

Supplementary

NMR spectra (in DMSO-d₆) of SCX4, TSCX4, SCX6 hosts, Rh6G and their complexes.

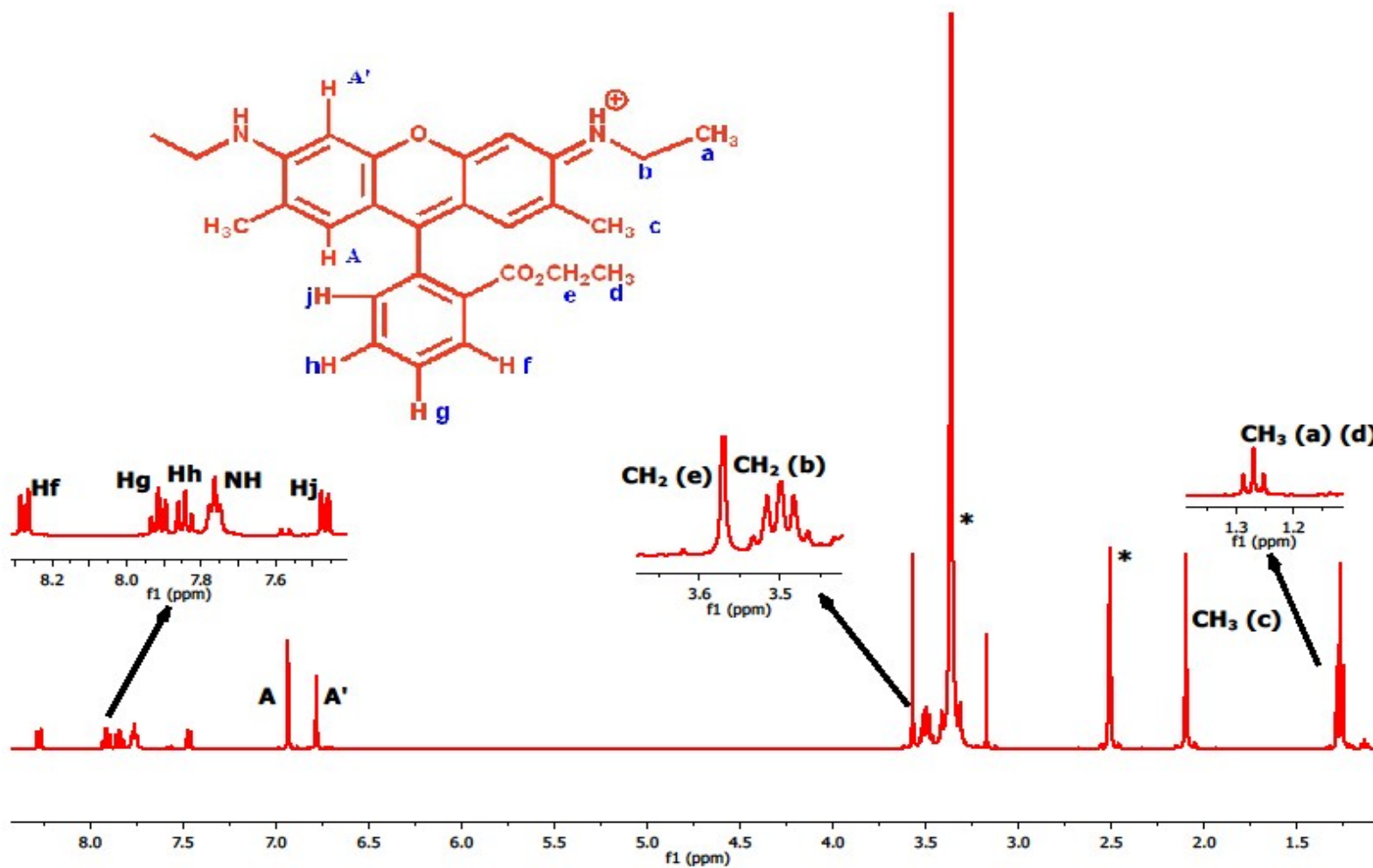


Fig. 1S: ¹H NMR spectrum of Rh6G in DMSO-d₆. (* indicates peaks of solvent)

