Supporting Information

A New Tetra-arylcyclopentadienone Based Low Molecular Weigth Gelator: Synthesis, Self-Assembly Properties and Anion Recognition

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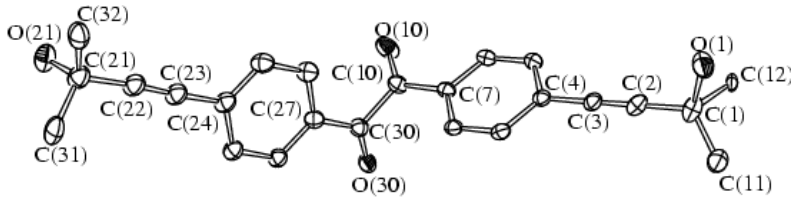


Figure 1S. ORTEP drawing of **6a** with key atoms labelled. Displacement ellipsoids are at the 30% probability level. H-atoms have been omitted for clarity. Only the main images of the disordered groups are represented.

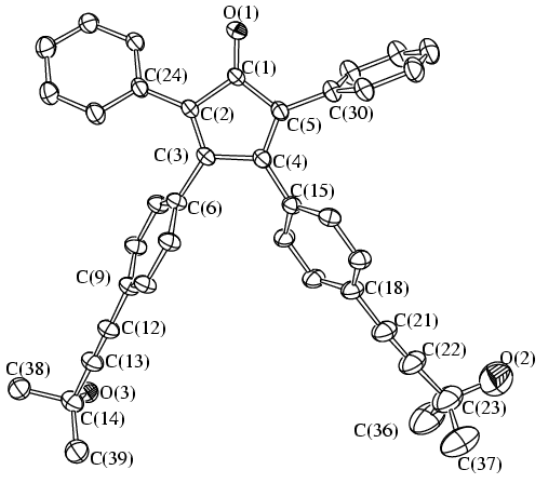


Figure 2S. ORTEP drawing of **1a** with key atoms labelled. Displacement ellipsoids are at the 30% probability level. H-atoms have been omitted for clarity. Only the main images of the disordered groups are represented.

Table 1S. Selected Bond Lengths (Å) and angles (°) for **6a**. Only the main images of disordered groups are considered.

C(10)-C(30)	1.538(6)		
C(10)-O(10)	1.211(5)	C(30)-O(30)	1.213(5)
C(7)-C(10)	1.466(6)	C(27)-C(30)	1.444(7)
C(3)-C(4)	1.434(6)	C(23)-C(24)	1.431(9)
C(2)-C(3)	1.193(6)	C(22)-C(23)	1.171(11)
C(1)-C(2)	1.471(6)	C(21)-C(22)	1.462(12)
O(10)-C(10)-C(7)	123.4(4)	O(30)-C(30)-C(27)	127.8(5)
O(10)-C(10)-C(30)	117.6(4)	O(30)-C(30)-C(10)	115.8(4)
C(7)-C(10)-C(30)	118.9(4)	C(27)-C(30)-C(10)	116.2(5)
C(2)-C(3)-C(4)	177.4(5)	C(22)-C(23)-C(24)	175.3(12)
C(3)-C(2)-C(1)	179.2(5)	C(23)-C(22)-C(21)	175.6(13)

Table 2S. Selected Bond Lengths (Å) and angles (°) for **1a**. Only the main images of disordered groups are considered.

C(1)-O(1)	1.221(9)	C(3)-C(4)	1.516(11)
C(1)-C(2)	1.520(10)	C(1)-C(5)	1.471(11)
C(2)-C(3)	1.337(10)	C(4)-C(5)	1.354(10)
C(3)-C(6)	1.499(11)	C(4)-C(15)	1.474(11)
C(9)-C(12)	1.438(11)	C(18)-C(21)	1.443(13)
C(12)-C(13)	1.186(11)	C(21)-C(22)	1.189(12)
C(13)-C(14)	1.487(12)	C(22)-C(23)	1.474(15)
C(5)-C(1)-C(2)	108.0(7)	C(3)-C(2)-C(1)	105.6(7)
C(2)-C(3)-C(4)	110.4(7)	C(5)-C(4)-C(3)	108.9(7)
C(4)-C(5)-C(1)	107.1(7)		
C(13)-C(12)-C(9)	173.7(11)	C(22)-C(21)-C(18)	175.1(12)
C(12)-C(13)-C(14)	179.8(12)	C(21)-C(22)-C(23)	176.5(14)

Crystal data and collection details for **1a** and **6a** are listed in Table 6.

Table 3S. Crystal data and details of the structure refinement for **1a** and **6a.**

	1a	**6a**
Formula	$C_{39}H_{32}O_3$	$C_{24}H_{22}O_4$
Fw	548.65	374.42
λ, Å	0.71073	0.71073
Temperature, K	293(2)	100(2)
Crystal system	Triclinic	Monoclinic
Space group	$P\bar{1}$	*C*2/c
a, Å	6.0489(17)	23.681(8)
b, Å	13.222(4)	4.9756(18)
c, Å	20.272(6)	33.914(12)
α, °	73.883(4)	90
β, °	86.839(4)	94.726(5)
γ, °	77.762(4)	90
Cell volume, Å^3	1522.3(7)	3983(2)
Z	2	8
D_c, g cm^{-3}	1.197	1.249
μ, mm^{-1}	0.074	0.084
F(000)	580	1584
θ limits, °	1.64-22.46	2.02-25.03
Reflections collected	11783	17291
Independent reflections	3958 (R_{int} = 0.1420)	3419 (R_{int} = 0.0479)
Data/restraints /parameters	3958/321/377	3419/622/366
Goodness on fit on F^2	1.008	1.020
R1 ($I > 2\sigma$(I))	0.1055	0.0986
wR2 (all data)	0.3554	0.2948
Largest diff. peak and hole, e.Å^{-3}	0.614 and –0.577	0.779 and –0.678

