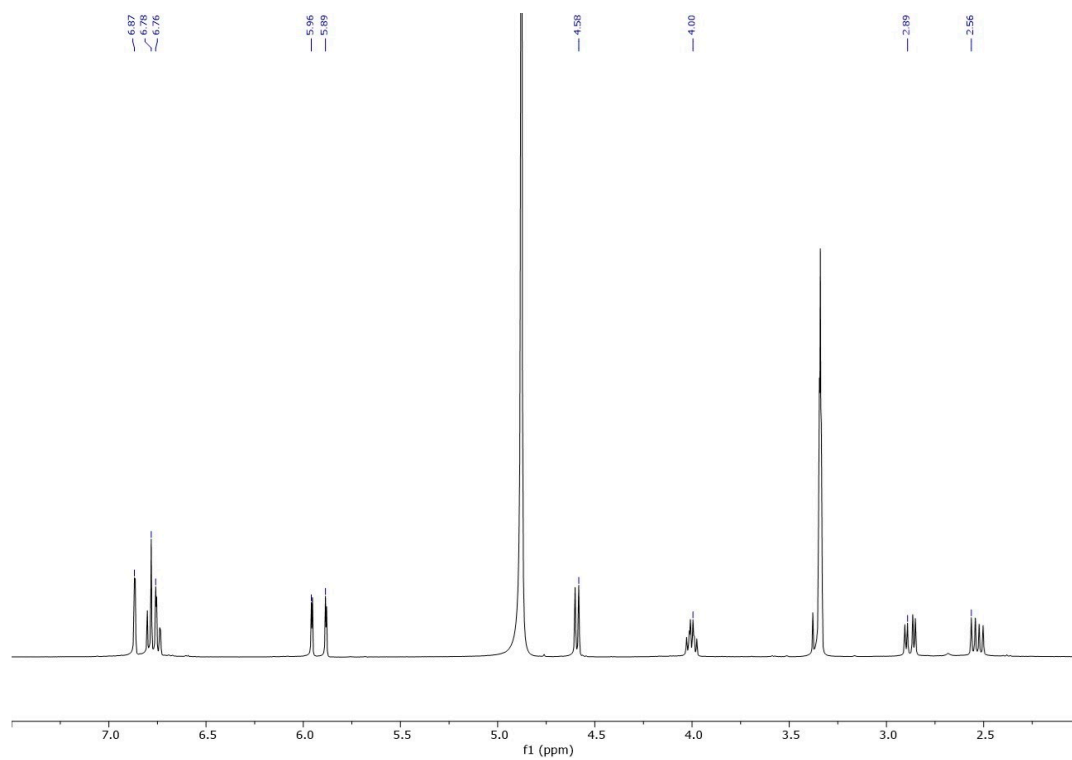


Figure S8. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **7**.

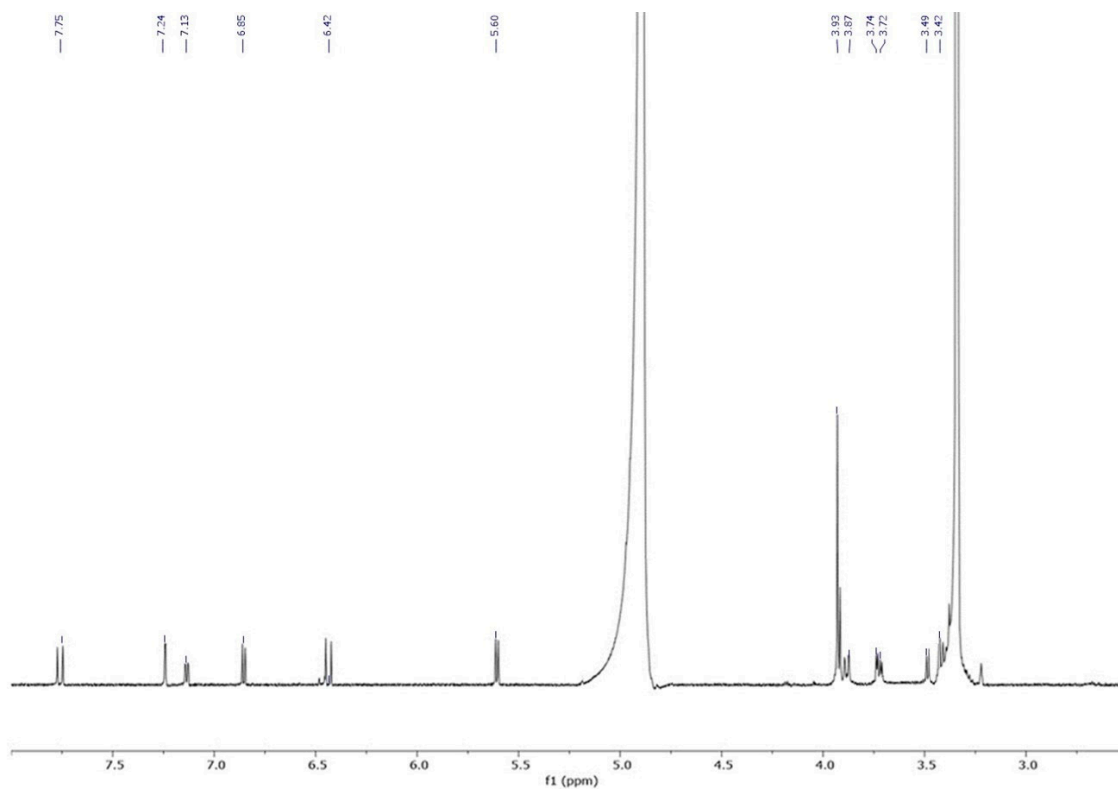


Figure S9. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **8**.

