Antimicrobial, antioxidant and antiproliferative secondary metabolites from *Inonotus nidus-pici*

Zsófia Garádi[1,2], Miklós Dékány [3], Ágnes M. Móricz[4], Anikó Gaál[5], Viktor Papp[6], Szabolcs Béni[1], and Attila Ványolós[1,*]

[1] *Department of Pharmacognosy, Semmelweis University, Üllői u. 26, H-1085 Budapest, Hungary; garadi.zsofia@pharma.semmelweis-univ.hu, beni.szabolcs@pharma.semmelweis-univ.hu,*
[2] *Directorate of Drug Substance Development, Egis Pharmaceuticals Plc, P. O. Box 100, H-1475 Budapest, Hungary;*
[3] *Spectroscopic Research, Gedeon Richter Plc., Gyömrői út 19-21, H-1103 Budapest, Hungary; m.dekany@richter.hu*
[4] *Plant Protection Institute, Centre for Agricultural Research, ELKH, 1022 Budapest, Herman Ottó út 15, Hungary; moricz.agnes@atk.hu*
[5] *Biological Nanochemistry Research Group, Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Magyar Tudósok Körútja 2, H-1117 Budapest, Hungary, gaal.aniko@ttk.hu*
[6] *Department of Botany, Hungarian University of Agriculture and Life Sciences, H-1118 Budapest, Villányi út 29-43, Hungary; papp.viktor@uni-mate.hu*

*Correspondence: vanyolosa@pharmacognosy.hu

Table of contents

NMR and MS spectra and spectral data of compound **1**

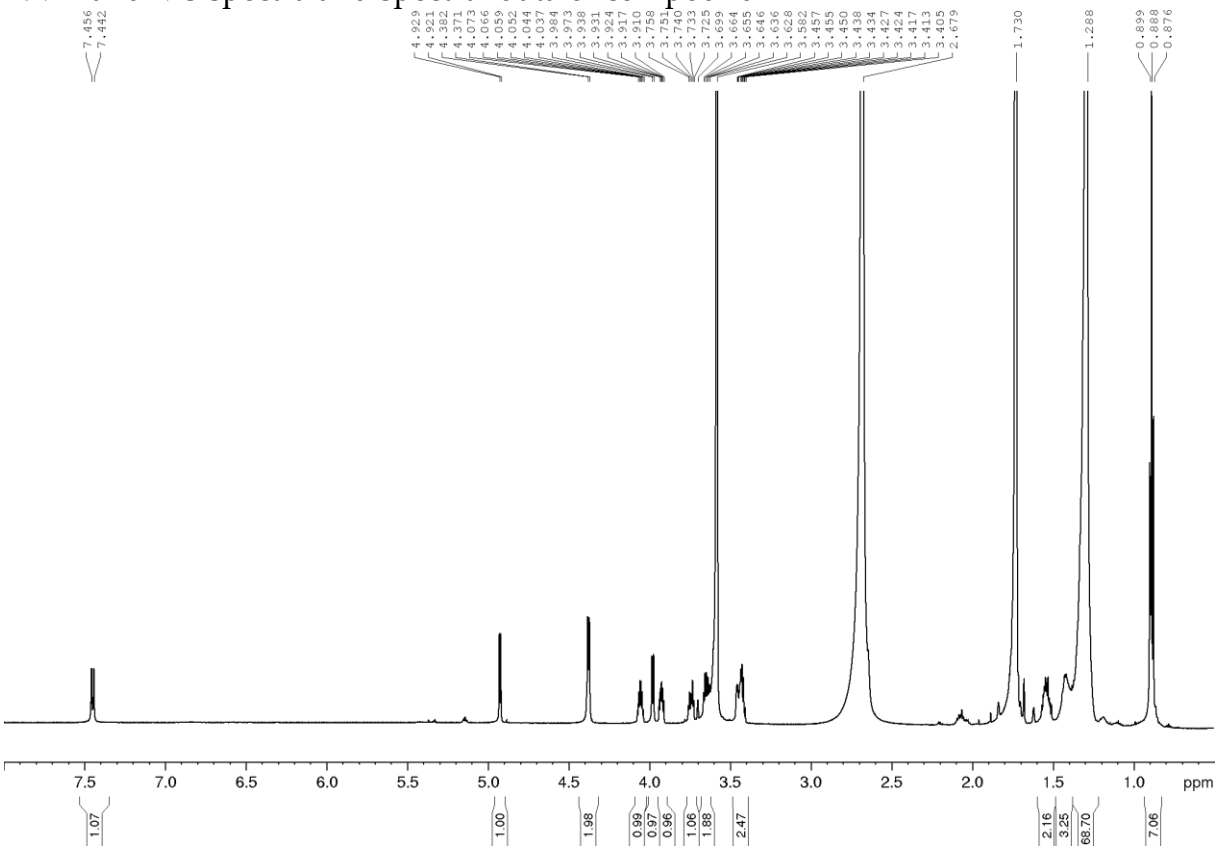

Figure S1. ^{1}H NMR spectrum of compound **1** (THF-d_8)

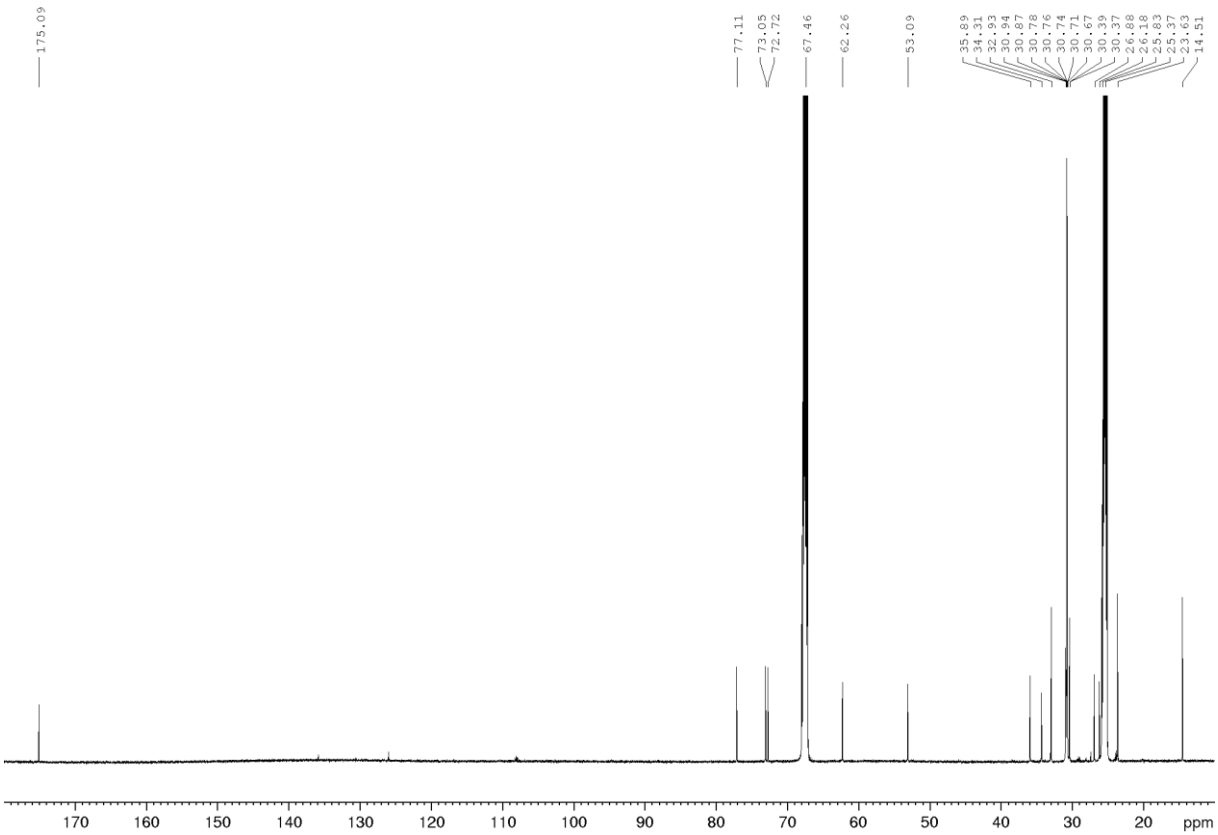

Figure S2. ^{13}C spectrum of compound **1** (THF-d_8)

