Electronic Supporting Information

An NMR insight into the solvatochromic behaviour of Brooker's merocyanine dyes

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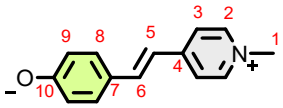
1. NMR tables

Compound **1a**.

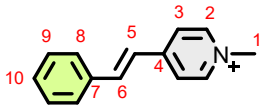


1a

solvent	**D_6-DMSO**	**CD_3CN**	**CD_3OD**	**D_2O**
colour	violet	purple	red-orange	orange
^{15}N				
^{+}N-CH_3	-211.0	-212.7	-197.3	-193.9
^{13}C				
1	44.99	45.88	46.77	46.90
2	141.57	142.39	144.50	143.88
3	118.05	119.49	122.67	122.77
4	152.76	154.67	156.36	154.80
5	106.88	108.75	115.12	116.83
6	143.94	145.52	145.62	142.78
7	115.65	118.20	122.06	122.15
8	133.20	134.54	132.69	131.62
9	121.64	122.74	121.20	120.18
10	179.85	180.42	175.27	171.47
^{1}H				
1-CH_3	3.88	3.83	4.08	3.99
2	3.88	3.83	4.08	3.99
3	8.04	7.72	8.24	8.16
5	7.42	7.31	7.71	7.67
6	6.40	6.45	6.77	6.77
8	7.61	7.58	7.65	7.50

Table S1: ^{1}H, ^{13}C and ^{15}N NMR values of compound **1a**.

Compound **1b**.



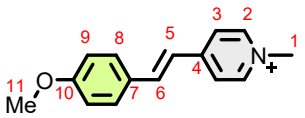
1b

solvent	**$CDCl_3$**	**D_6-DMSO**	**CD_3OD**	**D_2O**
colour	light orange[a]	dark orange[a]	dark orange[a]	orange[a]
^{15}N				
^{+}N-CH_3	-188.9	-184.6	-186.5	-187.6
^{13}C				
1	48.64	46.88	48.04	47.60
2	144.98	144.99	146.15	144.82
3	124.29	123.48	125.20	124.48
4	153.77	152.31	155.19	153.76
5	122.14	123.17	123.88	123.44
6	142.6	140.44	142.91	141.18
7	134.47	135.03	136.56	135.45
8	128.65	128.00	129.48	128.70
9	129.41	129.00	130.20	129.77
10	131.35	130.26	131.74	131.15
^{1}H				
1	4.54	4.28	4.32	4.16
2	8.99	8.89	8.72	8.41
3	8.06	8.26	8.26	7.90
5	7.19	7.56	7.56	7.19
6	7.73	8.04	8.04	7.63
8	7.66	7.78	7.78	7.60
9	7.44	7.50	7.50	7.44
10	7.44	7.46	7.46	7.45

[a] Colour intensity in this and other cases is probably mainly due to differences in concentration.

Table S2: ^{1}H, ^{13}C and ^{15}N NMR values of compound **1b**.

Compound **1c**.

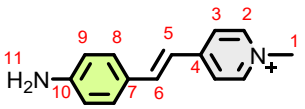


1c

solvent	**$CDCl_3$**	**acetone**	**D_6-DMSO**	**CD_3OD**	**D_2O**
colour	yellow	red-brown	red-brown	red-brown	red-brown
(^{15}N)					
^{+}N-CH_3	-191.6	-188.0	-186.4	-188.6	-189.1
^{13}C					
1	48.17	47.98	46.68	47.71	47.12
2	144.52	145.91	144.74	145.87	144.55
3	123.57	124.38	122.93	124.61	124.01
4	154.15	154.93	152.77	155.70	154.15
5	119.37	121.35	120.60	121.32	121.25
6	142.60	142.26	140.47	143.00	140.96
7	127.06	128.25	127.69	129.25	128.64
8	130.47	131.11	129.89	131.37	130.60
9	114.84	115.47	114.56	115.71	115.20
10	162.42	162.88	161.09	163.56	161.46
11	55.55	55.92	55.36	56.06	56.16
^{1}H					
1	4.52	4.52	4.25	4.29	4.13
2	8.91	8.99	8.82	8.65	8.37
3	7.95	8.31	8.18	8.10	7.81
5	7.01	7.46	7.38	7.27	6.99
6	7.68	8.10	7.99	7.89	7.55
8	7.61	7.79	7.74	7.71	7.54
9	6.97	7.05	7.07	7.01	6.95
11	3.88	3.88	3.83	3.86	3.82

Table S3: ^{1}H, ^{13}C and ^{15}N NMR values of compound **1c**.

Compound **1d**.

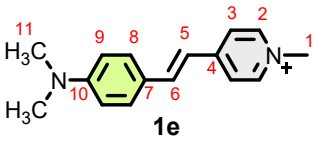


1d

solvent	**acetone**	**D_6-DMSO**	**CD_3OD**	**D_2O**
colour	yellow	dark orange	orange	yellow-orange
^{15}N				
^{+}N-CH_3	-191.6	-190.8	-192.6	-190.6
NH_2		-307.8	-318.3	-319.7
^{13}C				
1	47.55	46.23	47.20	47.19
2	145.32	144.16	145.30	144.37
3	123.43	121.89	123.64	123.53
4	155.60	153.39	156.31	154.54
5	117.55	116.28	117.72	119.31
6	143.89	142.20	144.58	141.85
7	124.32	122.34	125.06	126.06
8	131.57	130.39	131.84	130.68
9	115.09	113.67	115.60	116.46
10	153.33	151.93	153.48	150.31
^{1}H				
1	4.45	4.17	4.22	4.15
2	8.78	8.67	8.51	8.36
3	8.13	8.02	7.96	7.83
5	7.18	7.09	7.06	7.02
6	7.90	7.85	7.80	7.61
8	7.52	7.47	7.49	7.49
9	6.76	6.63	6.70	6.82
11	-	5.98	-	-

Table S4: ^{1}H, ^{13}C and ^{15}N NMR values of compound **1d**.

Compound **1e**.

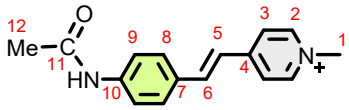


1e

solvent	**acetone**	**D_6-DMSO**	**CD_3OD**	**D_2O**
colour	orange	orange-red	orange	orange
^{15}N				
^{+}N-CH_3	-192.1	-190.4	-193.0	-191.7
$N(CH_3)_2$		-320.90	-325.40	
^{13}C				
1	47.53	46.27	47.19	47.15
2	145.30	144.23	145.27	144.38
3	123.39	122.02	123.59	123.38
4	155.49	153.26	156.22	154.75
5	117.71	117.02	117.77	118.77
6	143.67	141.79	144.39	141.98
7	123.63	122.36	124.19	124.35
8	131.29	130.02	131.62	130.64
9	112.88	111.85	113.51	113.98
10	153.47	151.79	154.07	153.40
11	40.15	39.59	40.26	40.47
^{1}H				
1	4.45	4.18	4.21	4.18
2	8.80	8.69	8.50	8.40
3	8.14	8.05	7.96	7.88
5	7.23	7.17	7.09	7.08
6	7.96	7.91	7.82	7.73
8	7.63	7.60	7.61	7.64
9	6.81	6.79	6.78	6.92
11	3.08	3.02	3.06	3.00

Table S5: ^{1}H, ^{13}C and ^{15}N NMR values of compound **1e**.

Compound **1f**.

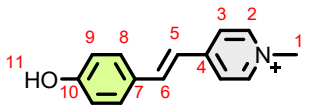


1f

solvent	**D_6-DMSO**	**CD_3OD**	**D_2O**
colour	orange	yellow	orange
^{15}N			
^{+}N-CH_3	-185.8	-187.3	-188.1
^{13}C			
1	46.71	47.72	47.51
2	144.82	146.04	144.88
3	123.07	124.82	124.33
4	152.6	155.49	154.12
5	121.32	122.56	122.89
6	140.32	142.58	140.70
7	129.66	132.06	132.30
8	128.94	130.33	129.60
9	118.94	121.10	122.15
10	141.28	142.53	140.70
11	168.59	171.89	173.59
12	24.04	24.03	23.61
^{1}H			
1	4.24	4.30	4.25
2	8.82	8.67	8.53
3	8.18	8.12	8.00
5	7.40	7.34	7.28
6	7.95	7.88	7.75
8	7.71	7.71	7.71
9	7.71	7.68	7.53
NH	10.20		
11	2.09	2.15	2.18

Table S6: ^{1}H, ^{13}C and ^{15}N NMR values of compound **1f**.

Compound **1g**.

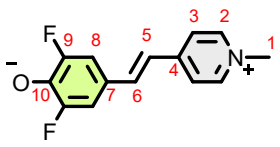


1g

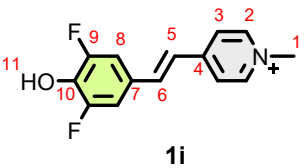
solvent	**D_6-DMSO**	**CD_3CN**	**CD_3OD**	**D_2O**
colour	purple	purple	red	yellow-orange
^{15}N				
^{+}N-CH_3	-193.1	-193.5	-192.4	-189.2
^{13}C				
1	46.04	47.63	47.24	47.36
2	143.91	144.88	145.38	144.54
3	121.55	123.30	123.82	123.92
4	153.13	155.35	156.13	154.40
5	116.09	117.73	118.66	120.78
6	142.12	143.67	144.27	141.34
7	122.68	125.15	126.14	127.91
8	130.87	132.06	131.97	130.90
9	117.52	118.52	118.47	116.76
10	166.27	166.60	166.23	159.15
^{1}H				
1	4.14	4.09	4.22	4.19
2	8.61	8.24	8.51	8.42
3	7.97	7.80	7.97	7.89
5	7.04	6.99	7.08	7.08
6	7.86	7.73	7.81	7.70
8	7.51	7.53	7.55	7.58
9	6.66	6.77	6.77	6.86
11	-	-	-	-

Table S7: ^{1}H, ^{13}C and ^{15}N NMR values of compound **1g**.[1]

Compounds **1h** and **1i**.



1h



1i

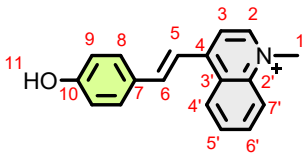
	1h		**1i**	
solvent	**D_6-DMSO**	**CD_3OD**	**D_6-DMSO**	**CD_3OD**
colour	purple	cherry red	brown-orange	brown-orange
^{15}N				
^{+}N-CH_3	-200.4	-193.8	-184.7	-186.5
^{13}C				
1	45.35	47.11	46.78	47.81
2	142.96	144.90	145.07	146.13
3	119.85	123.27	123.23	124.98
4	153.26	155.78	152.16	155.02
5	111.57	117.66	122.84	123.45
6[a]	143.28	143.93	138.68	141.04
7[b]	109.39	117.84	125.94	127.53
8[c]	112.02	112.78	111.56	112.72
9[d]	155.92	157.30	152.25	154.06
10[e]	156.48	152.28	135.73	137.93
^{1}H				
1	4.03	4.18	4.27	4.32
2	8.37	8.38	8.90	8.71
3	7.69	7.77	8.15	8.11
5	6.68	6.81	7.47	7.29
6	7.71	7.59	7.92	7.78
8	7.08	7.05	7.49	7.37

a. t, $^{4}J_{CF}$ = 3 Hz **b.** t, $^{3}J_{CF}$ = 9 Hz. **c.** 2nd order multiplet

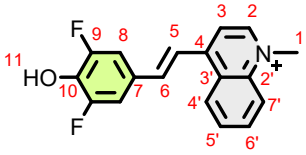
d. dd, $^{1}J_{CF}$ = 239 Hz, $^{3}J_{CF}$ = 12 Hz **e.** t, $^{2}J_{CF}$ = 17 Hz.

Table S8: ^{1}H, ^{13}C and ^{15}N NMR values of compound **1h** and **1i**.[3]

Compounds **2g** and **2i**.



2g



2i

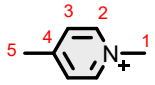
	2g		**2i**	
solvent	**D_6-DMSO**	**CD_3OD**	**D_6-DMSO**	**CD_3OD**
colour	dark green	purple	dark blue	violet
^{15}N				
^{+}N-CH_3	-213.6	-207.2	-220.6	-208.4
^{13}C				
1	43.18	44.91	42.58	44.76
2	145.25	147.81	144.18	147.45
3	112.12	115.47	110.12	114.99
4	151.67	155.97	151.71	155.60
5	111.05	114.86	108.19[c]	114.58[c]
6	144.38	146.47	145.84[c]	145.98
7	123.52	126.61	112.92[c]	119.77[c]
8	132.72	132.82	113.64[c]	113.49[b]
9	118.70	118.80	155.44[a]	156.86[a]
10	169.18	167.42	157.35[c]	151.56[c]
2'	138.70	140.69	138.73	140.67
3'	125.26	127.88	124.78	127.71
4'	125.94	127.39	126.00	127.38
5'	127.67	130.11	127.06	129.98
6'	133.91	136.17	133.60	136.08
7'	118.40	119.72	118.06	119.60
^{1}H				
1	4.27	4.47	4.20	4.45
2	8.78	8.88	8.59	8.80
3	8.04	8.19	7.85	8.12
5	7.75	7.91	7.55	7.77
6	8.03	8.01	8.05	7.90
8	7.74	7.71	7.48[c]	7.29

9	6.59	6.80	—	—
4'	8.85	8.84	8.89	8.81
5'	7.82	7.98	7.77	7.95
6'	8.06	8.19	8.03	8.16
7'	8.15	8.31	8.07	8.27

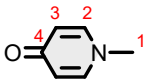
a. dd, $^{1}J_{CF}$ = 240 Hz, $^{3}J_{CF}$ = 10.5 Hz **b.** 2nd order multiplet **c.** broad signal

Table S9: ^{1}H, ^{13}C and ^{15}N NMR values of compound **2g** and **2i**.[3]

Compounds **3** and **4**.



3



4

	3		**4**		
solvent	**D_6-DMSO**	**CD_3OD**	**$CDCl_3$**	**D_6-DMSO**	**CD_3OD**
^{15}N					
$^{+}N\text{-}CH_3/N\text{-}CH_3$	-182.8	-183.7	-246.1	-242.1	-232.0
^{13}C					
1	47.11	48.31	43.53	42.50	44.27
2	144.37	145.80	140.41	141.52	144.06
3	127.85	129.69	118.92	117.18	118.39
4	158.10	160.89	178.65	176.75	180.59
5	21.26	22.03	—	—	—
^{1}H					
1	4.31	4.36	3.64	3.59	3.77
2	8.86	8.74	7.24	7.57	7.75
3	7.98	7.92	6.38	6.05	6.44
5	2.62	2.68	—	—	—

Table S10: ^{1}H, ^{13}C and ^{15}N NMR values of compound **3** and **4**.

	1a	1b	1c	1d	1e	1f	1g	2g	1h	1i	2i
C-5	8.24	0.71	0.72	1.44	0.75	1.24	2.57	3.81	6.09	0.61	6.00
C-7	6.41	1.53	1.56	2.72	1.83	2.40	3.46	2.09	8.45	2.36	6.25
C-10	-4.58	1.48	2.47	1.55	2.27	1.25	-0.04	-1.76	-4.20	2.19	-4.84
N-1	13.7	-1.9	-2.2	-1.8	-2.6	-1.5	0.8	6.4	6.6	-1.8	12.1

Table S11: $\delta_{methanol} - \delta_{DMSO}$ for selected nuclei.

solvent	E_T(30) (kcal.mol^{-1})	λ_{max} (nm)	λ_{max} (nm)
THF	37.4	611	400
$CHCl_3$	39.1	614	408
CH_2Cl_2	40.7	609	417
acetone	42.2	592	394
DMF	43.2	575	391
DMSO	45.1	577	395
CH_3CN	45.6	580	
2-propanol	48.4	548	405
ethanol	51.9	515	400
methanol	55.4		393
water	63.1		371

Table S12: λ_{max} values for **1a** in various solvents.