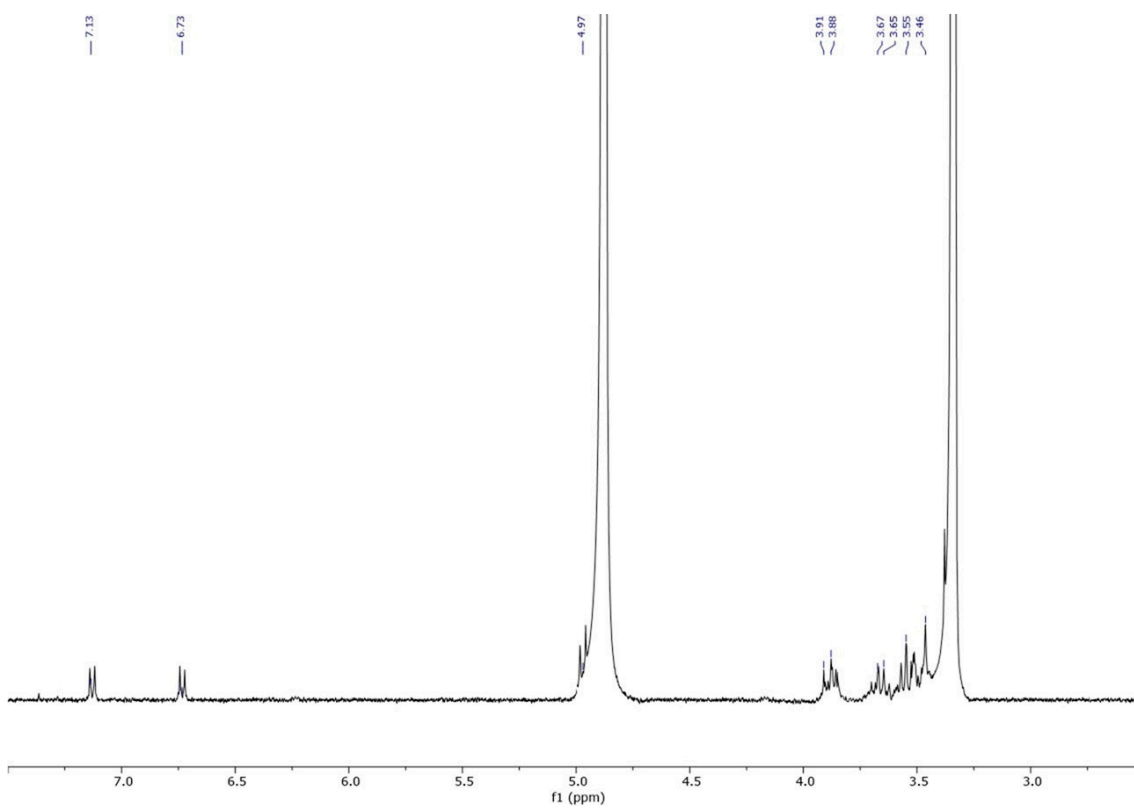


Figure S10. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **9**.

