Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Electronic Supplementary Information for:

Interactions between aromatic hydrocarbons and functionalized C_{60} fullerenes – insights from experimental data and molecular modelling

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Table S1: Selected quality parameters of the applied ASE-HPLC method**.**

Method parameter	Hydroxypyrene	Naphthylamine
Retention time [min]	10.68	7.88
LDR[a] [µg/L]	0.5 - 2500	800- 200000
LOD[b] [µg/L]	0.28	415
Recovery [%]	85 ± 4	93 ± 5

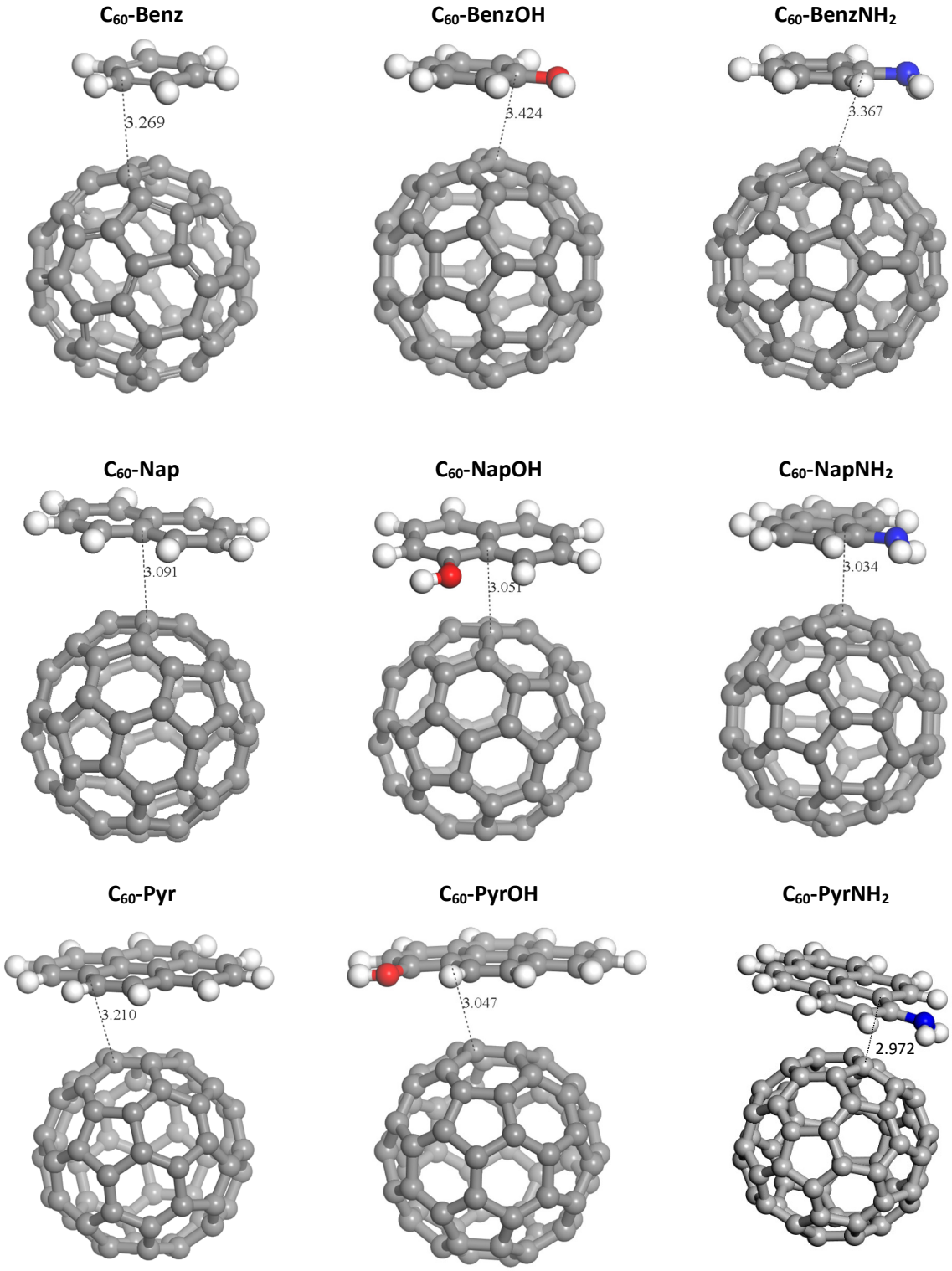
[a]LDR: linear dynamic range; [b]LOD: limit of detection.

Table S2: M05-2X/6-311+G(d,p) calculations in polarized continuum solvent listing model potential energies, potential energy differences for dimer formation, and experimentally determined phase-transfer free-energies.