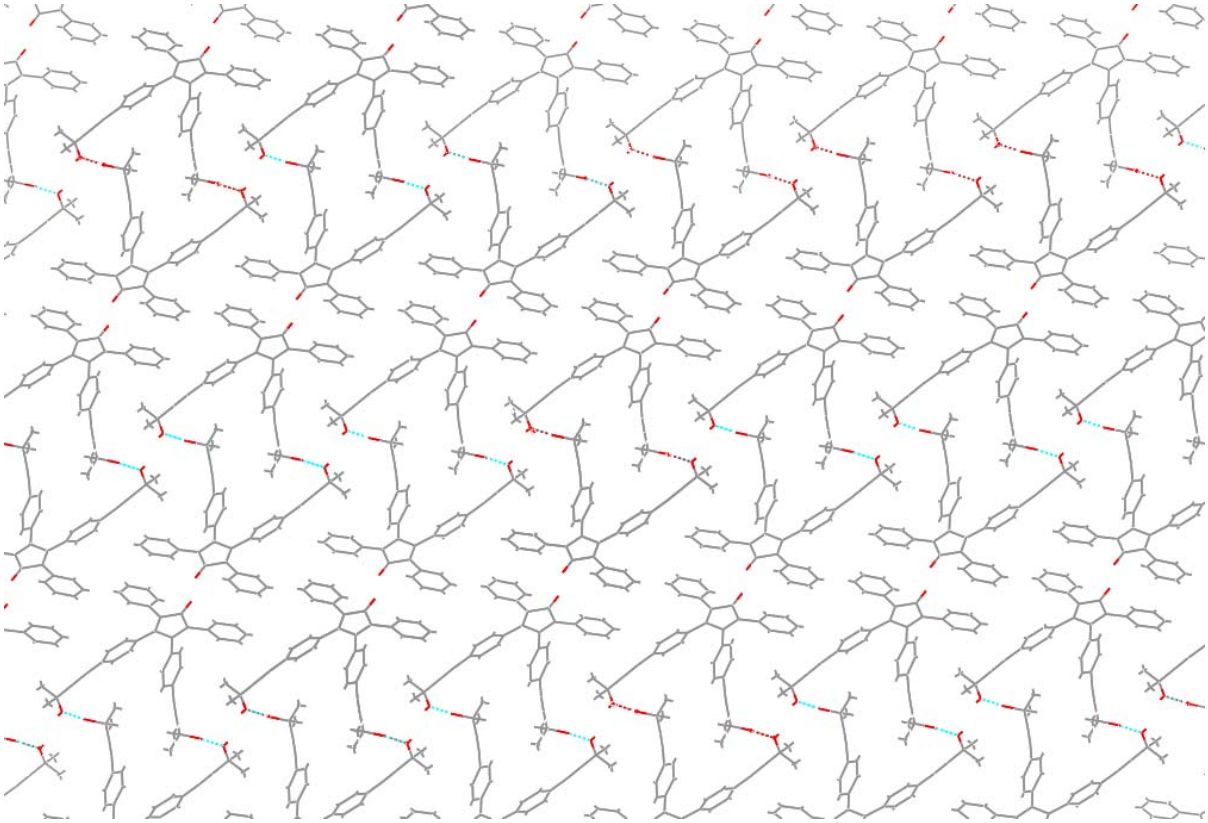


Figure 3S:View along the *a* axis of the crystal packing of **1a**. Oxygen atoms are in red; H-bonds dotted blue lines.

Table 4S: T_g of **1a**-gel in toluene at various concentrations (*c*) and the natural logarithm of the concentration and $1/T_g$ values.

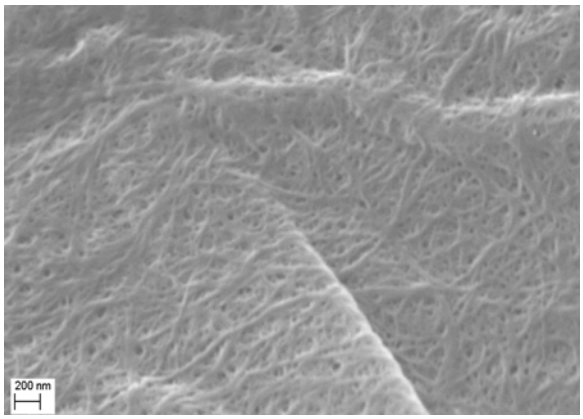
entry	***c* (M)**	**T_g (°K)**	**ln *c***	**1/T**
1	0.01260	323	-4.37406	0.003096
2	0.01360	324	-4.29769	0.003086
3	0.01800	326	-4.01738	0.003067
4	0.02500	329	-3.68888	0.00304
5	0.03650	332	-3.31044	0.003012
6	0.04500	335	-3.10109	0.002985

Table 5S: T_g of **1a**-gel in nitromethane at various concentrations (*c*) and the natural logarithm of the concentration and $1/T_g$ values.

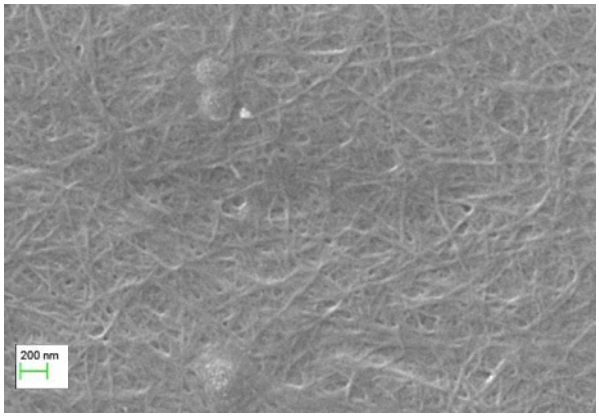
entry	***c* (M)**	**T_g (K)**	**ln *c***	**1/T**
1	0.00869	321	-4.74558	0.003115
2	0.01330	328	-4.31999	0.003049
3	0.02000	333	-3.91202	0.003003
4	0.02600	336	-3.64966	0.002976
5	0.03320	341	-3.40521	0.002933