2. NMR spectra

Compound **1a**.

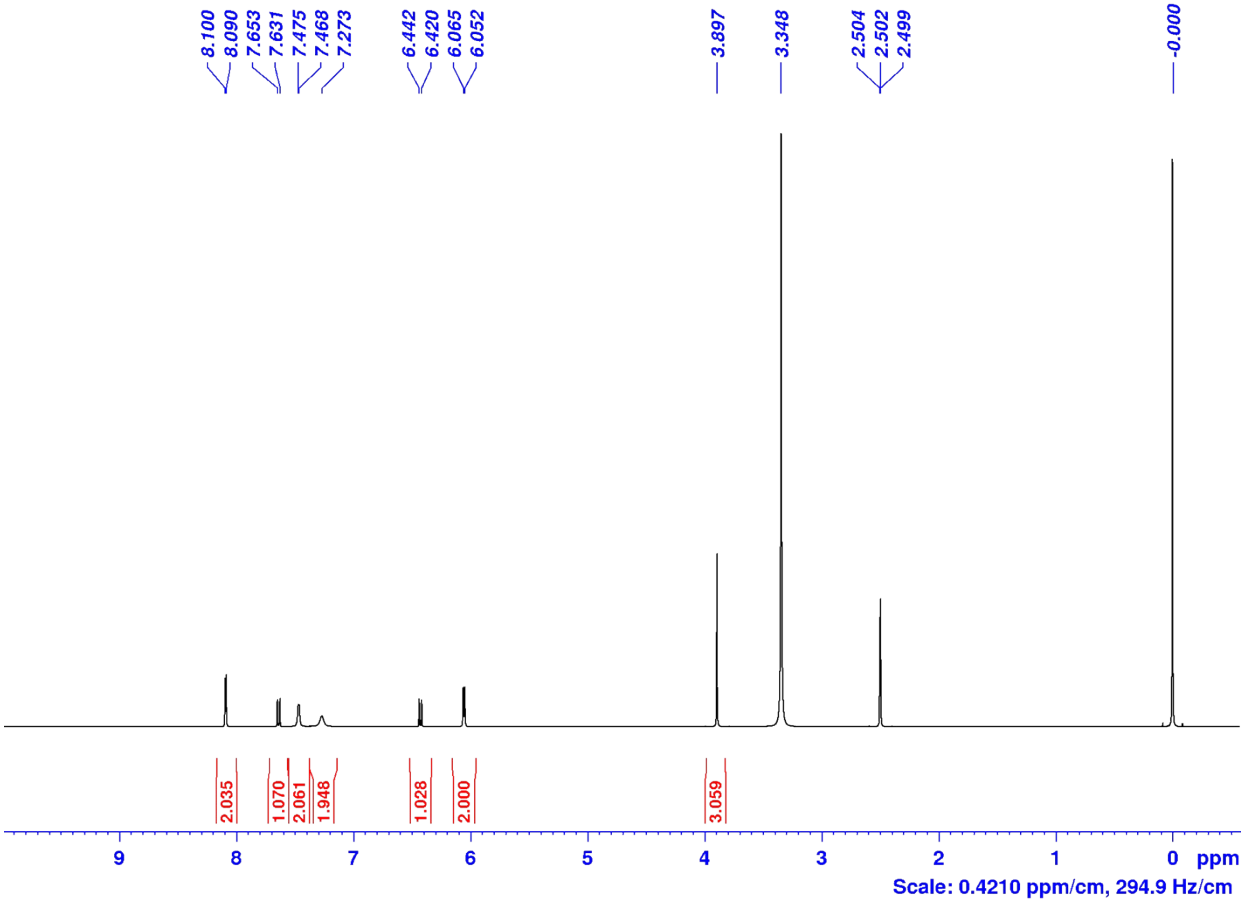


Figure S1: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **1a**.

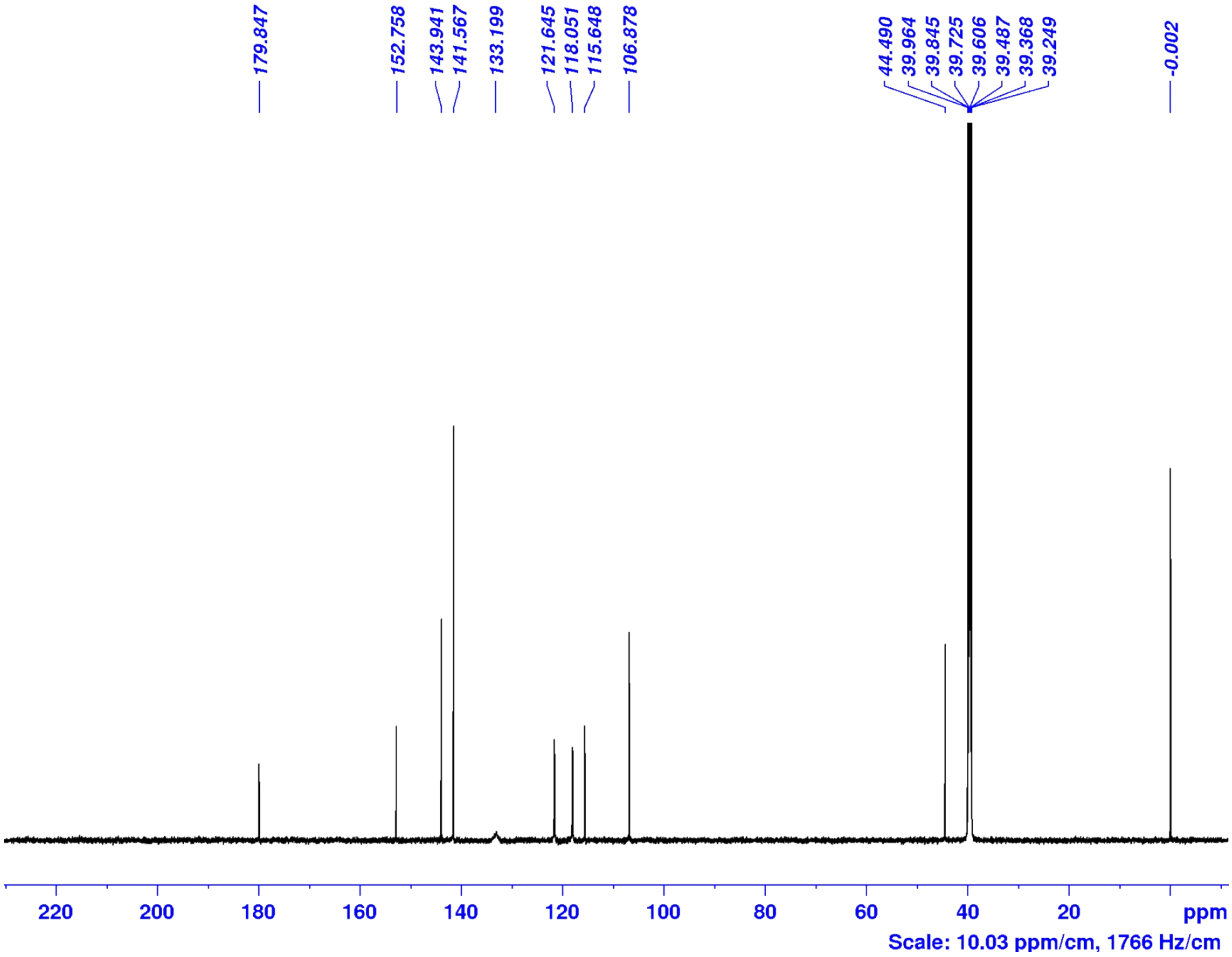


Figure S2: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **1a**.

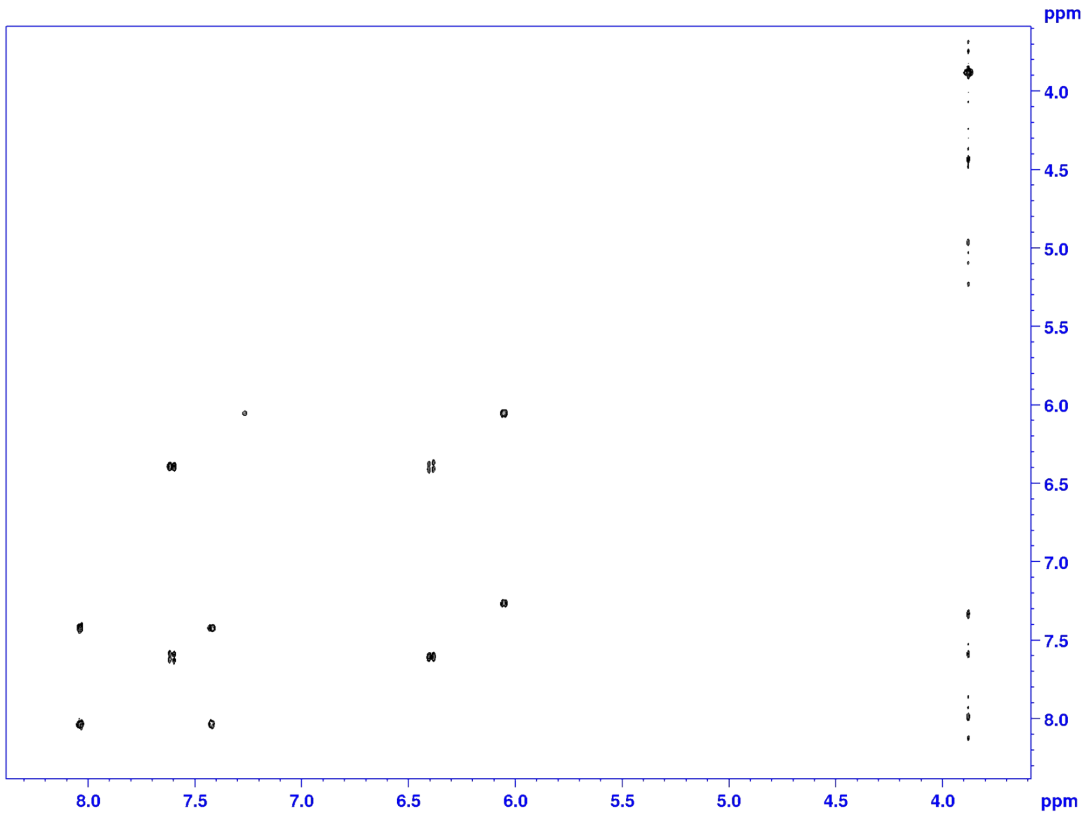


Figure S3: COSY NMR (DMSO, 298 K) of **1a**.

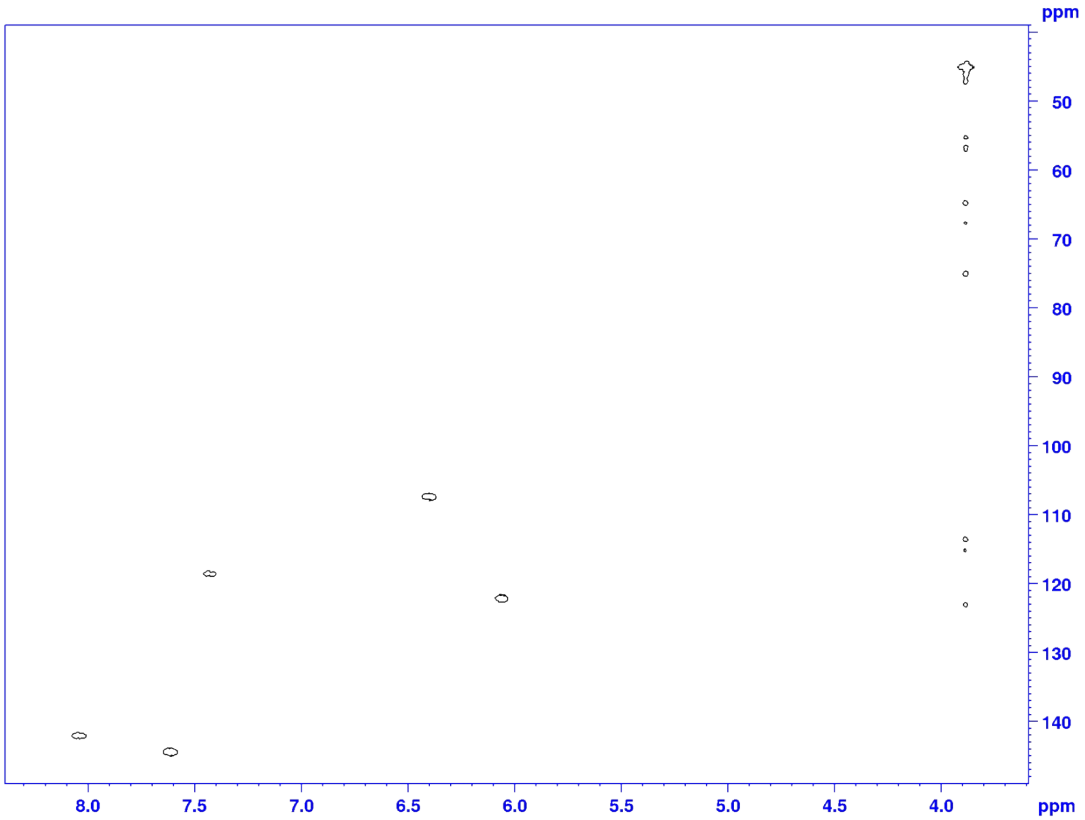


Figure S4: HMQC NMR (DMSO, 298 K) of **1a**.

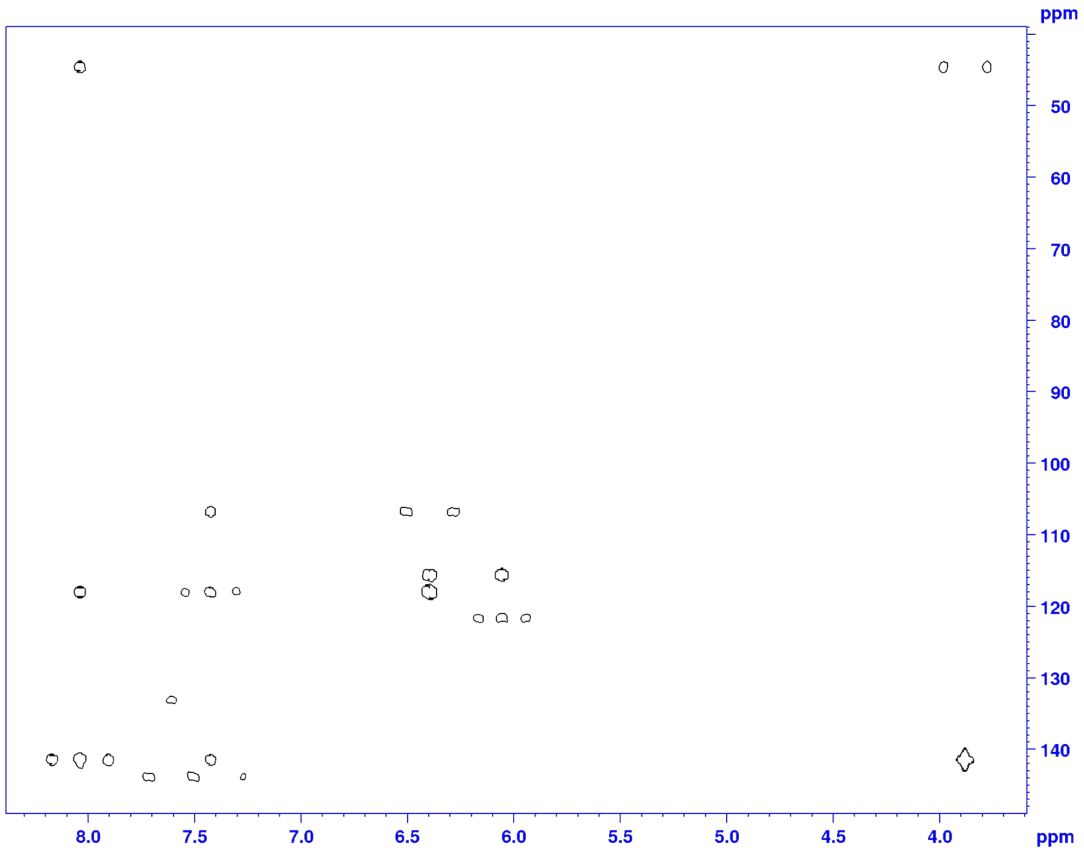


Figure S5: HMBC NMR (DMSO, 298 K) of **1a**.