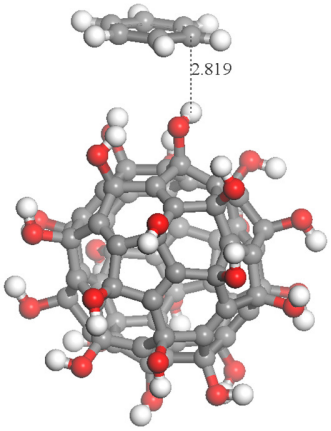
Model	ΔE_{calc} (kJ/mol)	ΔG_{exp} (kJ/mol)
C_{60}-Benzene	-16	-12.25
C_{60}-BenzeneOH	-20	-13.30
C_{60}-BenzeneNH_2	-25	-14.54
C_{60}-Napthalene	-29	-18.08
C_{60}-NapthaleneOH	-31	-18.45
C_{60}-NapthaleneNH_2	-32	-18.90
C_{60}-Pyrene	-41	n.a.[a]
C_{60}-PyreneOH	-42	n.a.[a]
C_{60}-OH-Benz	-26	-10.79
C_{60}-OH-BenzNH_2	-38	-14.38
C_{60}-OH-BenzOH	-46	-16.84
C_{60}-OH-Naph	-31	-13.53
C_{60}-OH-NaphNH_2	-55	-22.43
C_{60}-OH-NaphOH	-56	-24.66
C_{60}-OH-Pyr	-34	n.a.[a]
C_{60}-OH-PyrOH	-59	n.a.[a]

[a]n.a.: data not available.

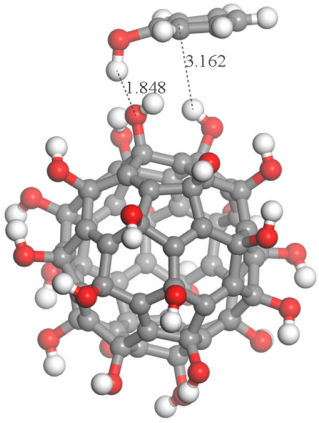
Figure S1: Configuration for each dimer after energy minimization with M05 -2x/6-311+G(d,p).



