Supporting Information

Dual Fluorescence of 4,4′-sulfonyldiphenol, 3,3'–dimethyl 4,4′-sulfonyldiphenol, 4,4′-sulfonyldibenzoic acid: Effects of cyclodextrin complexation

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Supporting Information

Table S1. Absorption and fluorescence maxima (nm) of SDP, DMSP and SDBA with different α-CD and β-CD concentrations.

Concentration of CD (M)	**SDP**						**DMSP**						**SDBA**					
	α-CD			**β-CD**			**α-CD**			**β-CD**			**α-CD**			**β-CD**		
	λ_{abs}	log ε	λ_{flu}	λ_{abs}	log ε	λ_{flu}	λ_{abs}	log ε	λ_{flu}	λ_{abs}	log ε	λ_{flu}	λ_{abs}	log ε	λ_{flu}	λ_{abs}	log ε	λ_{flu}
0 (without CD)	258 234	4.61	324 427	260 234	4.48	325 427	261 237	4.57	322 447	262 237	4.53	322 445	251 234	4.17	291 325 435	251 234	4.10	308 360 440
0.002	258 234	4.60	323 441	261 235	4.55	326 464	261 237	4.58	322 448	262 238	4.57	323 448	252 234	4.17	291 322 435	252 234	4.13	309 363 445
0.004	258 234	4.59	324 447	260 235	4.56	326 459	262 237	4.57	325 448	262 238	4.58	323 449	252 234	4.16	290 320 435	252 234	4.13	310 363 445
0.006	258 234	4.59	324 440	261 235	4.56	326 457	261 237	4.63	322 449	261 238	4.64	322 449	252 234	4.14	290 320 435	252 234	4.32	310 363 445
0.008	259 234	4.58	324 444	261 235	4.61	326 457	261 237	4.63	324 449	261 238	4.57	323 450	252 234	4.11	290 320 435	252 234	4.32	310 363 445
0.010	259 234	4.57	324 444	260 235	4.63	326 456	262 237	4.56	326 449	262 238	4.53	325 450	252 234	4.17	291 320 435	252 234	4.10	310 363 445
Excitation wavelength (nm)			260			260			260			260			260			260
K (M^{-1})	251		166	381		95	844		236	1564		1508	185		150	2369		2985
ΔG (-ve) (kJ mol^{-1})	3.32		3.07	3.58		2.74	4.05		3.28	4.42		4.40	3.14		3.01	4.67		4.81

Table S2. Energetic features, thermodynamic parameters and HOMO-LUMO energy calculations for SDBA, SDP, DMSP and its inclusion complexes by PM3 method.

Properties	**SDP**	**DMSP**	**SDBA**	**α-CD**	**β-CD**	**SDP/ α-CD**	**SDP/ β-CD**	**DMSP/ α-CD**	**DMSP/ β-CD**	**SDBA/ α-CD**	**SDBA/ β-CD**
E_{HOMO} (eV)	-9.72	-9.72	-10.66	-10.37	-10.35	-9.75	-9.58	-9.46	-9.34	-10.64	-10.56
E_{LUMO} (eV)	-0.49	-0.44	-1.39	1.26	1..23	-0.97	-0.62	-0.95	-0.71	-1.45	-1.42
E_{HOMO} – E_{LUMO} (eV)	-9.32	-9.28	-9.27	-11.63	-11.58	-8.78	-8.95	-8.51	-8.63	-9.18	-9.13
μ	-5.36	-5.08	-6.02	-4.56	-4.56	-5.36	-5.10	-5.20	-5.02	-6.05	-5.99
η	-4.39	-4.64	-4.63	5.81	5.79	-4.39	-4.47	-4.25	-4.31	-4.59	-4.56
ω	-3.28	-2.78	-3.92	1.78	1.79	-3.28	-2.91	-3.18	-2.93	-0.21	-3.94
S	-0.22	-0.21	-0.21	0.17	0.17	-0.22	-0.22	-0.23	-0.23	-3.99	-0.21
Dipole moment (D)	5.7079	5.881	1.146	11.34	12.29	15.087	3.03	16.45	15.43	4.7329	7.568
E*	-98.132	-114.77	-180.65	-1247.62	-1457.63	-1353.17	-1578.0	-1369.85	-1586.53	-1439.28	-1655.93
ΔE*						-7.41	-22.23	-7.45	-14.12	-11.01	-17.64
G *	-2.665	18.574	-77.37	-676.36	-789.52	-660.07	-793.32	-641.58	-766.31	-742.28	-861.257
ΔG *						18.94	-1.13	16.20	4.63	11.44	5.63
H *	35.96	56.475	-31.37	-570.84	-667.55	-540.28	-651.82	-518.87	-623.81	-611.624	-714.48
ΔH*						-5.40	-20.23	-4.51	-12.73	-9.40	-15.55
S **	0.129	0.14	0.154	0.35	0.40	0.401	0.474	0.411	0.478	0.43	0.49
ΔS**						-0.081	-0.064	-0.088	-0.077	-0.069	-0.070
ZPVE*	123.88	158.89	136.52	635.09	740.56	762.23	867.43	798.54	902.058	774.09	880.35

