Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

Photophysical, NMR studies of encapsulation of 2-cyano-6-hydroxy benzothiazole in p-sulfonatocalix[6]arene and its biological applications

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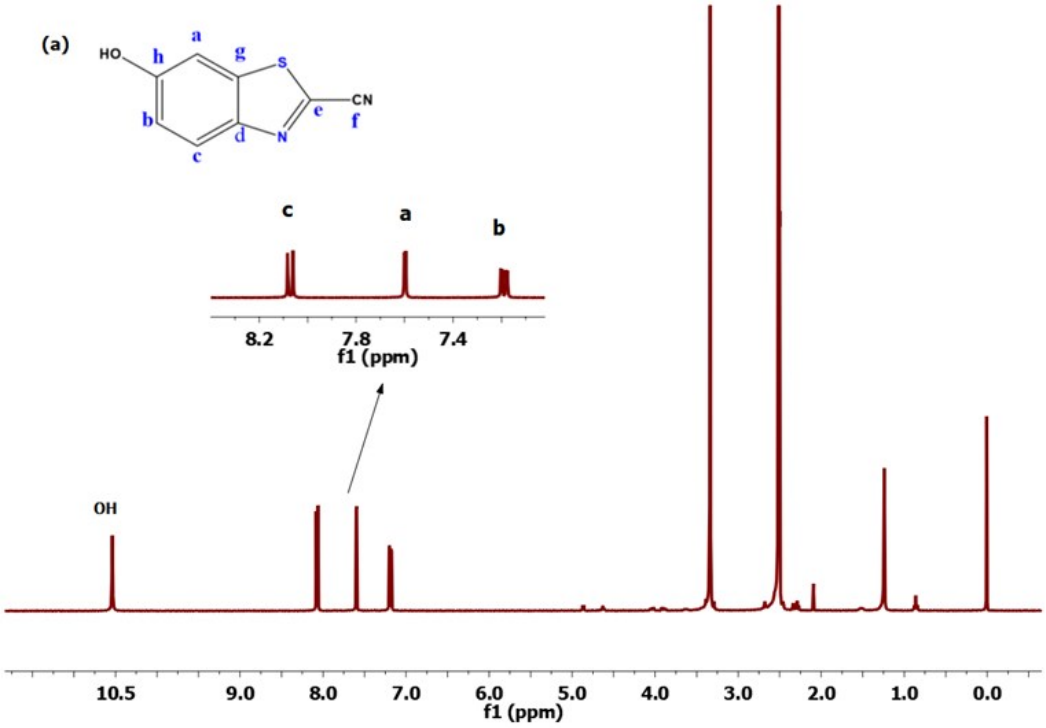
NMR spectra (in DMSO-d_6) of SCX6, CHBT and CHBT-SCX6 complex



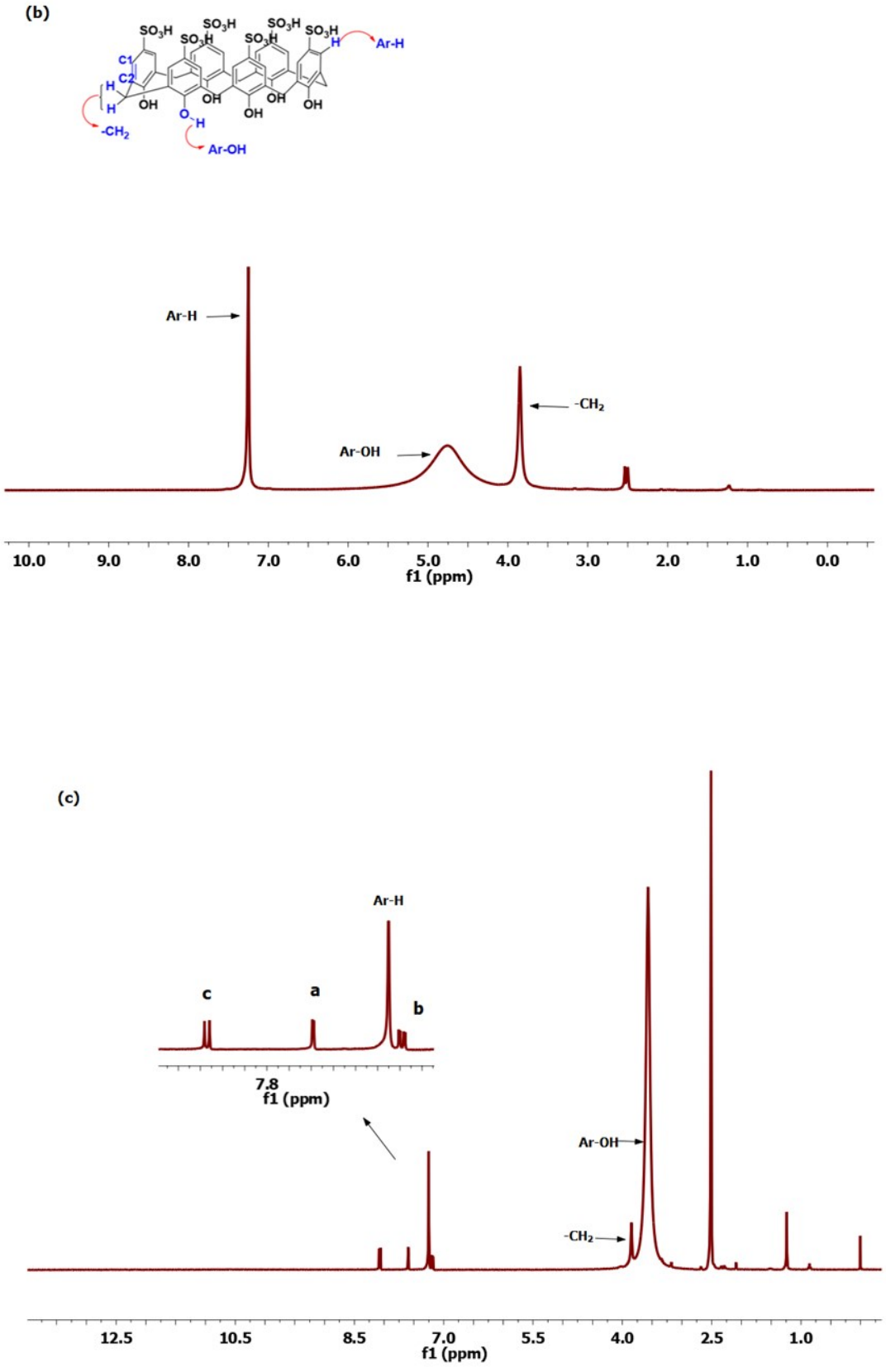


Fig.1S. ^{1}H NMR spectra of a) CHBT b) SCX6, and c) 1:1 mole ratio of CHBT-SCX6 complex in DMSO-d_6 at 25 ^{0}C.