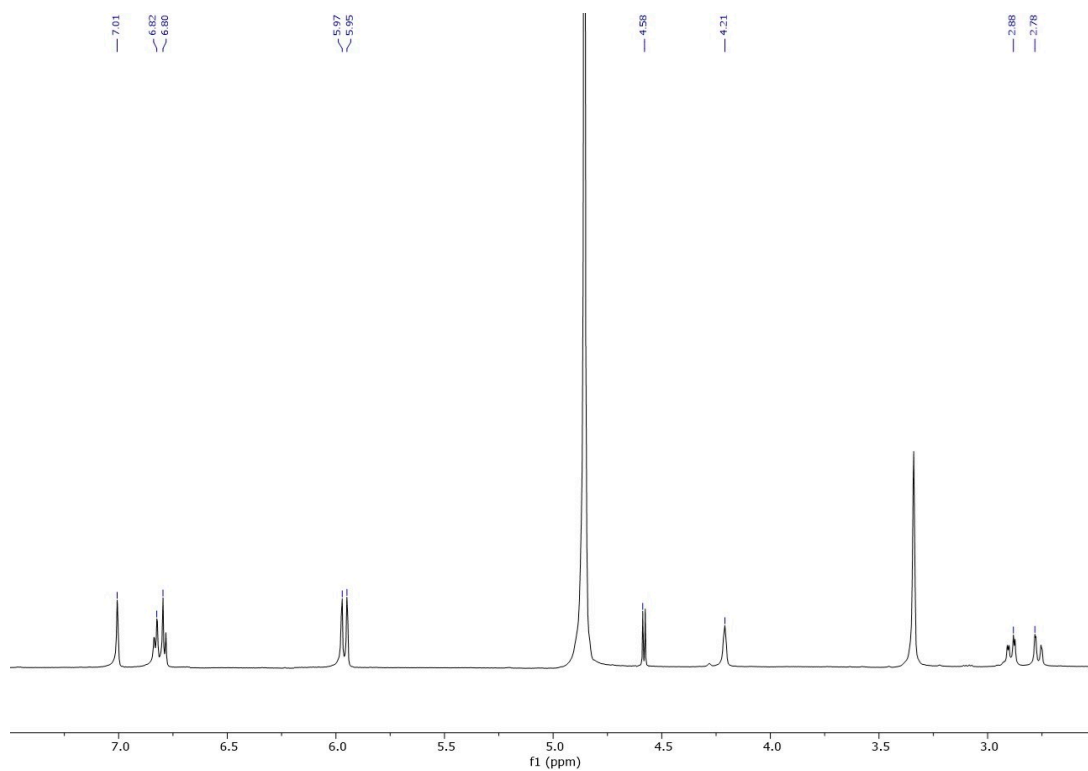


Figure S11. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **10**.

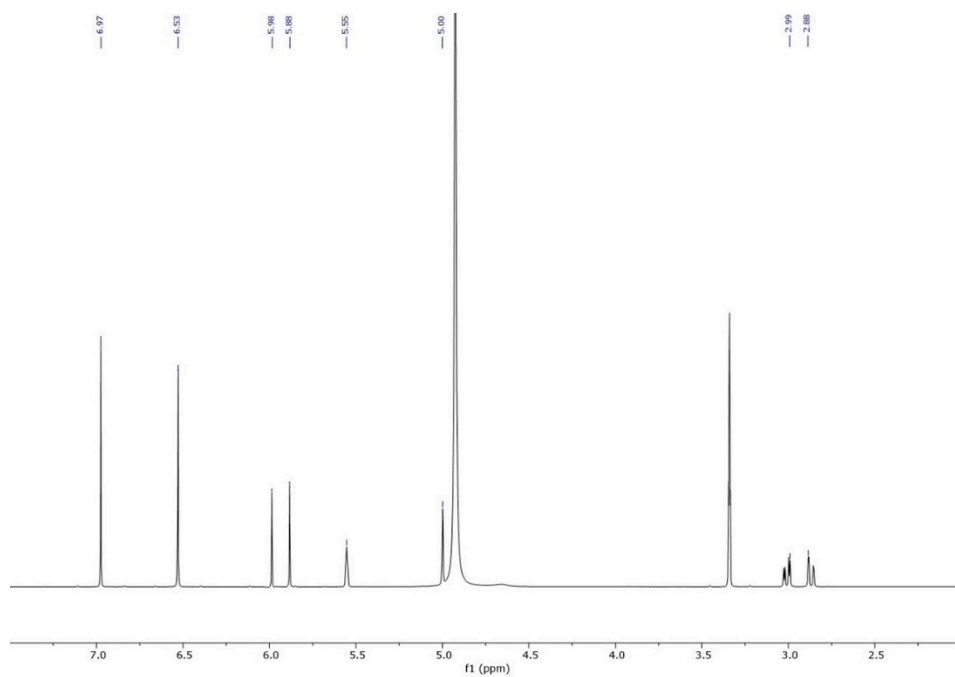


Figure S12. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **11**.