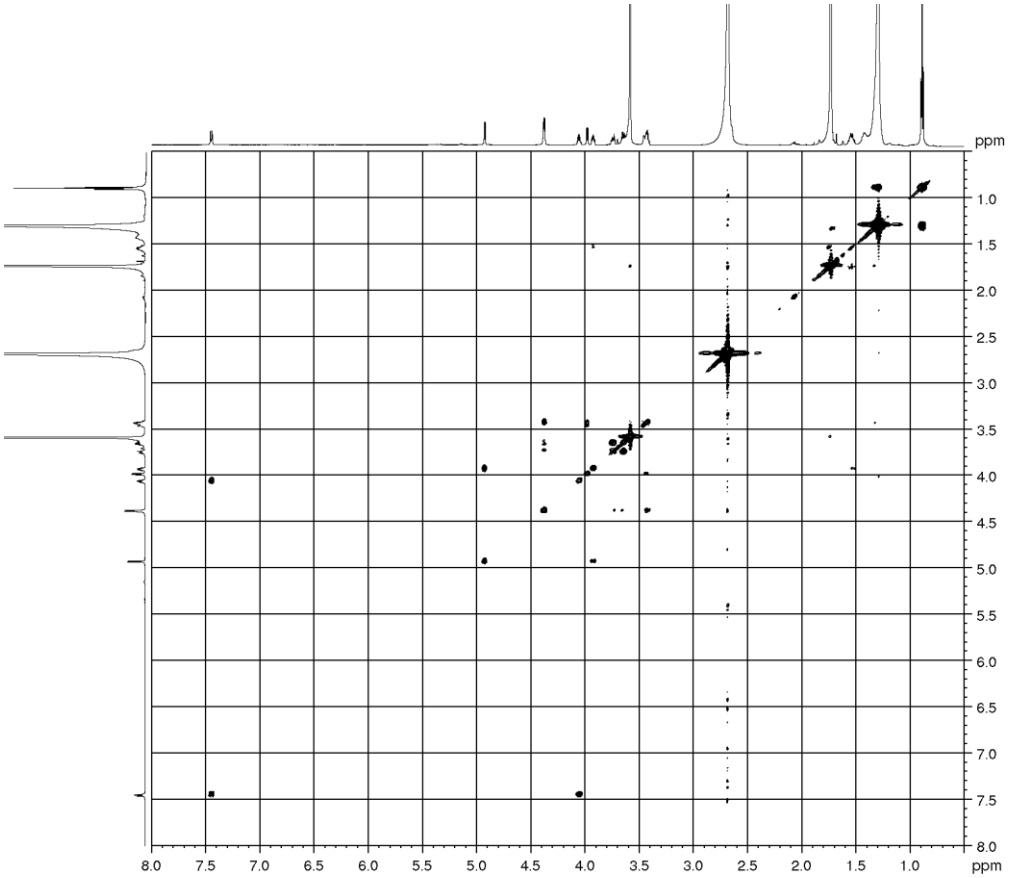

Figure S3. COSY spectrum of compound **1** (THF-d_8)

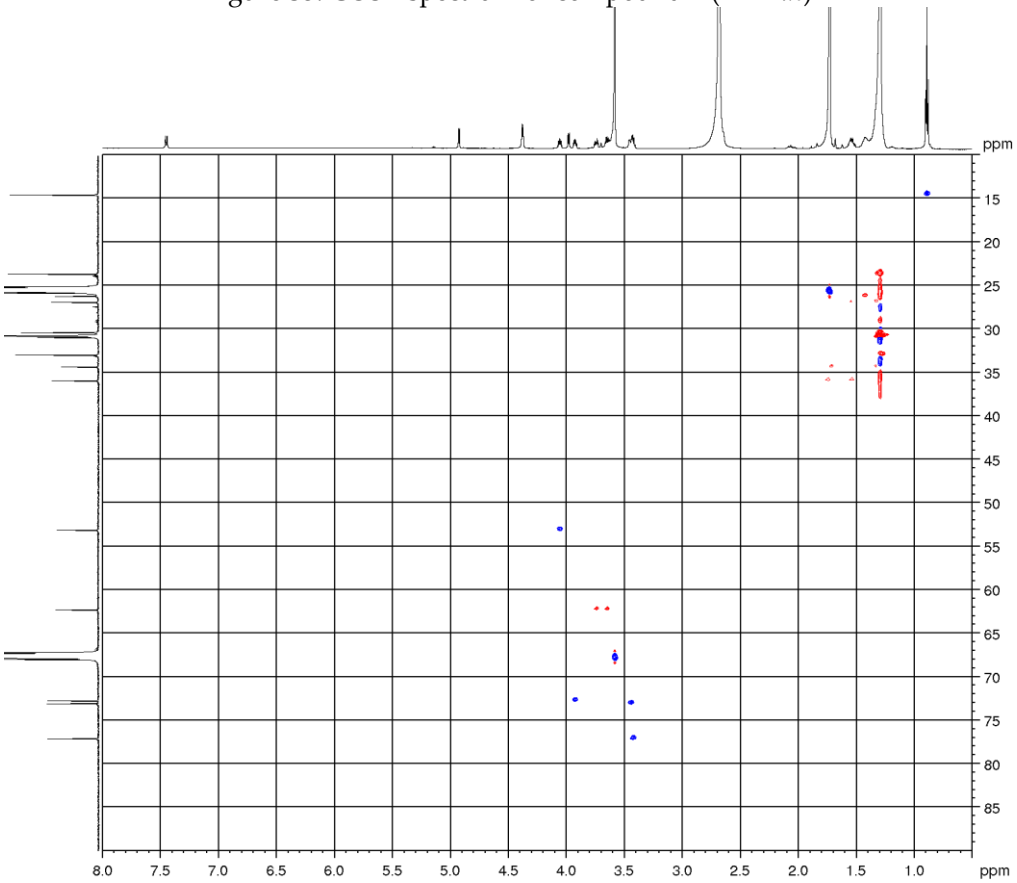

Figure S4. HSQC spectrum of compound **1** (THF-d_8)

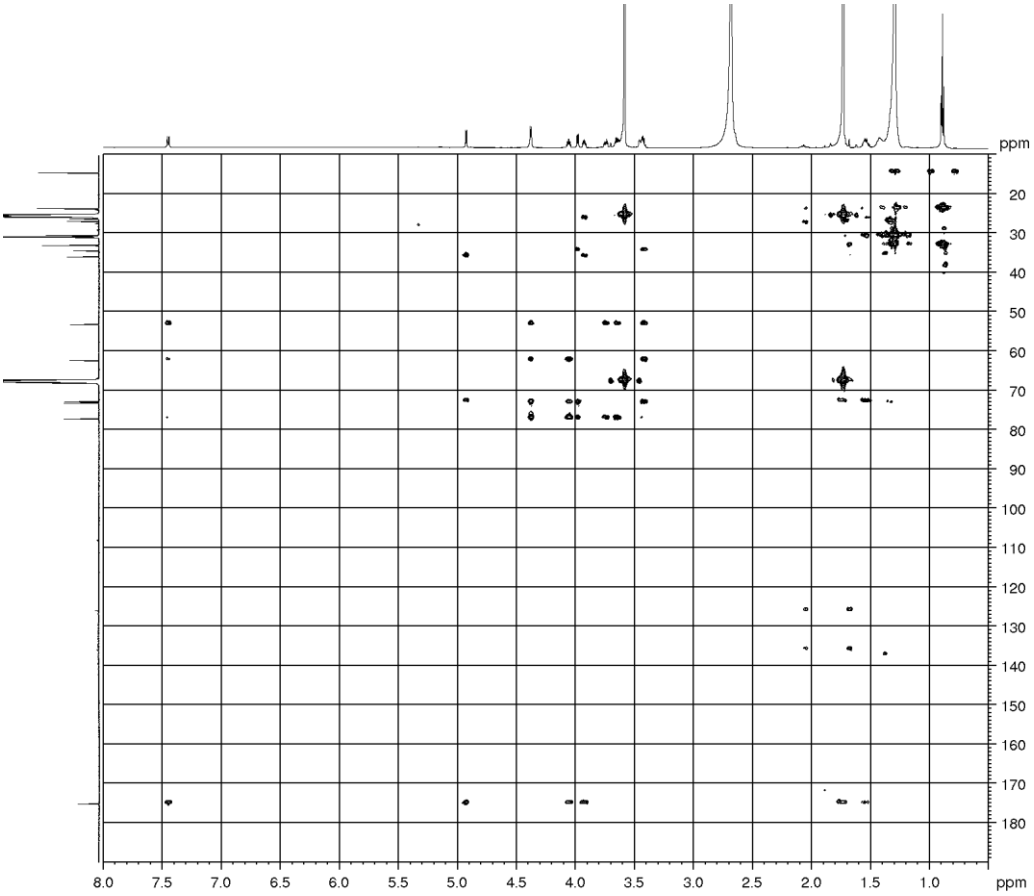

Figure S5. HMBC spectrum of compound **1** (THF-d_8)