Table 1S Chemical shifts along with Δδ for SCX6 (0.01M), CHBT (0.01M) and CHBT-SCX6 in DMSO-d_6.

Protons assignment	Chemical shift		(Δδ = δ –δ0) (ppm)
	δ0	δ	Δδ
a	7.59	7.58	-0.01
b	7.18	7.18	0
c	8.06	8.06	0
OH	10.53	Peak merge	
Ar-H	7.25	7.24	-0.01
Ar-OH	4.76	3.56	-1.19
Ar-CH_2	3.85	3.84	-0.01

^{1}H NMR spectra of CHBT-SCX6 complexes along with those of individual host and CHBT have been recorded and results are shown in figure 2S (supporting information). The NMR spectrum of SCX6 (figure 2S(a) and 3S(a) exhibit signals at δ = 3.82 ppm (-CH_2: methylene hydrogen), δ = 7.27 ppm (Ar-H: aromatic hydrogen). In the CHBT spectrum (figure 2S(b) and 3S(b), the doublet due to CH (c) (a) (δ = 8.03 ppm and δ = 7.48 ppm) and doublet of doublet (δ = 7.15 ppm) assigned to CH (b). Thus, figure 2S(c) and 3S(c) shows that there is a very small change in the chemical shift values of SCX6 and CHBT protons, table 2S (supporting information).

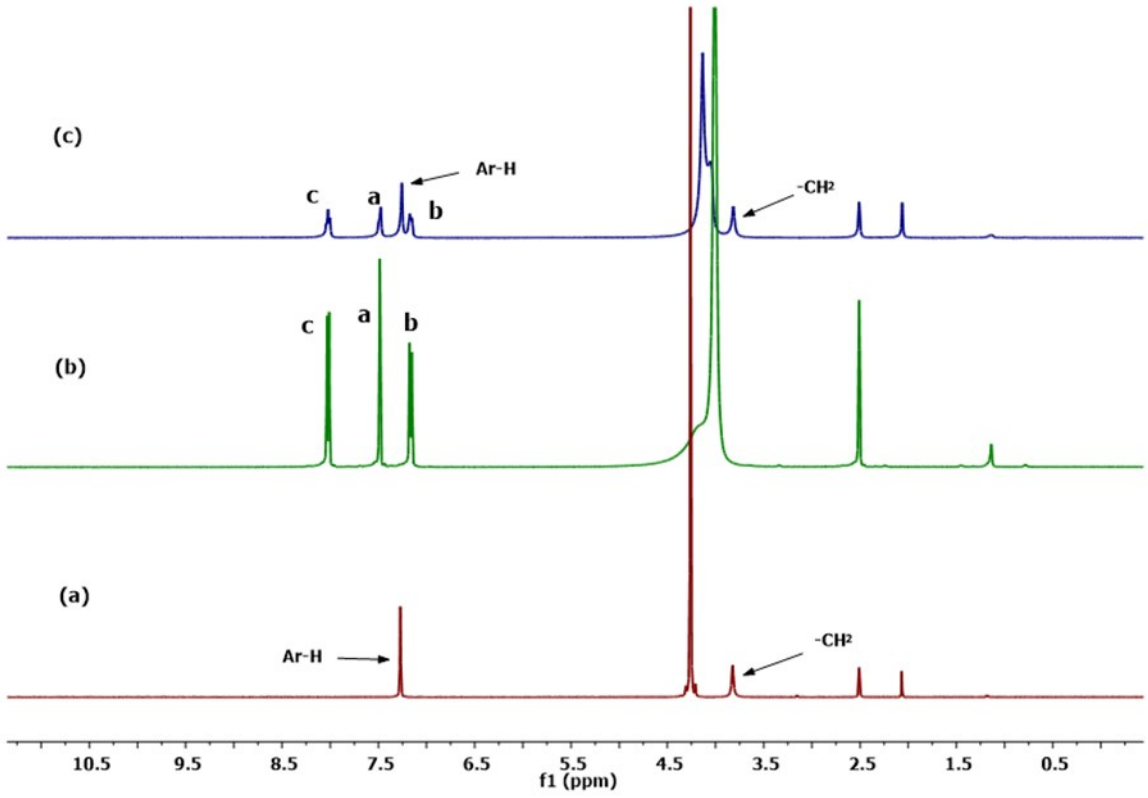


Fig. 2S ^{1}H NMR spectra of a) SCX6, b) CHBT and c) CHBT-SCX6 in small amount of DMSO-d_6 in D_2O.