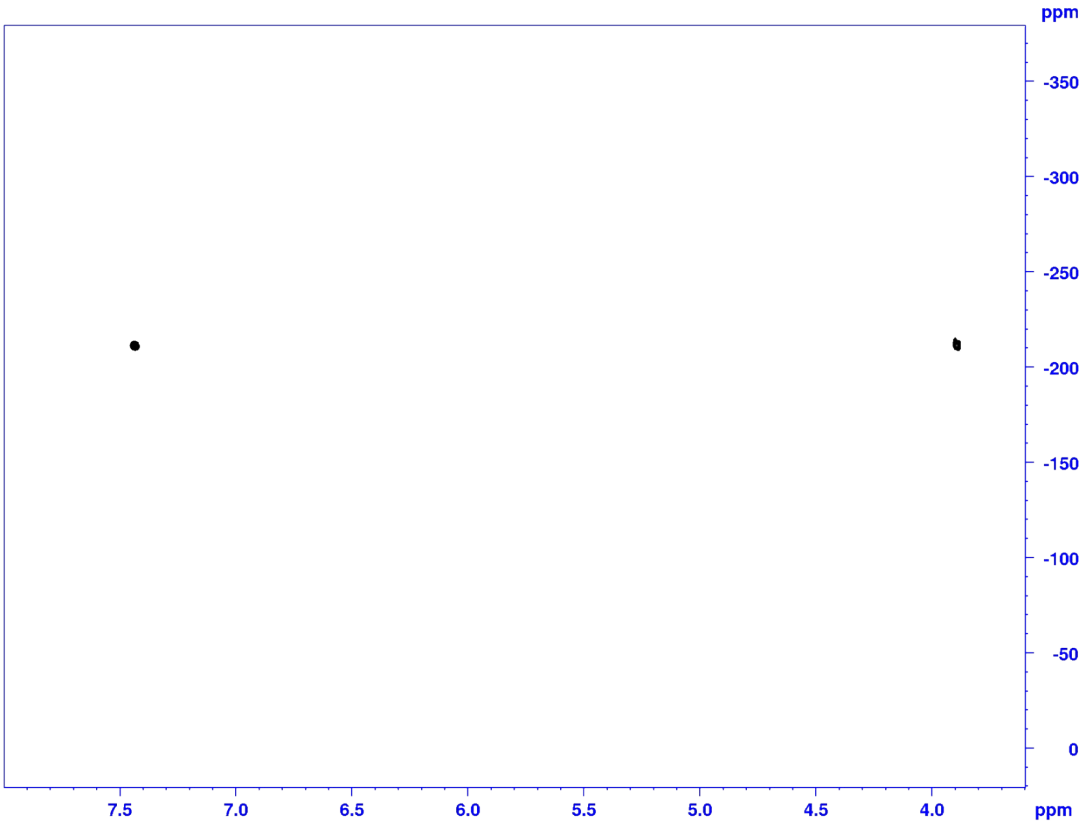


Figure S6: $^{1}H\times^{15}N$ HMBC NMR (DMSO, 298 K) of **1a**.

Compound **1b**.

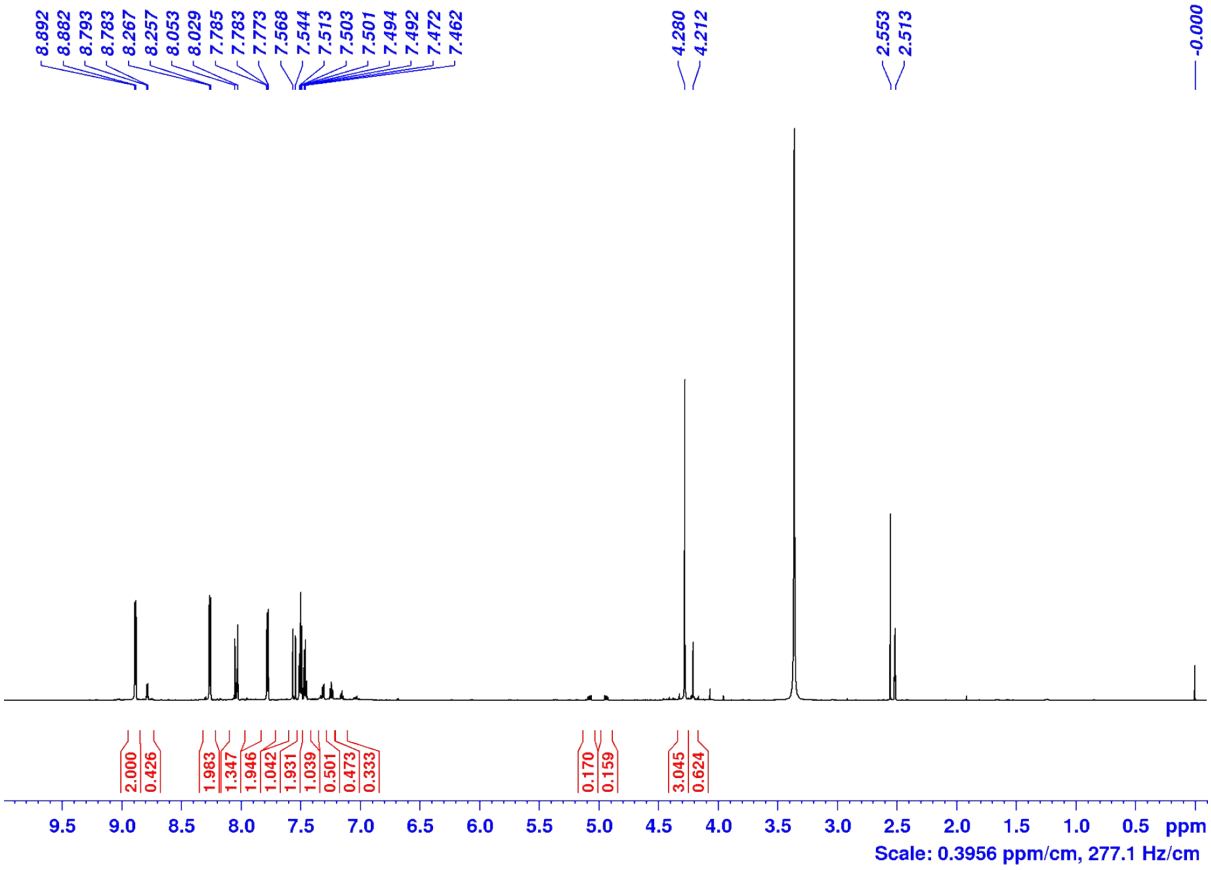


Figure S7: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **1b**.

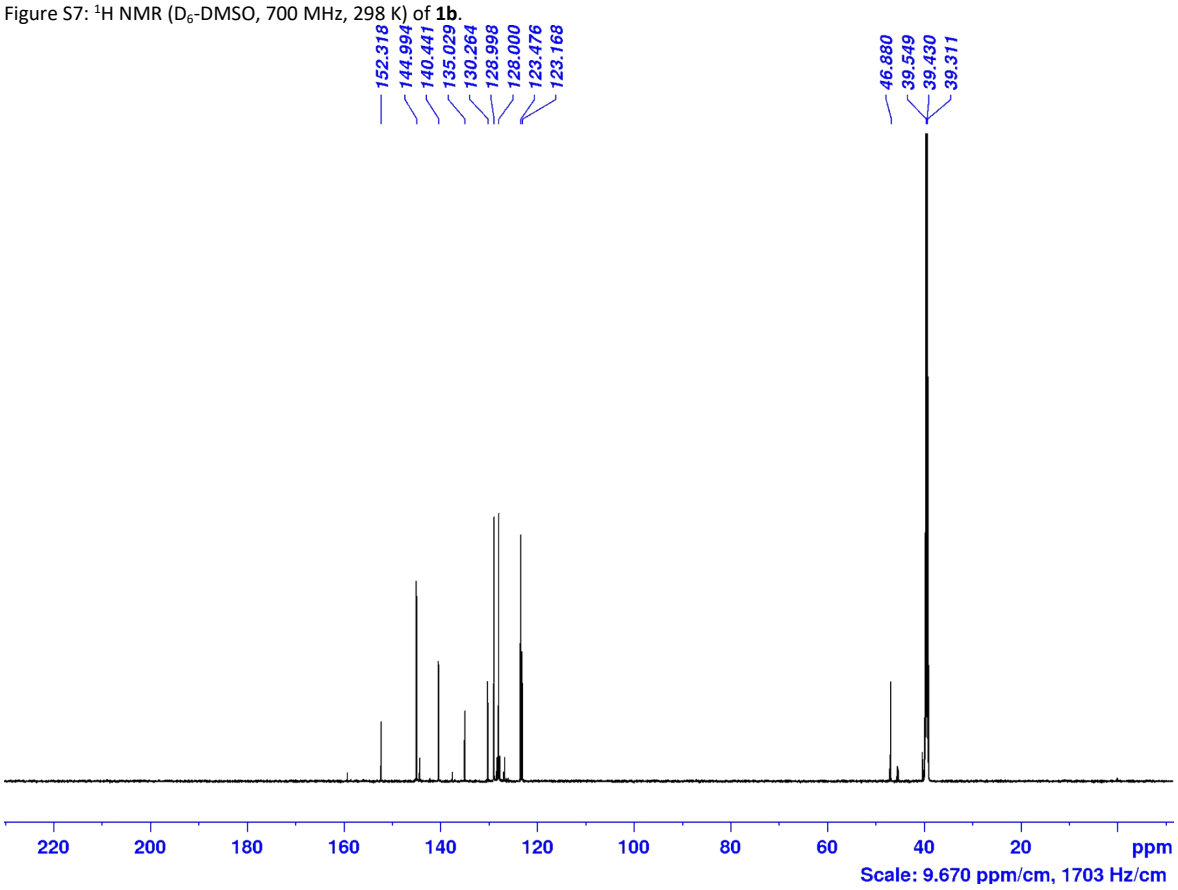


Figure S8: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **1b**.

Compound **1c**.

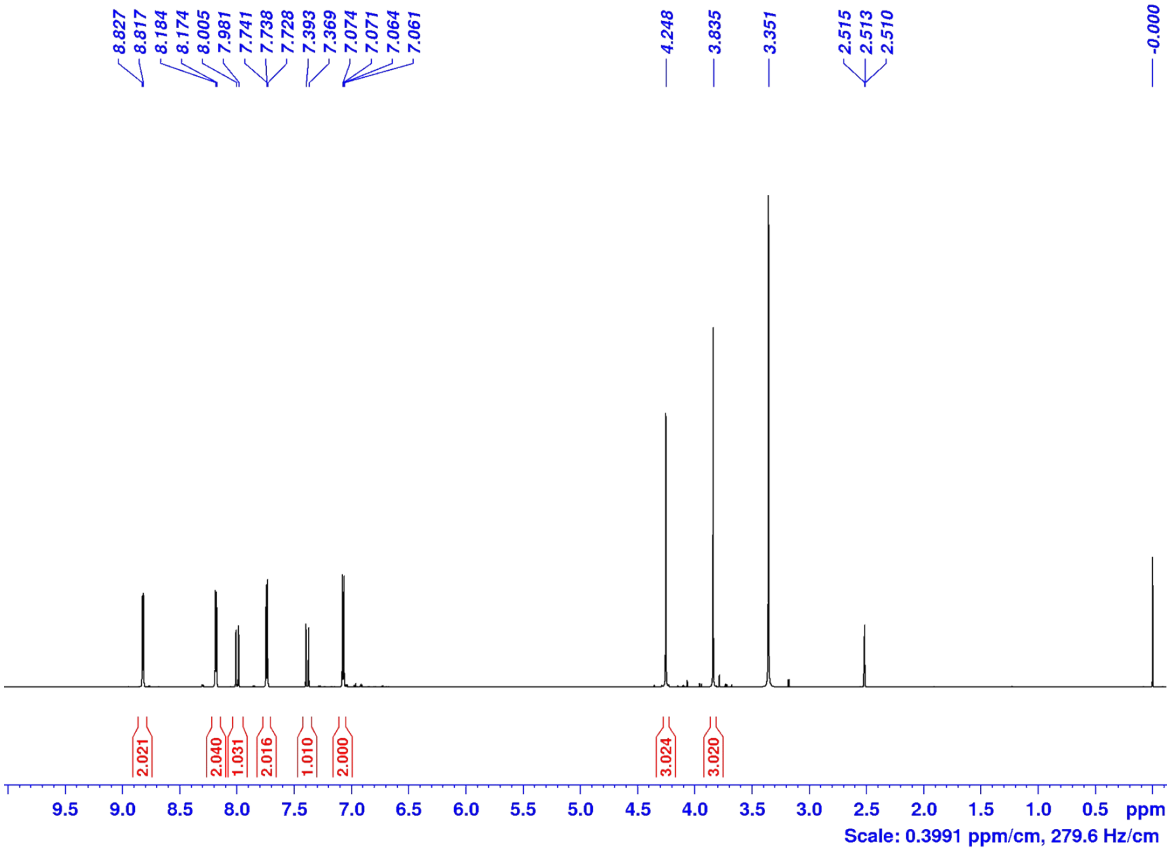


Figure S9: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **1c**.