Figure 4S: SEM images of xerogels of **1a** in various solvents

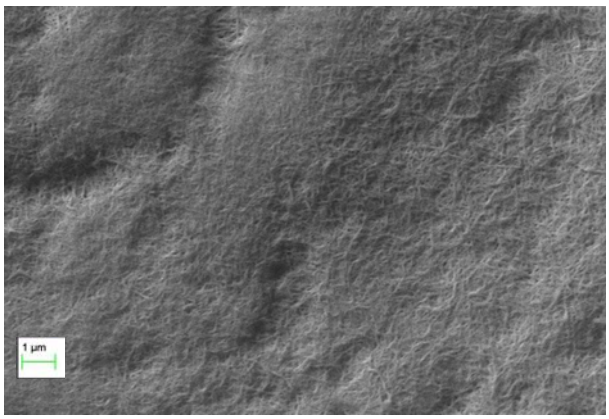
Acetonitrile



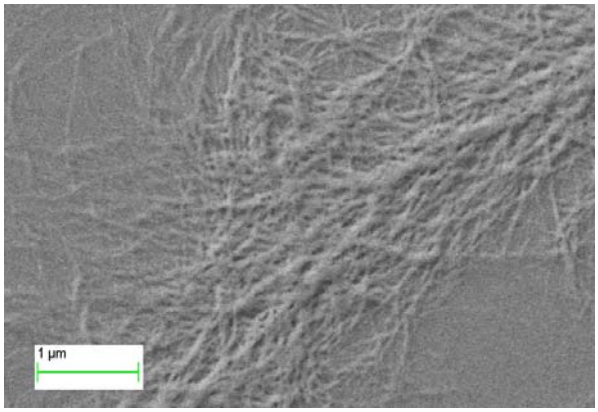
Nitromethane



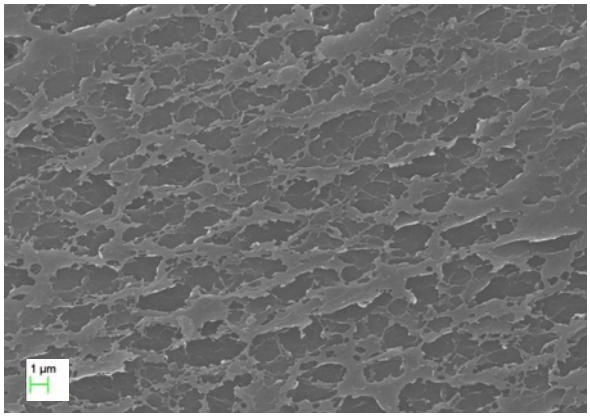
Benzene

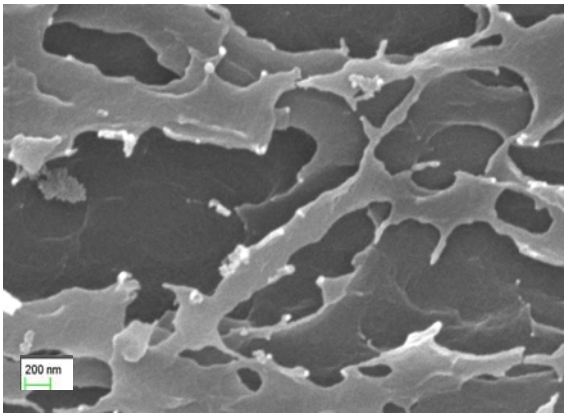


toluene

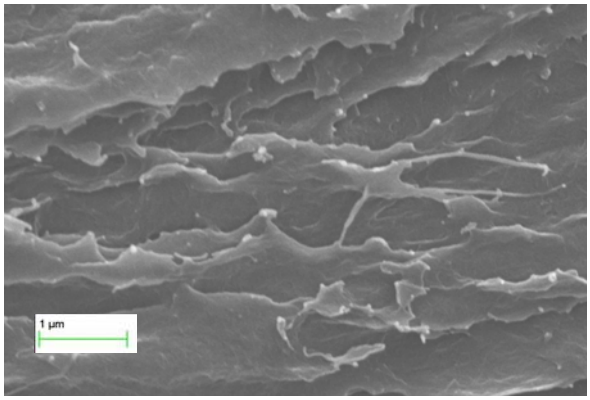


o-xylene

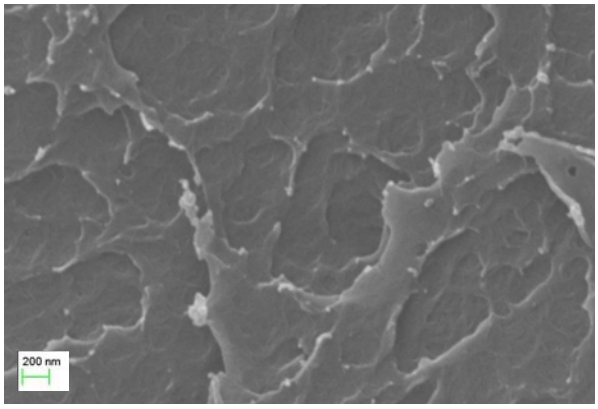


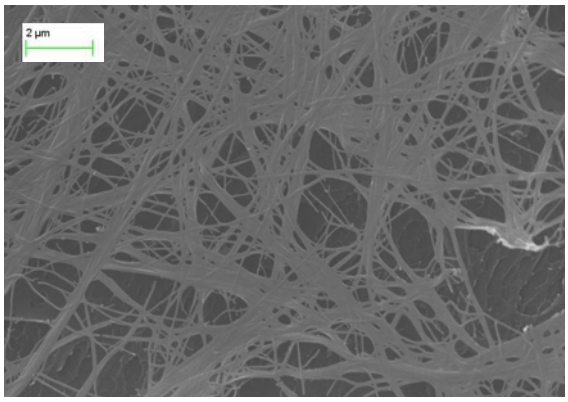


m-xylene



p-xylene





mesitilene

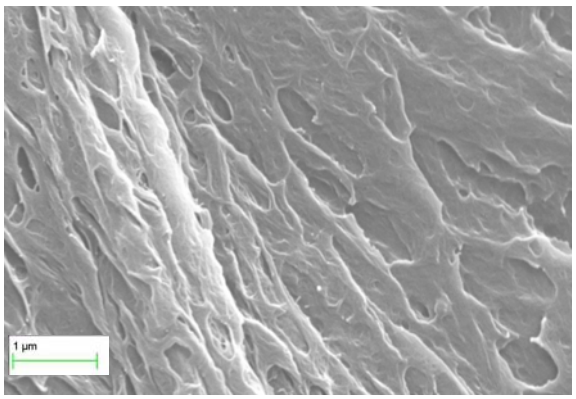


Figure 5S: ^{1}H NMR spectrum of **1a** in CD_3CN (a) and CD_3CN+D_2O (b).

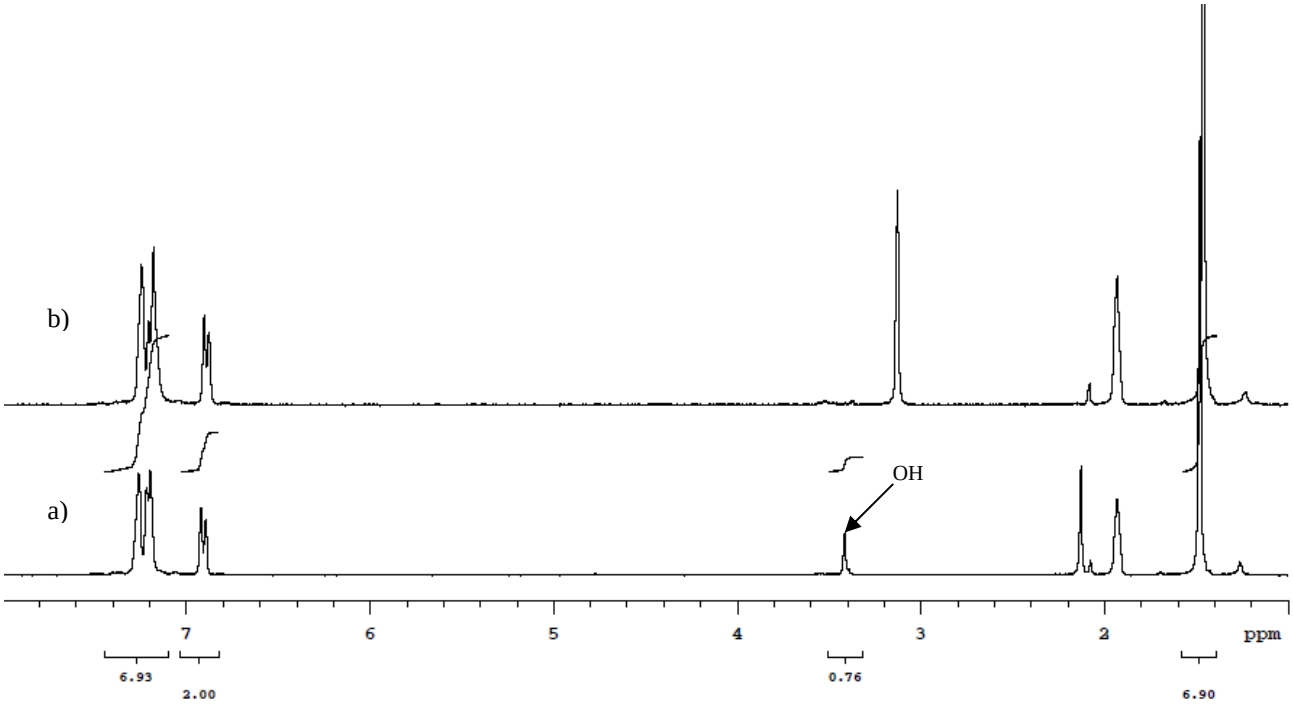


Figure 6S: ^{1}H NMR spectrum of **1a** in CD_3CN at different concentrations at 25°C