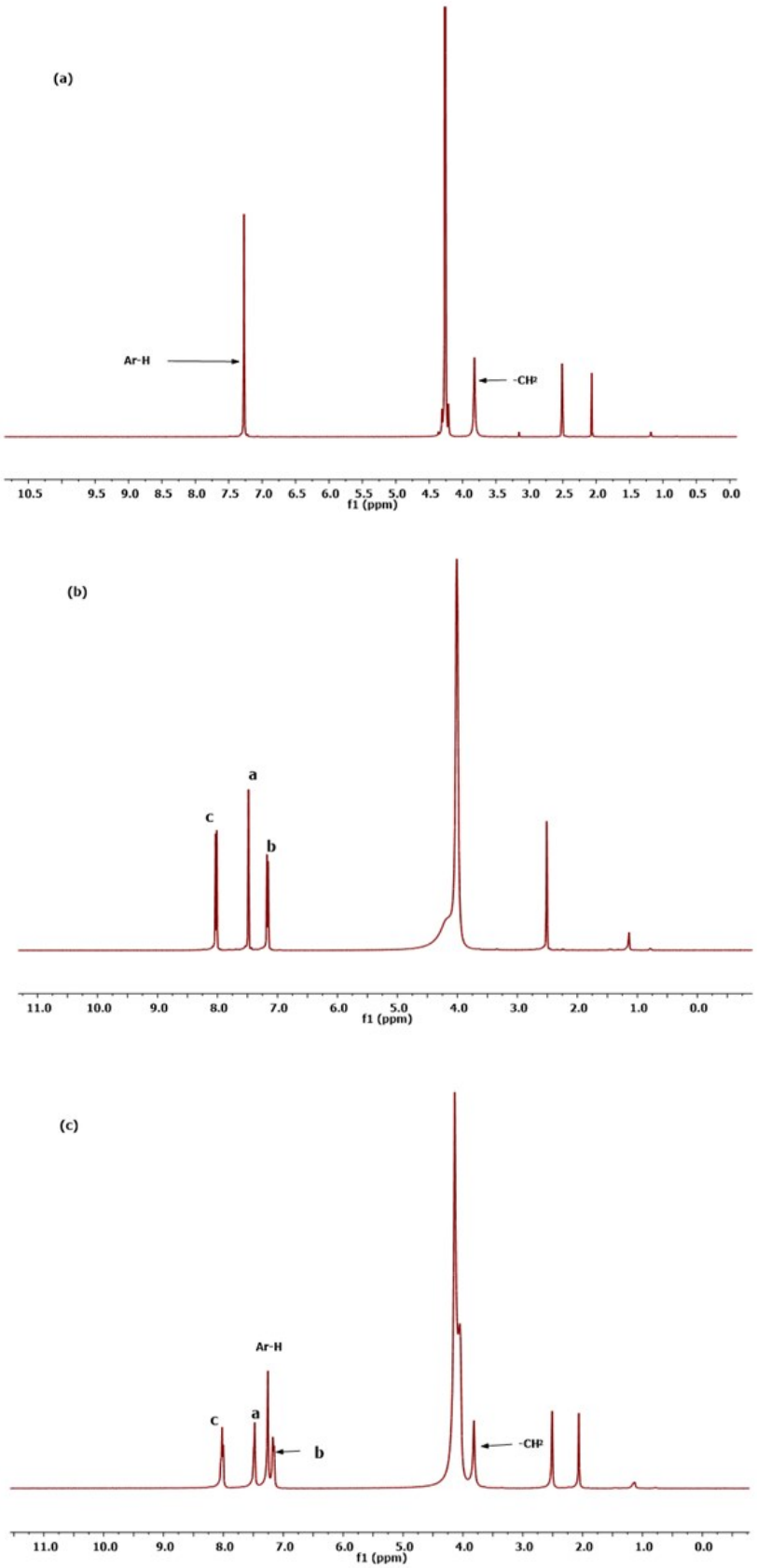


Fig.3S ^{1}H NMR spectra of a) SCX6, b) CHBT and c) 1:1 mole ratio of CHBT-SCX6 complex in small amount of DMSO-d_6 in D_2O.

Table. 2S ^{1}H NMR chemical shifts along with Δδ for SCX6 (0.01M), CHBT (0.01M) and CHBT-SCX6 in small amount of DMSO-d_6 in D_2O.

Proton assignment	Chemical shift		(Δδ = δ –δ0) (ppm)
	δ0	δ	Δδ
a	7.48	7.48	0
b	7.15	7.16	0.01
c	8.03	8.02	-0.01
Ar-H	7.27	7.26	-0.01
Ar-CH_2	3.82	3.81	-0.01

^{1}H NMR experiment of CHBT in DMSO-d_6 at pD 2.0 and pD 9.5 and results are shown in figure 4S, 5S (supporting information). The results match with the absorbance and fluorescence spectra. The CHBT remains neutral at pD 2.0, as there is no change in the chemical shift values of CHBT protons relative to neutral pD. While at pD = 9.5 there is change in chemical shift values (upfield shift) in the CHBT protons with deprotonation of hydroxyl proton shown in table 3S (supporting information).

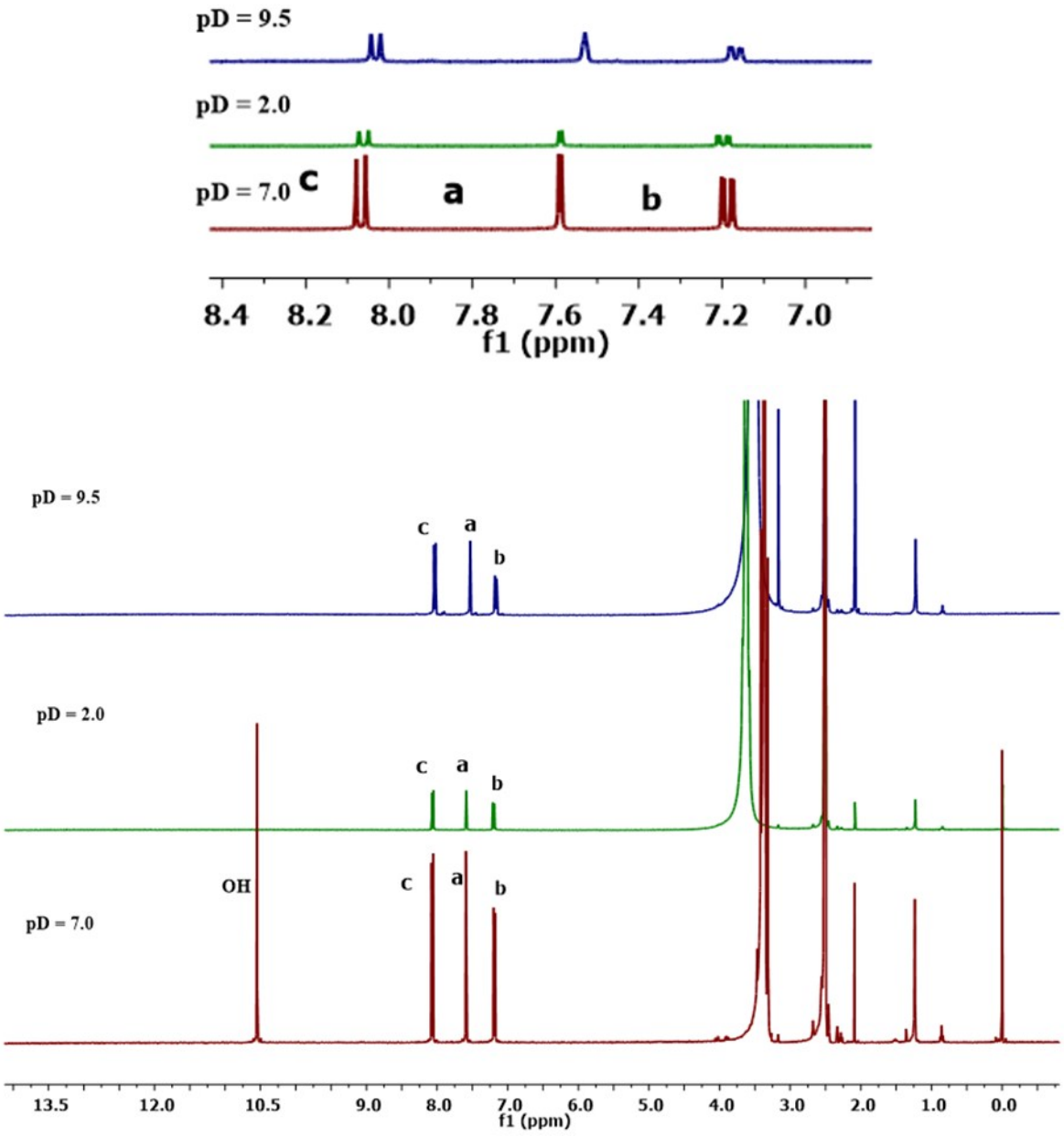


Fig. 4S. ^{1}H NMR spectra of CHBT (0.01 M) in DMSO-d_6 at pD 7.0, 2.0 and 9.5.