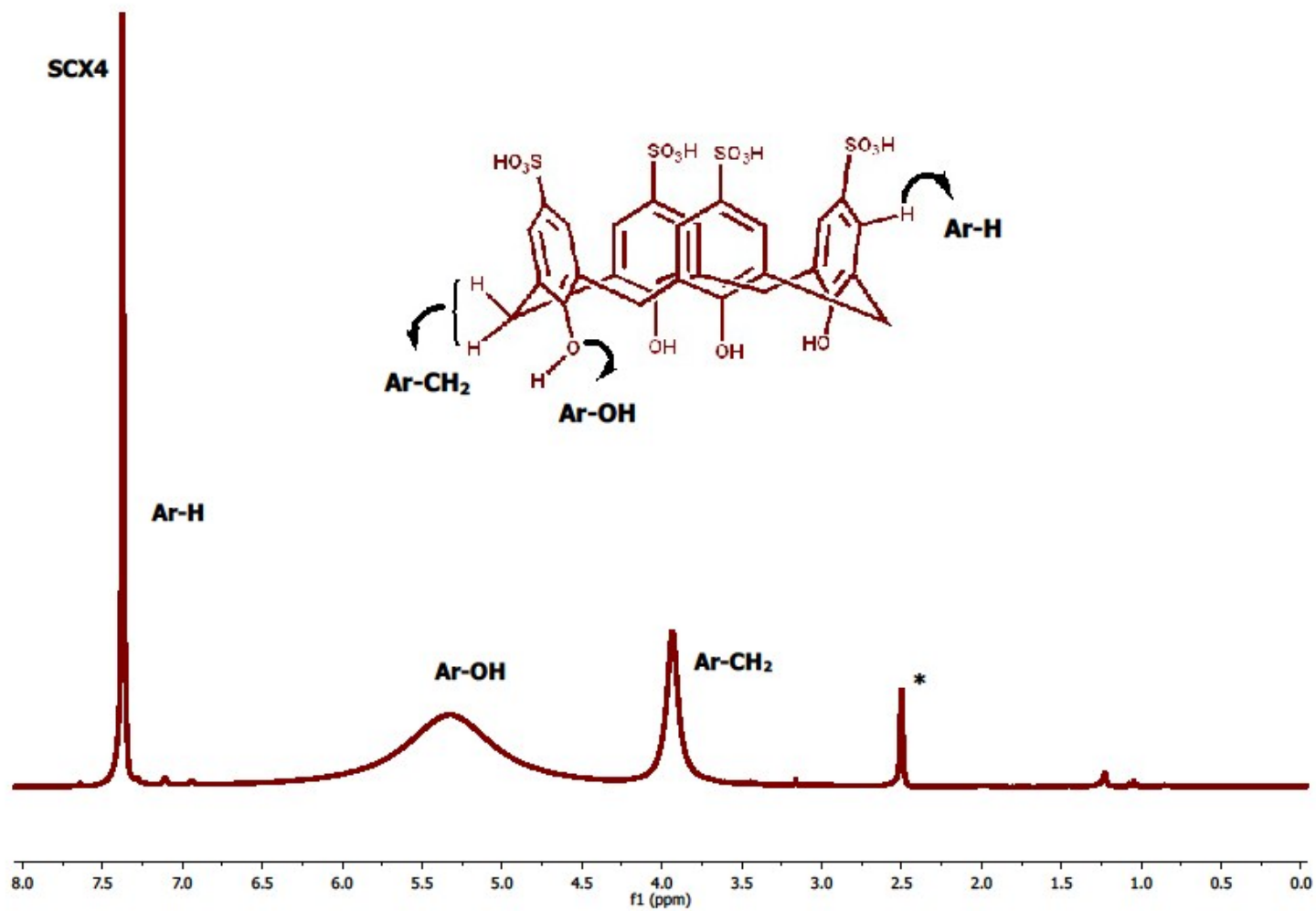


Fig. 2S: ^1H NMR spectrum of SCX4 in DMSO-d_6 . (* indicates peak of solvent)

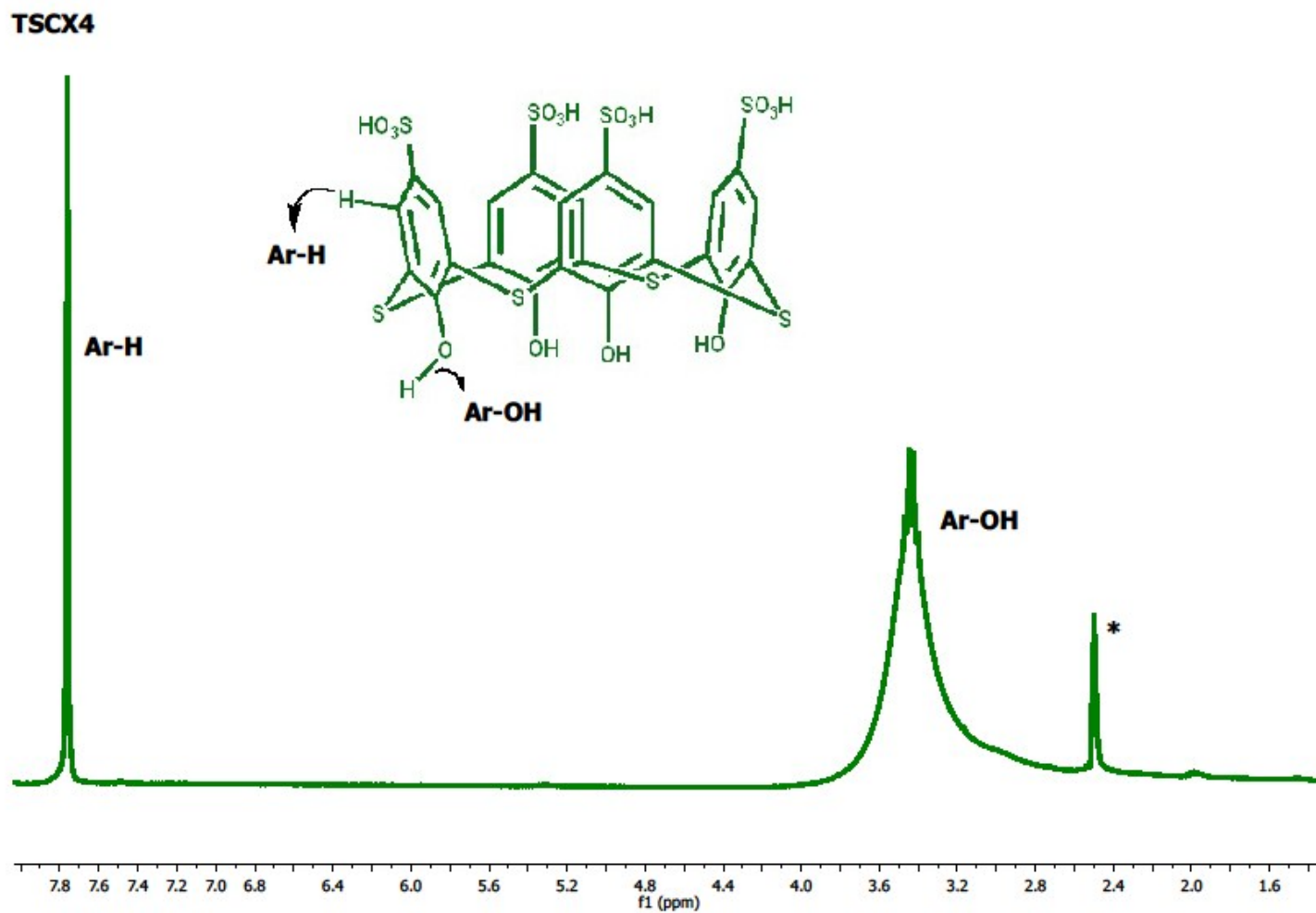


Fig. 3S: ^1H NMR spectrum of TSCX4 in $\text{DMSO-}d_6$. (* indicates peak of solvent)