* kcal $mole^{-1}$; ** kcal/mol-Kelvin, ZPVE- Zero point vibrational energy

Table S3. Geometrical parameters of SDP, DMSP and SDBA before and after inclusion with α-CD and β-CD for the most stable inclusion complexes.

	SDP	**SDP/ α-CD**	**SDP/ β-CD**		**DMSP**	**DMSP/ α-CD**	**DMSP/ β-CD**		**SDBA**	**SDBA/ α-CD**	**SDBA/ β-CD**
Bond length (Å)											
H_1-O_2	2.65	2.68	2.92	H_1-O_2	2.67	2.61	2.55	O_1-H_5	2.65	2.62	2.75
H_4-O_1	2.66	2.58	2.59	H_3-O_1	2.63	2.70	2.85	O_2-H_1	2.65	2.58	3.02
C_4-O_3	1.36	1.35	1.35	O_3-H_{13}	2.78	2.72	2.55	O_3-O_4	2.11	2.19	2.12
H_1-H_8	3.00	2.98	3.30	O_4-H_9	2.97	2.81	2.83	O_6-H_7	2.64	2.88	2.72
H_3-O_3	2.57	2.72	2.58	H_1-H_6	3.14	3.63	3.20	H_9-H_6	3.01	3.35	2.92
Bond angle (°)											
C_1-S-O_1	109.4	108.6	110.5	C_1-S-O_1	109.37	109.01	109.31	C_1-S-O_1	109.40	107.31	108.32
O_1-S-O_2	117.7	117.7	115.8	C_4-O_3-H_{14}	108.09	108.08	108.18	C_1-S-C_{12}	99.09	101.95	100.19
C_4-O_3-H_{10}	108.2	108.3	108.6	C_1-S-C_{12}	99.84	101.73	100.60	H_1-O_2-H_8	68.80	73.10	61.70
C_9-O_4-H_9	108.2	109.2	109.0	H_1-O_2-H_6	73.33	87.59	71.90	O_4-C_{13}-O_3	110.86	108.02	116.92
Dihedral angle (°)											
C_3-C_4-O_3-H_{10}	178.8	179.14	173.80	C_1-C_2-C_3-C_{13}	179.93	179.47	176.67	S-C_1-C_2- C_3	179.34	172.80	179.39
C_2-C_3-S-O_1	157.0	148.39	179.90	C_1-S-C_{12}-C_7	94.19	118.36	105.71	C_6-C_1-S- O_2	155.92	175.76	165.65
O_2-C_7-C_8-C_9	166.8	170.27	169.79	C_8-C_9-O_4-H_7	178.63	167.85	178.40	O_1-S-C_{12}-C_{11}	155.79	179.46	176.23