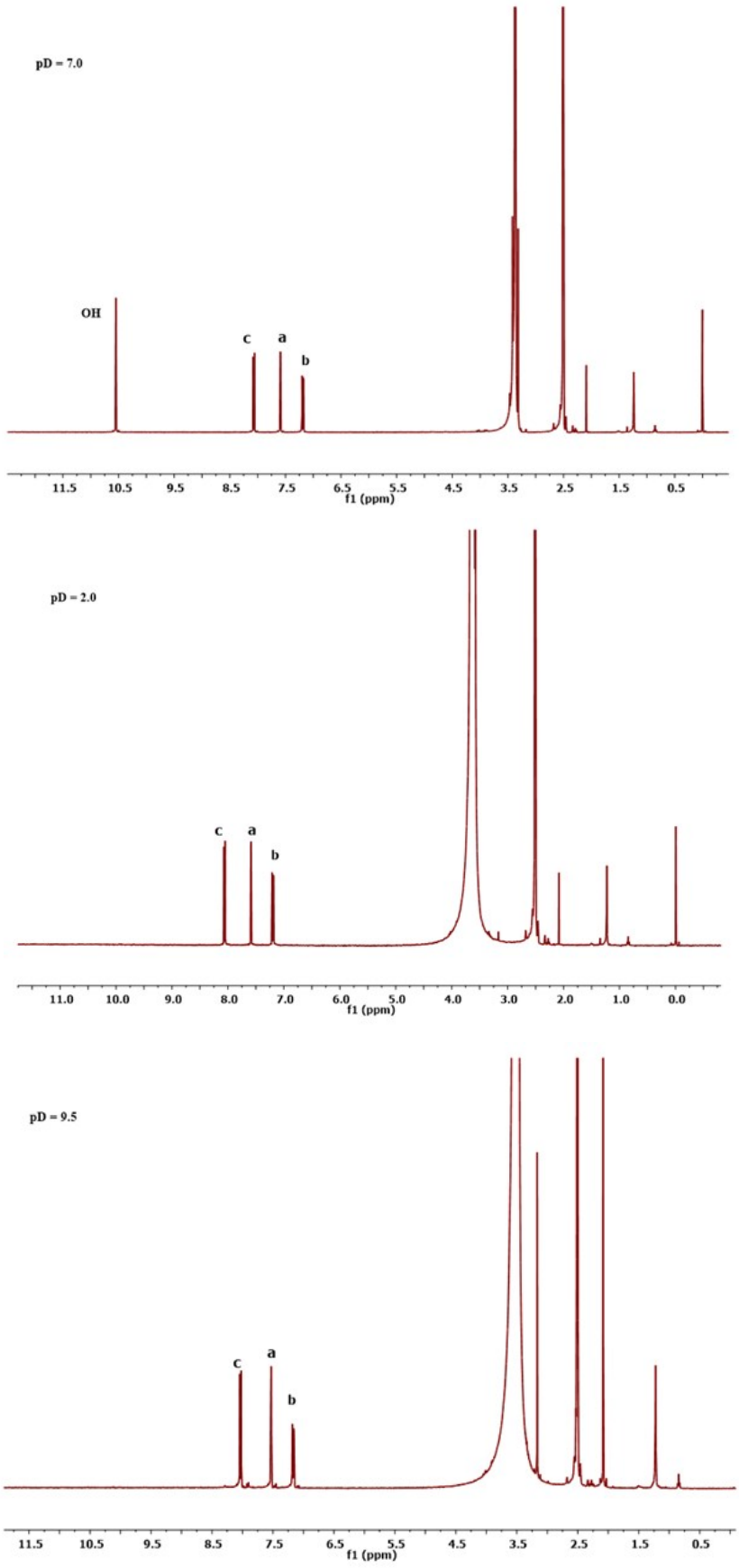


Fig. 5S ^{1}H NMR spectra of CHBT (0.01 M) in DMSO-d_6 at pD 7.0, 2.0 and 9.5.

Table 3S ^{1}H NMR chemical shifts along with the change from neutral to basic conditions (Δδ) for CHBT (0.01M) in DMSO-d_6 at pD 7.0, 2.0 and 9.5.

Proton assignment	Chemical shift			(Δδ = δ –δ0) (ppm)
	δ0 (pD 7.0)	δ (pD 2.0)	δ (pD 9.5)	Δδ (pD 9.5)
a	7.59	7.59	7.49	-0.1
b	7.19	7.19	7.13	-0.06
c	8.06	8.06	8.03	-0.03
OH	10.55	-	-	-