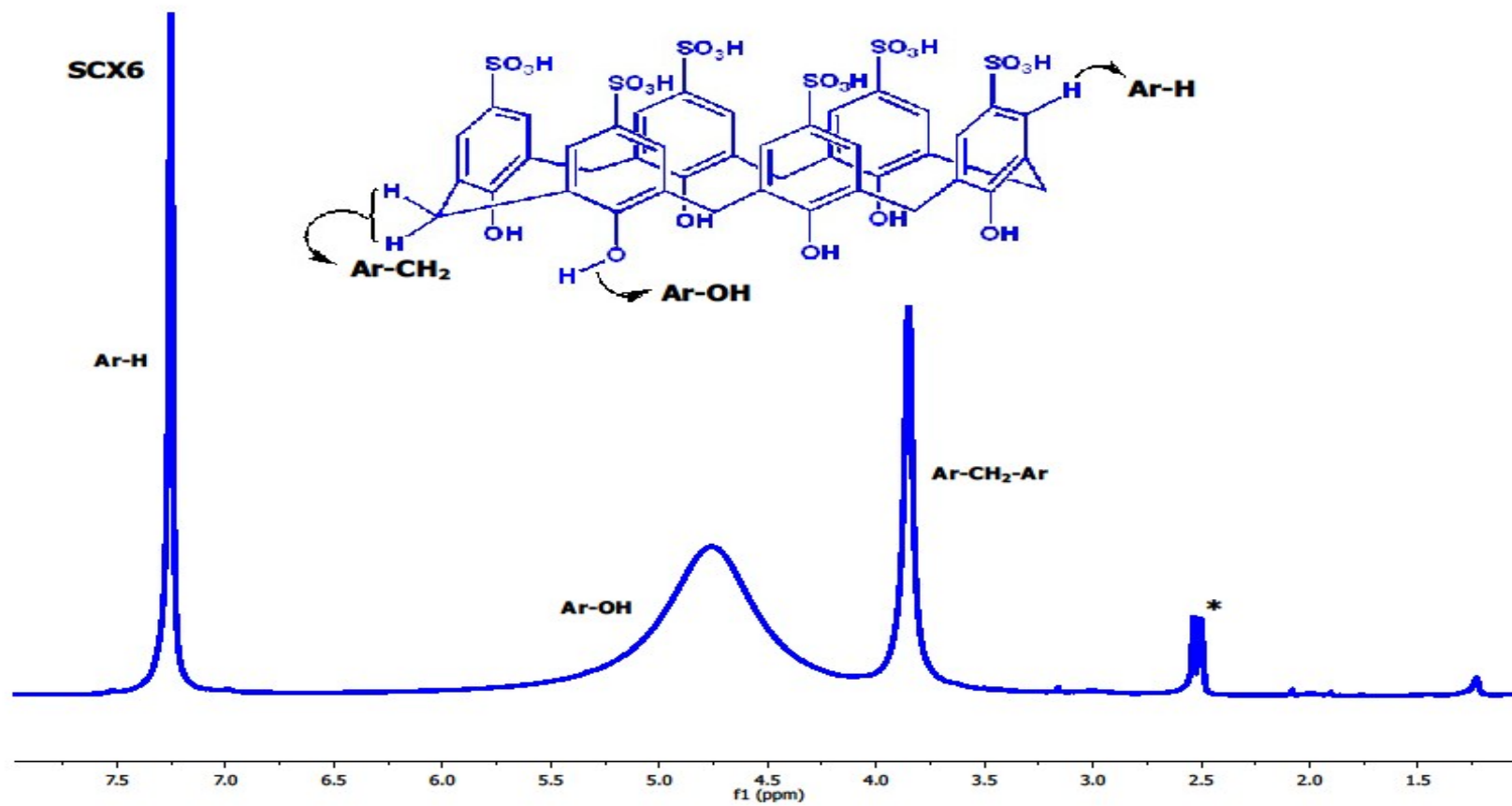


Fig. 4S: ^1H NMR spectrum of SCX6 in DMSO-d_6 . (* indicates peak of solvent)

Table 1S: Chemical shifts along with $\Delta\delta$ for TSCX4 (0.01 mM), Rh6G (0.01 mM) and Rh6G \subset TSCX4 in DMSO-d₆.

Proton assignment	Chemical shift		$(\Delta\delta = \delta - \delta_0)$
	δ_0	δ	(ppm) $\Delta\delta$
H _f	8.27	8.26	-0.01
H _g	7.91	7.93	0.02
H _h	7.84	7.84	0
H _j	7.72	7.48	-0.24
NH	7.46	-	-
A	6.94	6.89	-0.05
A'	6.78	6.76	-0.02
CH ₂ (e)	3.53	3.56	0.03
CH ₂ (b)	2.14	3.45	1.31
CH ₃ (c)	2.08	2.09	0.01
CH ₃ (a)(d)	1.27	1.26	-0.01
Ar-H	7.76	7.8	0.04
Ar-OH	3.38	4.04	0.66

Table 2S: Chemical shifts along with $\Delta\delta$ for SCX6 (0.01 mM) and Rh6G (0.01 mM) and Rh6G \subset SCX6 in DMSO-d₆.

Proton assignment	Chemical Shift		$(\Delta\delta = \delta - \delta_0)$
	δ_0	δ	(ppm) $\Delta\delta$
H _f	8.27	8.23	-0.04
H _g	7.91	7.88	0.03
H _h	7.84	7.8	-0.04
H _j	7.72	7.41	-0.31
NH	7.46	-	-
A	6.94	6.86	-0.08
A'	6.78	6.75	-0.03
CH ₂ (e)	3.53	3.53	0
CH ₂ (b)	2.14	3.43	1.29
CH ₃ (c)	2.08	2.04	-0.04
CH ₃ (a)(d)	1.27	1.22	-0.05
Ar-H	7.25	7.26	0.01
Ar-OH	4.76	5.39	0.63
Ar-CH ₂ -Ar	3.85	3.84	-0.01