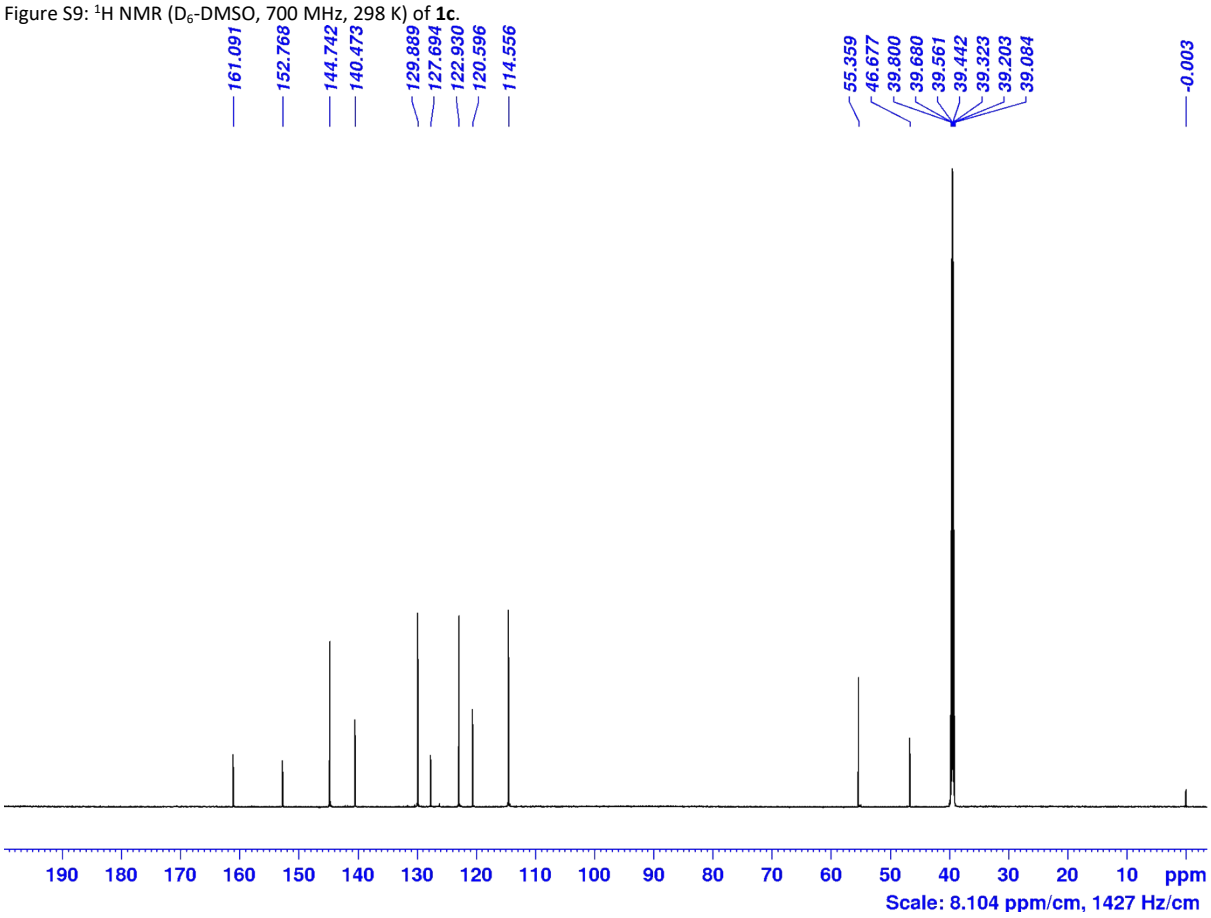


Figure S10: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **1c**.

Compound **1d**.

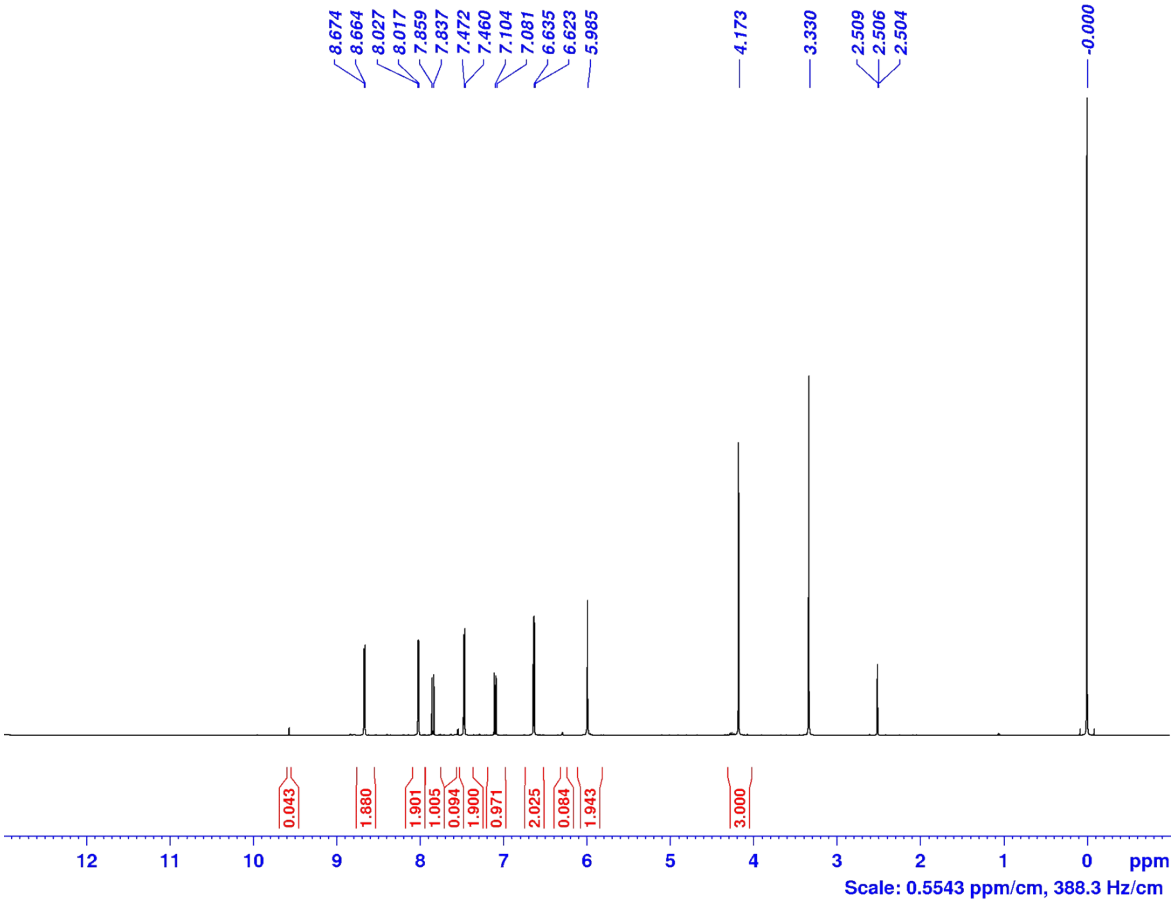


Figure S11: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **1d**.

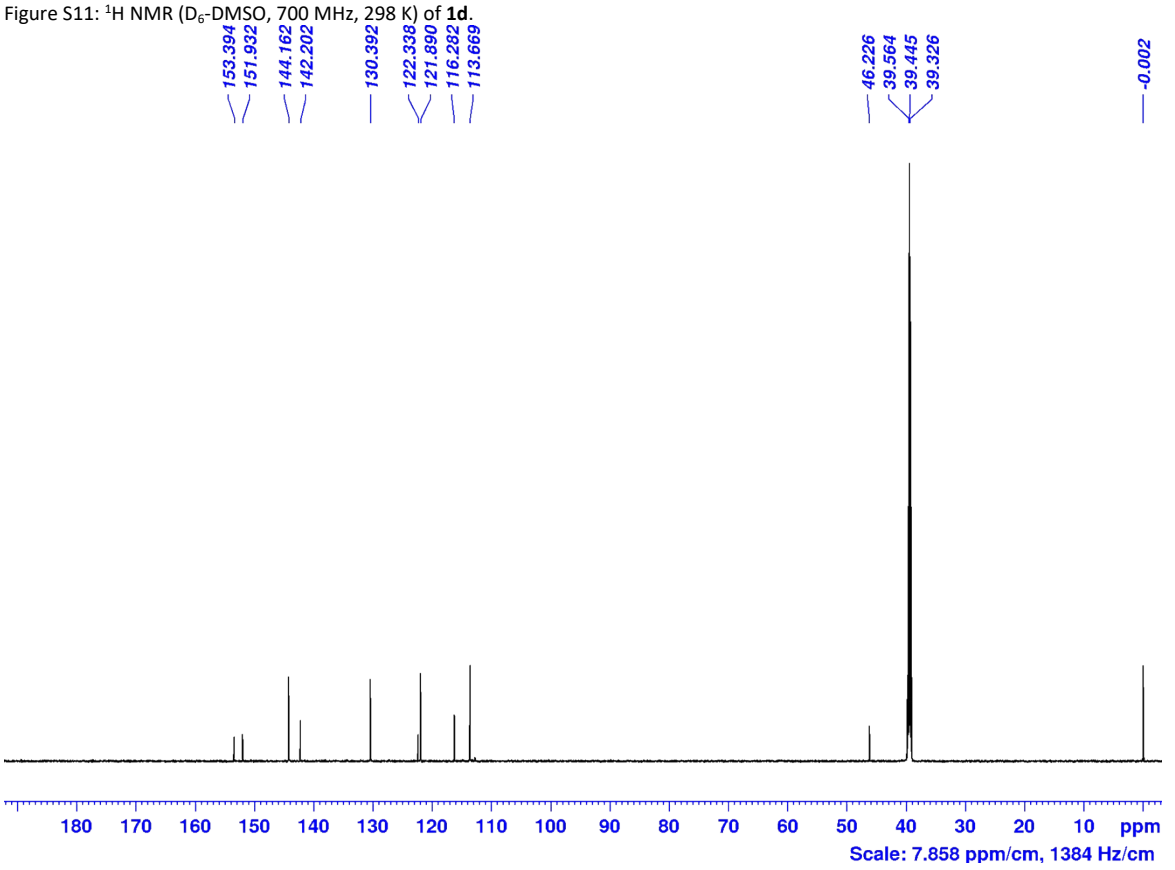


Figure S12: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **1d**.

Compound **1e**.

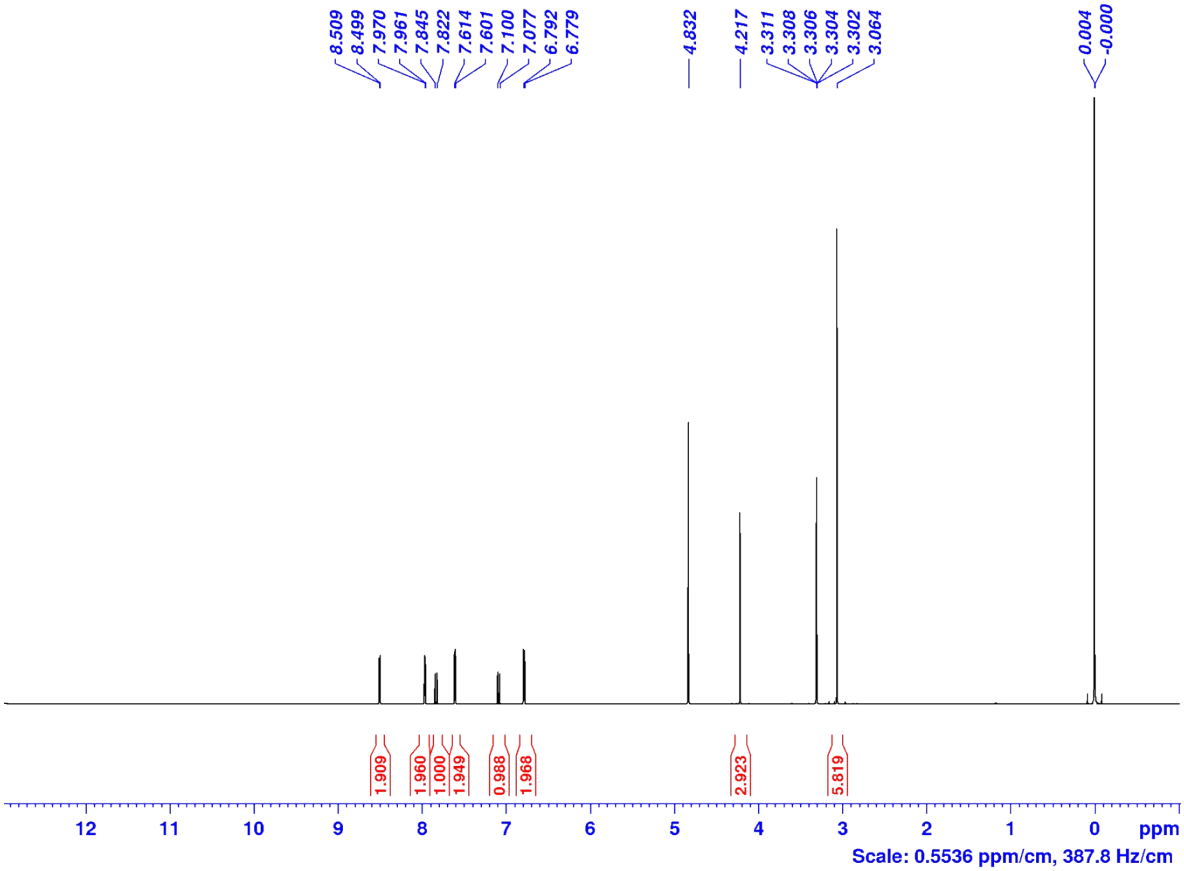


Figure S13: ^{1}H NMR (CD_3OD, 700 MHz, 298 K) of **1e**.

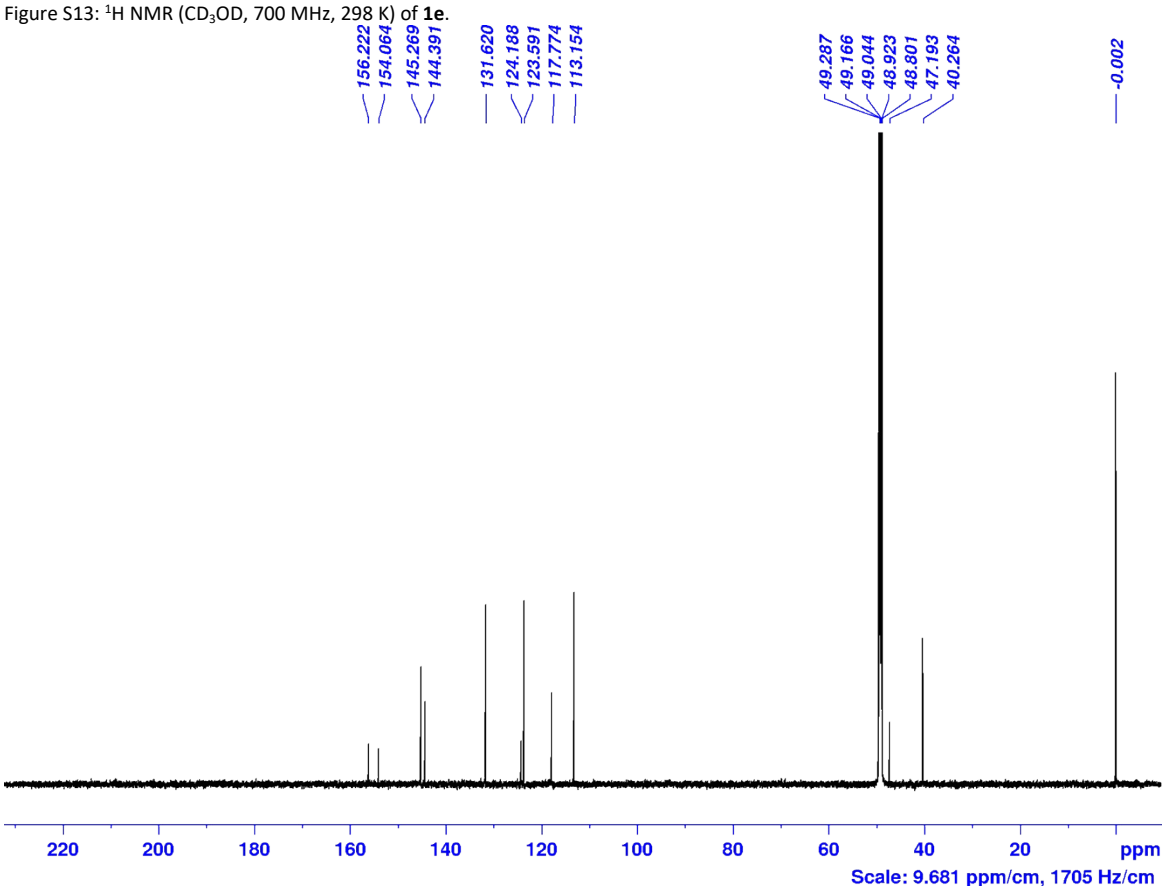


Figure S14: ^{13}C NMR (CD_3OD, 176 MHz, 298 K) of **1e**.