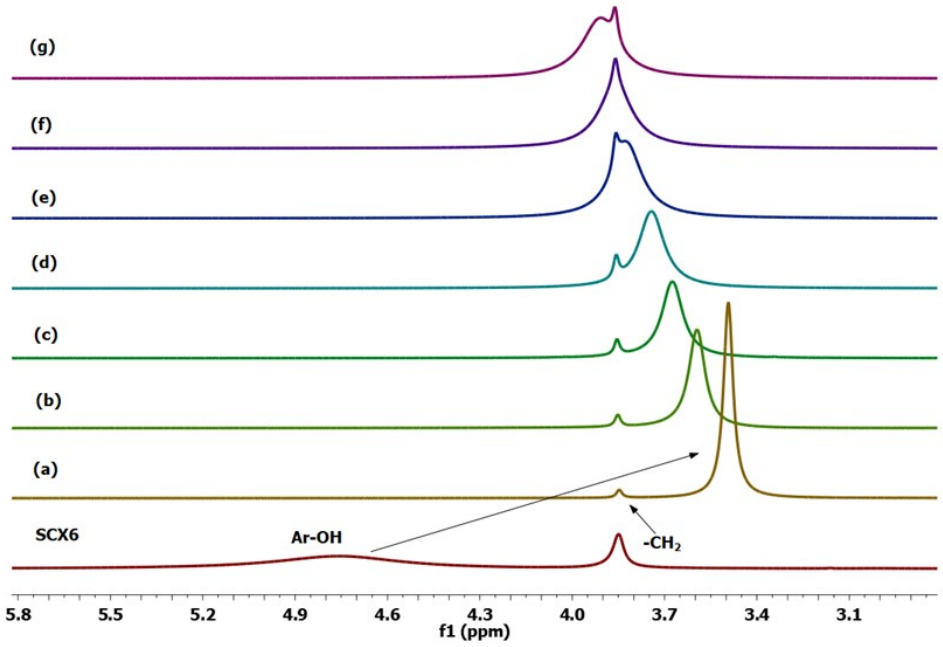


Fig.6S. Partial ^{1}H NMR spectra titration spectra (400 MHz, 25^{0}C) recorded in DMSO-d_6 of CHBT at the concentration of 0.01 M upon addition of SCX6 (0.01M), SCX6, (a) 5:1 equi., (b) 3:1 equi., (c) 2:1 equi., (d)1:1 equi., (e) 1:2 equi., (f) 1:3 equi., (g) 1:5 equi.

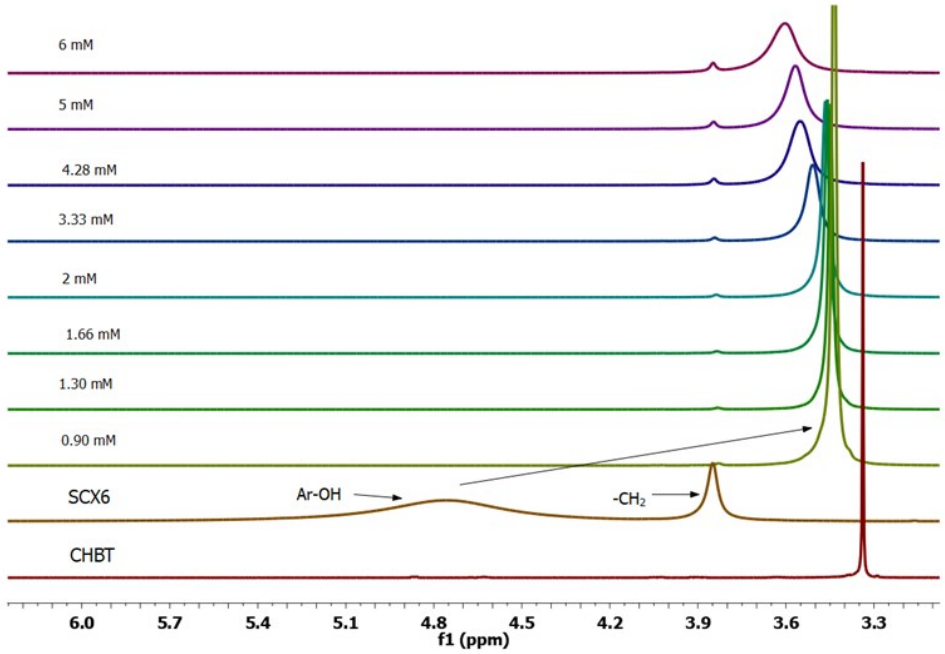
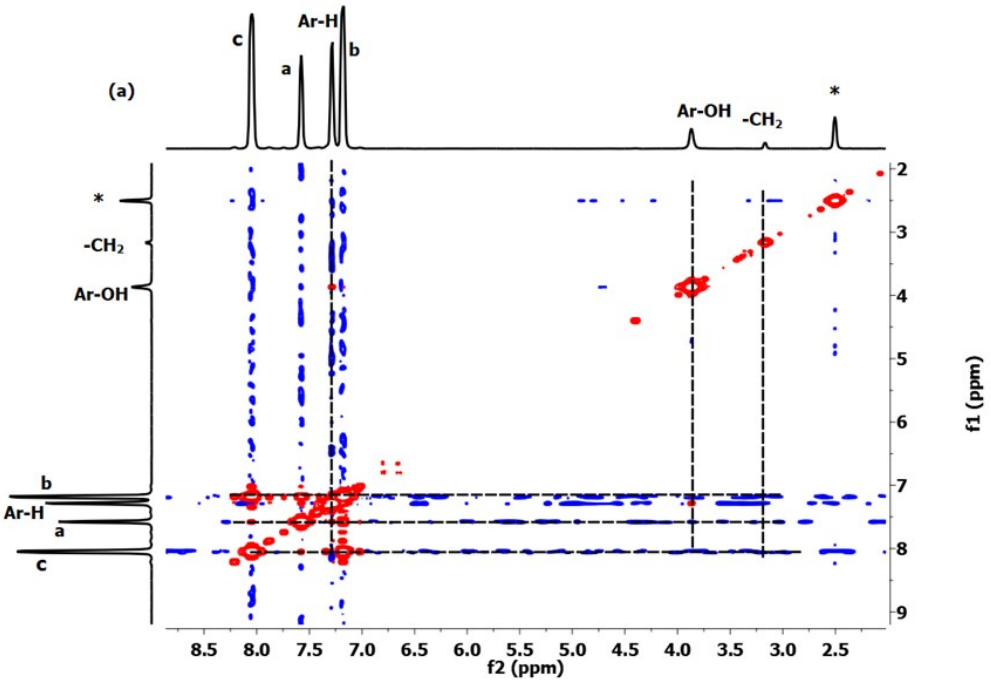


Fig.7S. Partial ^{1}H NMR spectra (400 MHz, DMSO-d_6, 298 K) of SCX6 at the concentration of 6 mM upon addition of CHBT: (1) 0.90 mM; (2) 1.30 mM; (3) 1.66 mM; (4) 2 mM; (5) 3.33 mM; (6)4.28 mM; (7) 5 mM; (8) 6 mM.



