Predicting Adsorption of Organic Pollutants on Boron Nitride Nanosheets via *in silico* Techniques: DFT Computations and QSAR Modeling

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The SI consists of three tables and three figures. There are 14 pages in total.

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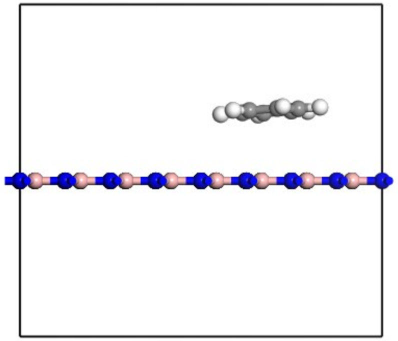
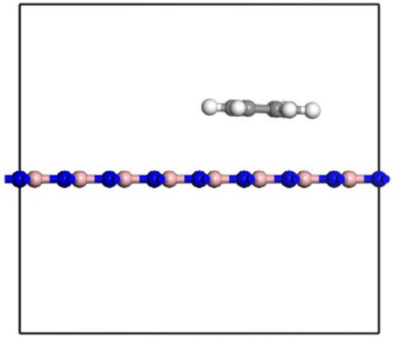
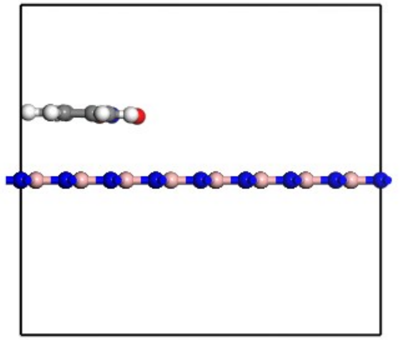
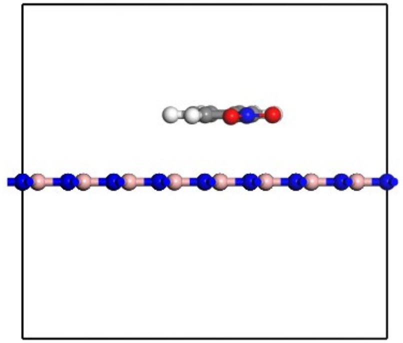
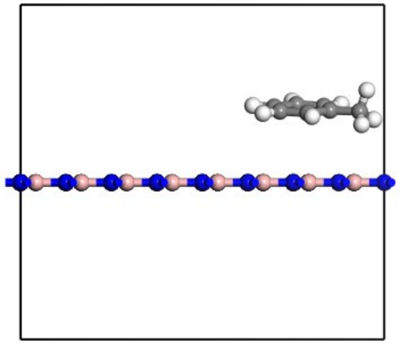
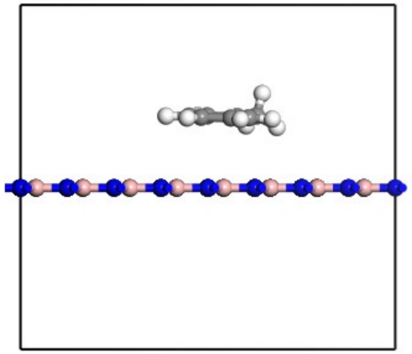