Compound **1f**.

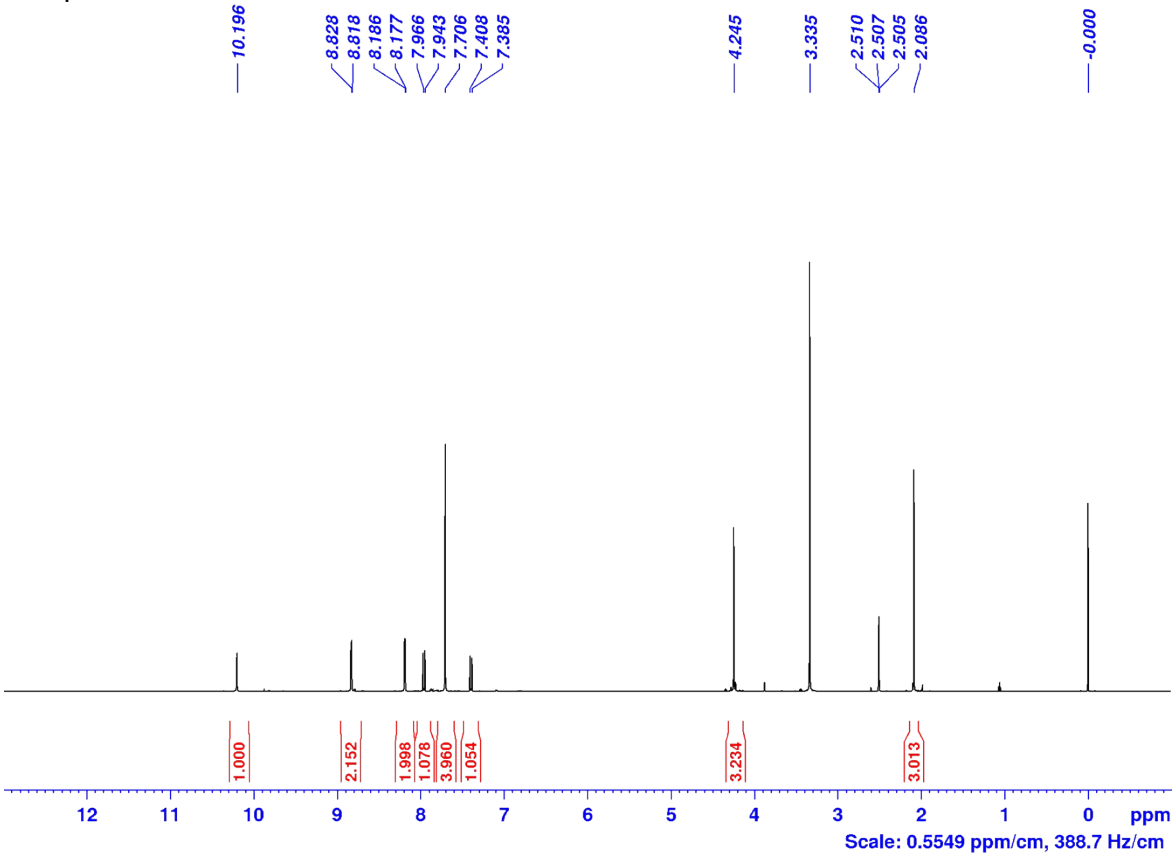


Figure S15: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **1f**.

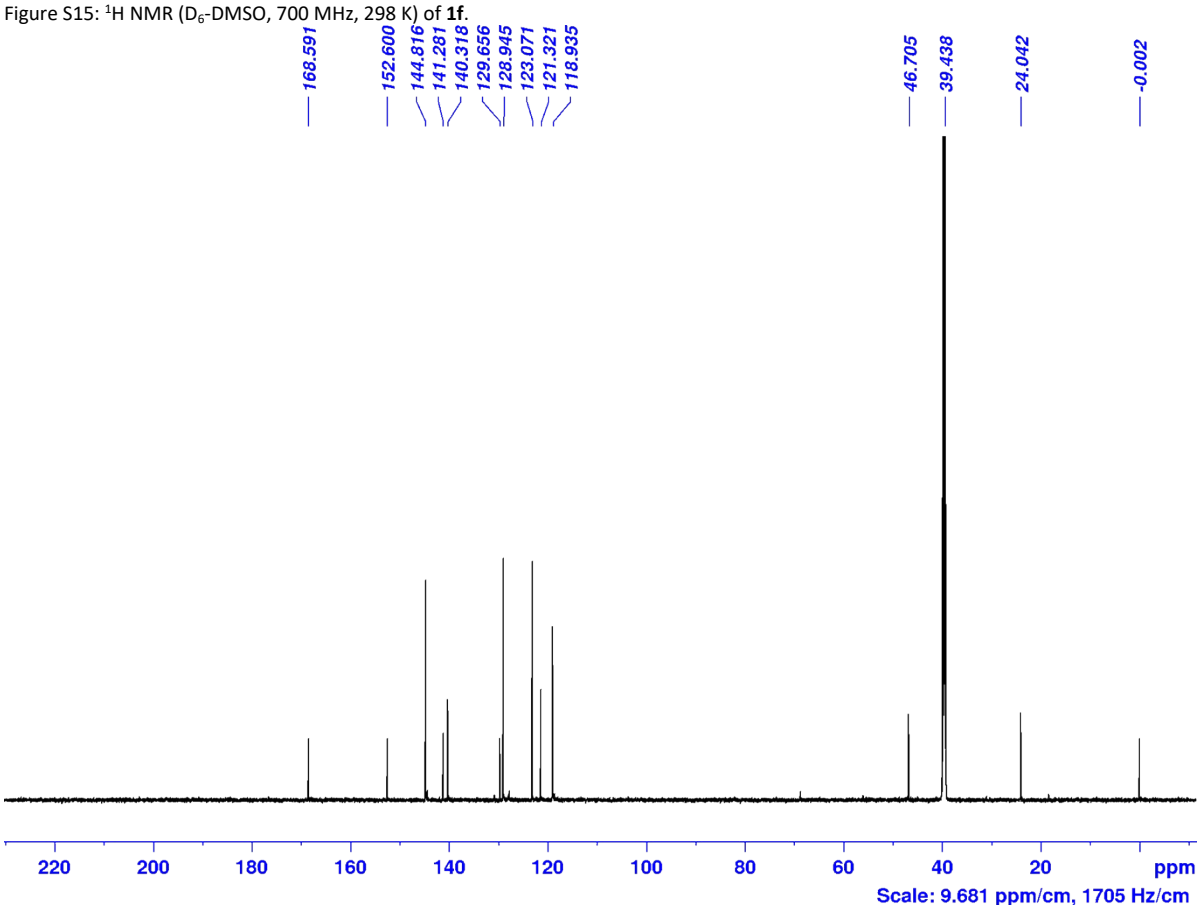


Figure S16: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **1f**.

Compound **1g**.

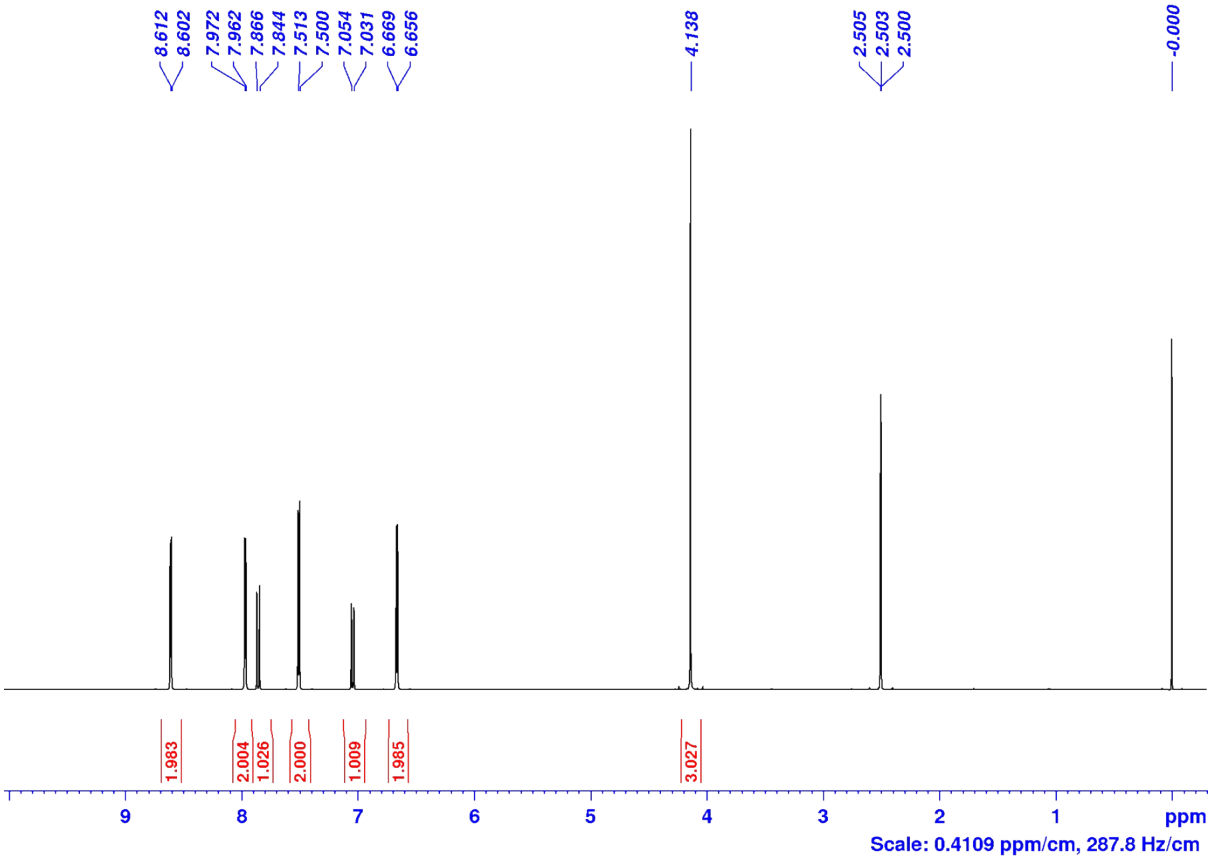


Figure S17: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **1g**.

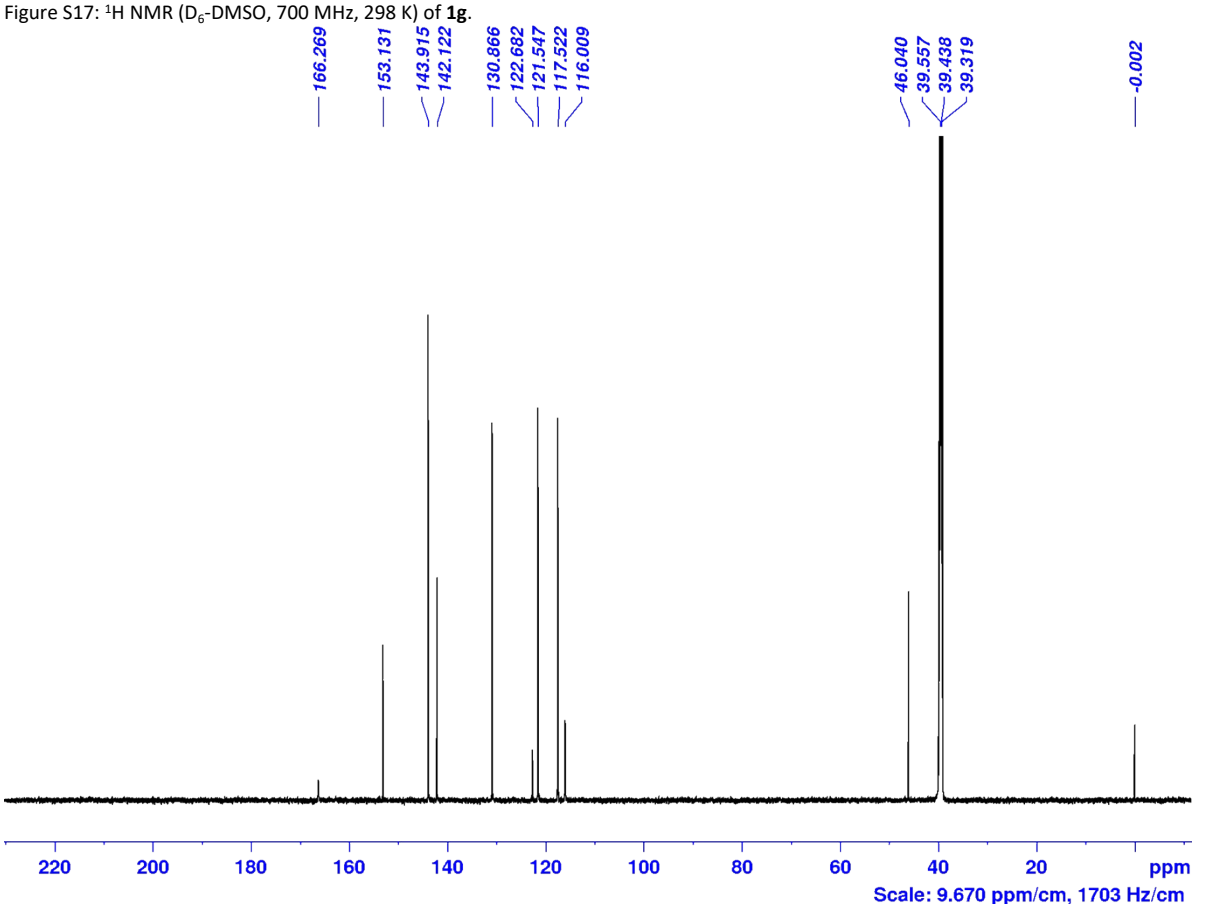


Figure S18: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **1g**.

Compound **1h**.