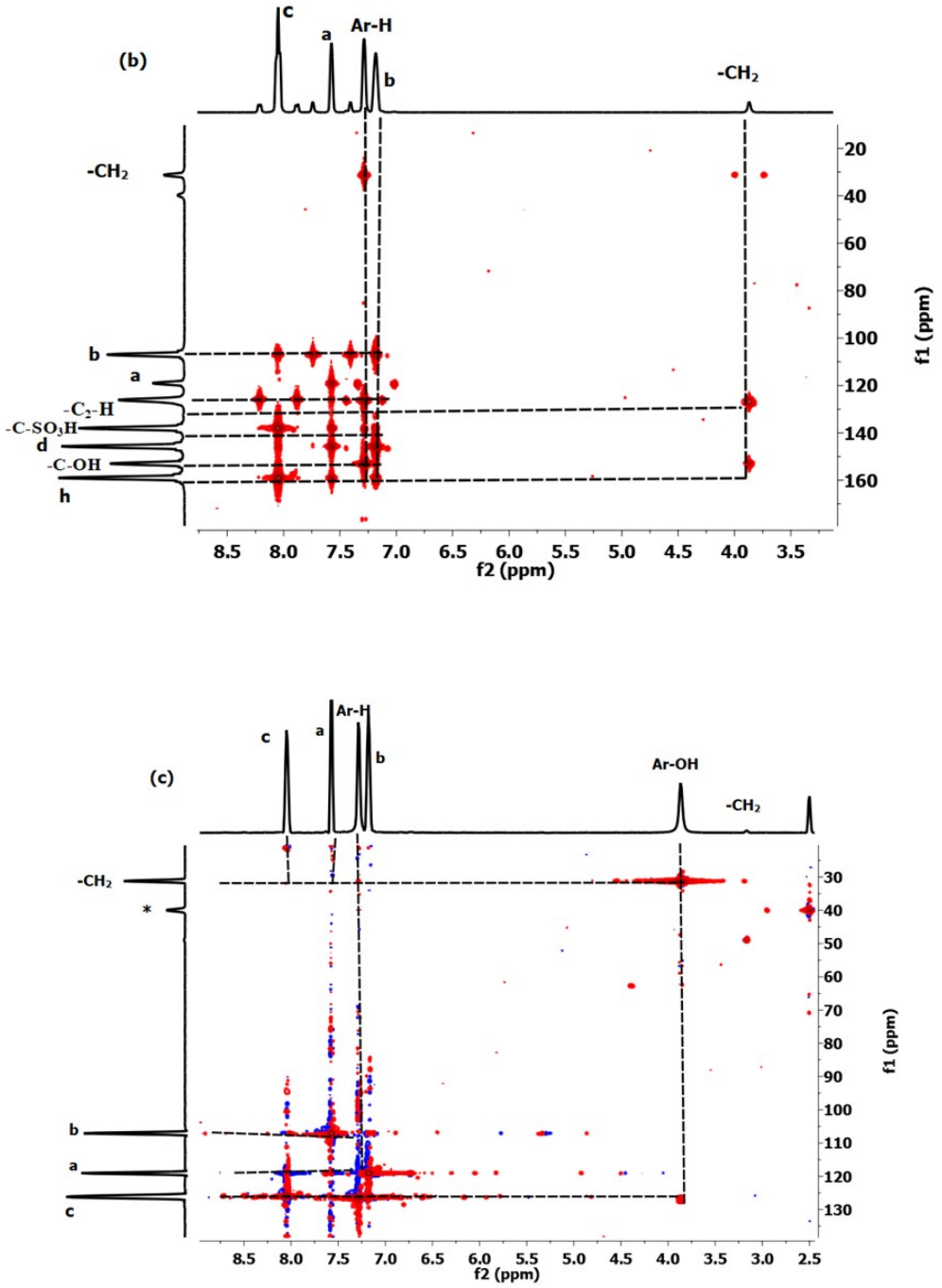


Fig.8S. 2D a) COSY b) HMBC and c) HSQC spectrum of CHBT-SCX6 1:1 complex in DMSO-d_6.

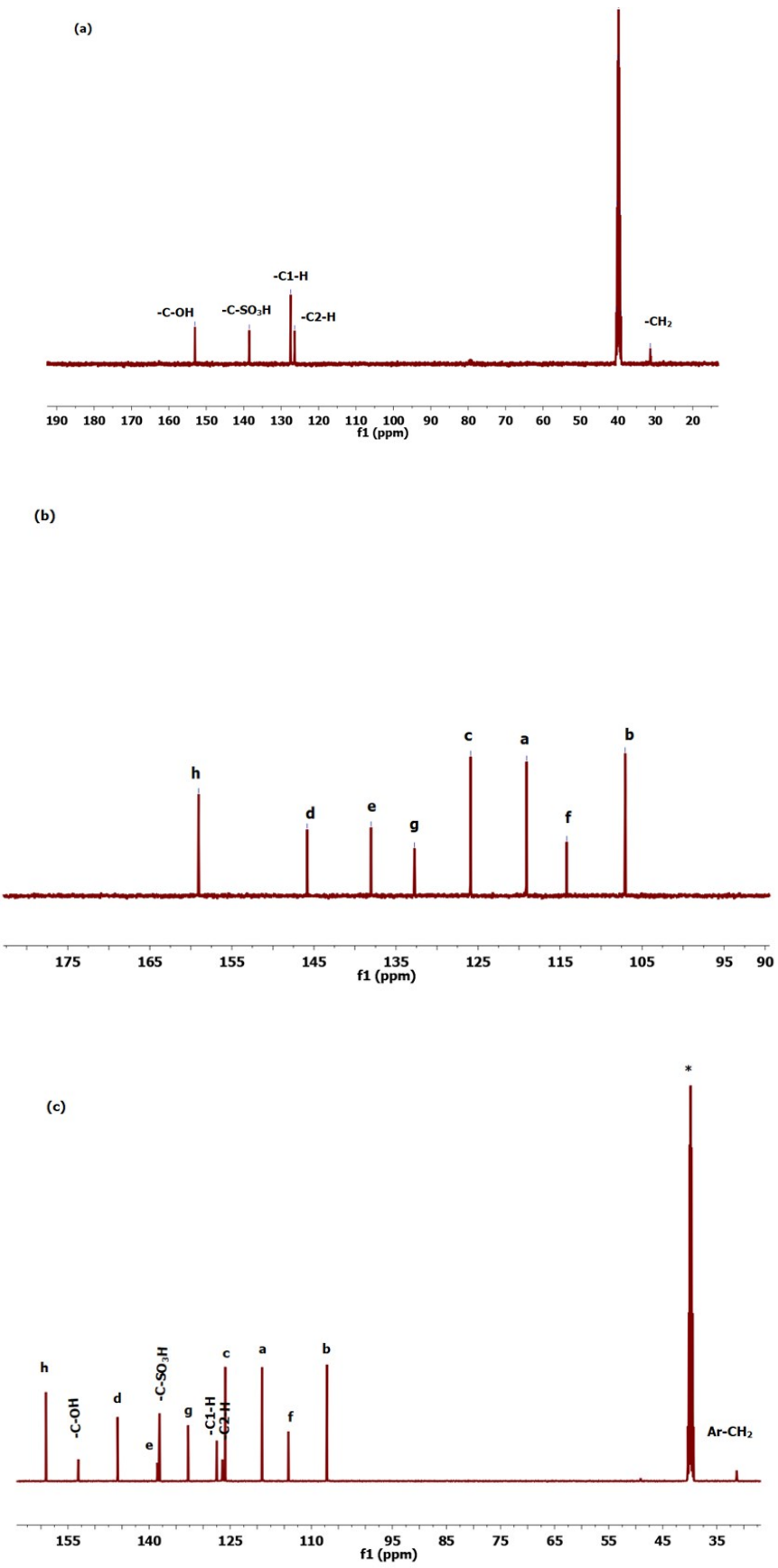
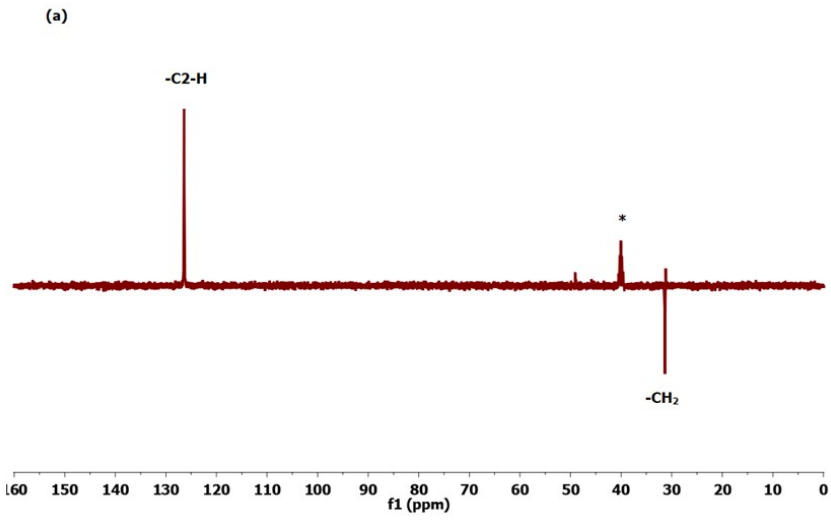