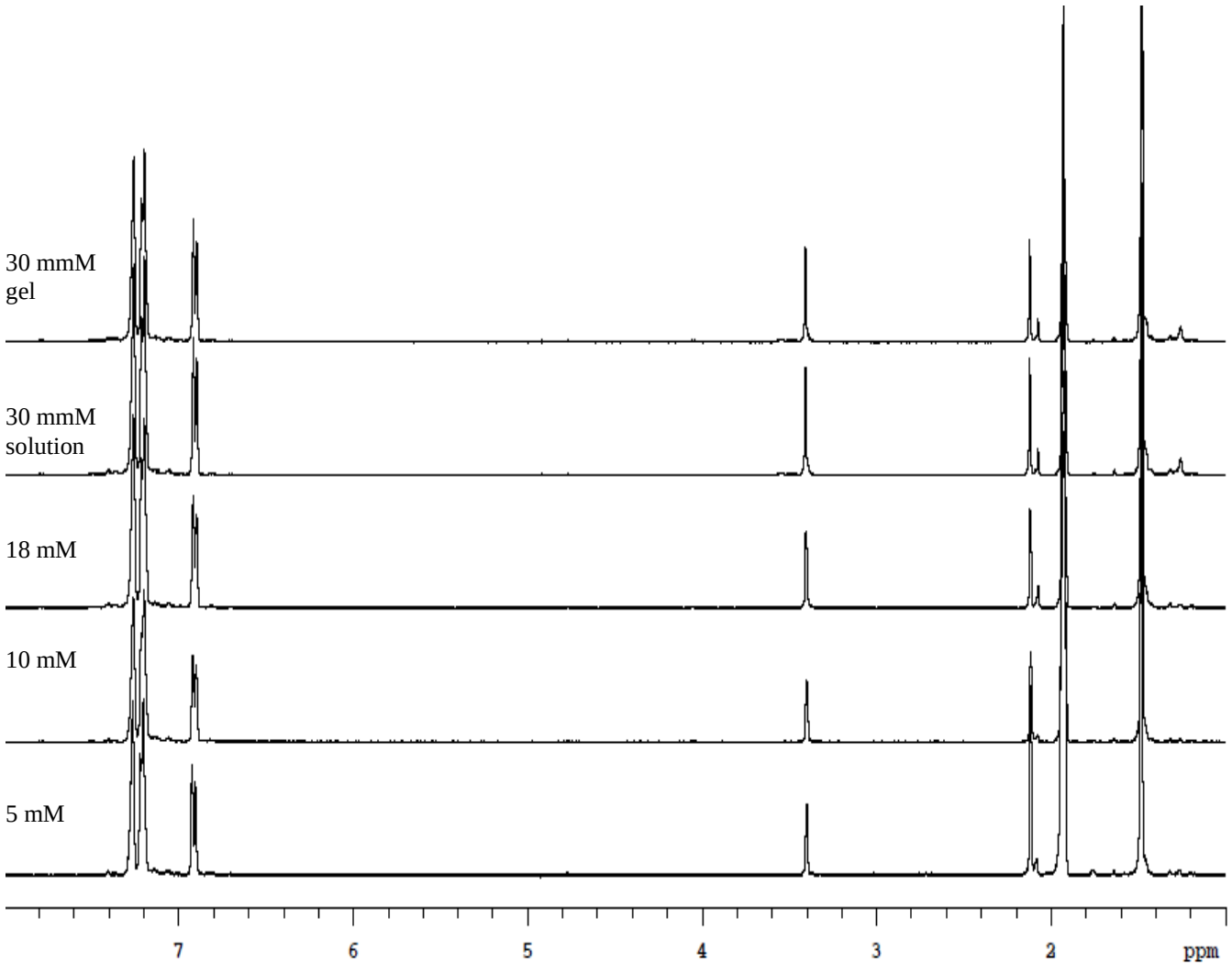


Figure 7S: ^{1}H NMR spectrum of **1a** in CD_3NO_2 at different concentrations at 25°C

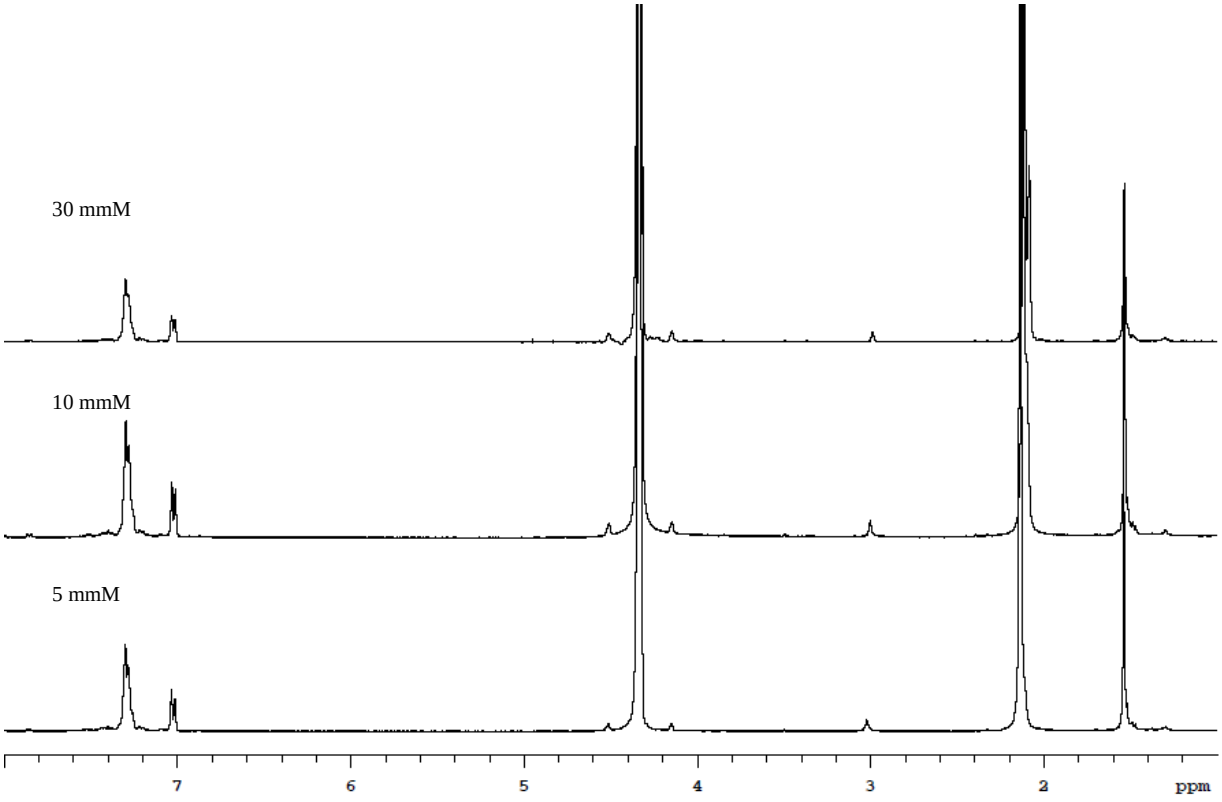


Figure 8S-a, b, c: VT-^{1}H NMR spectra of **1a** in CD_3NO_2 (10mM) ranging from 25 to 85°C