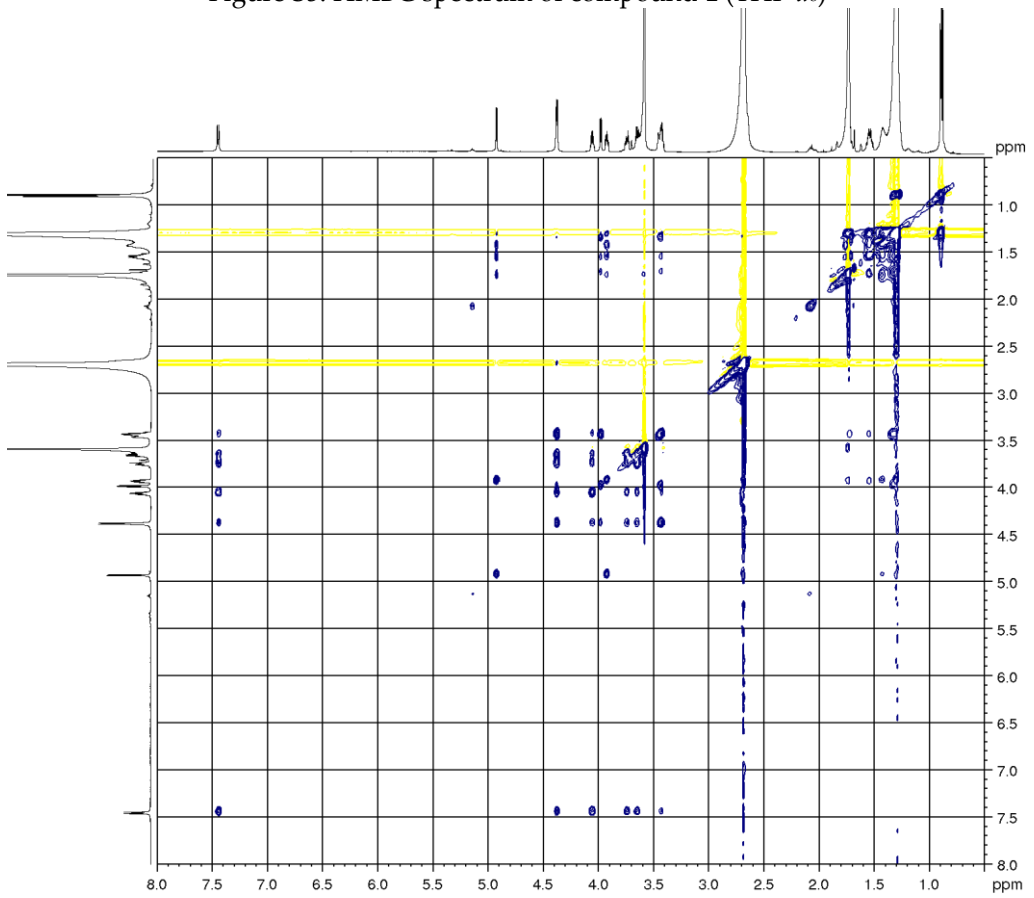

Figure S6. TOCSY spectrum of compound **1** (THF-d_8)

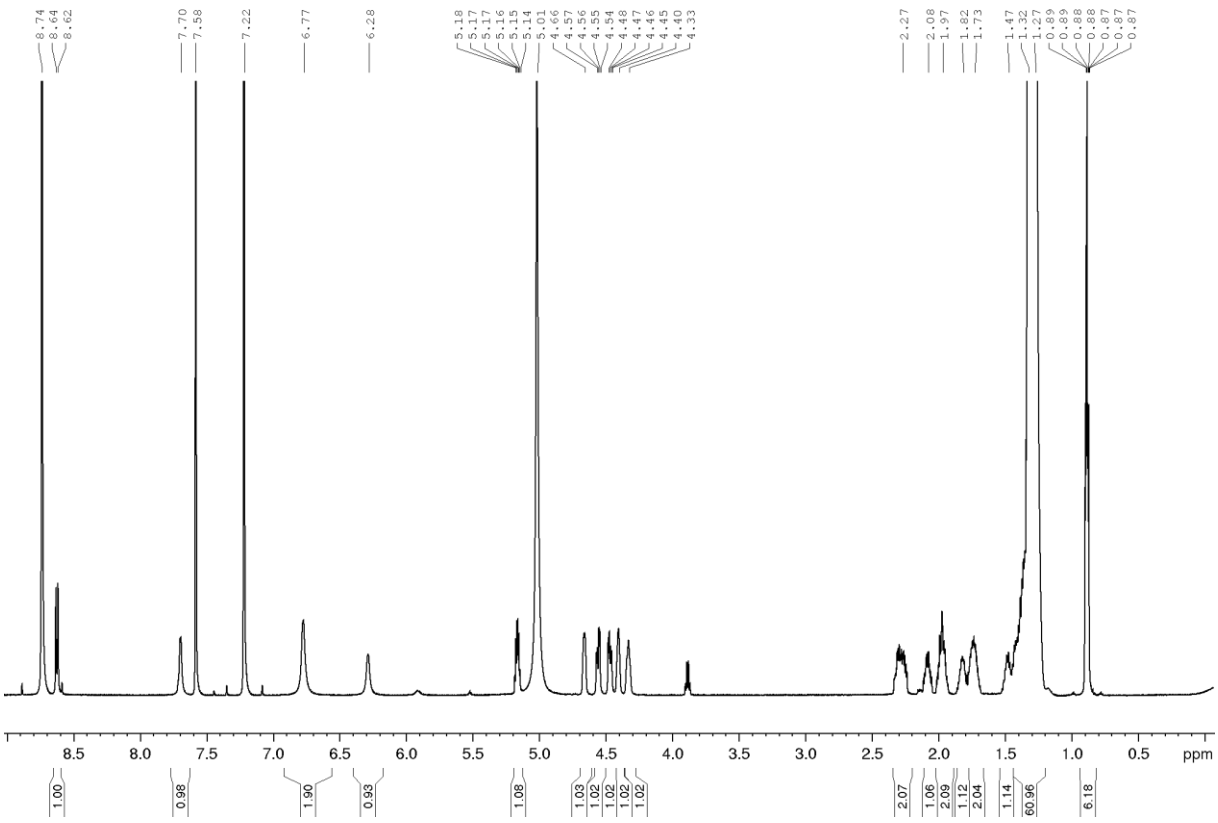

Figure S7. ^{1}H NMR spectrum of compound **1** (pyridine-d_5)