Fig.9S. ^{13}C NMR spectrum of (a) SCX6, (b) CHBT, and (c) CHBT-SCX6 in DMSO-d_6.

Table 4S Chemical shifts along with Δδ for CHBT, SCX6 and CHBT-SCX6 in DMSO-d_6

Carbon Assignment	Chemical Shift		(Δδ=δ-δ0) (ppm)
	δ0	δ	Δδ
a	119.08	119.11	0.03
b	107.06	107.11	0.05
c	125.90	125.91	0.01
d	145.83	145.82	-0.01
e	138.03	138.06	0.03
f	114.18	114.23	0.05
g	132.75	132.79	0.04
h	159.05	159.07	0.02
-C-OH	153.03	153.09	0.06
-C-SO_3H	138.51	138.47	-0.04
-C_1-H	127.45	127.48	0.03
-C_2-H	126.40	126.42	0.02
Ar-CH_2	31.24	31.32	0.08



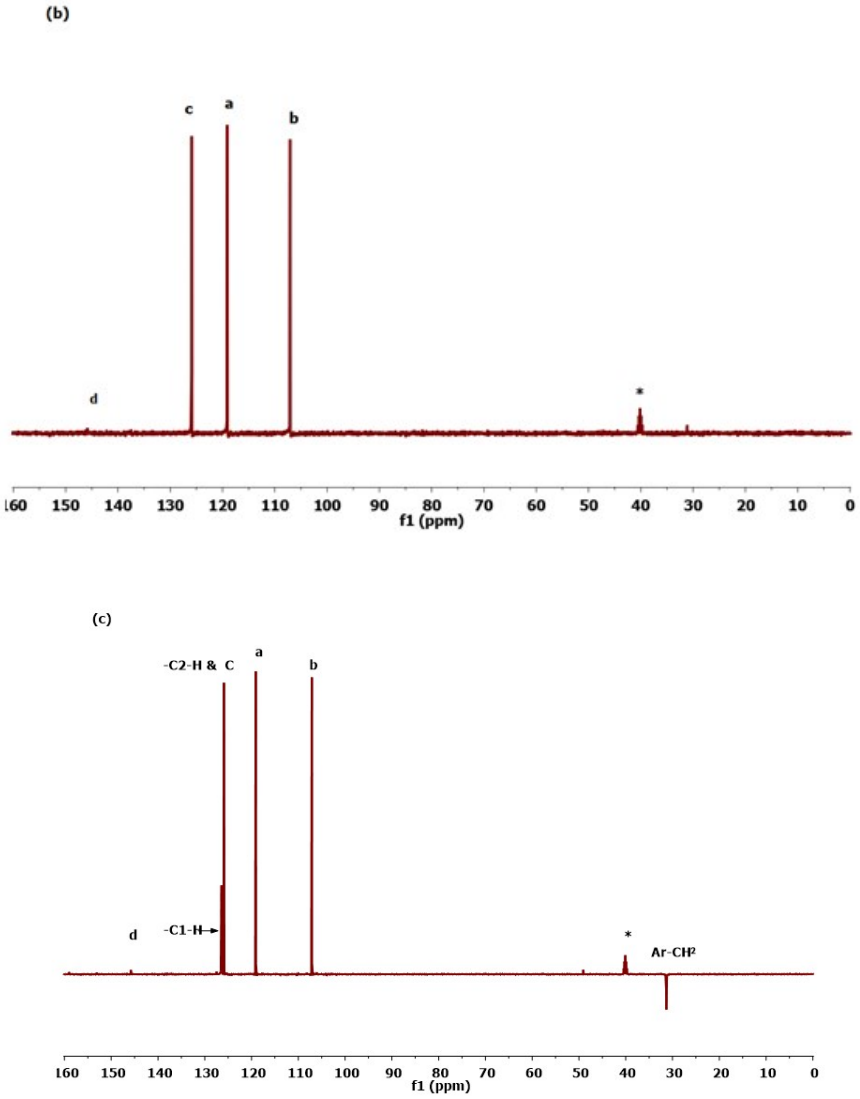


Fig.10S. DEPT spectra of (a) SCX6, (b) CHBT, and CHBT-SCX6 complex.

Table 5S Chemical shifts along with Δδ for CHBT, SCX6 and CHBT-SCX6 in DMSO-d_6.

