Supplementary Information

Binding modes of environmental endocrine disruptors to human serum albumin: insights from STD-NMR, ITC, spectroscopic and molecular docking studies

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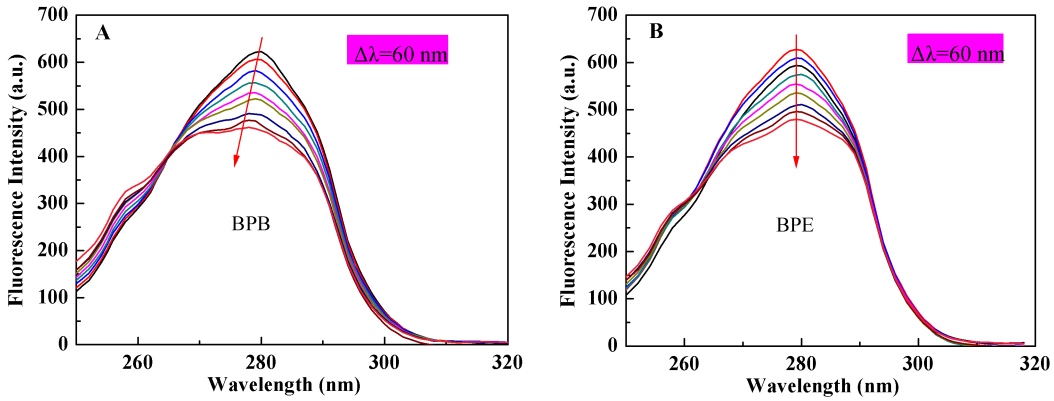
Table S1. Relative degrees of saturation of protons in STD-NMR spectra for BPB and BPE. The proton of H1/3/10/12 with the strongest STD effect was assigned with a value of 100%.

Hydrogen	H1/3/10/12	H4/6/9/13	H14	H15	H16
BPB-R_{STD}	100	61	25	59	55
BPE-R_{STD}	100	73	54	-	-

Table S2 Three-dimensional fluorescence spectral parameters of HSA alone and in the presence of BPB/BPE.

System	Peak No.	Peak position [λ_{ex} / λ_{em} (nm/nm)]	Δλ (nm)	Intensity
HSA	A	280/280→350/350	0	212.99→307.99
	1	280/338	58	621.95
	2	225/332	107	710.67
HSA–BPB	A	280/280→350/350	0	192.86→300.76
	1	280/337	57	633.01
	2	225/330	105	662.56
HSA–BPE	A	280/280→350/350	0	194.09→333.07
	1	280/333	53	647.29
	2	225/334	109	692.05



Supplementary Figure 1. Synchronous fluorescence spectra of HSA in the presence of different concentrations of BPB **(A)** and BPE **(B)** at Δλ = 60 nm. Concentrations of BPB/BPE were in the range of 0–120 μM.