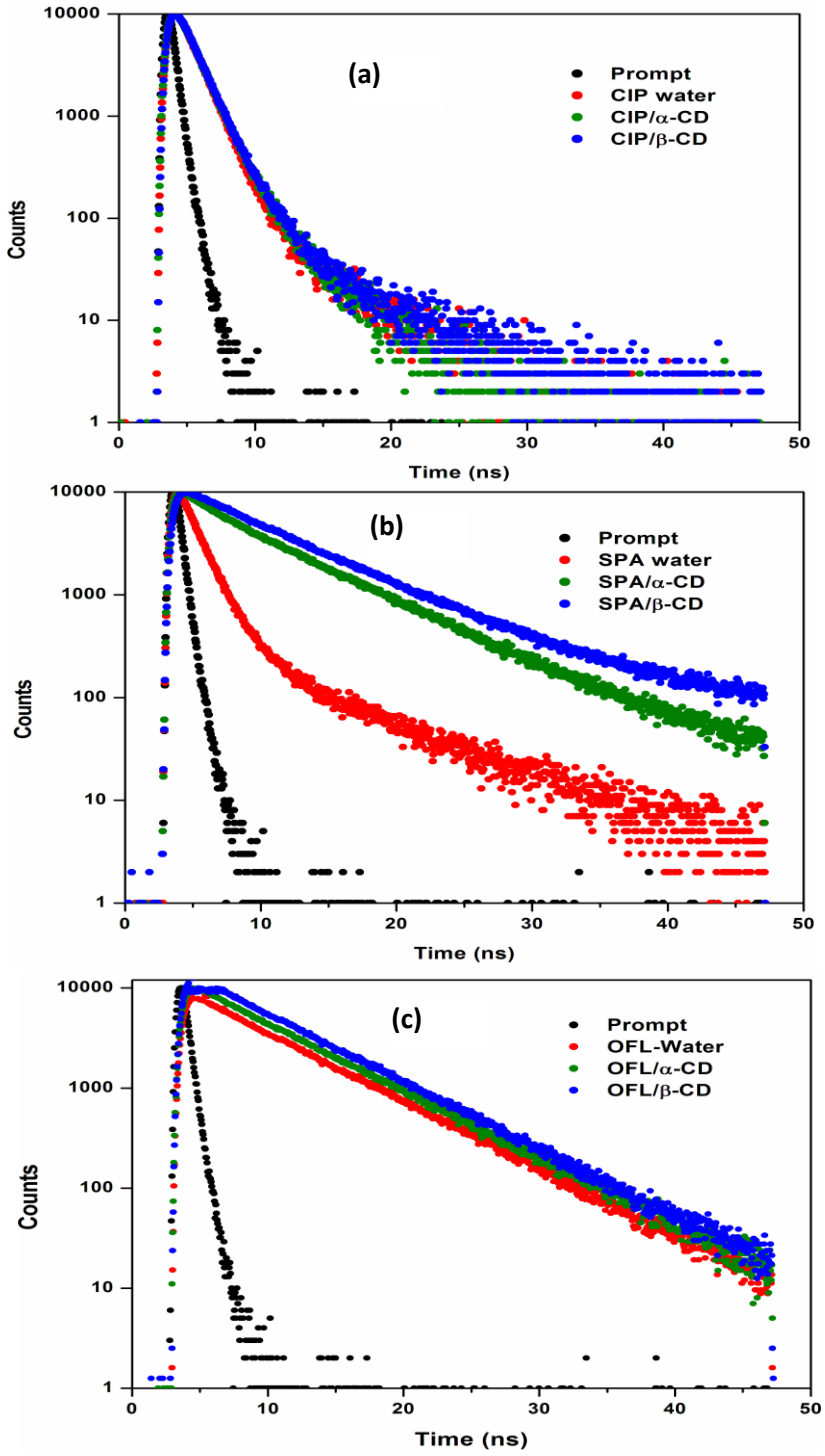

Fig. S1 Fluorescence decay cures of (a) SDP, (b) DMSP and (c) SDBA in water and 0.01 M CD solution.