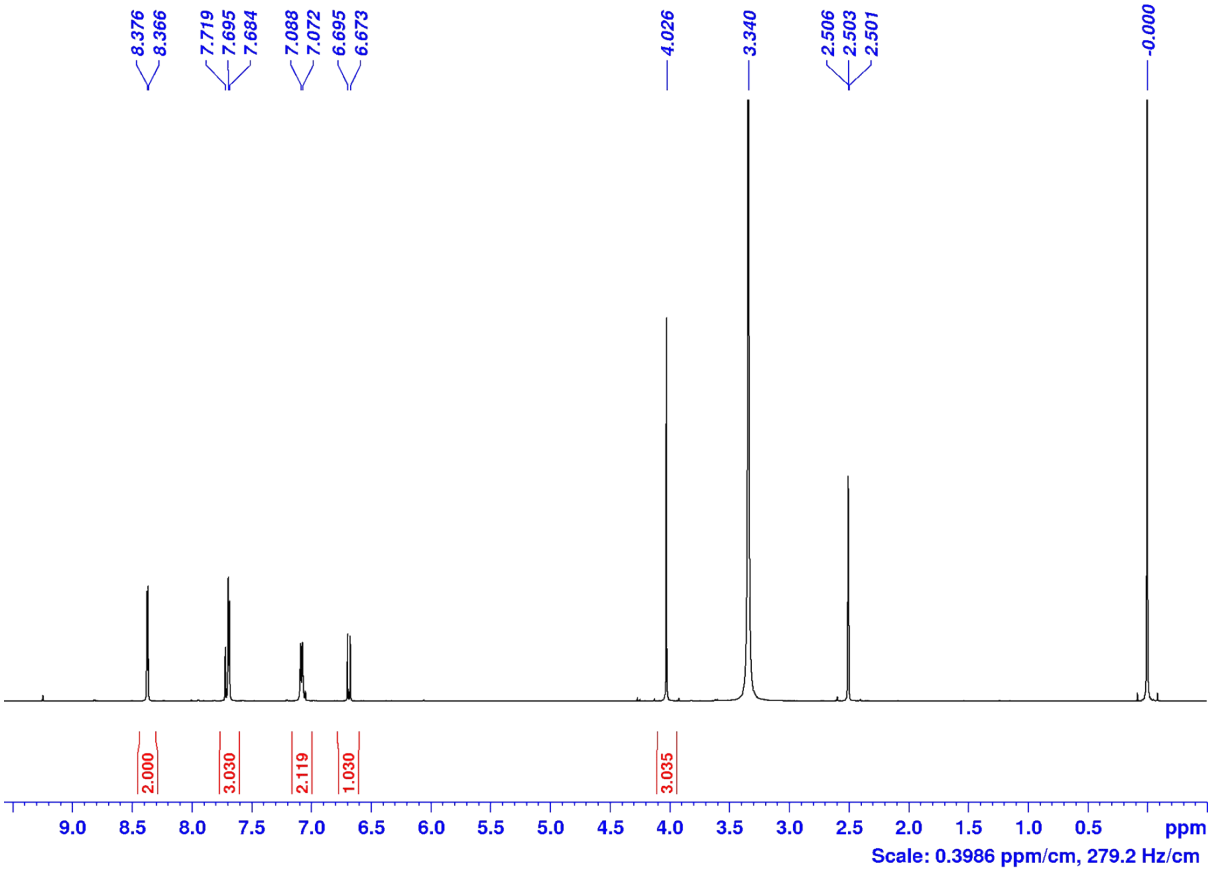


Figure S19: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **1h**.

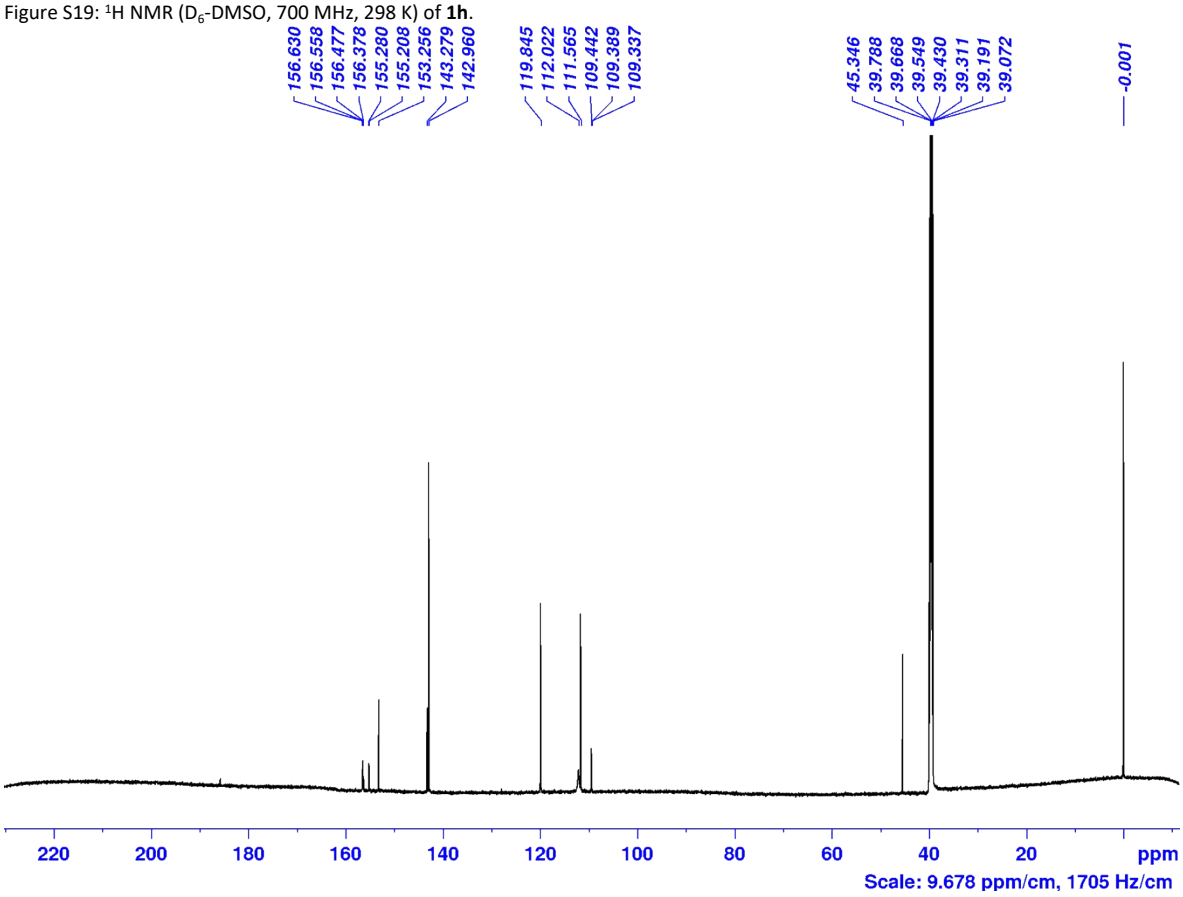


Figure S20: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **1h**.

Compound **1i**.

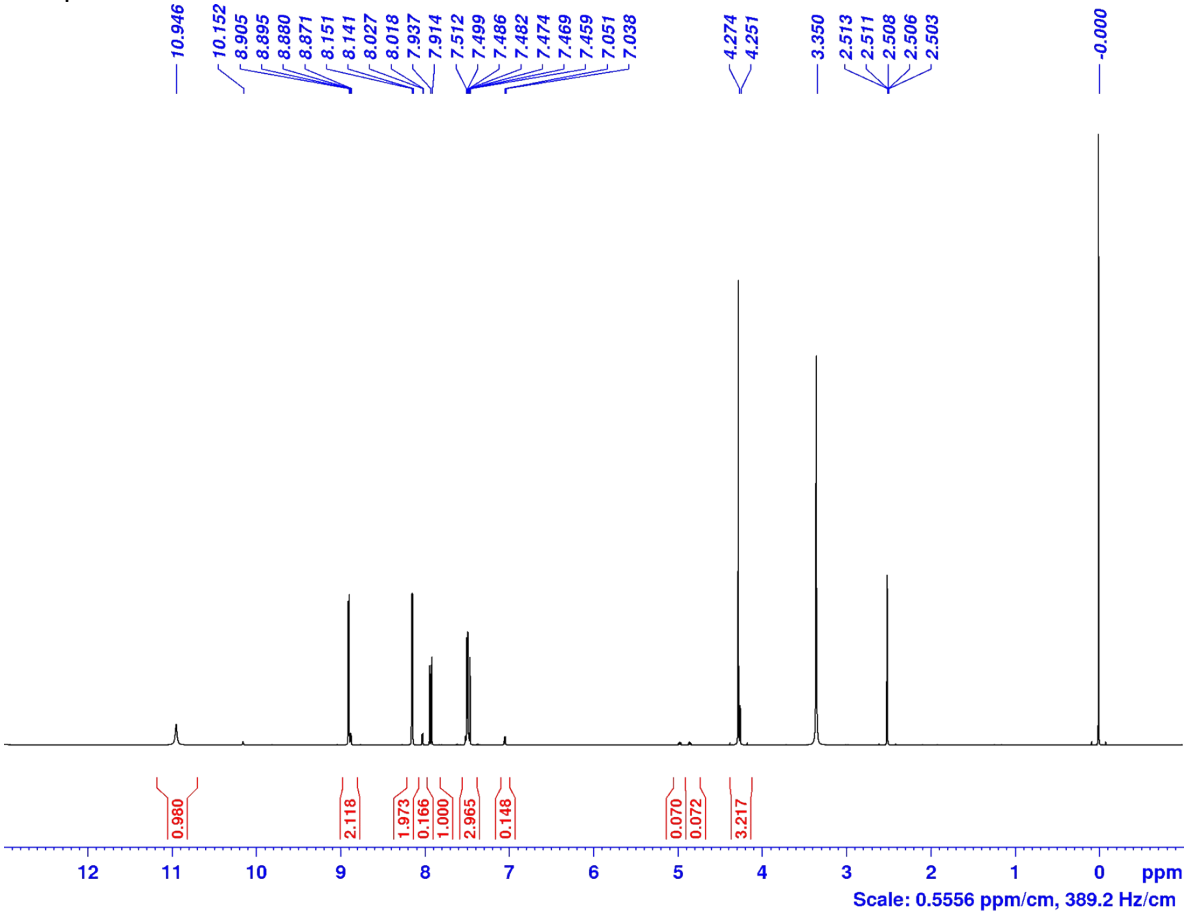


Figure S21: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **1i**.

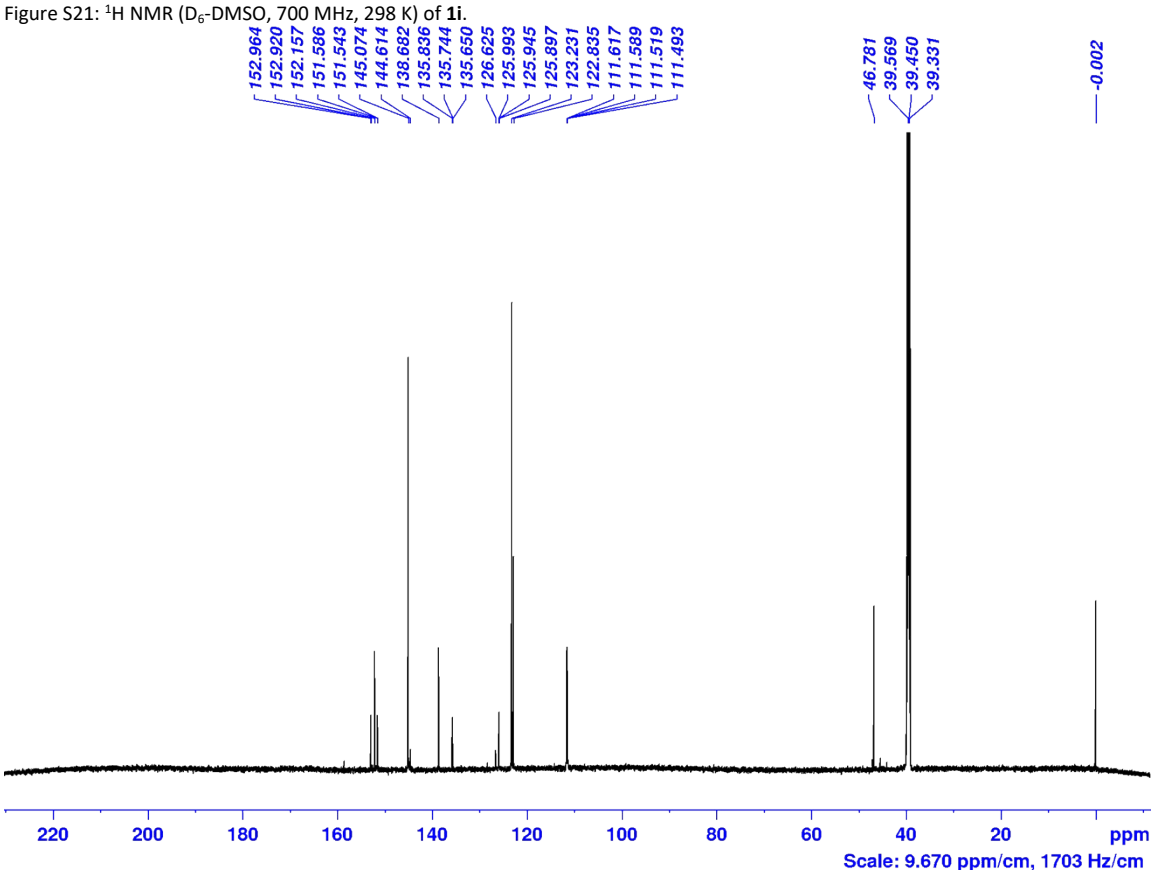


Figure S22: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **1i**.

Compound **2g**.

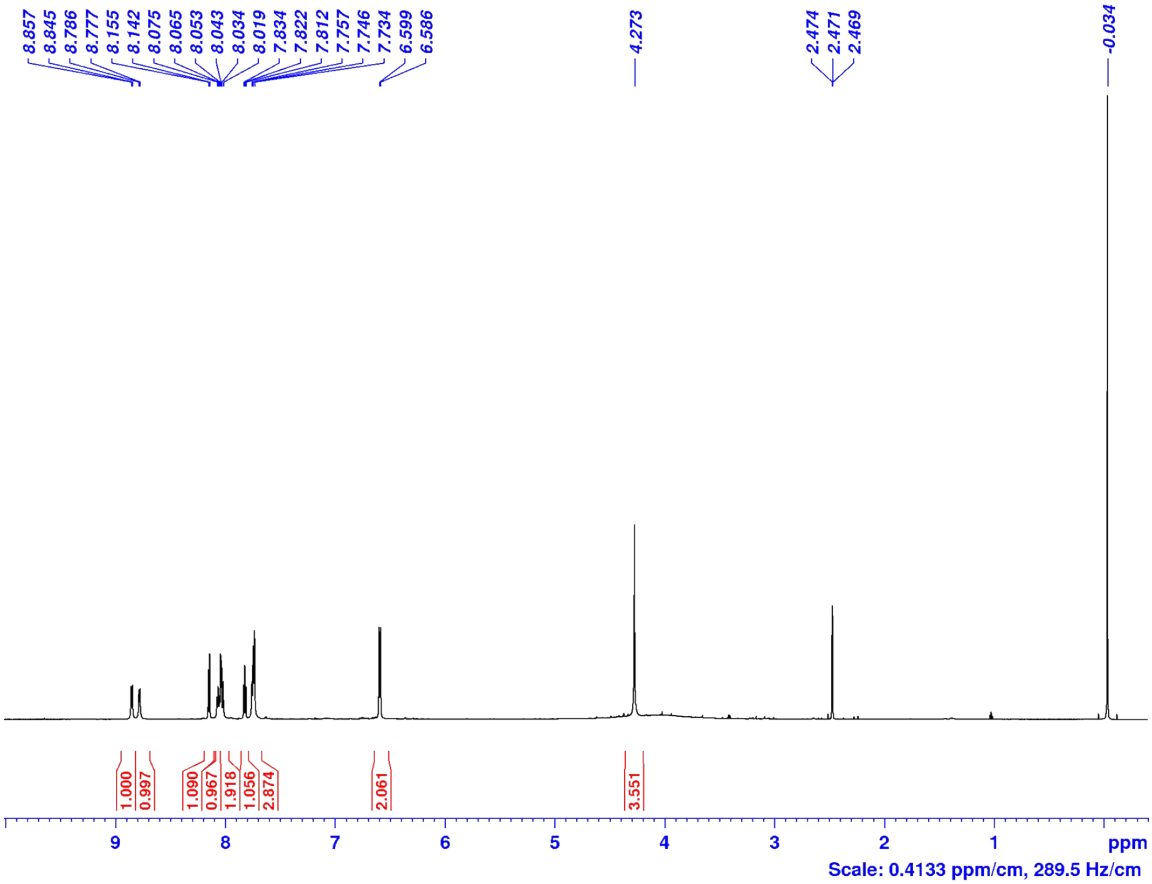


Figure S23: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **2g**.