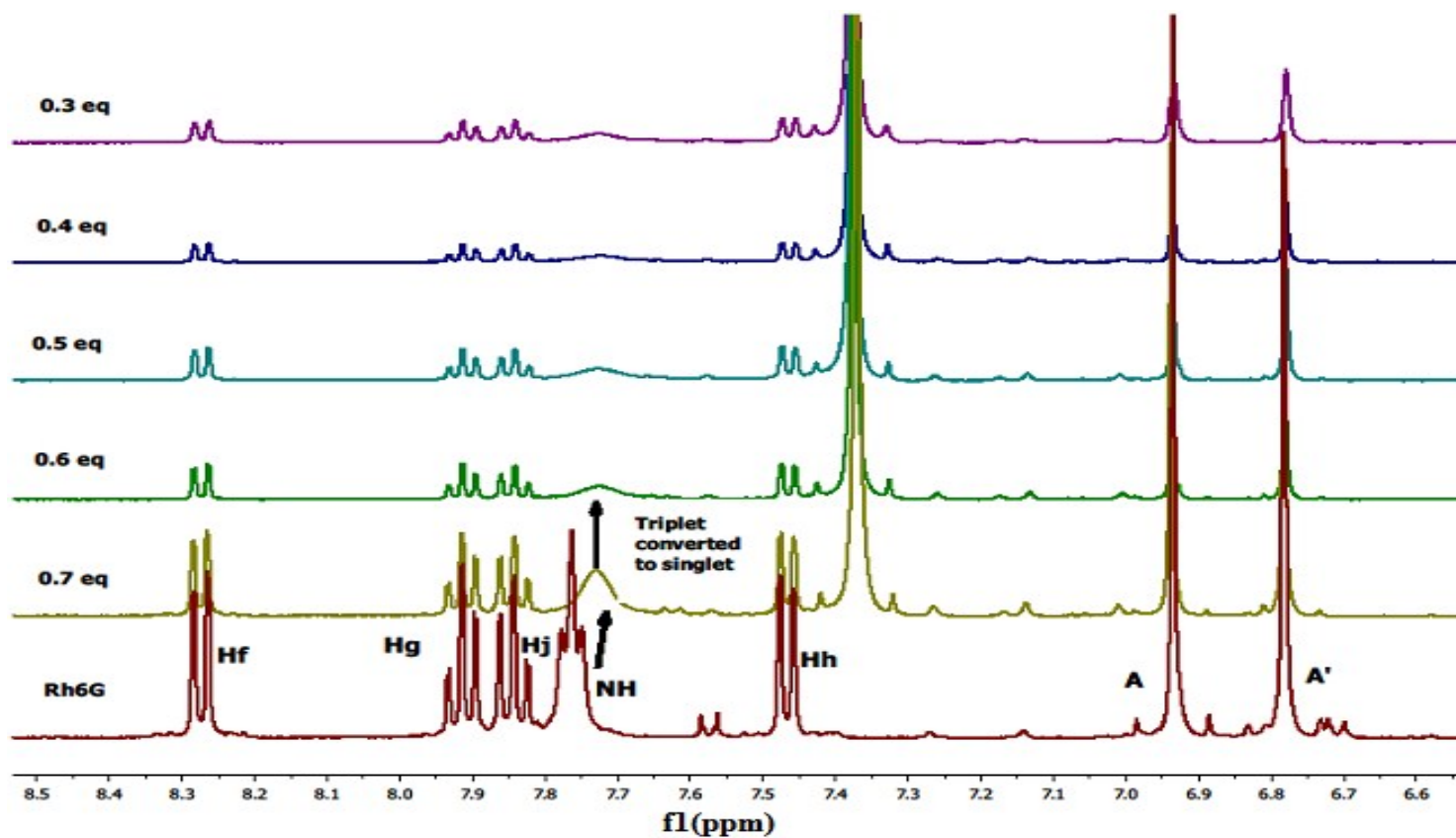


Fig. 5S: ¹H NMR spectra showing aromatic region of Rh6G (0.01 mM) and (Rh6G⊂SCX4) complex with different mole ratio (0.3, 0.4, 0.5, 0.6, and 0.7) in DMSO-d₆ at room temperature.

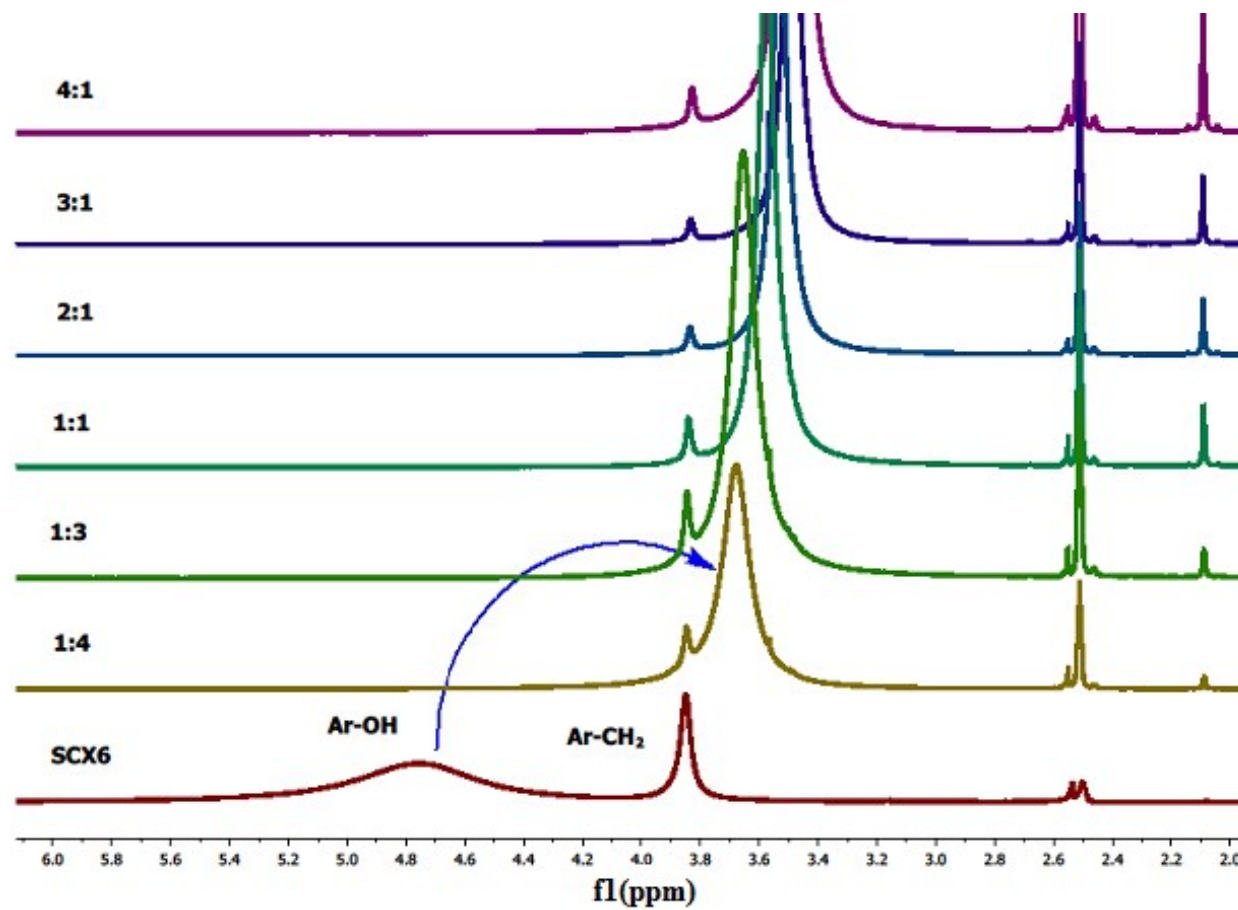
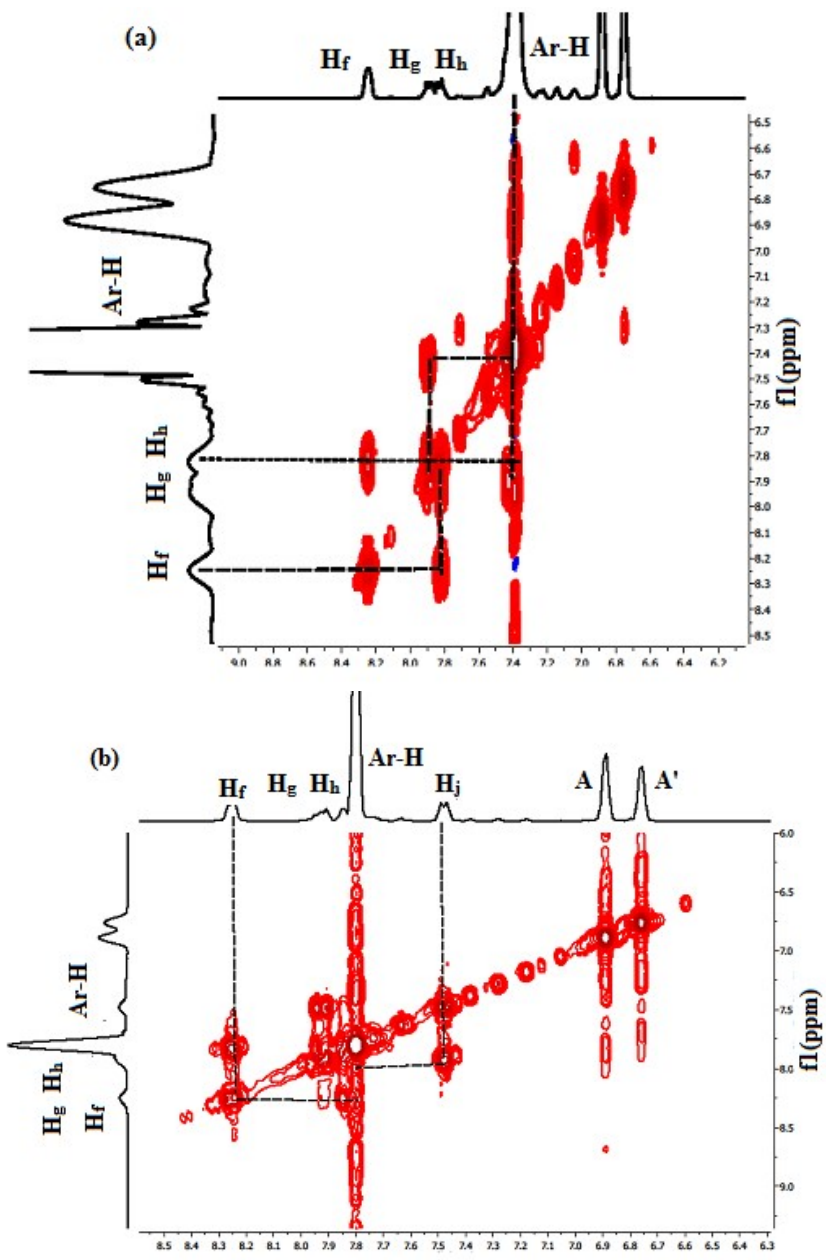