Fig 8S-a

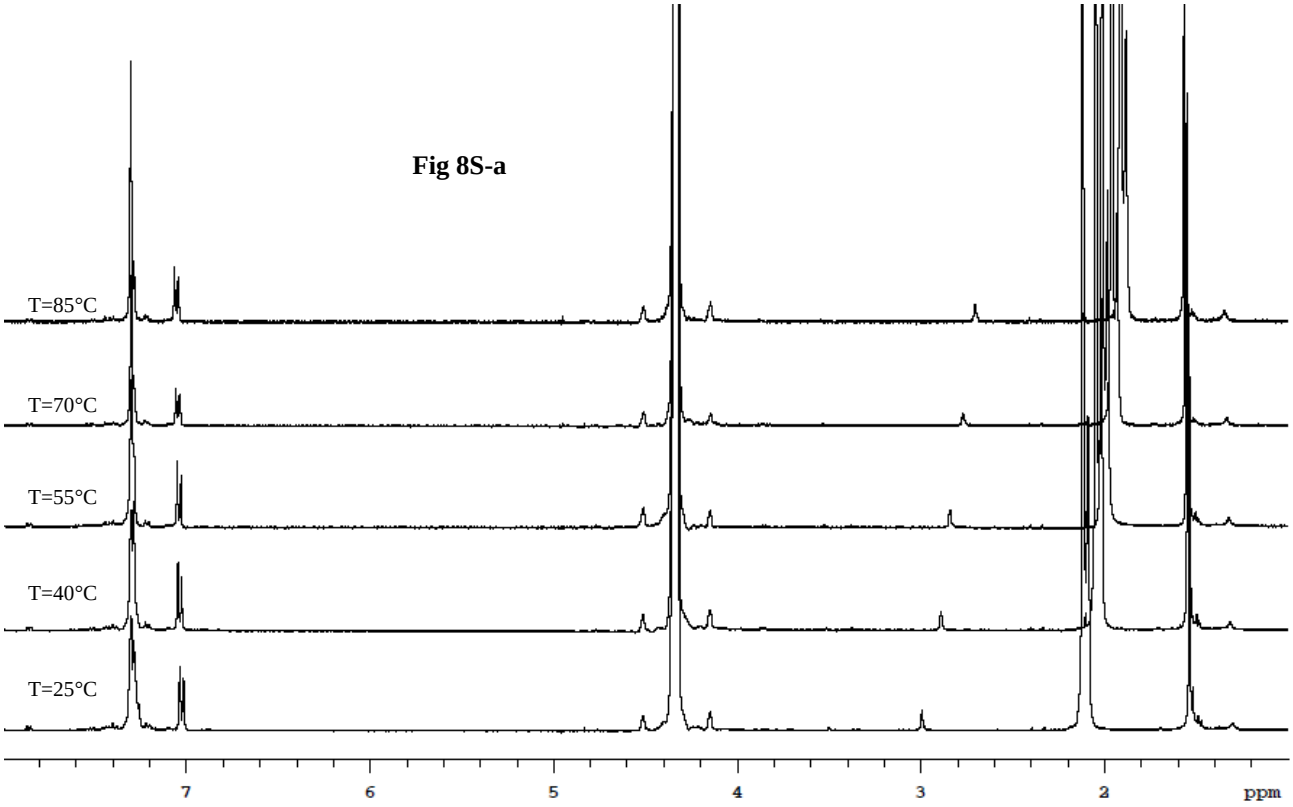


Fig 8S-b

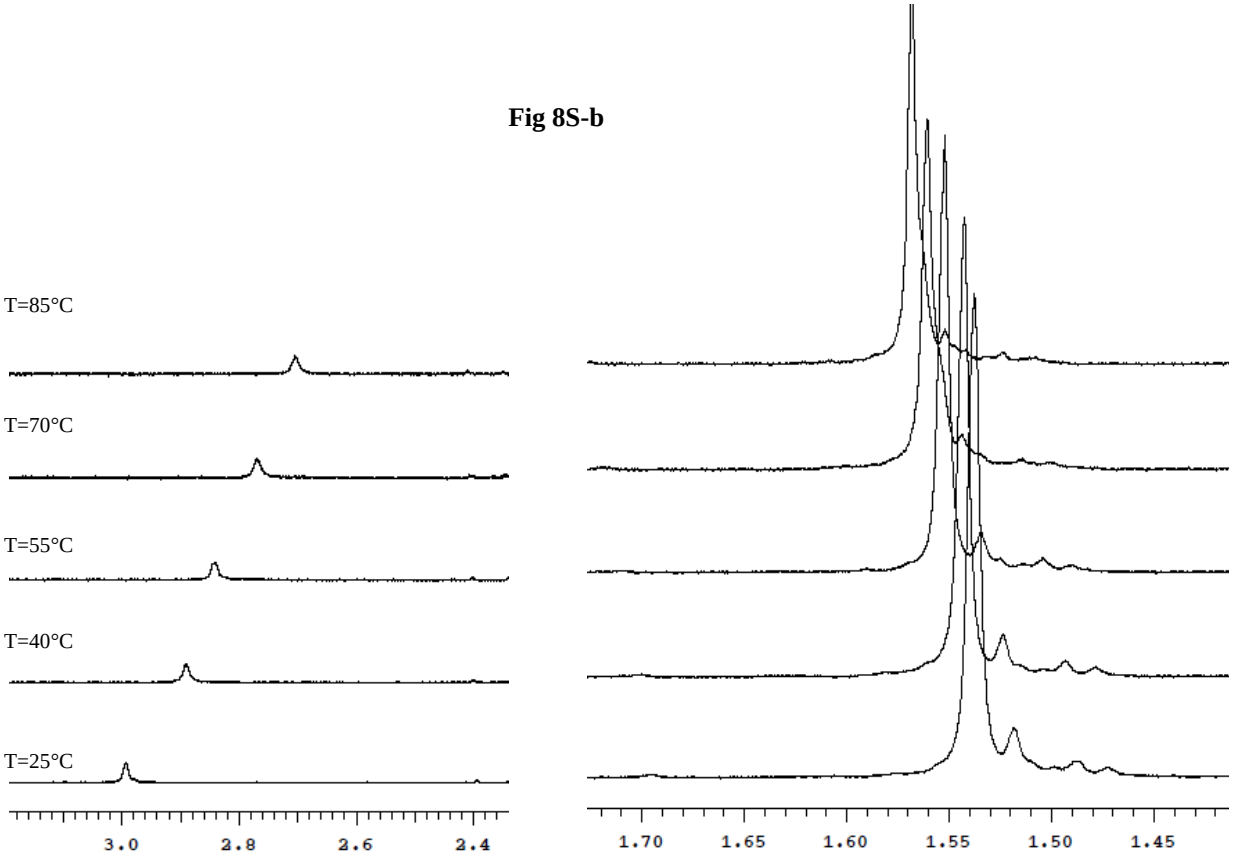


Fig 8S-c

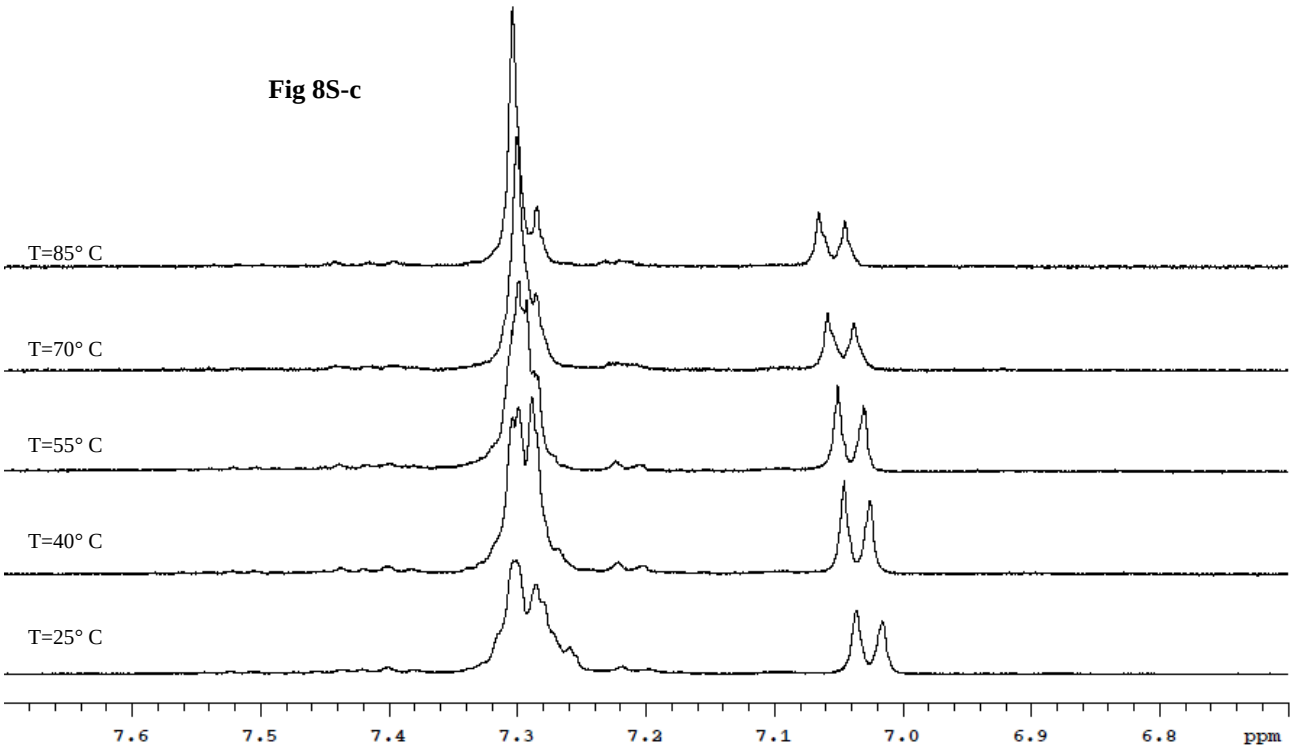


Figure 9S: ^{1}H NMR spectrum of **1a** in toluene at different concentrations at 25°C