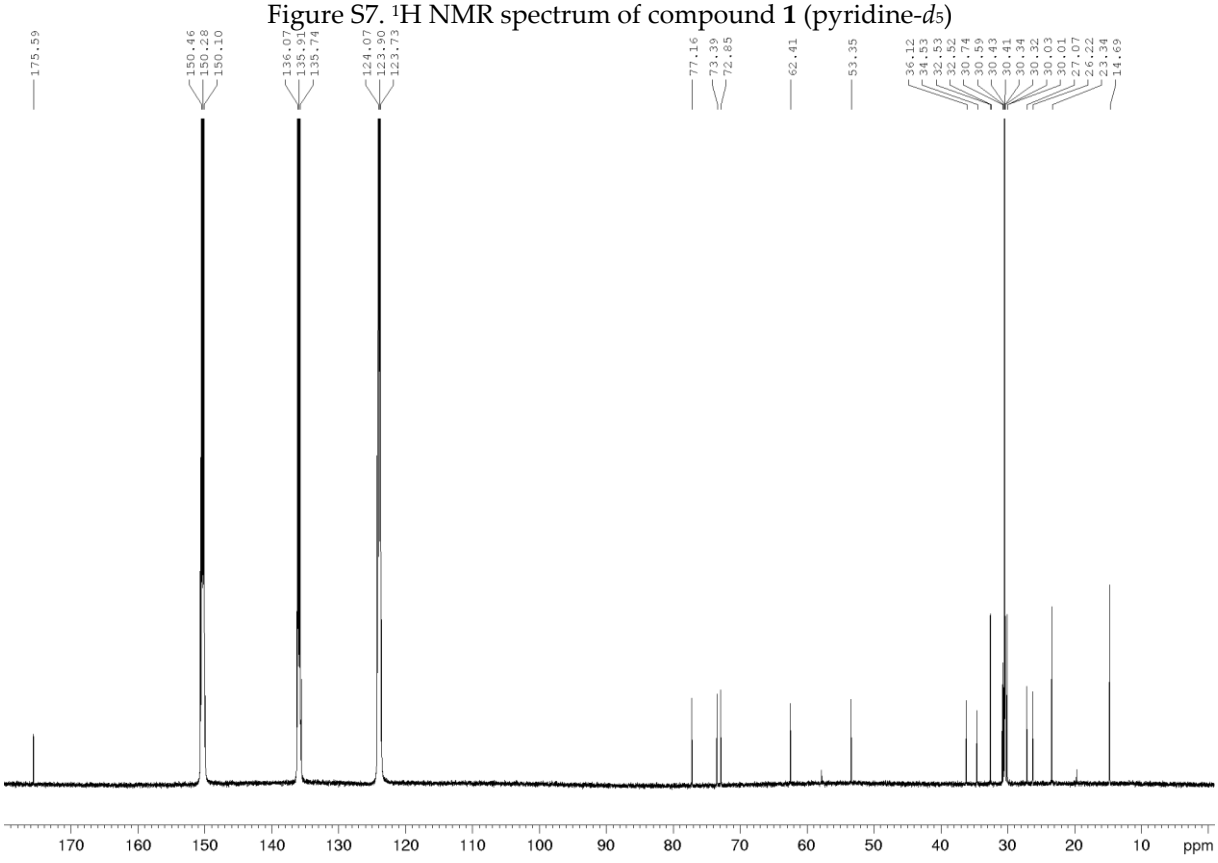

Figure S8. ^{13}C NMR spectrum of compound **1** (pyridine-d_5)