Fig. 6S: ^1H NMR spectra (500 MHz, 298K) recorded in DMSO-d_6 for a) SCX6, b) 1:4 Rh6G \subset SCX6, c) 1:3 Rh6G \subset SCX6, d) 1:1 Rh6G \subset SCX6, e) 2:1 Rh6G \subset SCX6, f) 3:1 Rh6G \subset SCX6 and g) 4:1 Rh6G \subset SCX6.



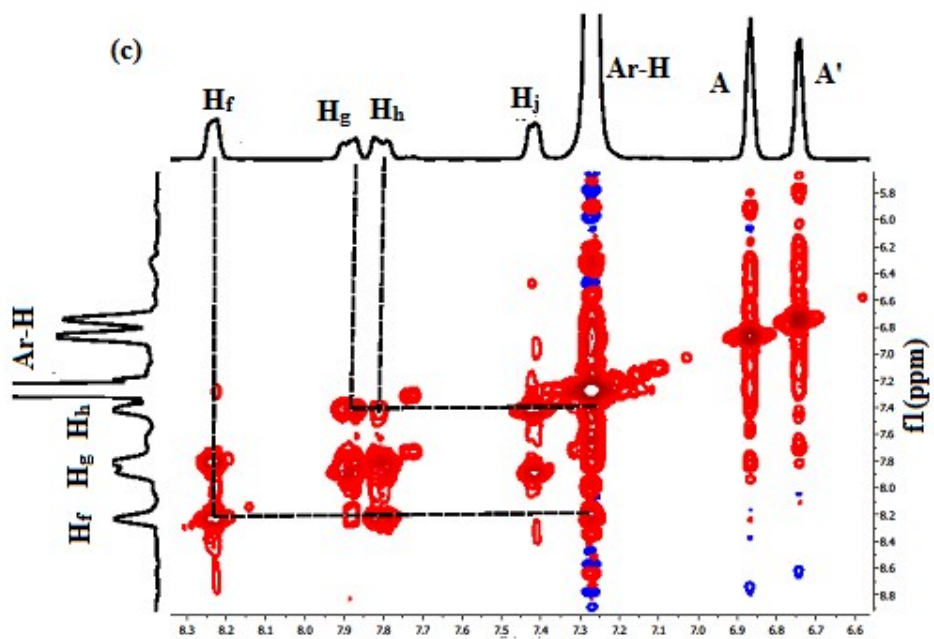


Fig. 7S: 2D COSY spectrum of a) Rh6G \subset SCX4, b) Rh6G \subset TSCX4, and c) Rh6G \subset SCX6 1:1 complexes in DMSO- d_6 .