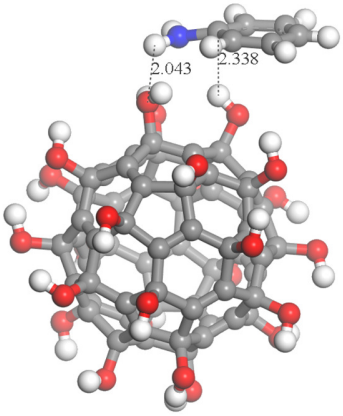
C_{60}-OH-Benz



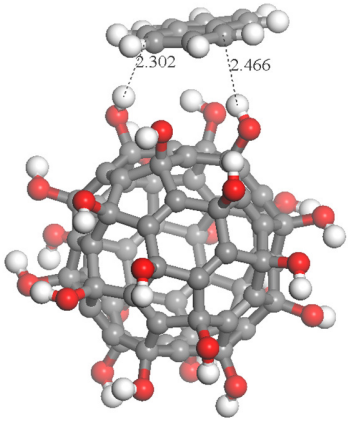
C_{60}-OH-BenzOH



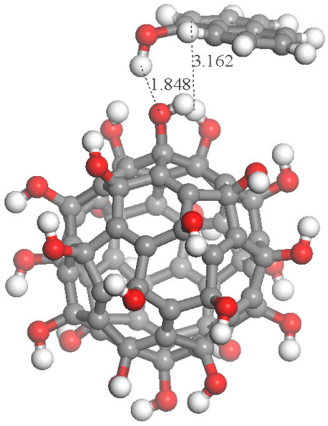
C_{60}-OH-BenzNH_2



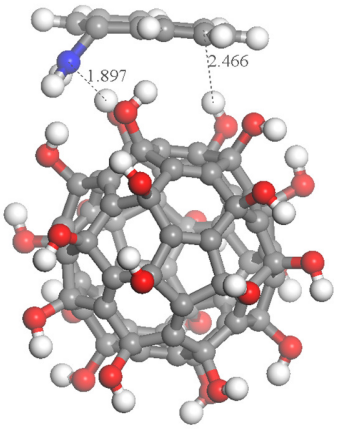
C_{60}-OH-Nap



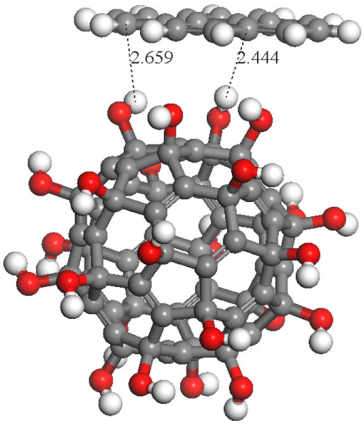
C_{60}-OH-NapOH



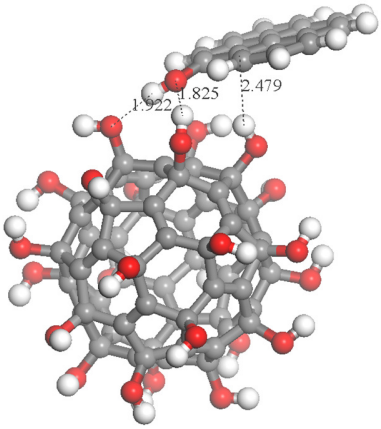
C_{60}-OH-NapNH_2



C_{60}-OH-Pyr



C_{60}-OH-PyrOH



C_{60}-OH-PyrNH_2

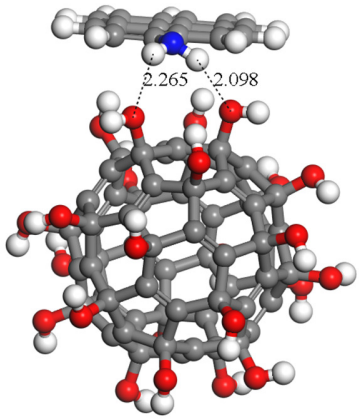


Figure S2: Sorption isotherms of benzene, naphthalene, and pyrene.

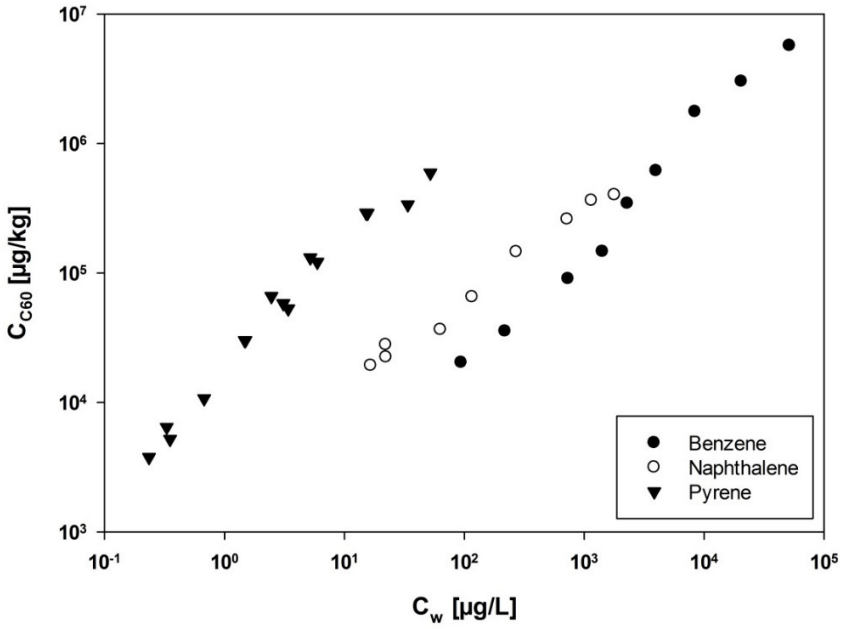


Figure S3: Comparison between sorption energies obtained in this study for C_{60} and sorption energies obtained by Zou et al.[1] for carbon nanotubes.

