

Table S1 Structures of PAHs and their derivatives.

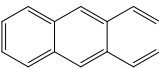
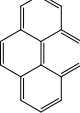
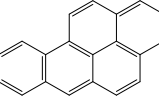
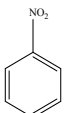
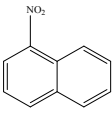
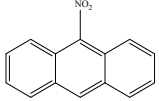
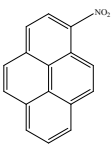
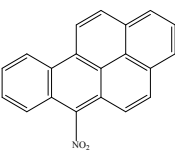
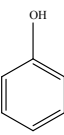
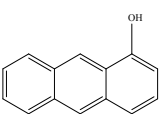
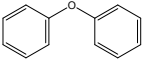
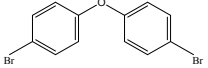
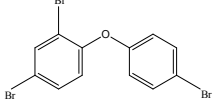
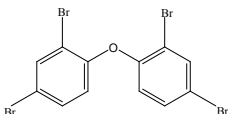
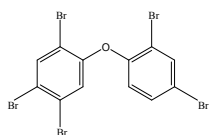
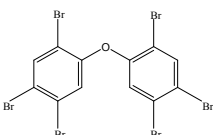
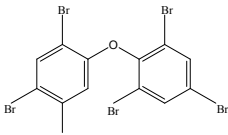
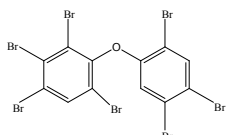
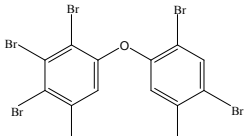
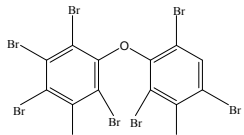
Analyte	Structure
benzene	
naphthalene	
Anthracene	
Pyrene	
Benzo[a]pyrene	
Nitrobenzene	
1-Nitronaphthalene	
9-Nitroanthracene	
1-Nitropyrene	
6-Nitrobenzo[a]pyrene	
Phenol	
1-Anthrol	

Table S2 Structures of PBDEs.

Analyte	Structure
DE	
BDE 15	
BDE 28	
BDE 47	
BDE 99	
BDE 153	
BDE 154	
BDE 183	
BDE 194	
BDE 209	

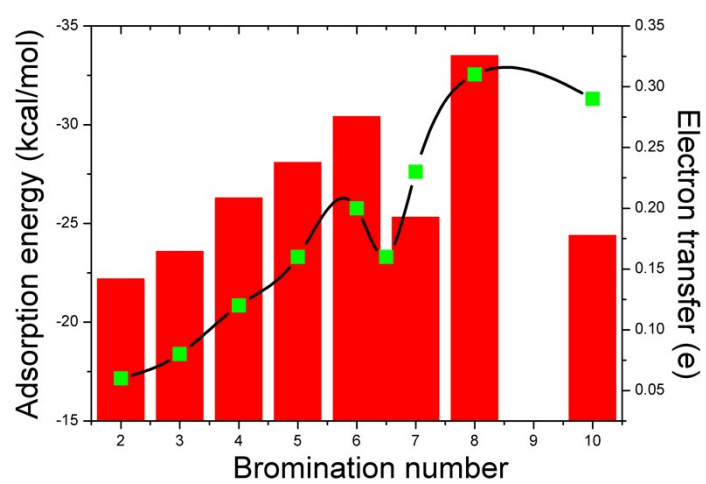


Fig. S1 The relationship between the adsorption energy and bromination degree (left-hand scale); and amount of electron transfer (right-hand scale)