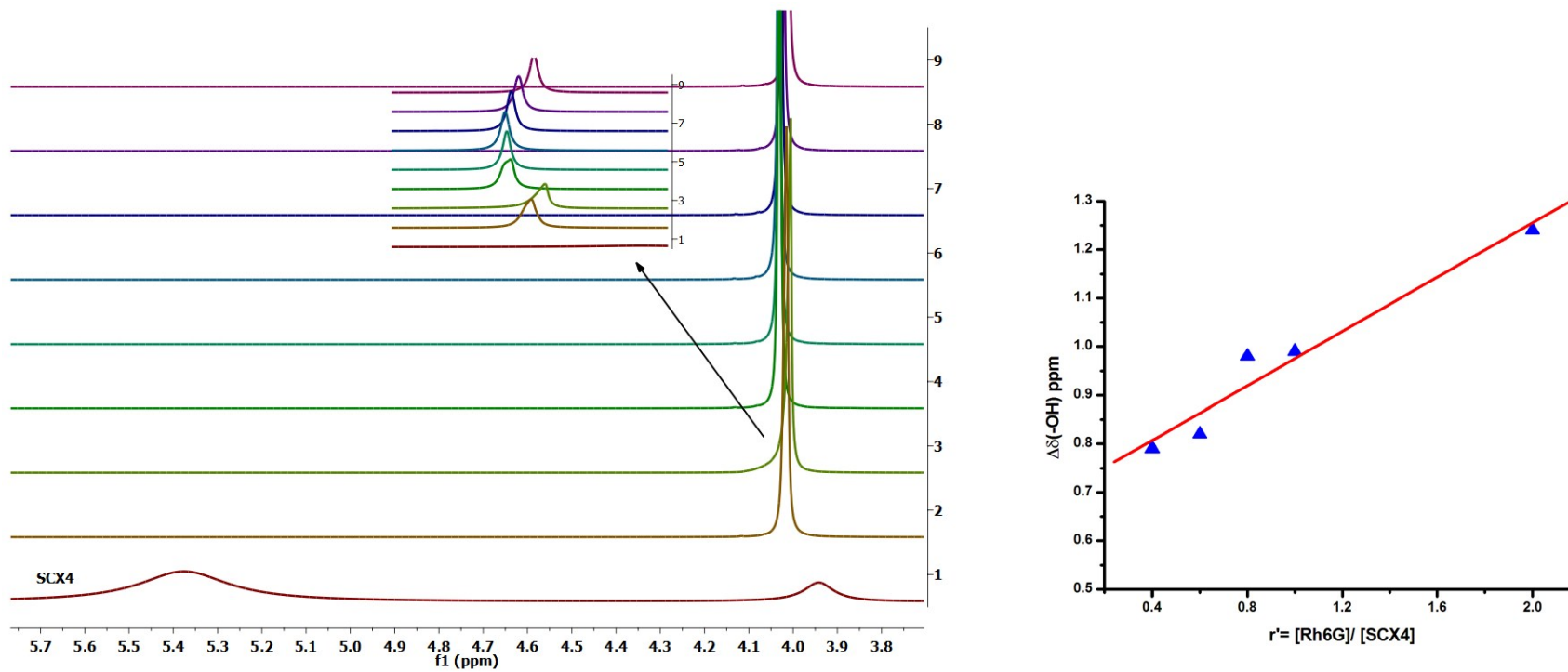


Fig 8S: (a) Partial ¹H NMR spectra (400 MHz, DMSO-d₆, 298 K) of SCX4 at the concentration of 5mM upon addition of Rh6G; (1) 0 mM; (2) 1 mM; (3) 2 mM; (4) 3 mM; (5) 5 mM; (6) 10mM; (7) 20mM; (8) 30 mM (b) Titration curve of SCX4 with Rh6G showing changes in the chemical shifts of -OH against an increasing amount of Rh6G.

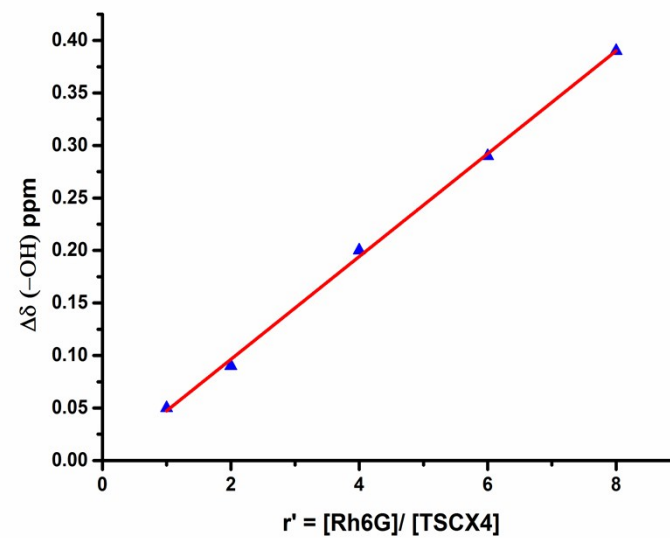
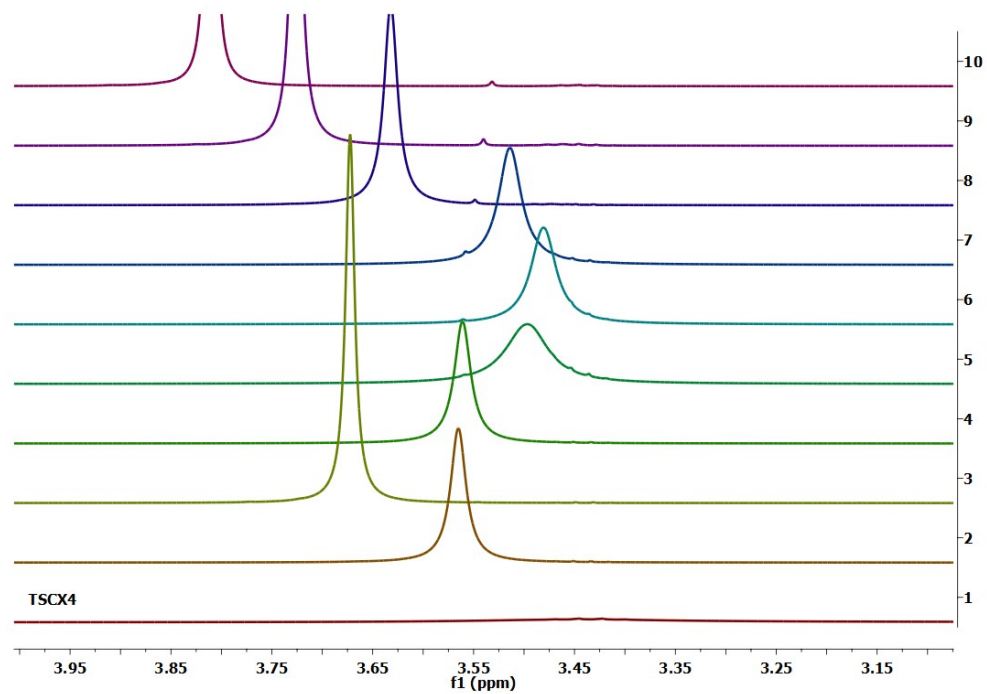
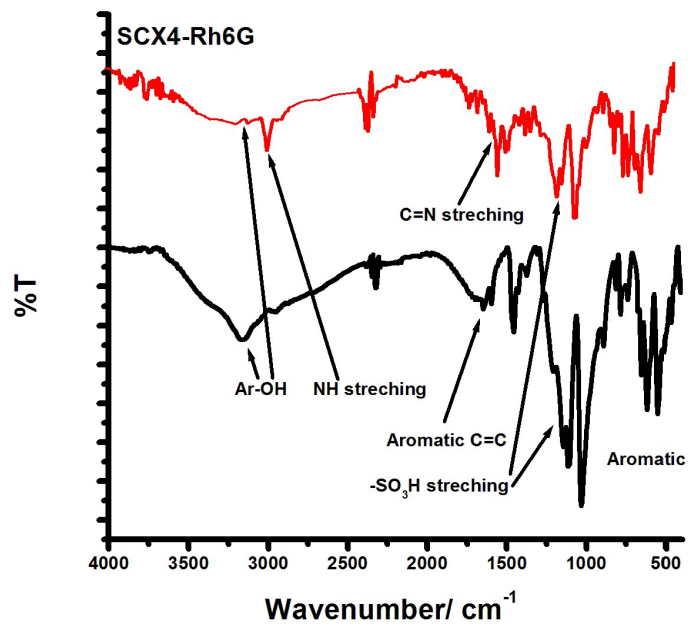
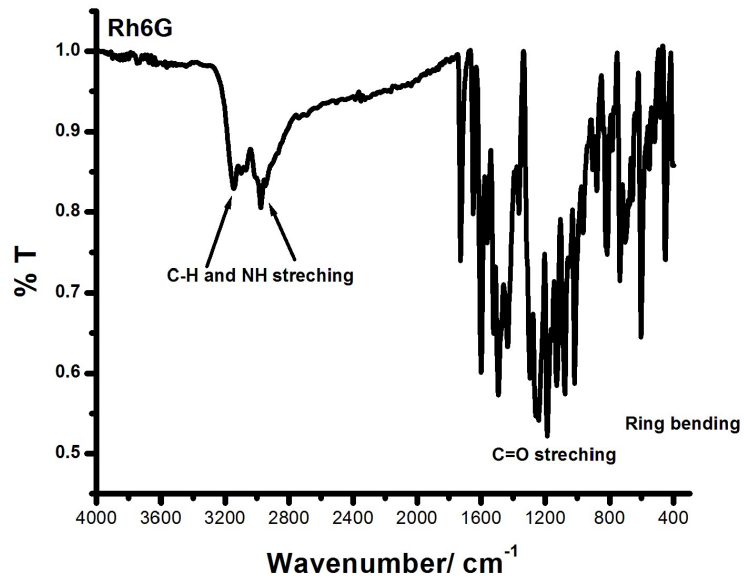


Fig 9S: Partial ^1H NMR spectra (400 MHz, DMSO- d_6 , 298 K) of TSCX4 at the concentration of 5mM upon addition of Rh6G; (1) 0 mM; (2) 1 mM; (3) 2 mM; (4) 3 mM; (5) 4 mM; (6) 5mM; (7) 10mM; (8) 20 mM; (9) 30 mM (b) Titration curve of TSCX4 with Rh6G showing changes in the chemical shifts of -OH against an increasing amount of Rh6G.