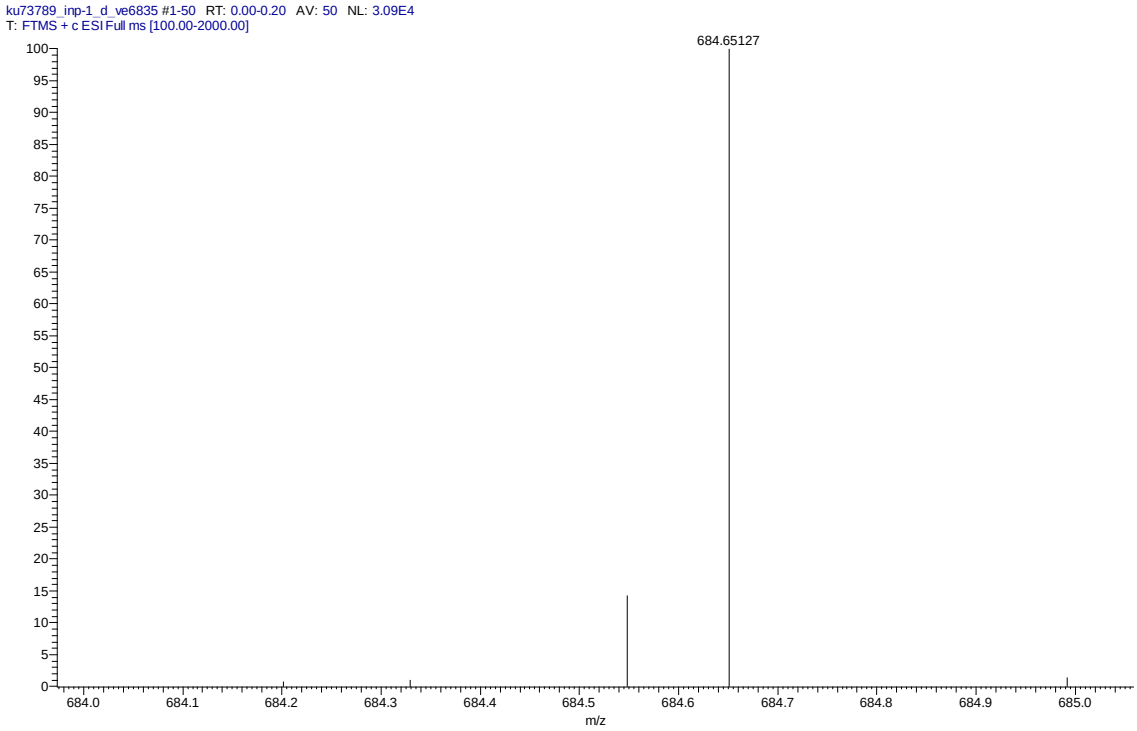

Figure S9. HRMS spectrum of compound **1**

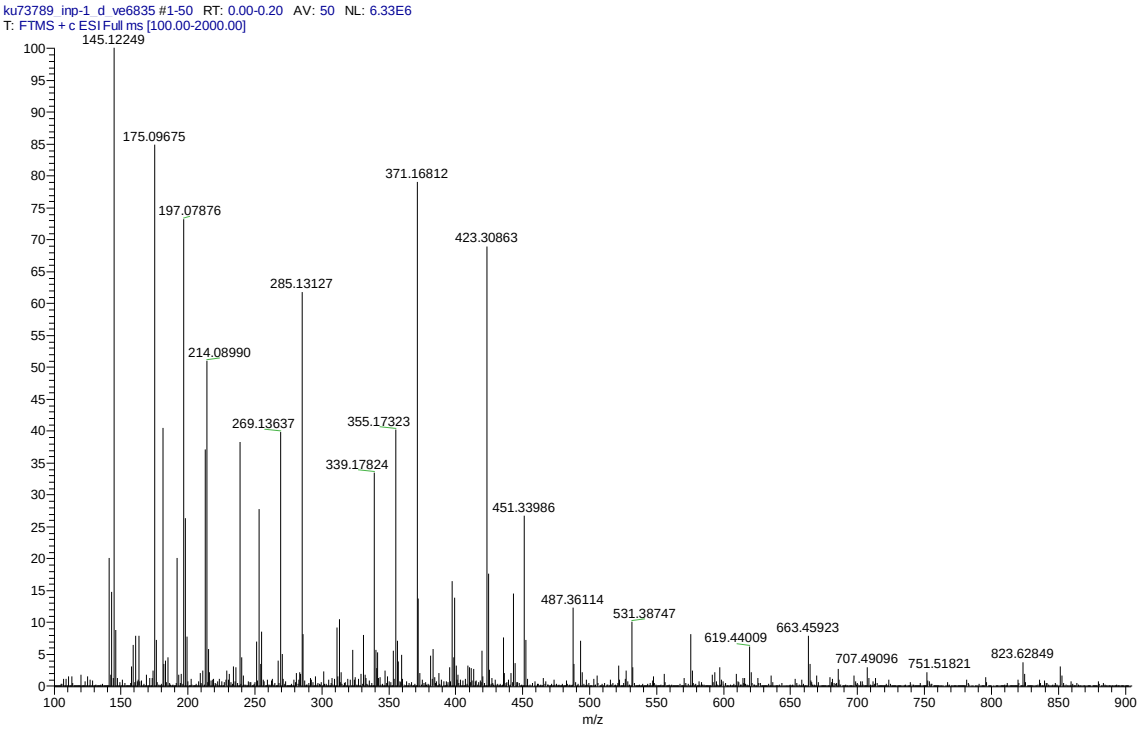

Figure S10. Full HRMS spectrum of compound **1**

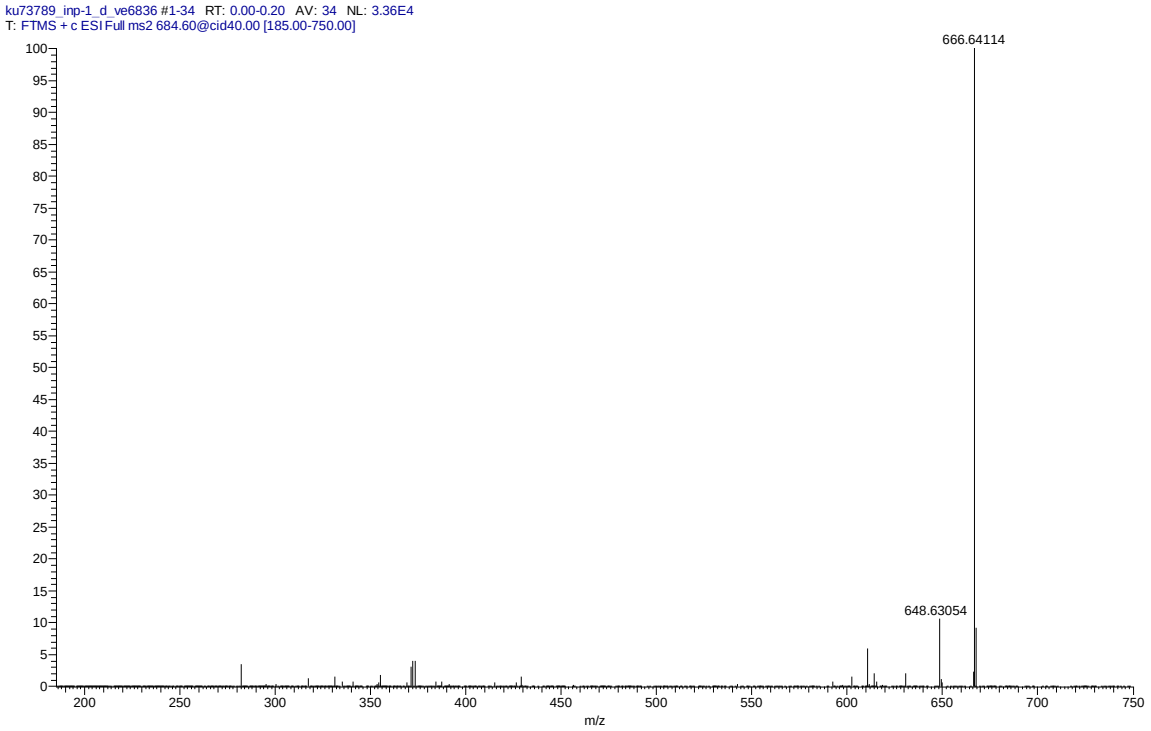

Figure S11. HR-MS/MS spectrum of compound **1**

HRMS: M+H=684.65127 (delta=1.8 ppm; $C_{42}H_{86}O_5N$). HR-ESI-MS-MS (CID=40%; rel. int. %): 666(100); 648(11); 300(<1); 282(3).

666.64114	666.63949	2.48	1.5	C42 H84 O4 N
648.63054	648.62892	2.49	2.5	C42 H82 O3 N
300.29071	300.28971	3.34	0.5	C18 H38 O2 N
282.28014	282.27914	3.54	1.5	C18 H36 O N

Table S1. HRMS spectral data of compound **1**

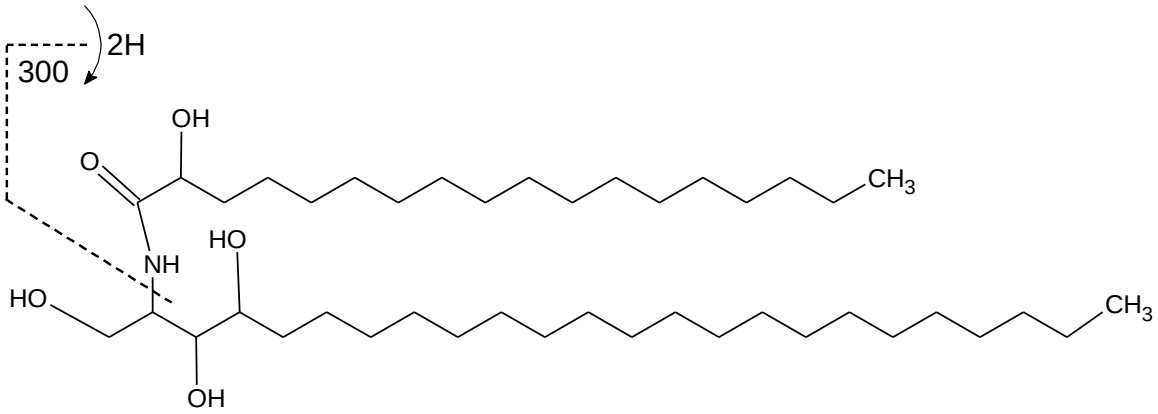

Figure S12. Mass fragmentation of compound **1**

NMR spectra and spectral data of compound **2**

No.	**Compound 2**		
	δ ^{13}C	**δ ^{1}H**	**multiplicity**
1	127.7	-	-
2	115.3	7.08	d (*J*=1.6 Hz)
3	146.9	-	-
4	150.0	-	-
5	116.5	6.80	d (*J*=8.2 Hz)
6	123.5	7.00	dd (*J*=8.2, 1.6 Hz)
7	146.9	7.52	d (*J*=16.2 Hz)
8	124.7	6.54	d (*J*=16.2 Hz)
9	201.6	-	-
10	27.0	2.33	s

Table S2. Complete ^{1}H and ^{13}C NMR resosnance assignments for compound **2** (methanol-d_4)

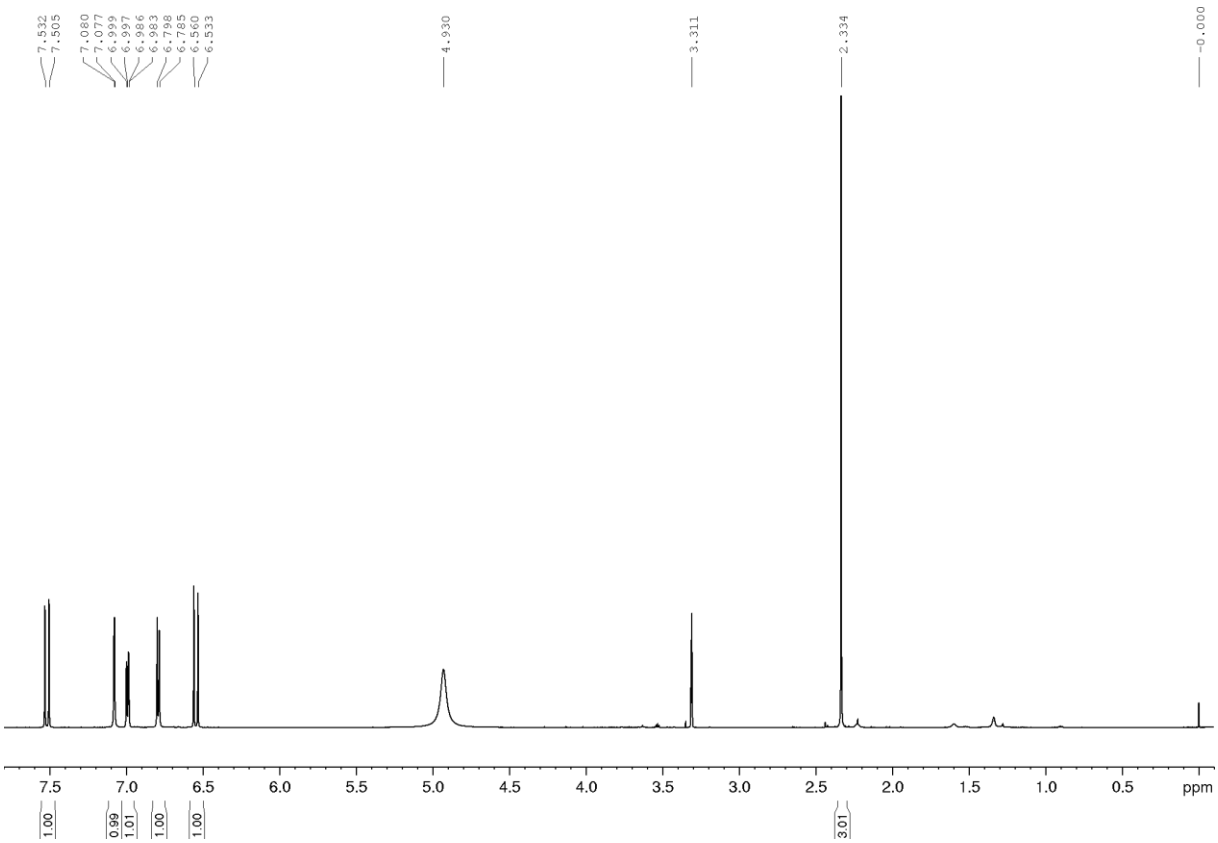

Figure S13.[1]H NMR spectrum of compound **2** (methanol-d_4)