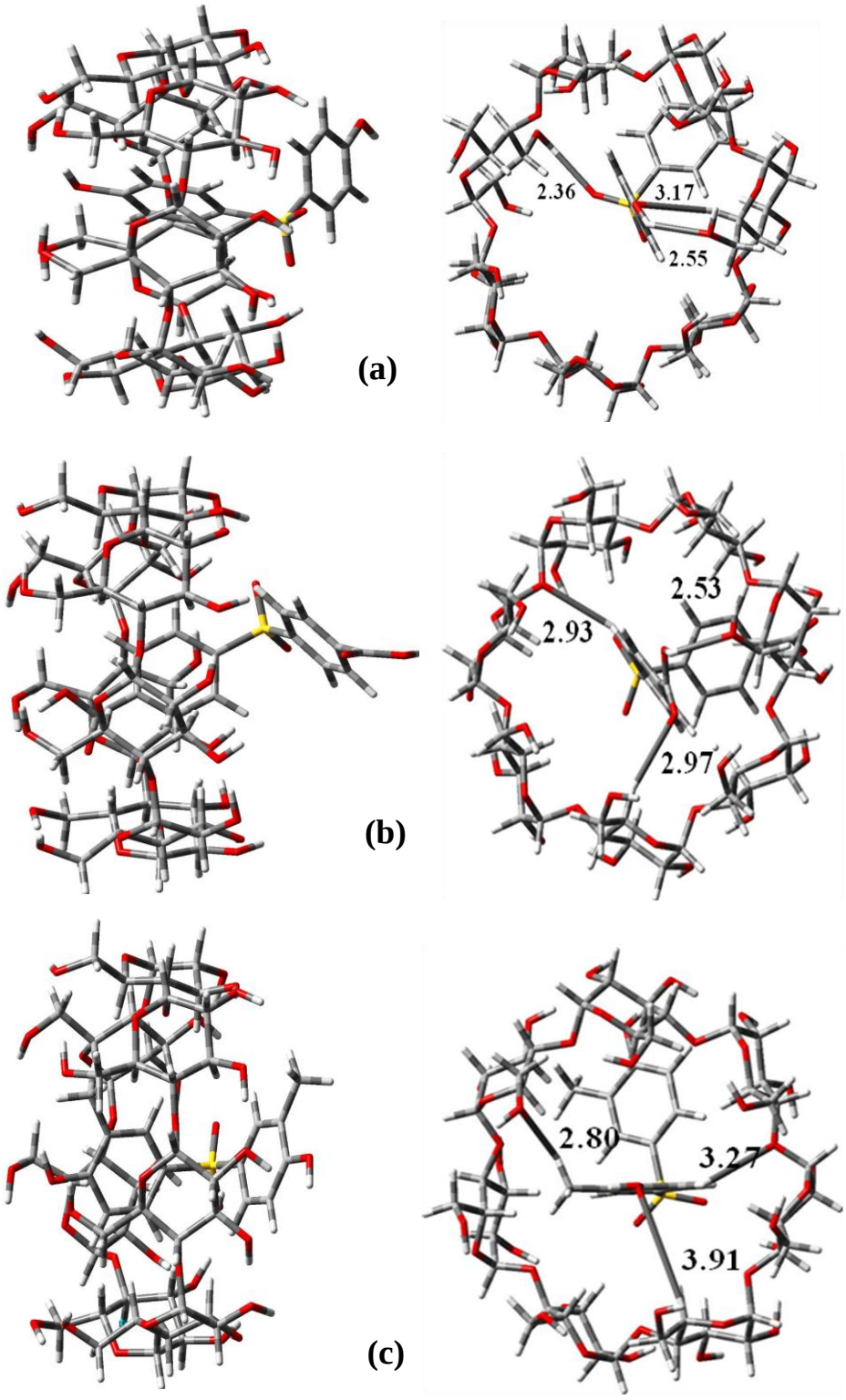

Fig. S2 Upper and side views of PM3 optimized structures of (a) SDP/β-CD, (b) SDBA/β-CD, and (c) DMSP/β-CD inclusion complex.