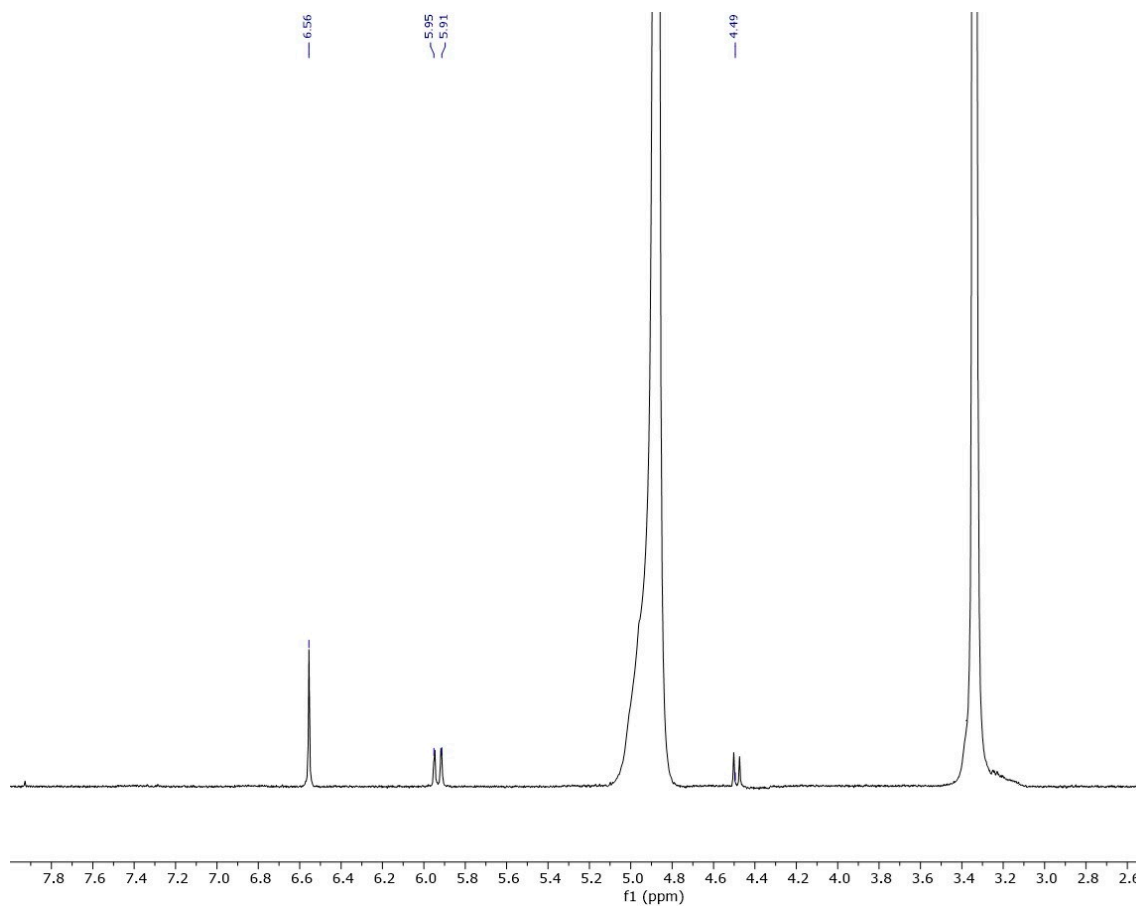


Figure S13. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **12**.

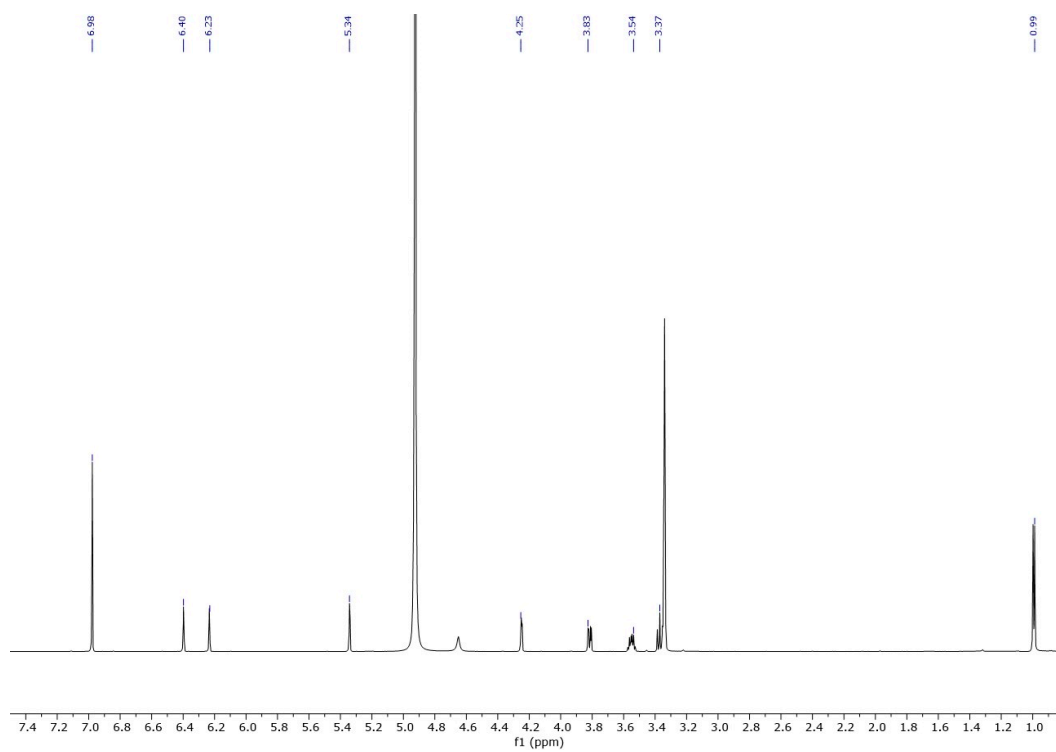


Figure S14. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **13**.