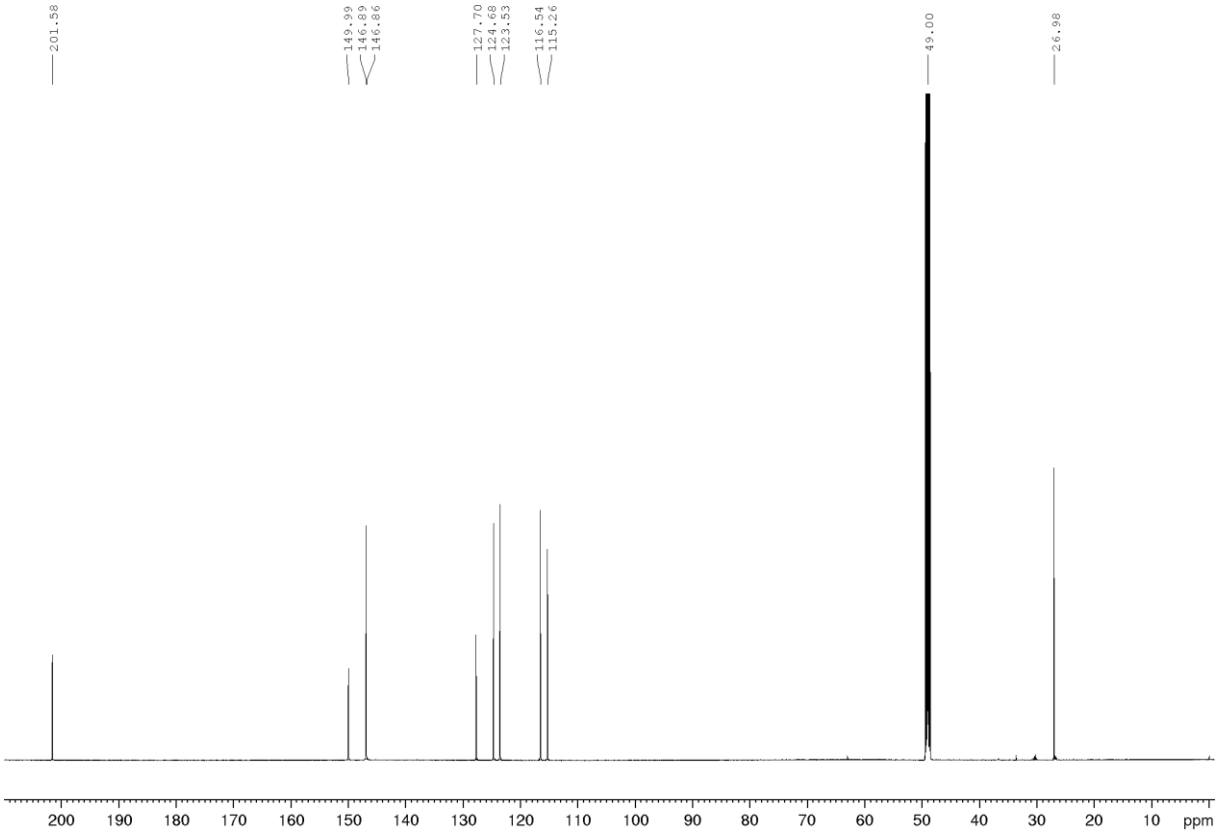

Figure S14.[13]C NMR spectrum of compound **2** (methanol-d_4)

NMR spectra and spectral data of compound **3, 4 and 5**

No.	Compound 3			Compound 4			Compound 5		
	δ ^{13}C	**δ ^{1}H**	**multiplicity**	**δ ^{13}C**	**δ ^{1}H**	**multiplicity**	**δ ^{13}C**	**δ ^{1}H**	**multiplicity**
1	35.6	1.73 1.23	m m	38.3	1.89 1.31	m m	34.6	1.95 1.70	m m
2	27.8	1.66 1.59	m m	32.0	1.88 1.50	m m	30.1	1.84 1.54	m m
3	79.0	3.24	dd, *J*=11.7, 4.4 Hz	70.4	3.64	m	66.5	3.97	m
4	38.9	-	-	40.8	2.47 2.29	m m	36.9	2.11 1.91	m m
5	50.4	1.05	m	46.2	1.97	m	82.1	-	-
6	18.2	1.68 1.51	m m	119.6	5.57	dd, *J*=5.8, 2.5 Hz	135.4	6.24	d, *J*=8.5 Hz
7	26.5	2.04	m	116.3	5.39	m	130.7	6.51	d, *J*=8.5 Hz
8	134.4	-	-	141.4	-	-	79.4	-	-
9	134.4	-	-	139.8	-	-	51.0	1.50	m
10	37.0	-	-	37.0	-	-	36.9	-	-
11	21.0	2.00	m	21.1	1.72 1.59	m m	23.4	1.51 1.23	m m
12	30.9	1.69	m	39.0	2.06 1.26	m m	39.3	1.95 1.23	m m
13	44.4	-	-	42.8	-	-	44.5	-	-
14	49.8	-	-	54.5	1.89	m	51.6	1.22	m
15	30.8	1.59	m	28.3	1.76	m	20.6	1.59	m

		1.17	m					1.41	m
16	28.2	1.92	m	23.0	1.66	m	28.6	1.75	m
		1.32	m		1.36	m		1.35	m
17	50.4	1.48	m	55.7	1.26	m	56.1	1.22	m
18	15.7	0.69	s	12.0	0.63	s	12.8	0.82	s
19	19.1	0.98	s	16.3	0.95	s	18.2	0.88	s
20	36.2	1.38		40.4	2.04	m	39.7	2.02	m
21	18.6	0.91	d, *J*=6.4 Hz	21.1	1.04	d, *J*=6.7 Hz	20.9	1.00	d, *J*=6.6 Hz
22	36.3	1.43	m	135.6	5.18	dd, *J*=15.3, 7.3 Hz	135.2	5.14	dd, *J*=15.5, 8.4 Hz
		1.04	m						
23	24.9	2.03	m	131.9	5.21	dd, *J*=15.3, 7.3 Hz	132.3	5.22	dd, *J*=15.5, 7.7 Hz
		1.86	m						
24	125.2	5.10	m	42.8	1.85	m	42.7	1.85	m
25	130.9	-	-	33.1	1.47	m	33.0	1.47	m
26	17.6	1.60	s	19.9	0.84	d, *J*=6.8 Hz	19.6	0.82	d, *J*=6.8 Hz
27	25.7	1.68	s	19.6	0.82	d, *J*=6.8 Hz	19.9	0.83	d, *J*=6.8 Hz
28	27.9	1.00	s	17.6	0.92	d, *J*=6.8 Hz	17.5	0.91	d, *J*=6.8 Hz
29	15.4	0.81	s						
30	24.2	0.87	s						

Table S3. Complete ^{1}H and ^{13}C NMR resosnance assignments for compounds **3, 4 and 5** ($CDCl_3$)

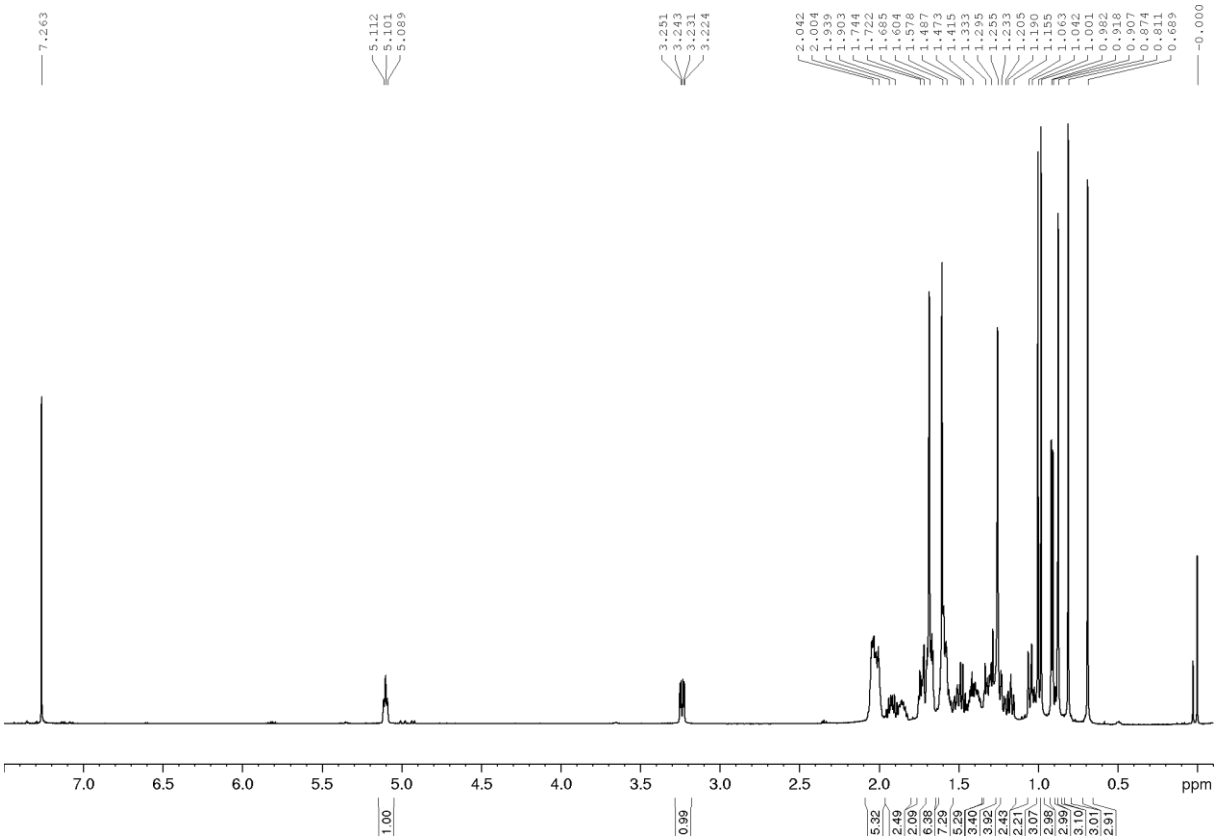

Figure S15.[1]H NMR spectrum of compound **3** ($CDCl_3$)