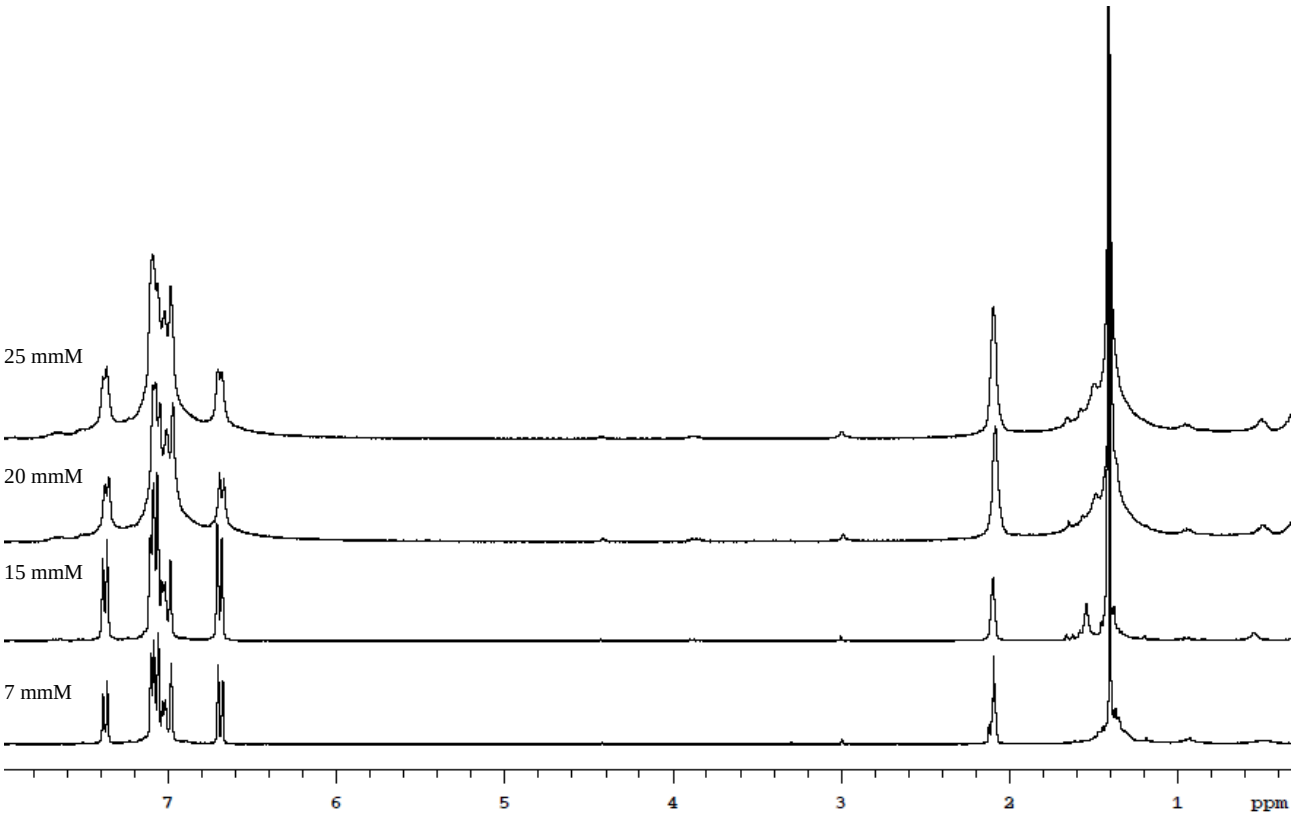


Figure 10S-a, b, c: VT-^{1}H NMR spectra of **1a** in toluene (14.3 mM) ranging from 25 to 85°C