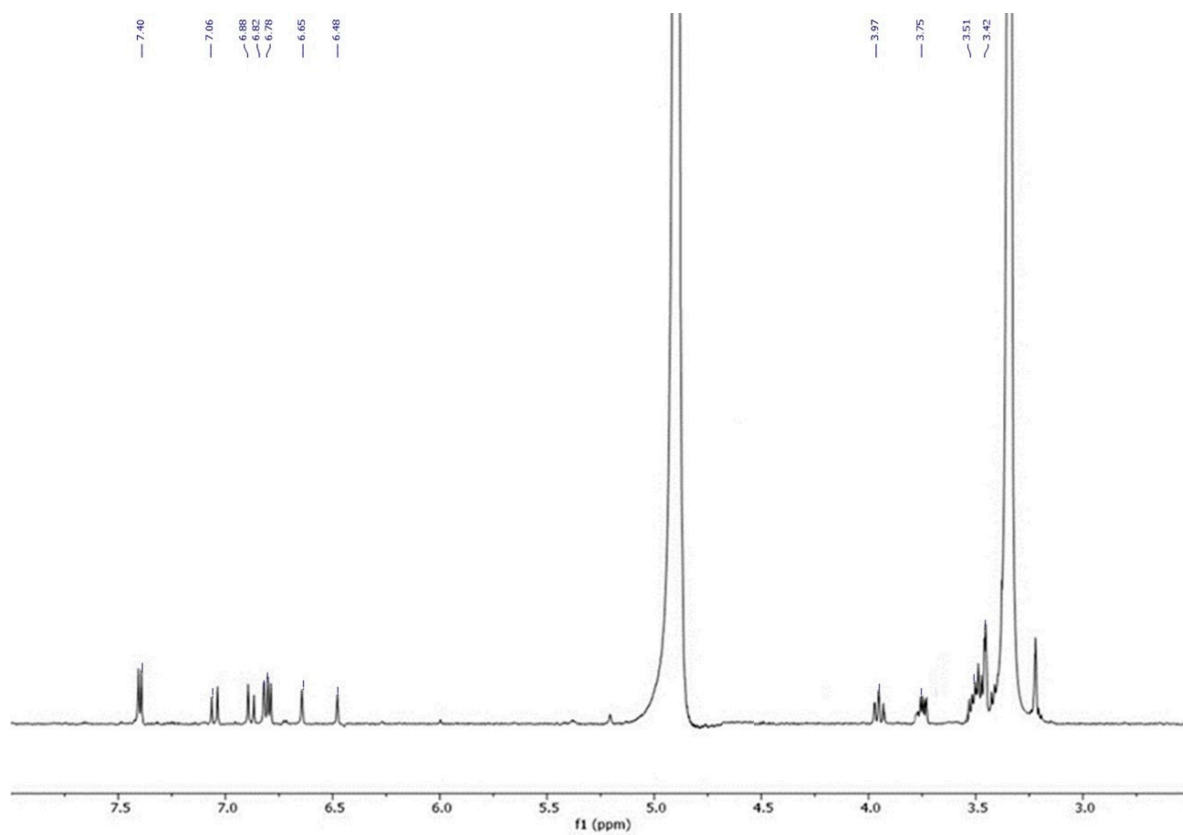


Figure S15. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **14**.

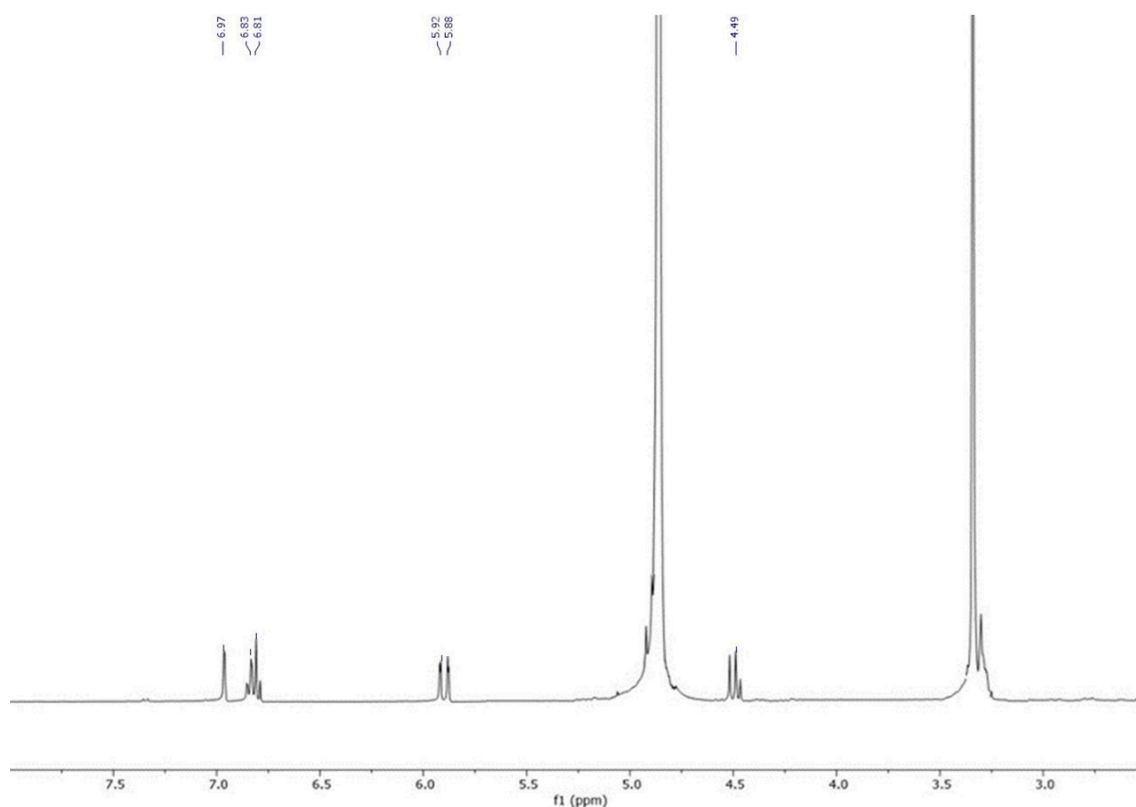


Figure S16. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **15**.