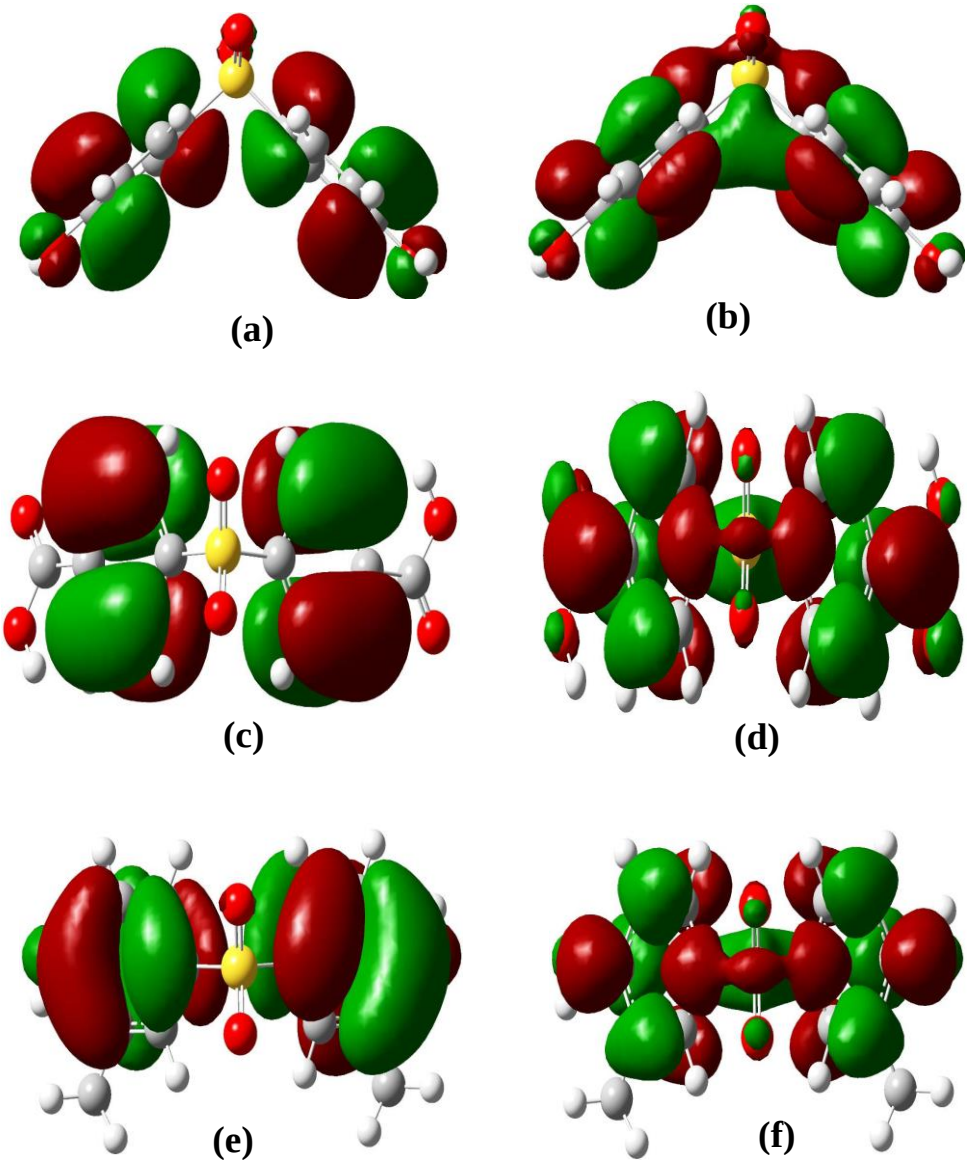

Fig. S3 HOMO, LUMO molecular orbital pictures of (a) SDP-HOMO, (b) SDP-LUMO, (c) SDBA-HOMO, (d) SDBA LUMO, (e) DMSP-HOMO and (f) DMSP -LUMO.