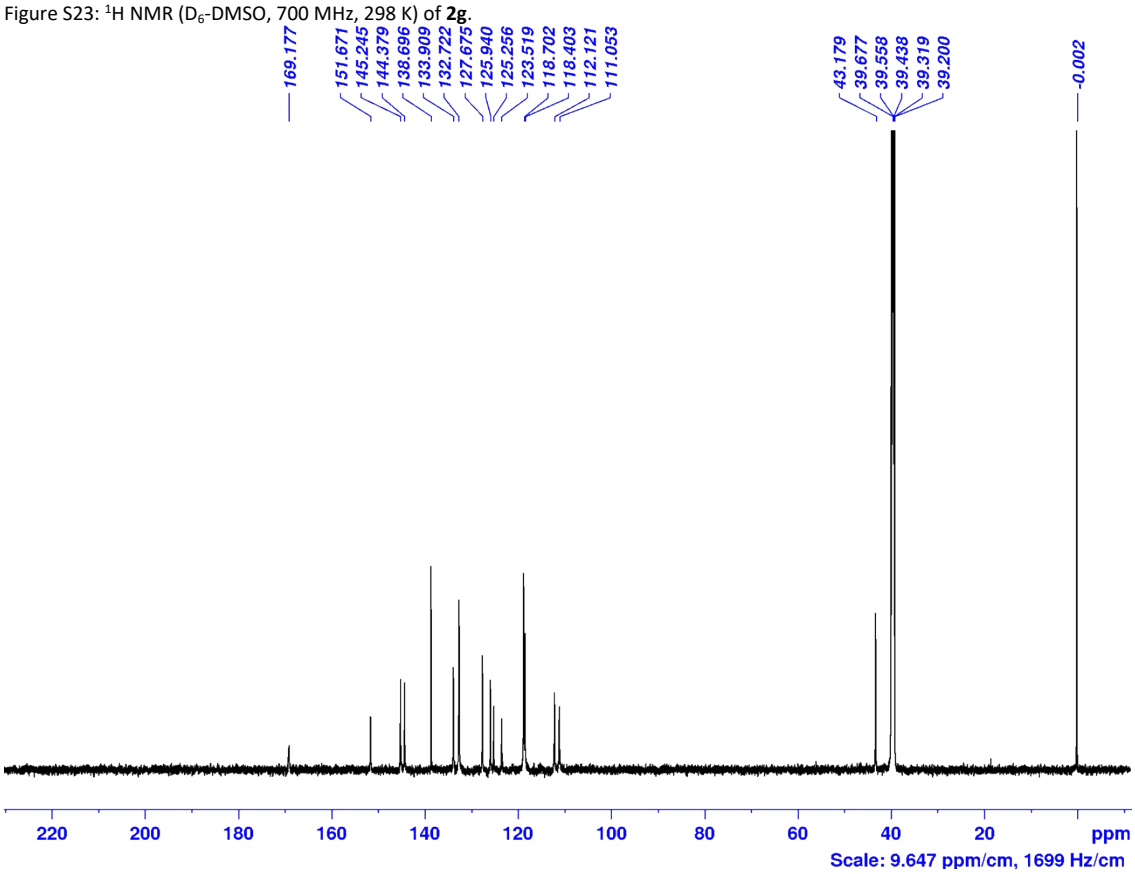


Figure S24: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **2g**.

Compound **2i**.

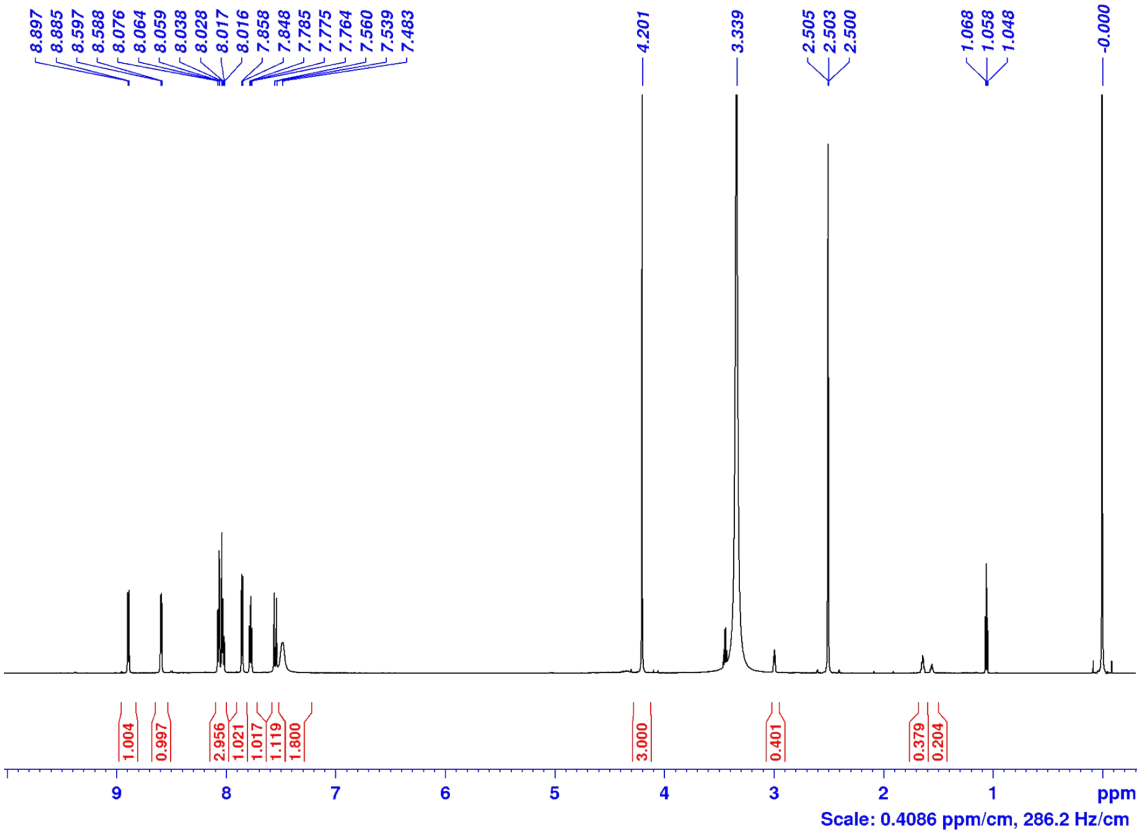


Figure S25: ^{1}H NMR (D_6-DMSO, 700 MHz, 298 K) of **2i**.

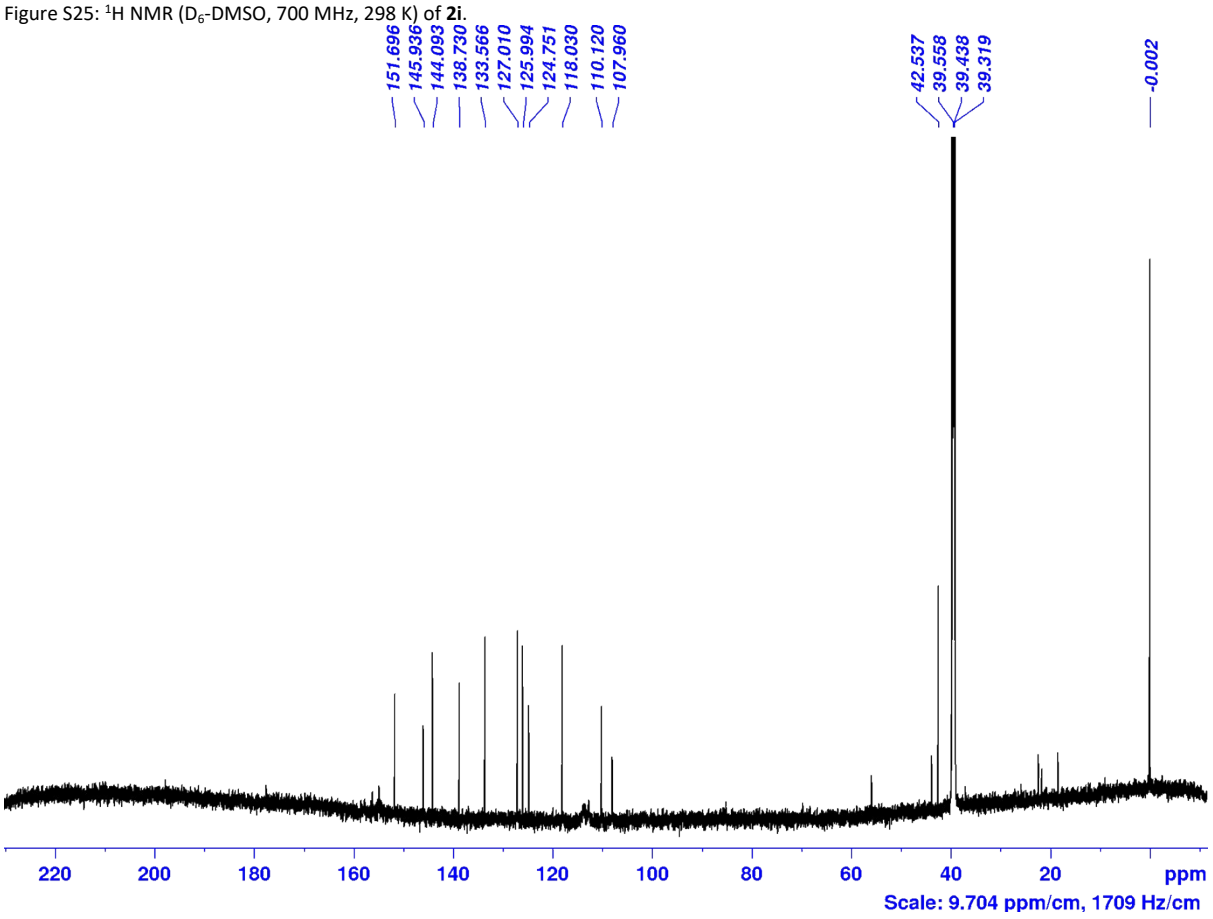


Figure S26: ^{13}C NMR (D_6-DMSO, 176 MHz, 298 K) of **2i**.

3. UV-visible absorbance

Compound **1a**.

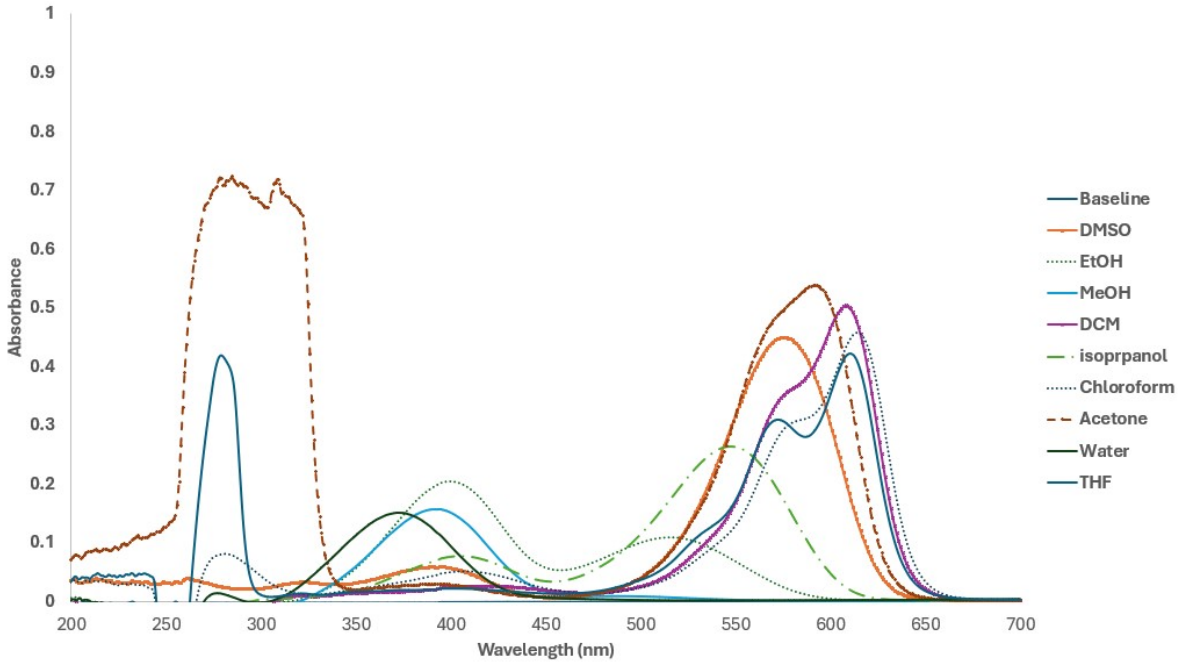


Figure S27: UV–vis absorption spectrum of compound **1a**, recorded in various solvents at 10 µM.

Compound **1b**.

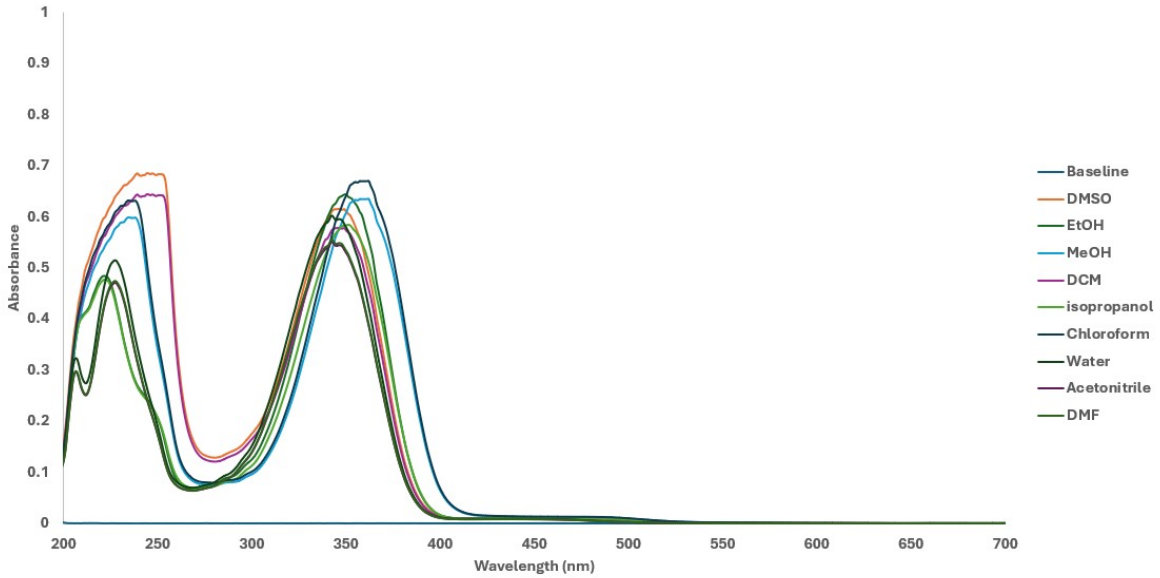


Figure S28: UV–vis absorption spectrum of compound **1b**, recorded in various solvents at 10 µM.