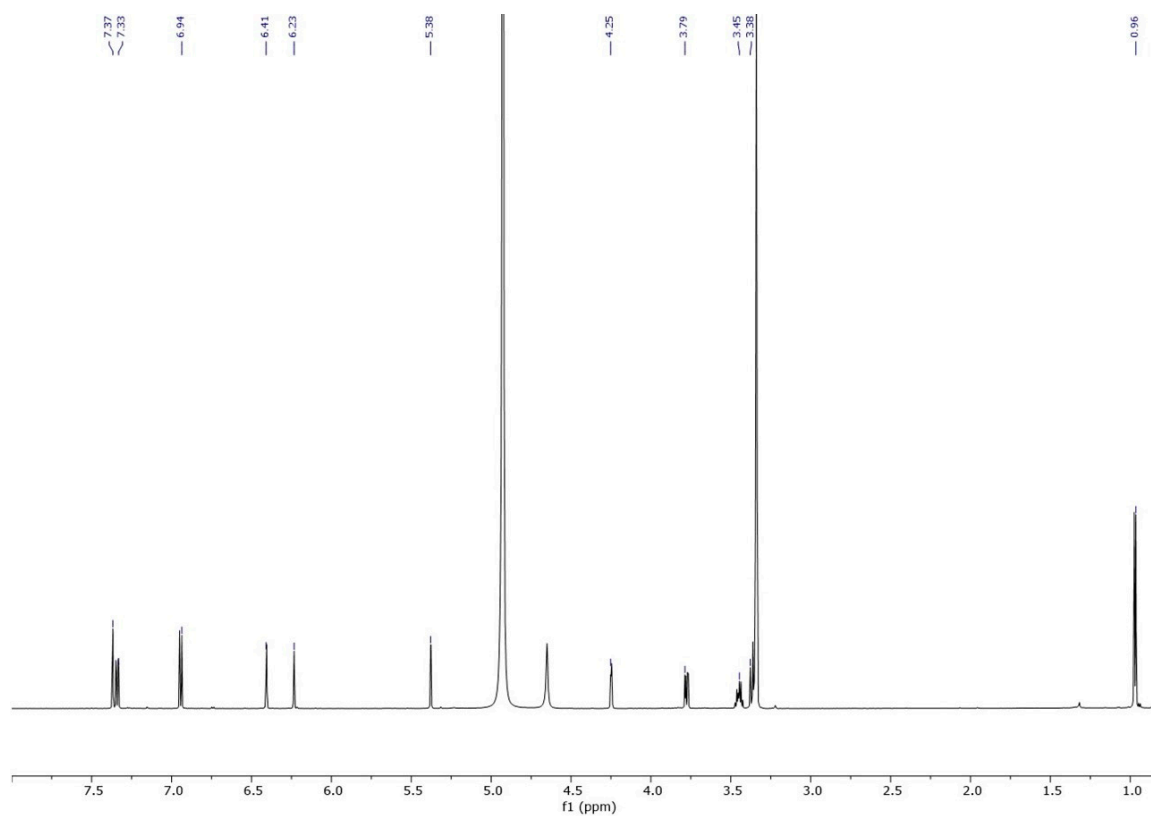


Figure S17. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **16**.

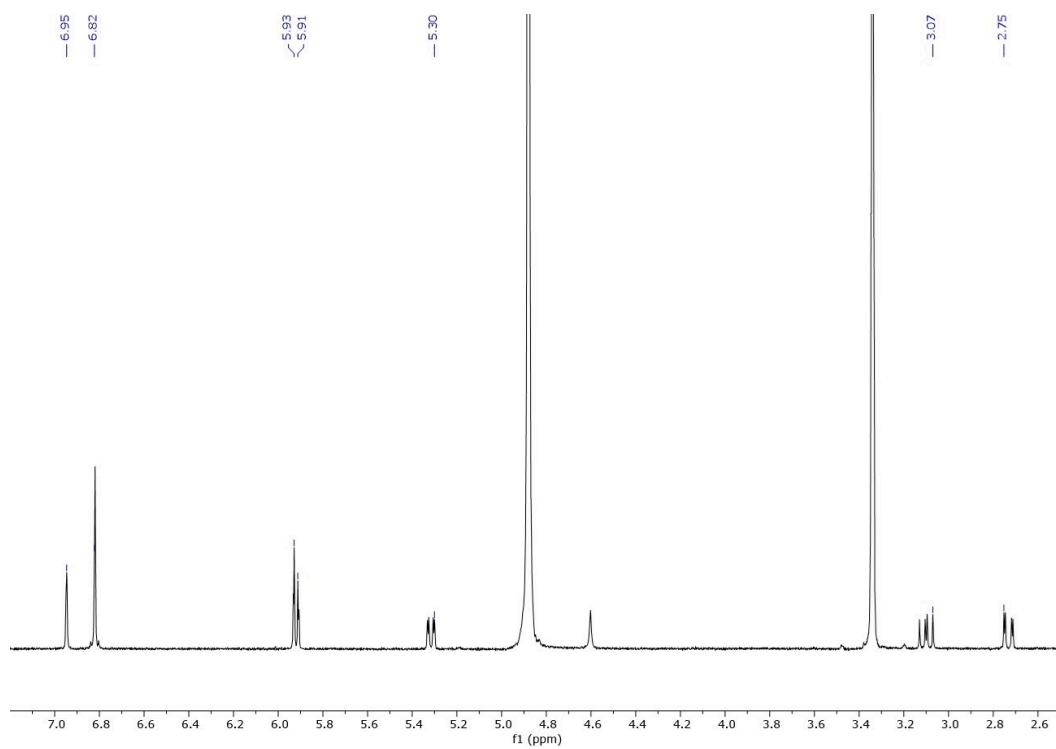


Figure S18. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **17**.