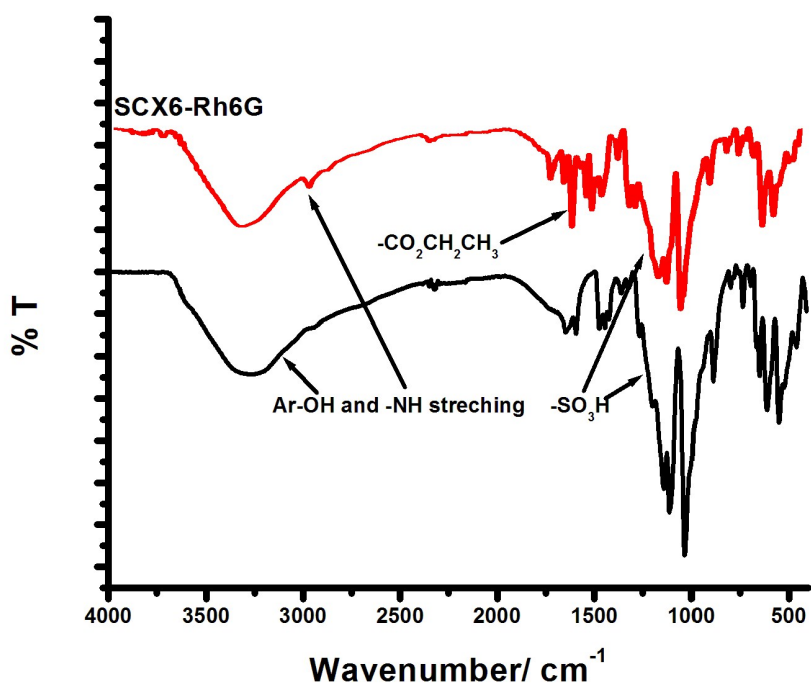
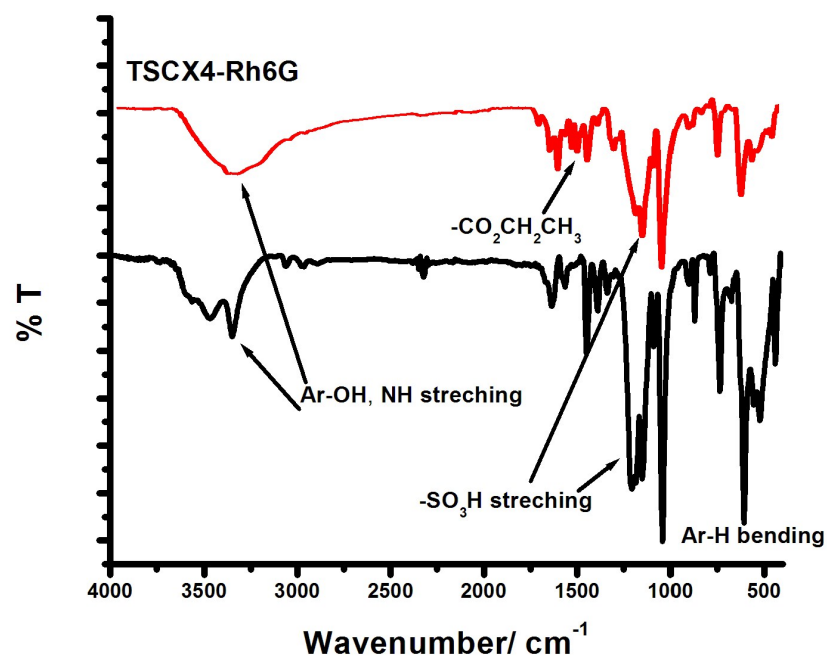
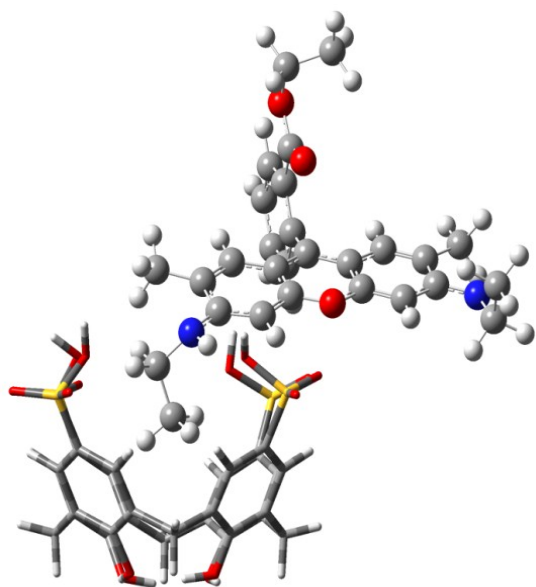
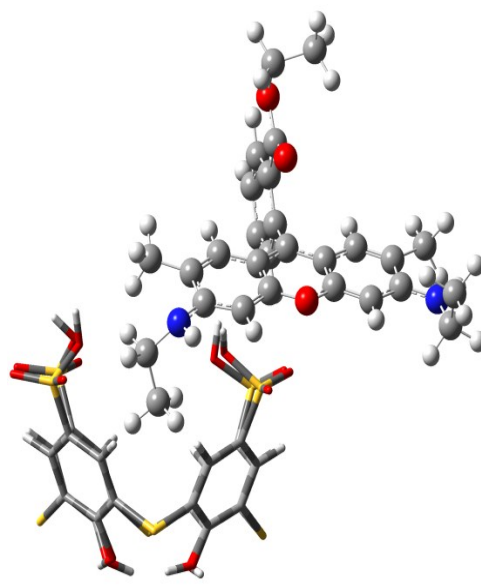


Fig. 10S: FT-IR spectra of a) Rh6G, b) SCX4 and Rh6G \subset SCX4 c) TSCX4 and Rh6G \subset TSCX4, and d) SCX6 and Rh6G \subset SCX6 complex in 1:1 mole ratio.