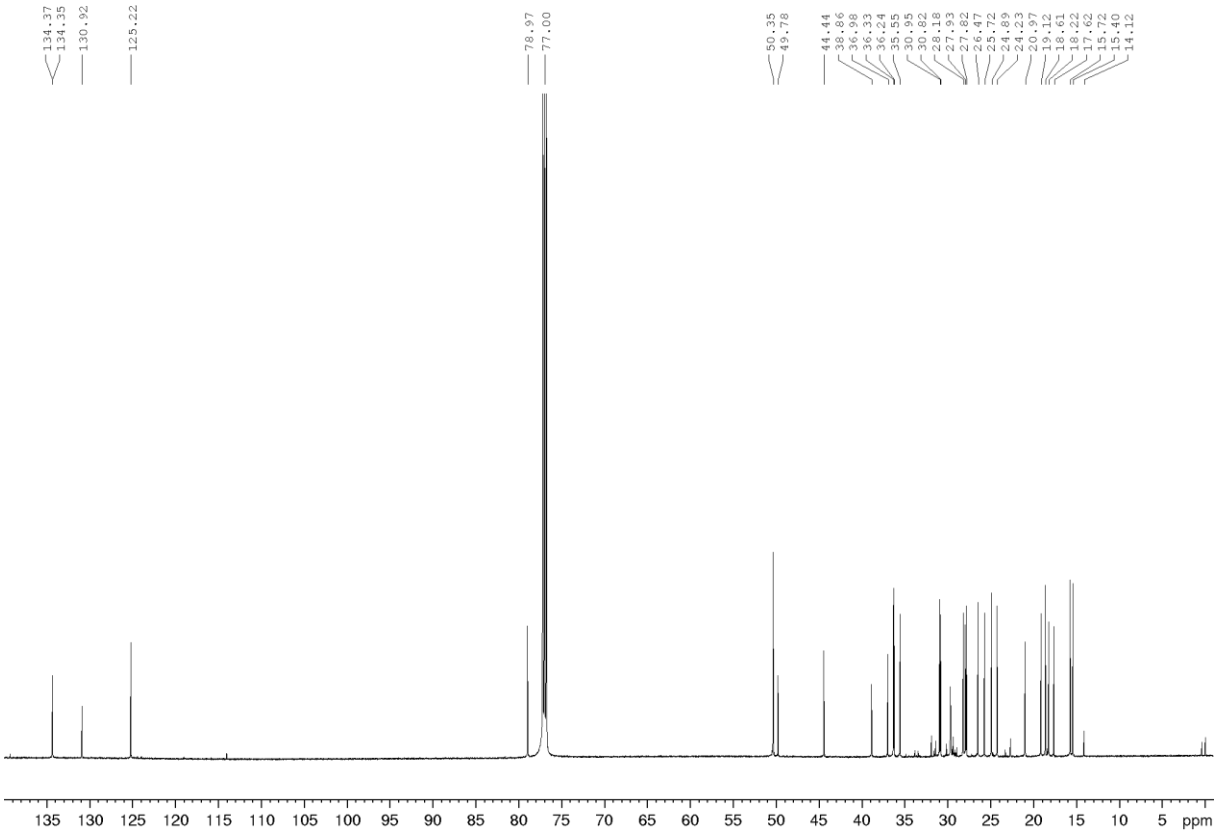

Figure S16.[13]C NMR spectrum of compound **3** ($CDCl_3$)

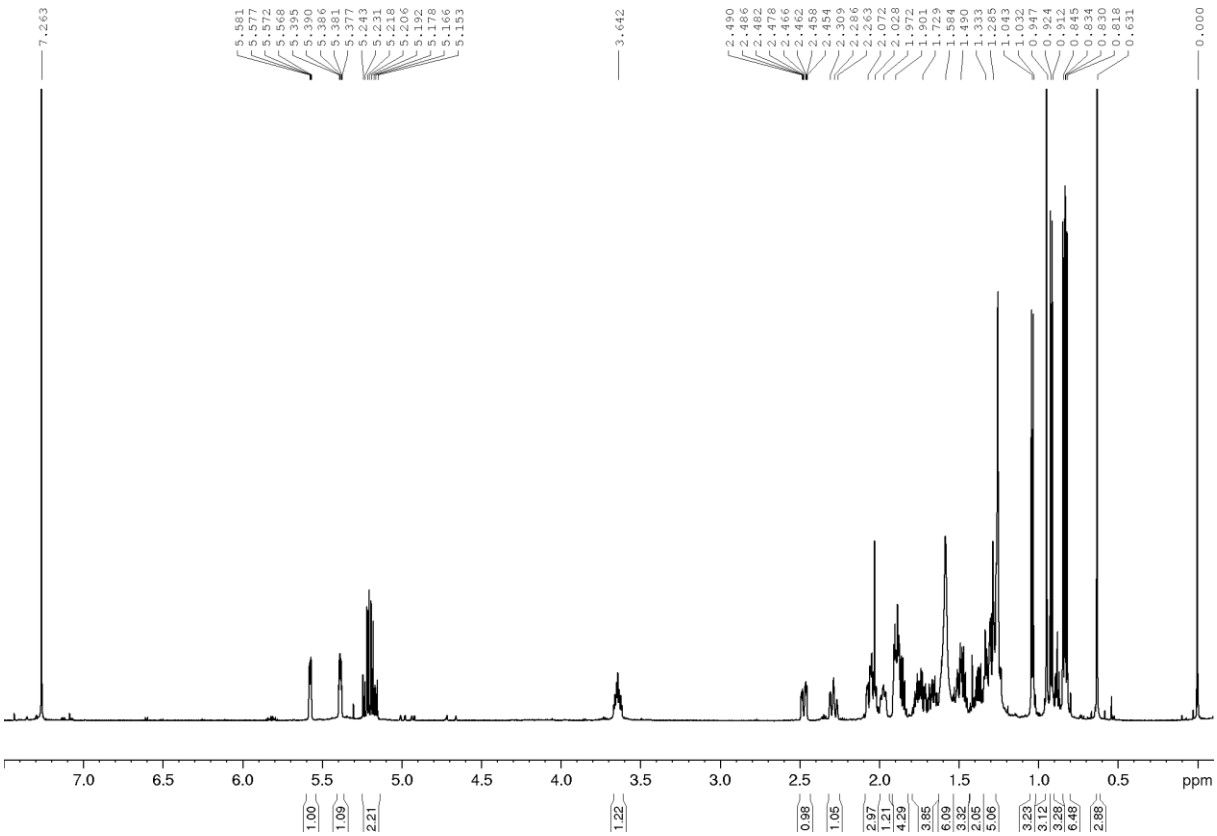

Figure S17.[1]H NMR spectrum of compound **4** ($CDCl_3$)