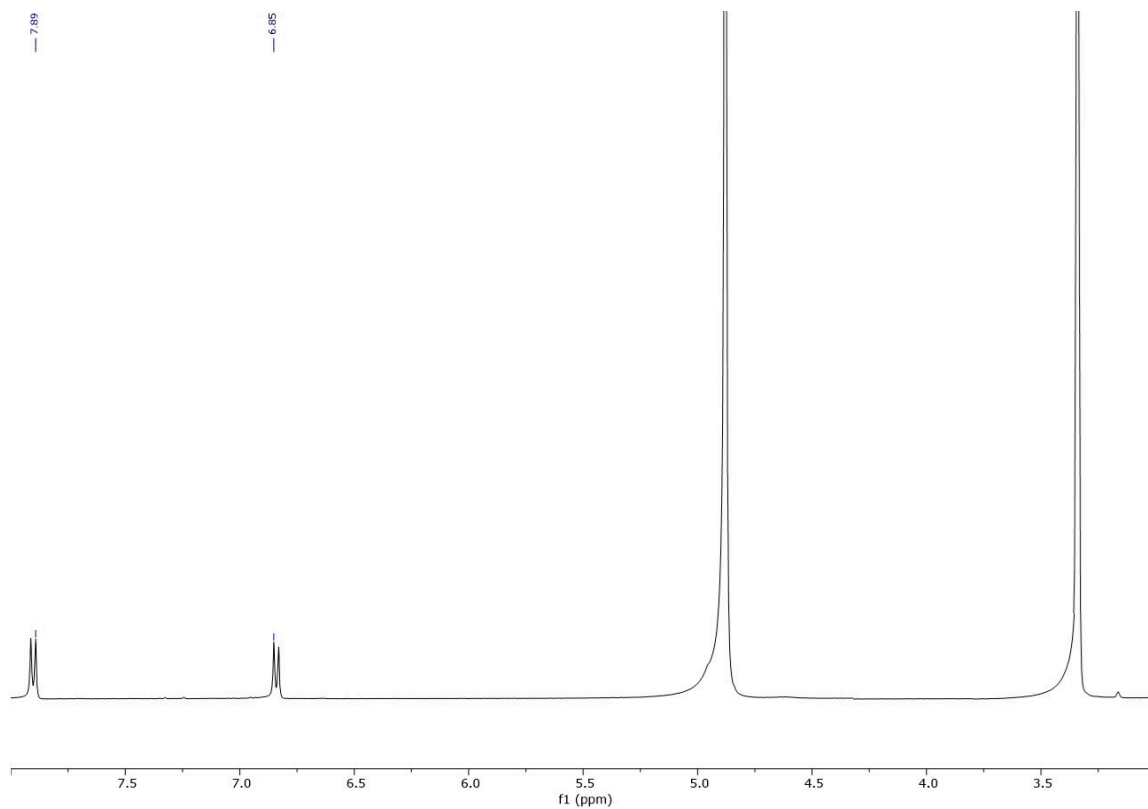


Figure S19. ¹H NMR Spectrum (600 MHz, CD₃OD) of compound **18**.