Compound **1c**.

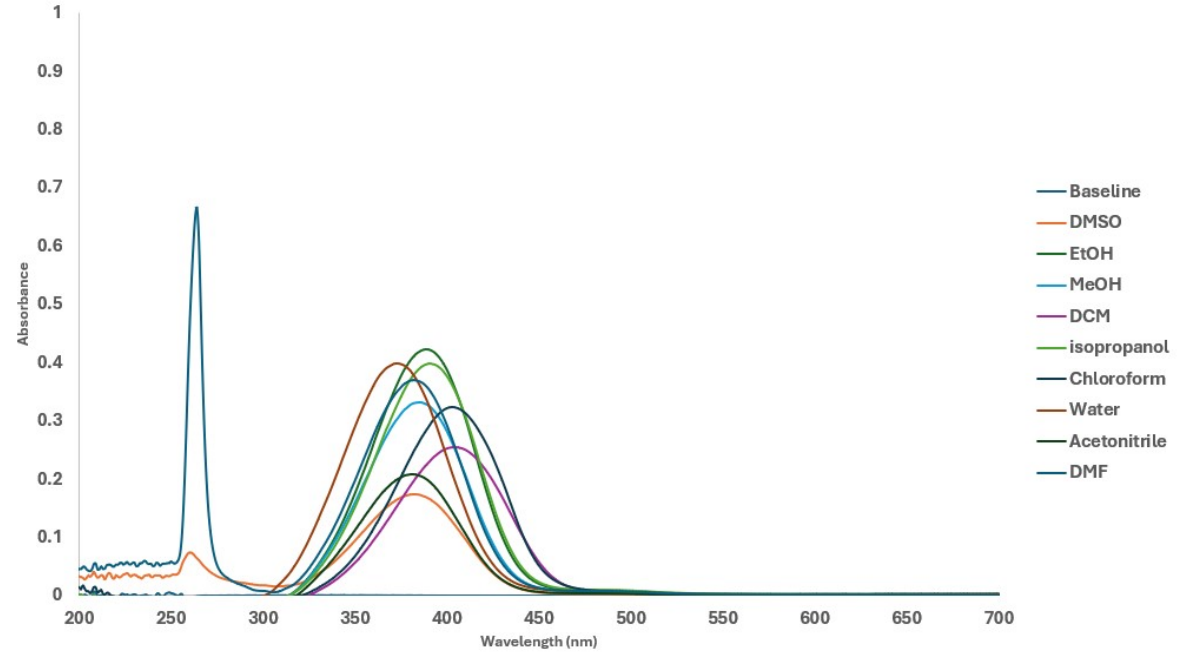


Figure S29: UV–vis absorption spectrum of compound **1c**, recorded in various solvents at 10 µM.

Compound **1e**.

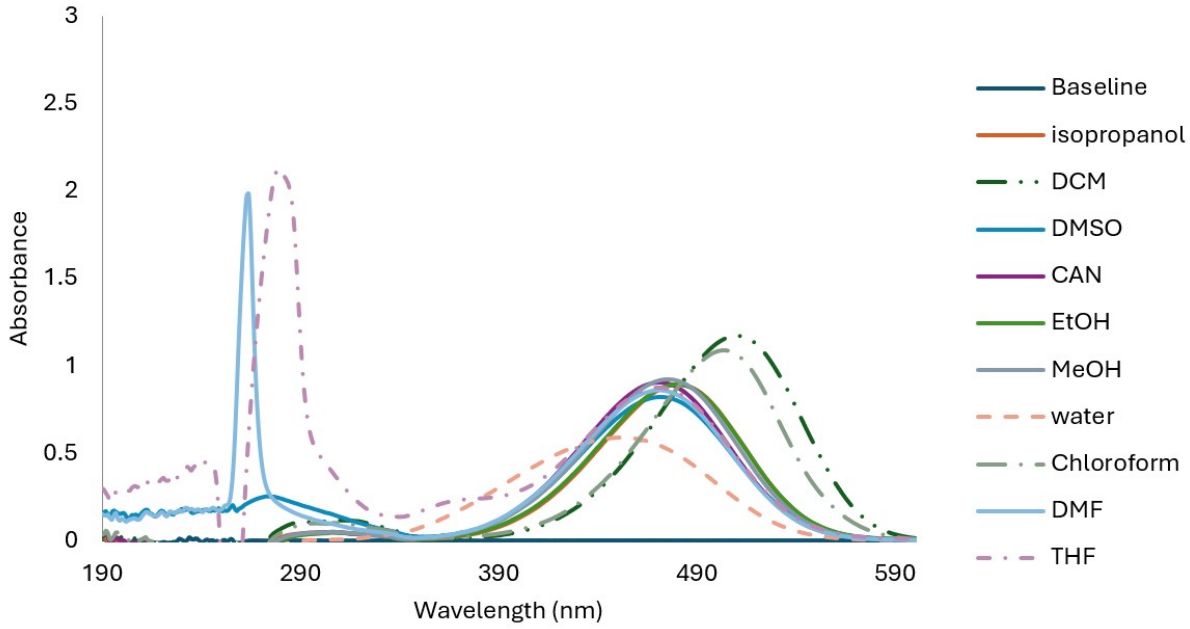


Figure S30: UV–vis absorption spectrum of compound **1e**, recorded in various solvents at 50 µM.

4. Additional graphs

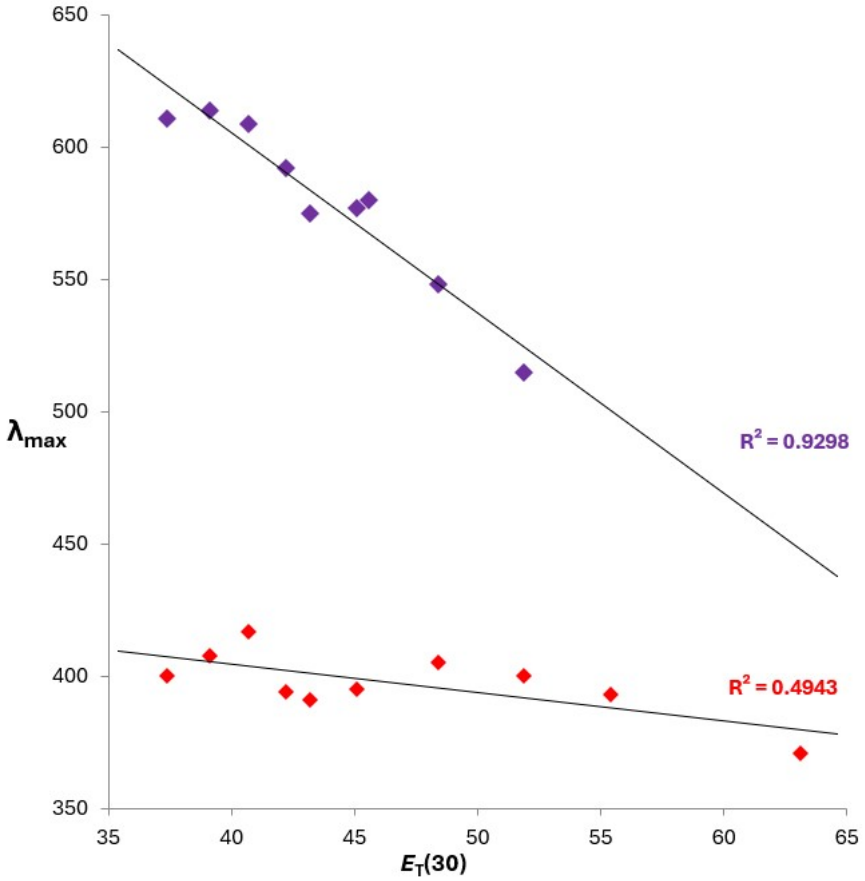


Figure S31: λ_{max} (nm) values for **1a**, as a function of the polarity of the solvent [$E_T(30)$ values, in kcal.mol^{-1}]. ranging from THF (least polar) to water (most polar).

5. Crystallographic data

Compound 1b

The single-crystal of orange block material of **compound 1b** was recrystallised by vapour diffusion of Et_2O into a saturated solution in $CHCl_3$. A suitable crystal was selected and mounted on a Paratone–N oil and mounted on a Rigaku Oxford Diffraction - XtaLAB Synergy-S at 100K. Data collection was performed using monochromated Mo Kα radiation, λ = 0.71073 Å using ϕ and ω scans to cover the Ewald sphere. Accurate cell parameters were obtained with the amount of indicated reflections. Using Olex2,[2] the structure was solved with the olex2.solve,[3] structure solution program using Charge Flipping and refined with the ShelXL[4] refinement package using Least Squares minimization. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Software used for molecular graphics: Mercury 2022.3.0.

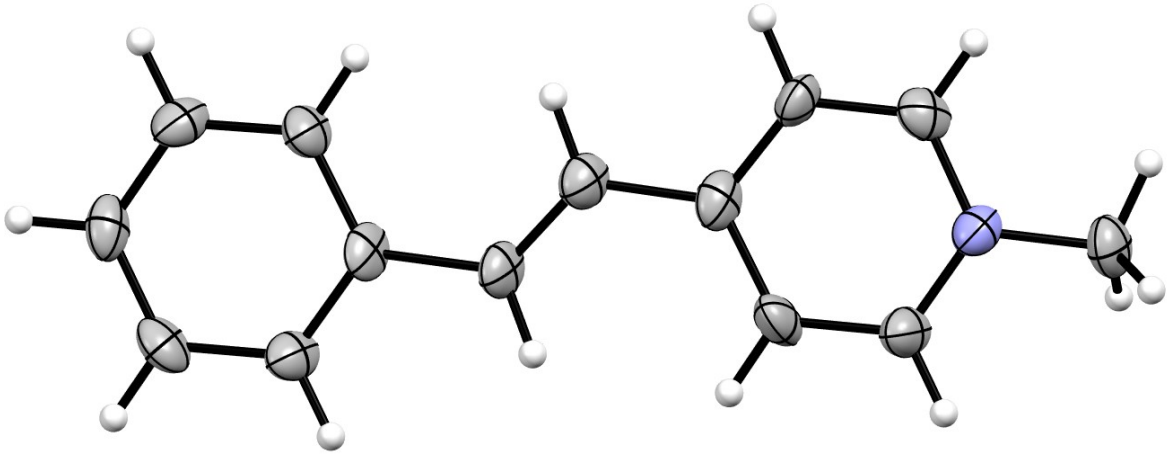


Figure S32: Solid state structure of **compound 1b** shown in ORTEP mode. Ellipsoids are shown at 50% probability.

Crystal data	**1 b**
Empirical formula	$C_{14}H_{16}INO$
Formula weight	341.18
Temperature (K)	100.15
Wavelength (Å)	1.54184
Crystal system,	monoclinic
space group	$P2_1/n$
a (Å)	7.3941(10)
b (Å)	10.5533(14)
c (Å)	17.659(2)
alpha	90
beta	96.310(12)
gamma	90
Volume (Å3)	1369.6(3)
Z	4
Calculated density (mg/m3)	1.655
Absorption coefficient (mm-1)	18.238
F(000)	672
Crystal size (mm)	0.18 × 0.18 × 0.15
2Theta range	9.78 - 141.984
Reflection collected/unique	5658 / 2433
Rint	0.0893
Completeness (%)	96.4
Absorption correction	semi-empirical
Data/restraints/ parameters	2433/151/164
Goodness-of-fit on F^2	1.095
R1, wR2 [I>2sigma(I)]	0.0798, 0.2147
R1, wR2 (all data)	0.0972, 0.2404
Largest diff. peak and hole	1.68/-2.34
Diffractometer	XtaLAB Synergy-S

Compound 3

The single-crystal of colorless block material of **compound 3** was recrystallised by slow evaporation of saturated solution in $CHCl_3$. A suitable crystal was selected and mounted on a Paratone–N oil and mounted on a Rigaku Oxford Diffraction - XtaLAB Synergy-S at 100K. Data collection was performed using monochromated Mo Kα radiation, λ = 0.71073 Å using ϕ and ω scans to cover the Ewald sphere. Accurate cell parameters were obtained with the amount of indicated reflections. Using Olex2,[2] the structure was solved with the olex2.solve,[3] structure solution program using Charge Flipping and refined with the ShelXL[4] refinement package using Least Squares minimization. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Software used for molecular graphics: Mercury 2022.3.0.

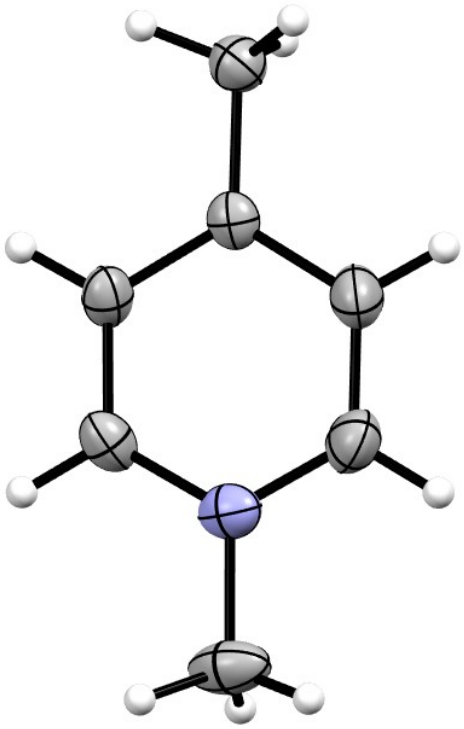


Figure S33: Solid state structure of **compound 3** shown in ORTEP mode. Ellipsoids are shown at 50% probability.

Crystal data	**3**
Empirical formula	$C_7H_{10}IN$
Formula weight	235.06
Temperature (K)	100.15
Wavelength (Å)	0.71073
Crystal system,	monoclinic
space group	$P2_1/c$
a (Å)	13.7854(6)
b (Å)	19.6358(7)
c (Å)	10.1873(5)
alpha	90
beta	109.428(5)
gamma	90
Volume (Å3)	2600.5(2)
Z	12
Calculated density (mg/m3)	1.801
Absorption coefficient (mm-1)	3.616
F(000)	1344
Crystal size (mm)	0.33 × 0.33 × 0.3
2Theta range	4.72 - 60.026
Reflection collected/unique	22226 / 5941
Rint	0.0451
Completeness (%)	99.7
Absorption correction	semi-empirical
Data/restraints/ parameters	5941/0/250
Goodness-of-fit on F^2	1.033
R1, wR2 [I>2sigma(I)]	0.0376, 0.0915
R1, wR2 (all data)	0.0451, 0.0951
Largest diff. peak and hole	0.87/-1.93
Diffractometer	XtaLAB Synergy-S

6. References and Notes

1. The OH proton (11) signals were not detected in the NMR spectra of this compound even in DMSO-d_6, likely due to rapid exchange and/or broadening effects.
2. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A.; Puschmann, H., OLEX2: a complete structure solution, refinement and analysis program. *Applied Crystallography* **2009,** *42*, 339-341.
3. Bourhis, L. J.; Dolomanov, O. V.; Gildea, R. J.; Howard, J. A.; Puschmann, H., The anatomy of a comprehensive constrained, restrained refinement program for the modern computing environment–Olex2 dissected. *Foundations of Crystallography* **2015,** *71*, 59-75.
4. Sheldrick, G. M., Crystal structure refinement with SHELXL. *Crystal Structure Communications* **2015,** *71*, 3-8.