Fig 10S-a

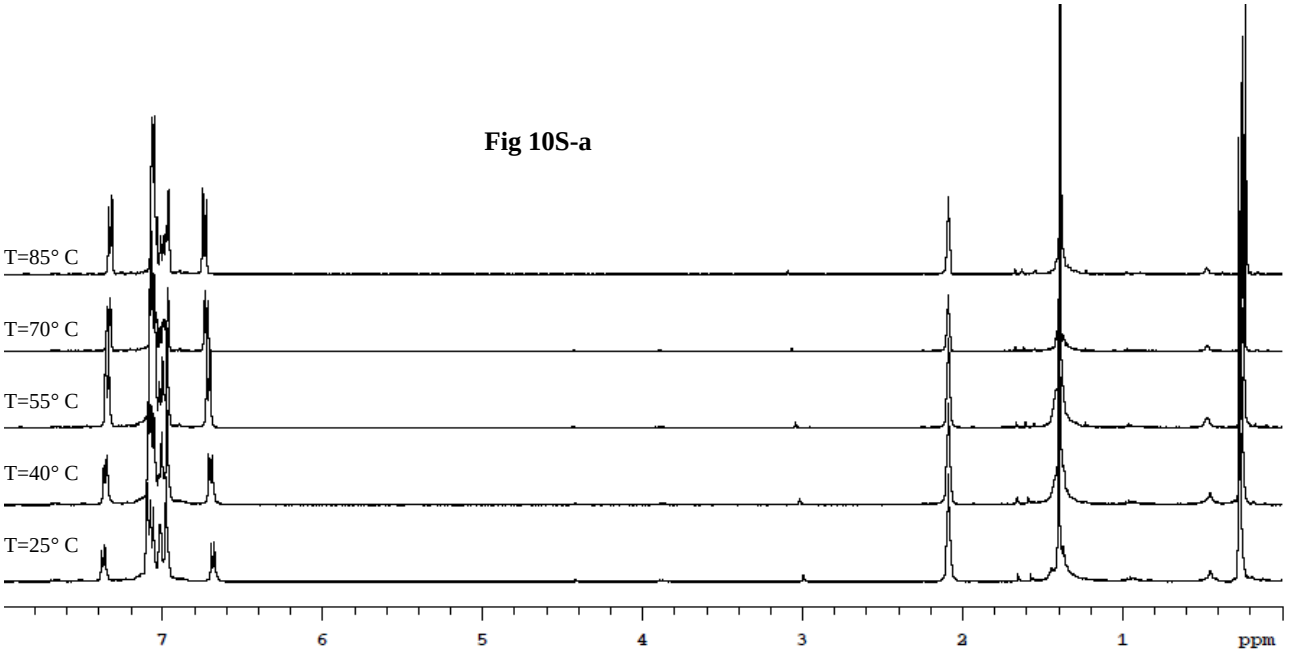


Fig 10S-b

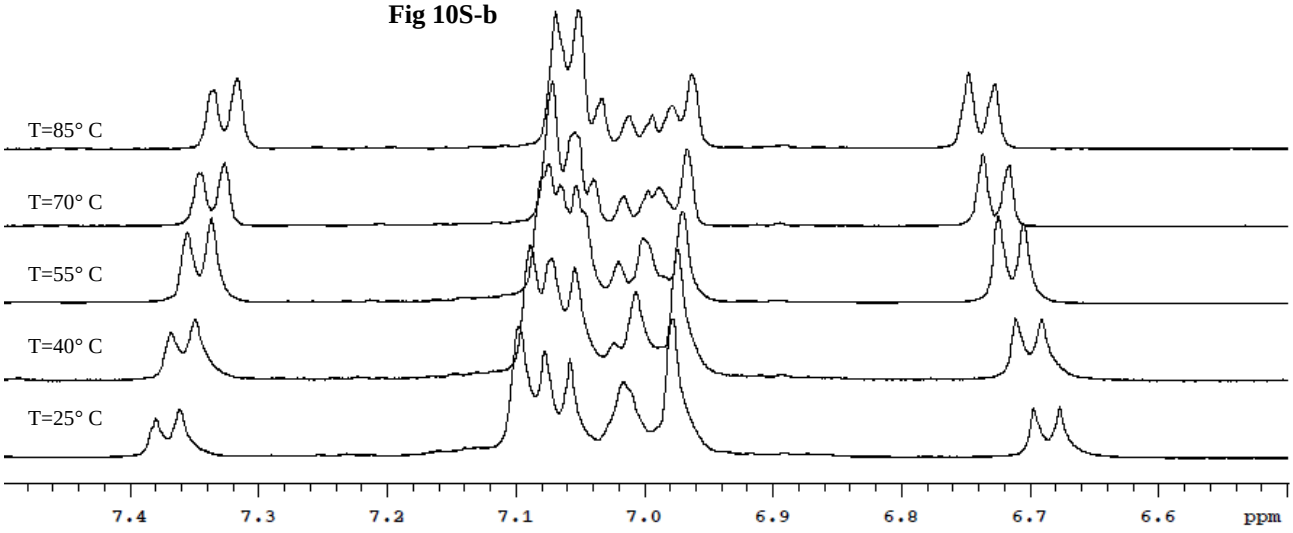


Fig 10S-c

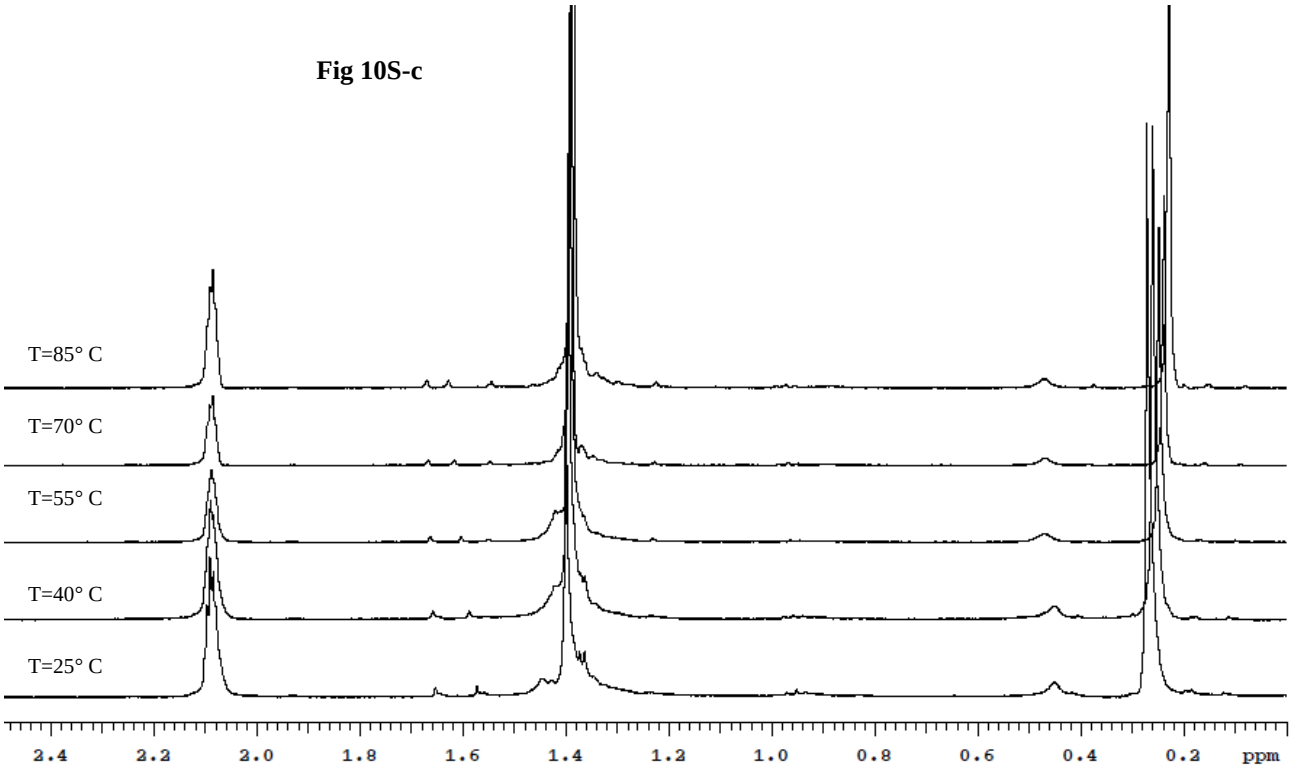
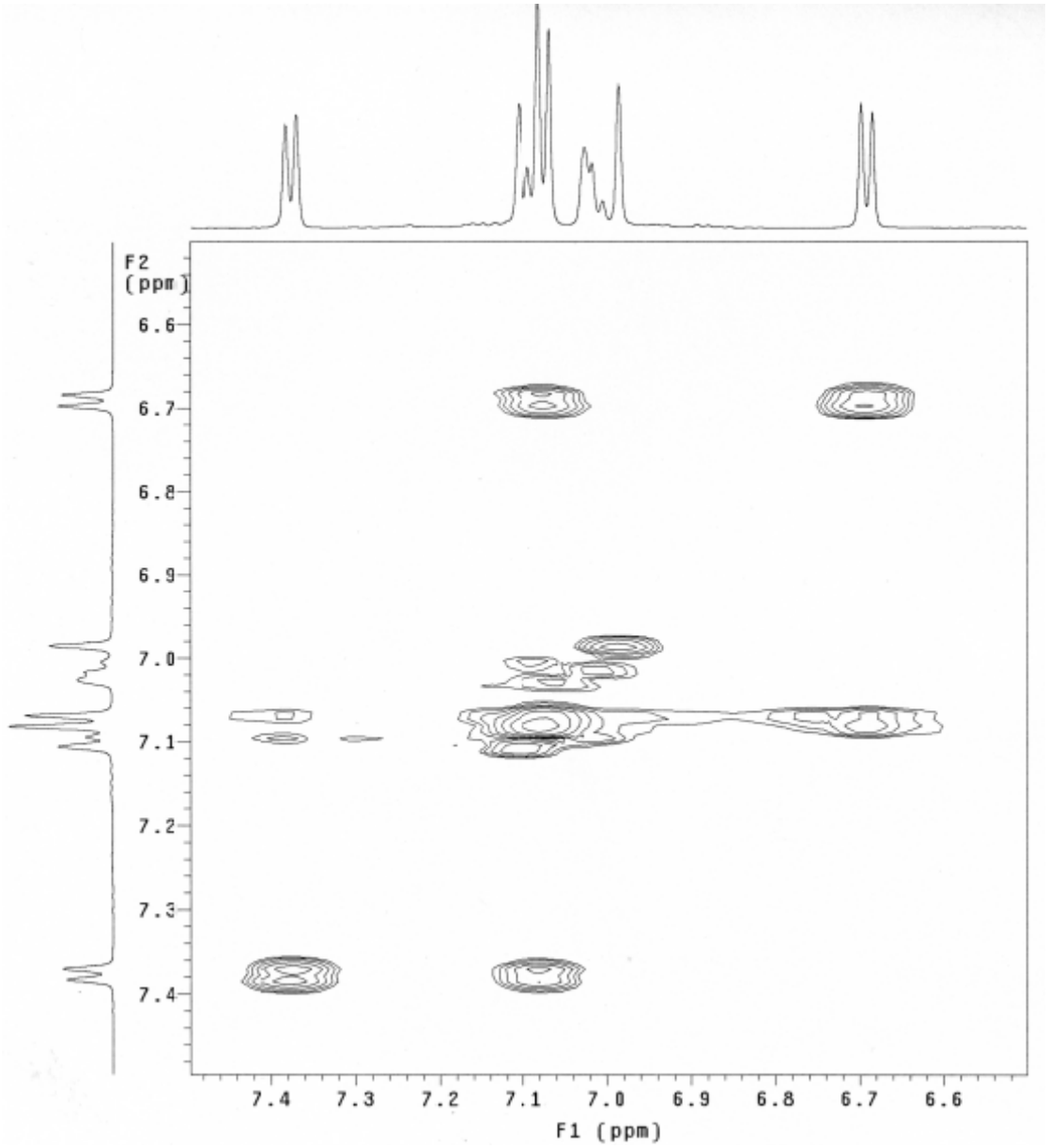