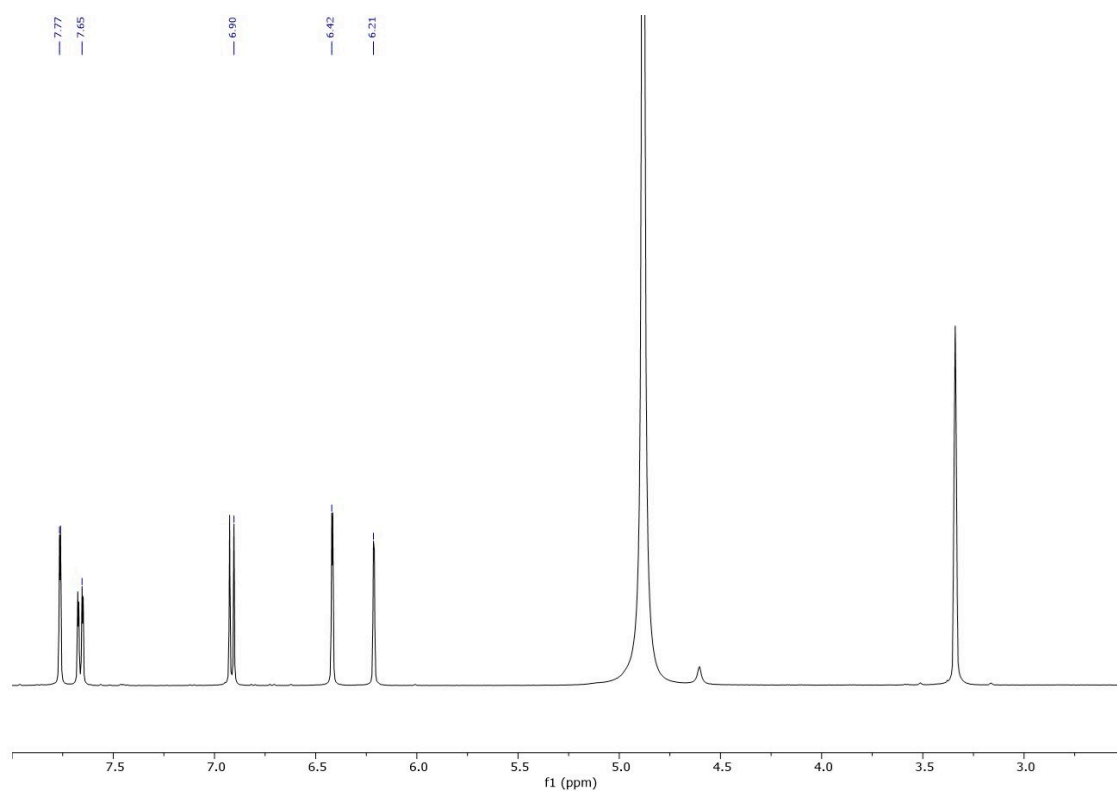


Figure S20. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **19**.

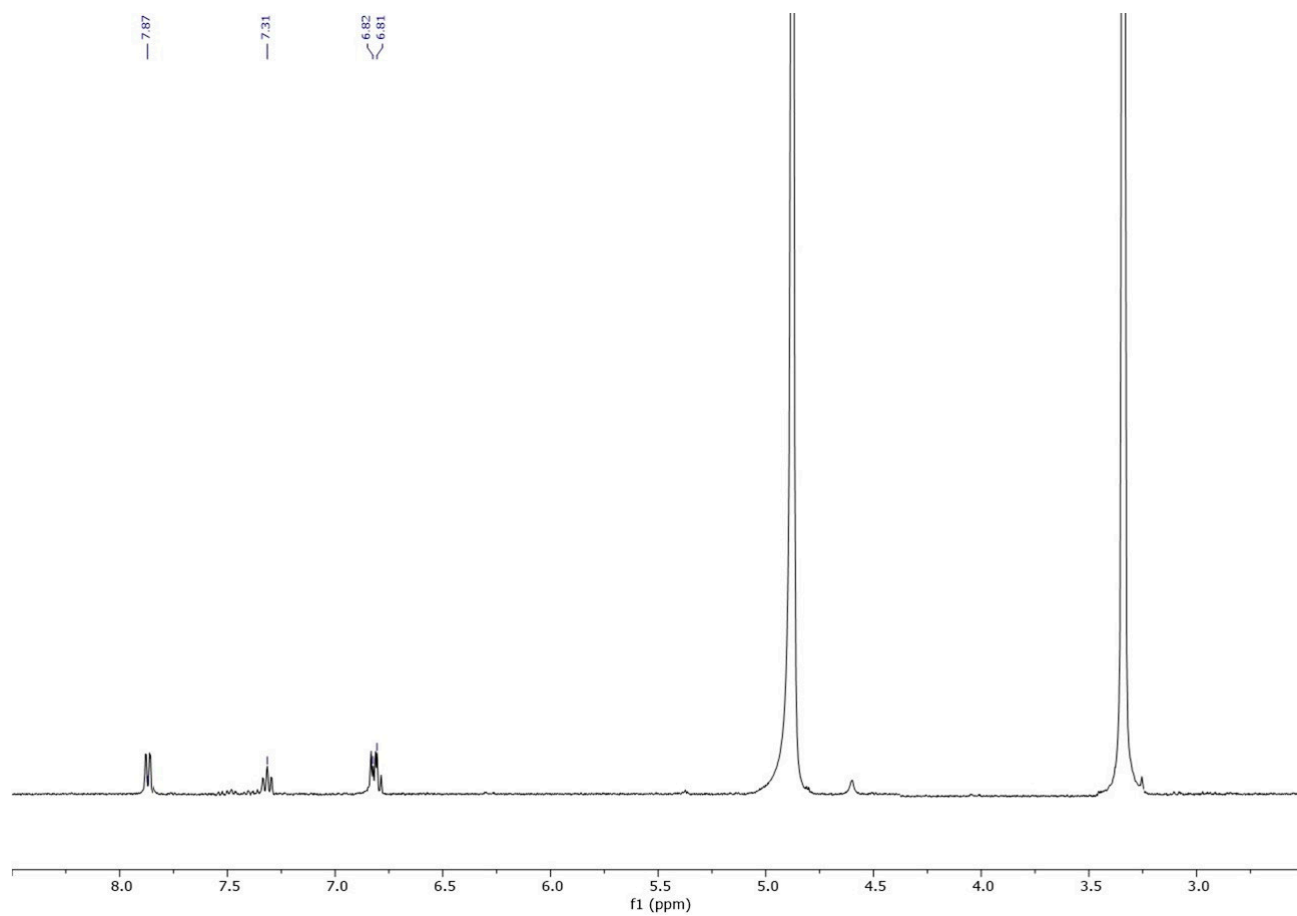


Figure S21. ^1H NMR Spectrum (600 MHz, CD_3OD) of compound **20**.