Carbon Assignment	**Chemical Shift**		**(Δδ=δ-δ0) (ppm)**
	δ0	**δ**	**Δδ**
a	119.08	119.11	0.03
b	107.06	107.11	0.05
c	125.90	125.91	0.01
d	145.79	145.82	0.03
$-C_2-H$	126.39	126.42	0.03
$Ar-CH_2$	31.25	31.32	0.07

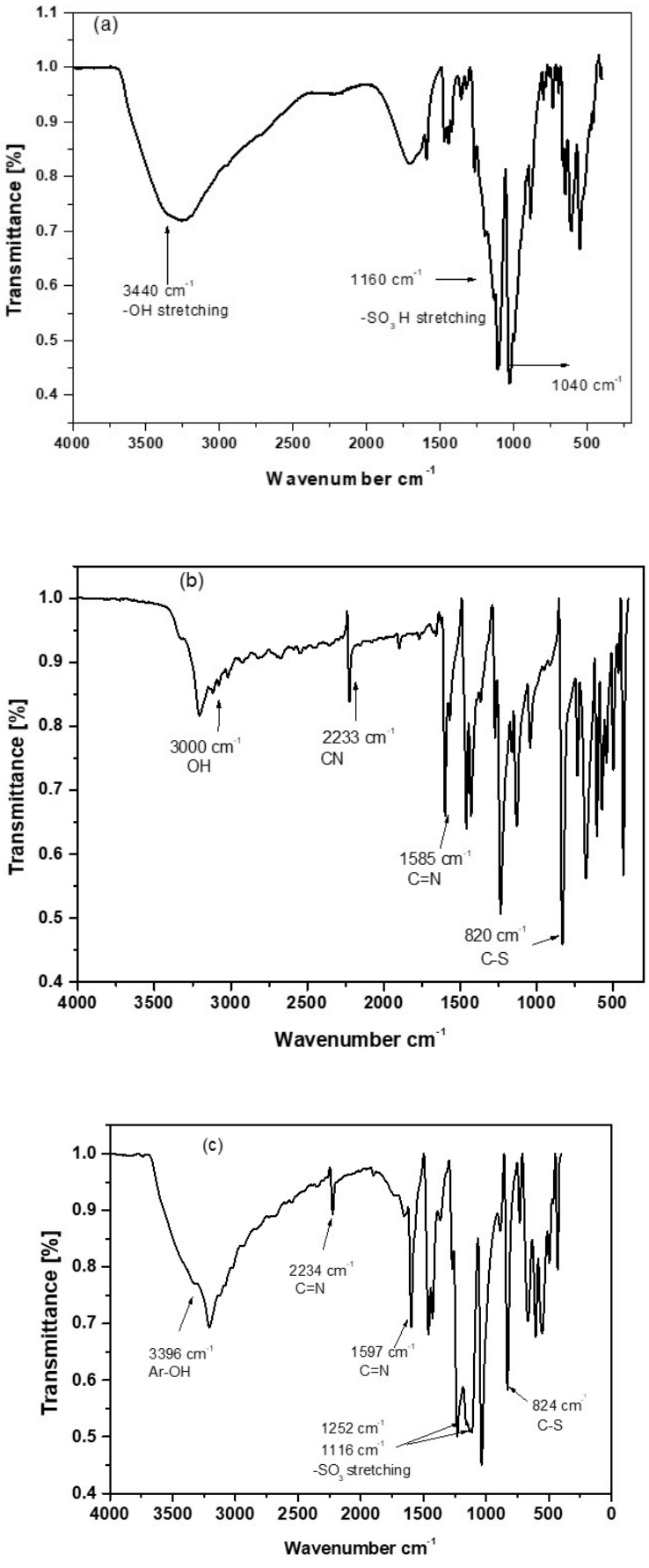


Fig.11S. FT-IR spectra of (a) SCX6 (b) CHBT and (c) CHBT-SCX6 complex in 1:1 mole ratio.

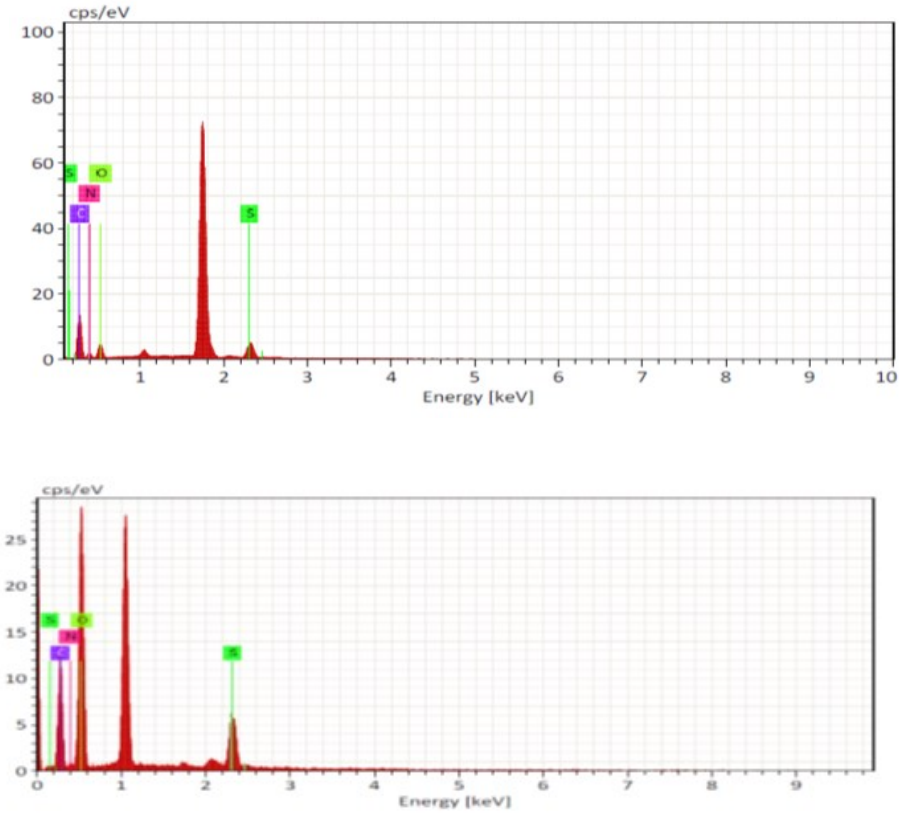


Fig.12S. EDS of (a) CHBT and (b) CHBT-SCX6 complex.

Table.6S EDS

	C (Atom %)	N (Atom %)	O (Atom %)	S (Atom %)
CHBT	57.88	17.33	19.19	5.60
CHBT-SCX6	37.27	2.56	55.16	5.01