Figure 11S: Particular of COSY-NMR spectrum of **1a**-toluene gel (14.3 mM) at 25°C



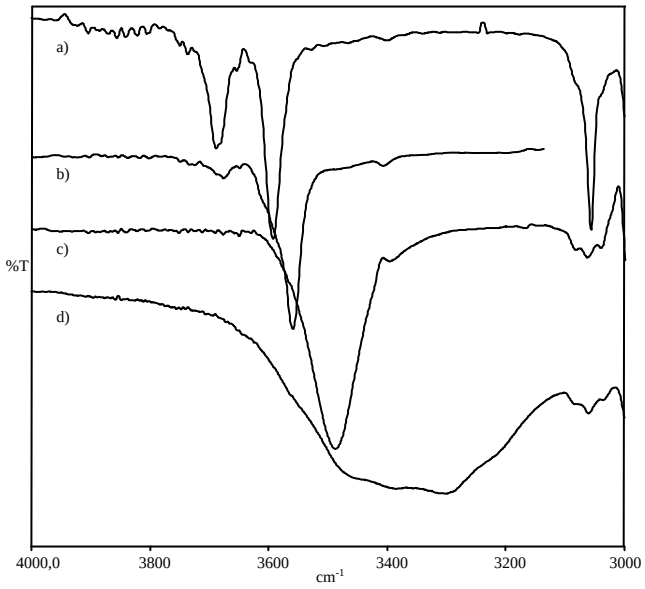
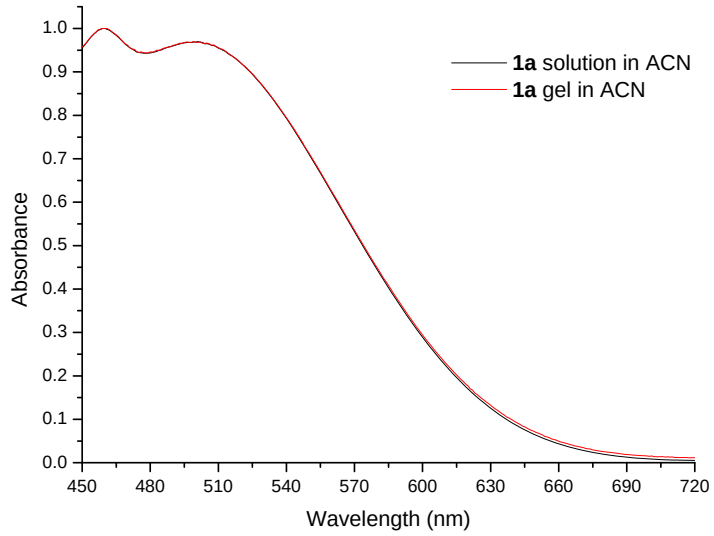


Figure 12S. FT-IR spectra of **1a**: a) in DCM solution, b) in *o*-xylene solution; c) in ACN solution and d) xerogel from *o*-xylene.

a)



b)

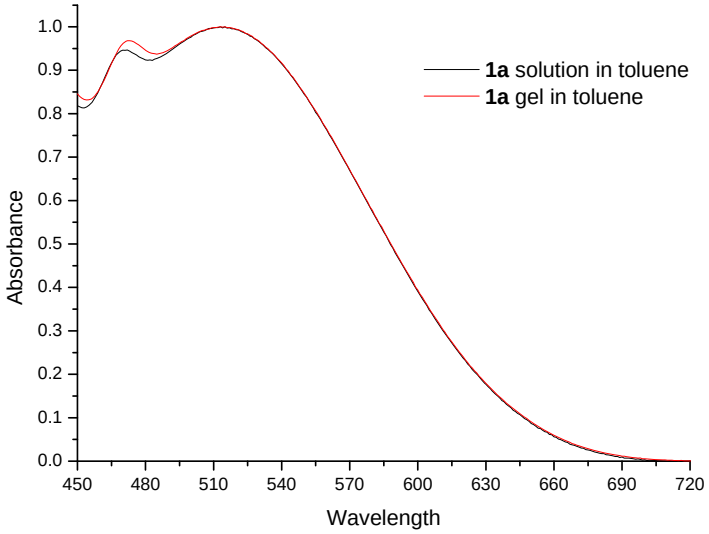
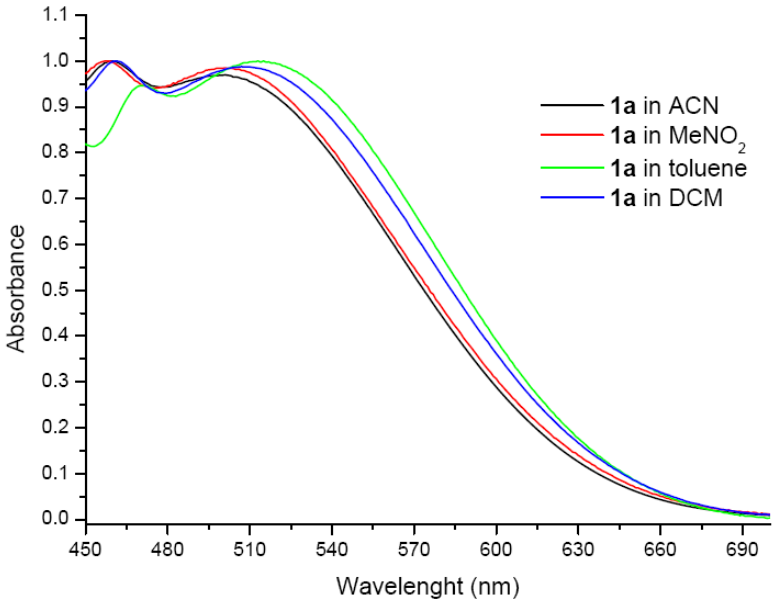


Figure 13S: Normalized UV/Vis absorption spectra at room temperature of **1a** in solution (1.0 mM) and in gel in different solvents. a) in ACN, **1a**-gel =24.0 mM, b) in toluene, **1a**-gel =12.6 mM.

a)



b)

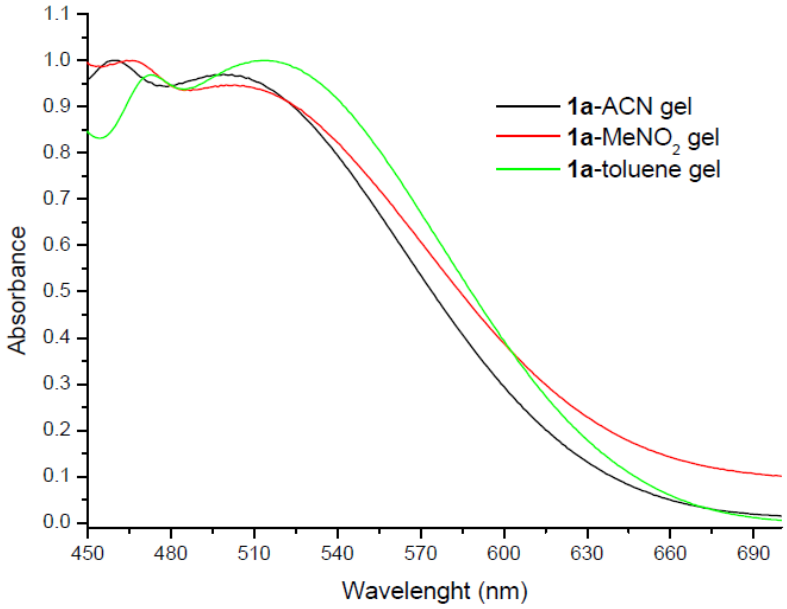


Figure 14S. Normalized UV/Vis absorption spectra at room temperature. a) **1a**-solutions (1.0 mM) in ACN, $MeNO_2$, toluene and DCM; b) **1a**-gel in ACN (24.0 mM), $MeNO_2$ (8.7 mM) and toluene (12.6 mM)