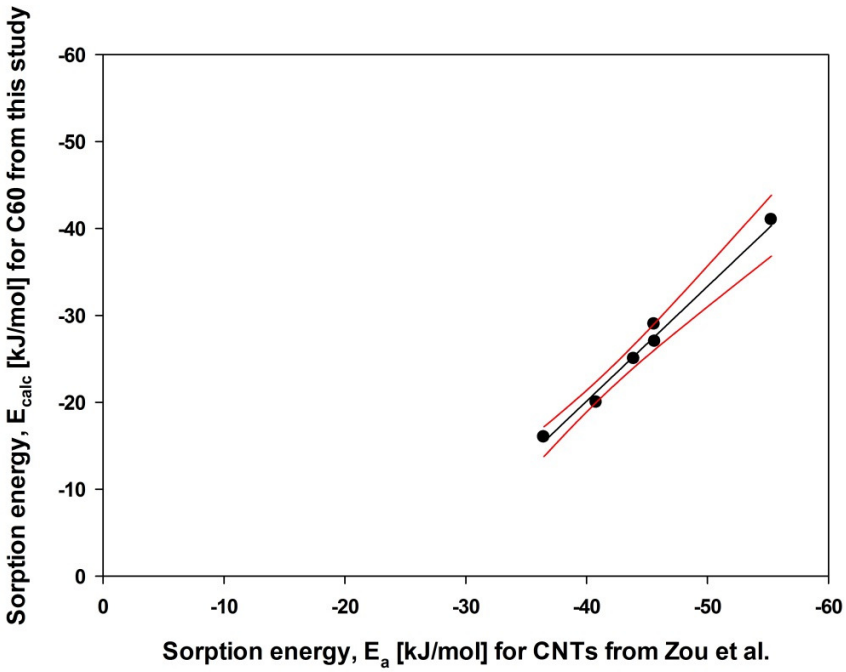


Figure S4: Comparison between the experimental distribution coefficients (log K_d) and the hydrophobicity of the sorbates (log K_{ow})

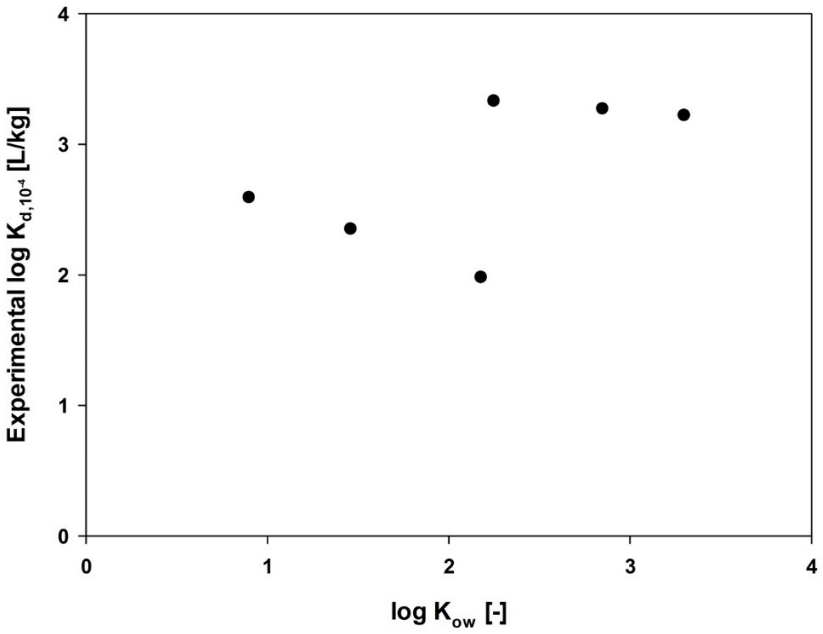
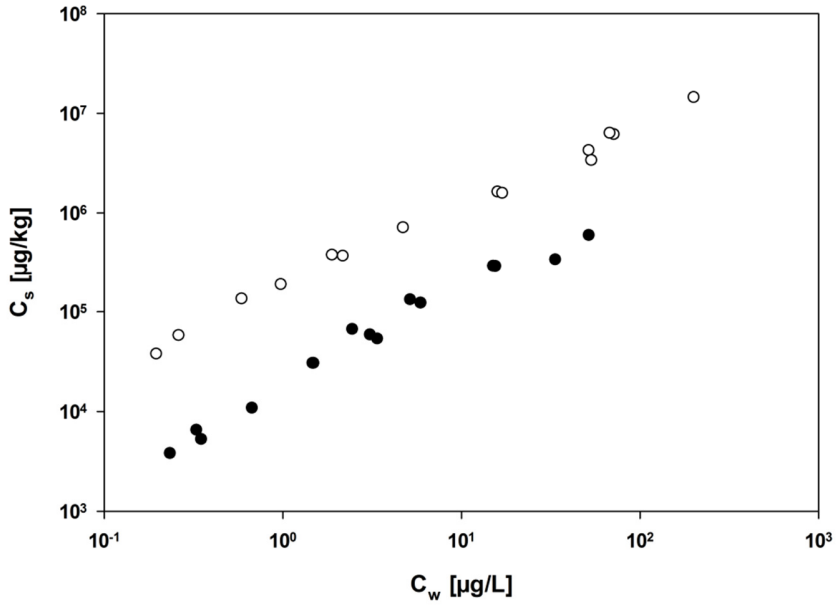


Figure S5: Sorption isotherms of (•) pyrene and (○) hydroxypyrene by C_{60} using POM method.



References

1. Zou, M. Y.; Zhang, J. D.; Chen, J. W.; Li, X. H., Simulating Adsorption of Organic Pollutants on Finite (8,0) Single-Walled Carbon Nanotubes in Water. *Environ. Sci. Technol.* **2012,** *46*, (16), 8887-8894.