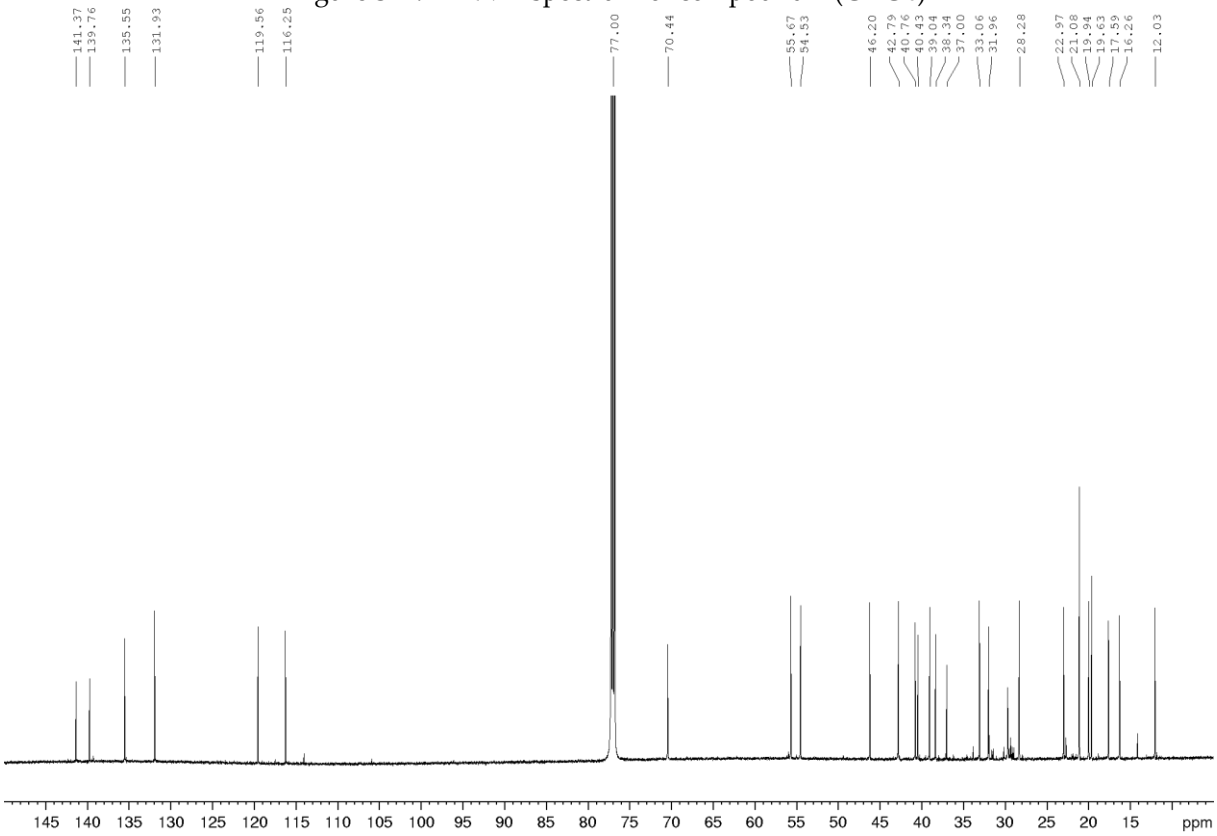

Figure S18.[13]C NMR spectrum of compound **4** ($CDCl_3$)

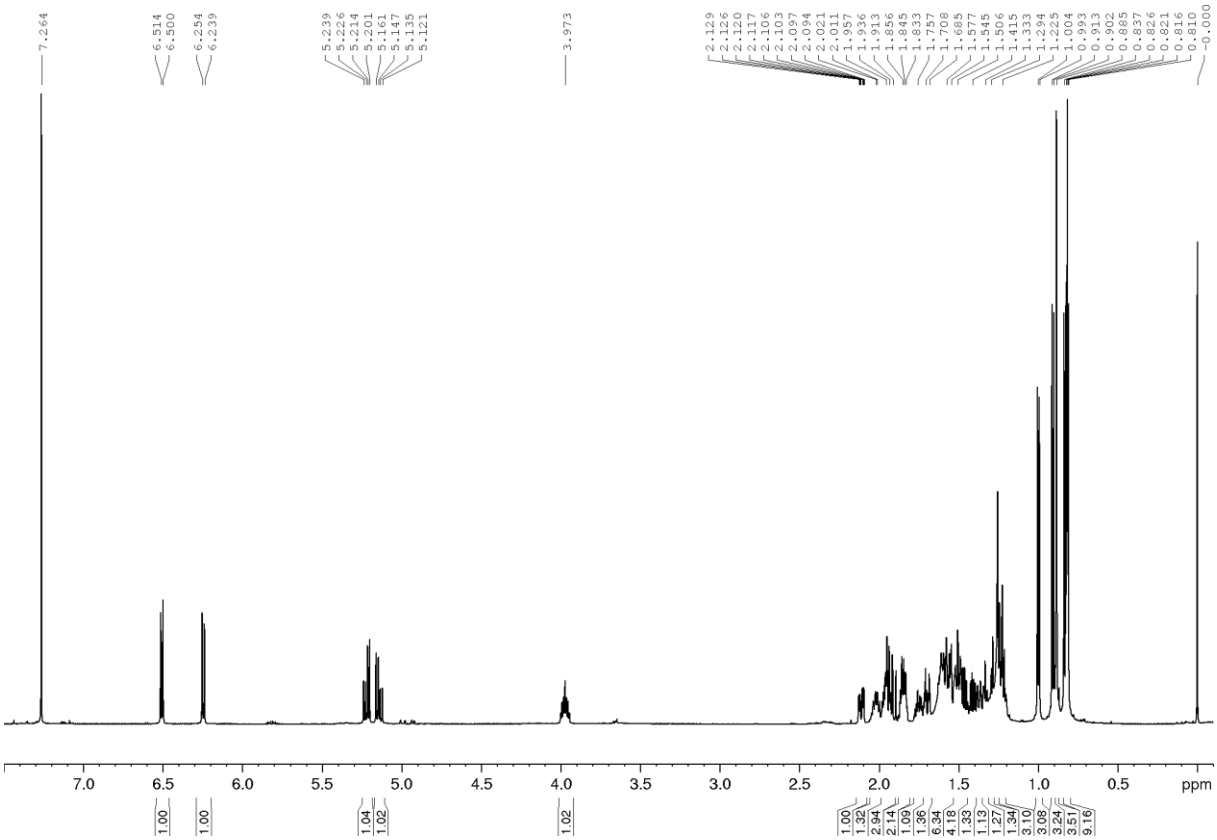

Figure S19.[1]H NMR spectrum of compound **5** ($CDCl_3$)

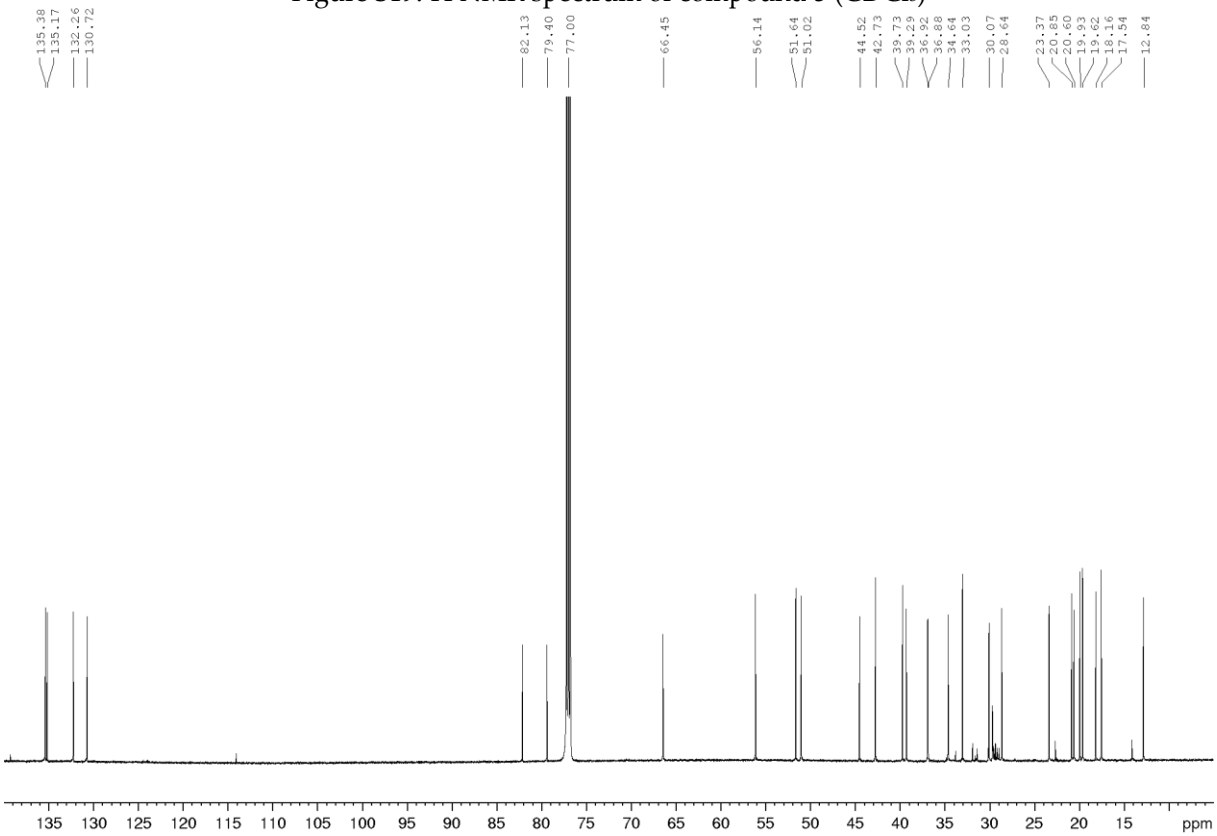

Figure S20.[13]C NMR spectrum of compound **5** ($CDCl_3$)