Rh6G@SCX4



Rh6G@TSCX4

Fig. 11S: ω B97x/6-31G(d,p) optimized high energy complexes

Table 3S: A comparison of ¹H NMR chemical shifts in the free Rhodamine-6G, SCX4, TSCX4 and their complexes (Solvent=DMSO)

Proton	Rh6G		SCX4		Rh6G⊂SCX4		TSCX4		Rh6G⊂TSCX4	
	Theory	Experiment	Theory	Experiment	Theory	Experiment	Theory	Experiment	Theory	Experiment
ArCH2	–	–	3.8	3.9	4.0	3.9	–	–	–	–
Ar-H	–	–	8	7.3	8.1	7.4	8.8	7.8	8.8	7.8
A	7.2	6.9	–	–	6.9	6.9	–	–	6.9	6.9
A'	6.8	6.8	–	–	6.8	6.8	–	–	6.8	6.8
a	1.3	1.3	–	–	1.3	1.2	–	–	1.3	1.3
b	3.6	2.1	–	–	3.7	3.5	–	–	3.7	3.5
c	2.2	2.1	–	–	2.4	2.1	–	–	2.4	2.1
d	1.4	1.3	–	–	2.0	1.2	–	–	2.0	1.3
e	4	3.5	–	–	4.6	3.6	–	–	4.6	3.6
f	8.8	8.3	–	–	6.3	8.3	–	–	6.2	8.3
g	8.2	7.9	–	–	3.8	7.9	–	–	4.3	7.9
h	8.2	7.8	–	–	6.6	7.8	–	–	6.3	7.8
i=k	4.7	7.5	–	–	4.9	2.5	–	–	6.6	-

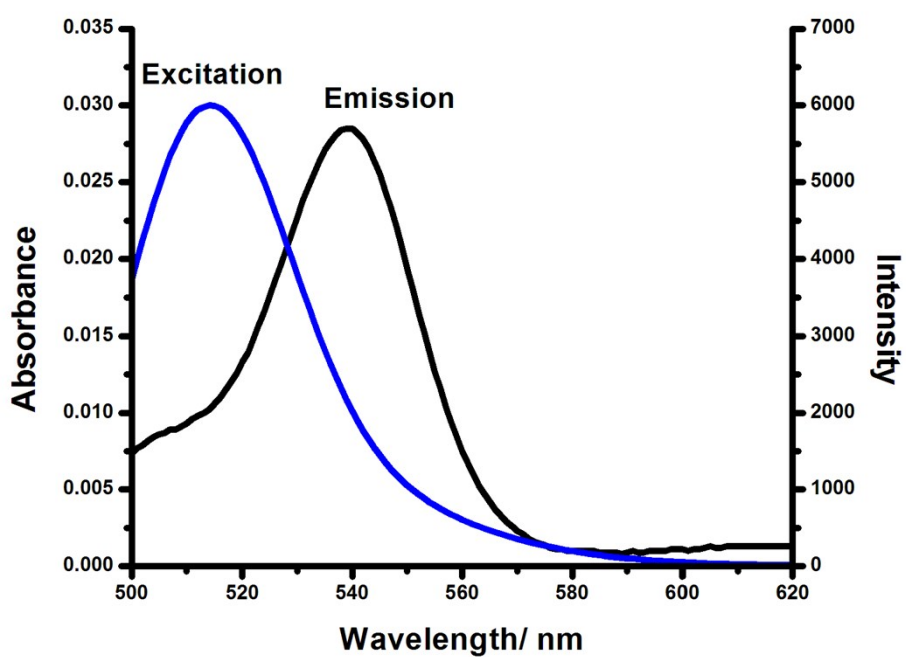


Fig. 12S: Spectral overlap between excitation and emission spectrum of Rh6G $\lambda_{\text{ex}} = 535 \text{ nm}$, $\lambda_{\text{em}} = 563 \text{ nm}$.

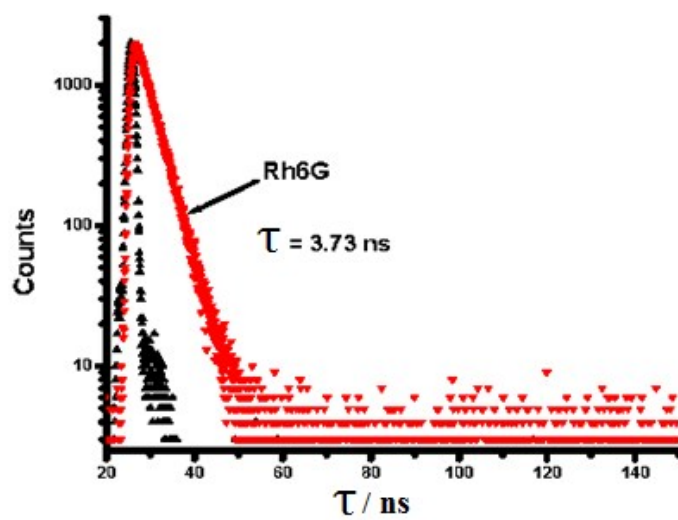


Fig. 13S: Decay traces of Rh6G (0.001 M) in DMSO $\lambda_{\text{ex}} = 535 \text{ nm}$.

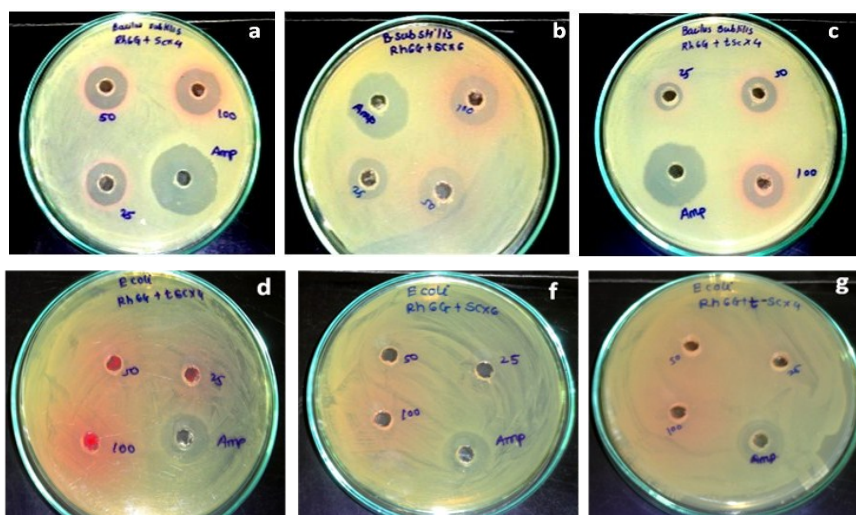


Fig. 14S: Antimicrobial activity of sulfonated calixarenes derivatives Rh6G-SCX4, Rh6G-TSCX4 and Rh6G-SCX6 with varying concentrations (25, 50, 100 ppm) against (a, b and c) *B. subtilis* ATCC 6633 and (d,e and f) *E. coli* ATCC 8739 at 37 °C after 24 h.