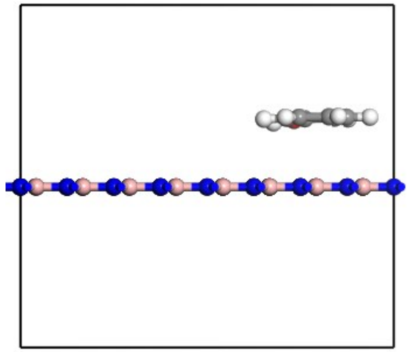
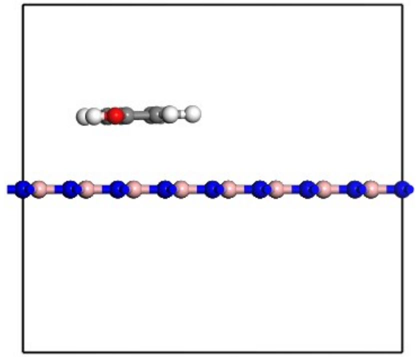
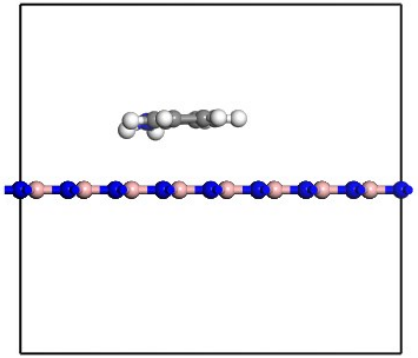
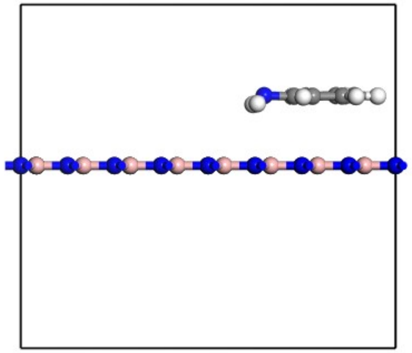
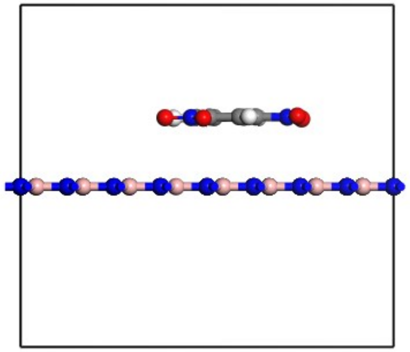
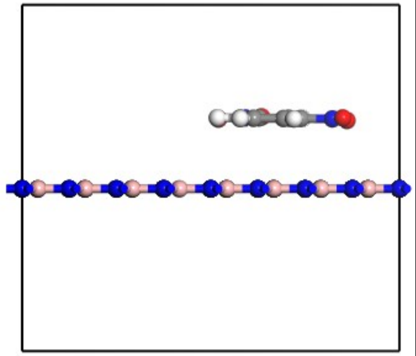
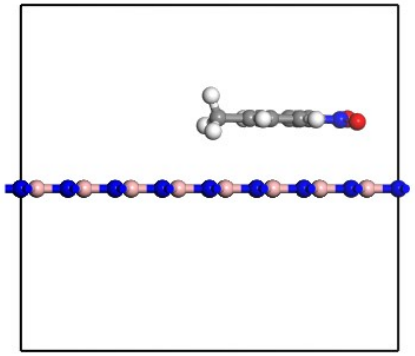
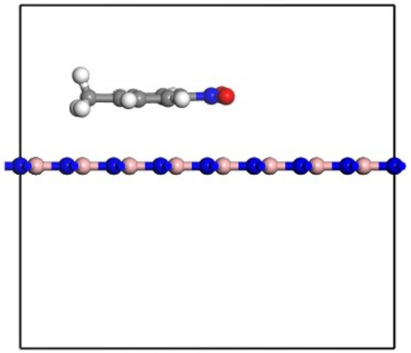
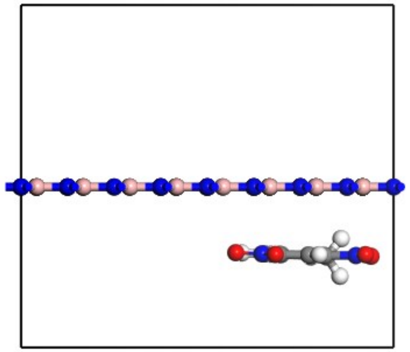
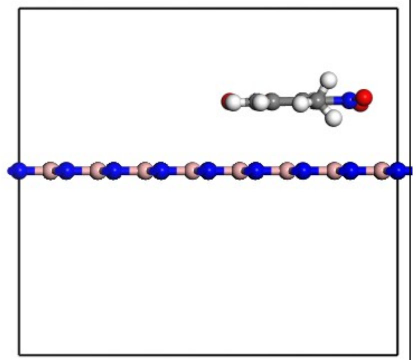
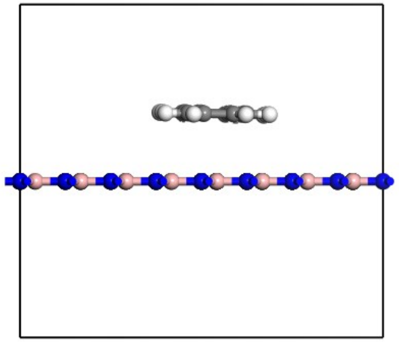
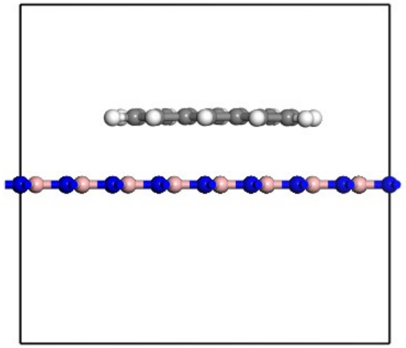
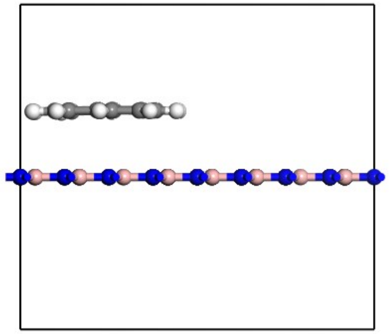
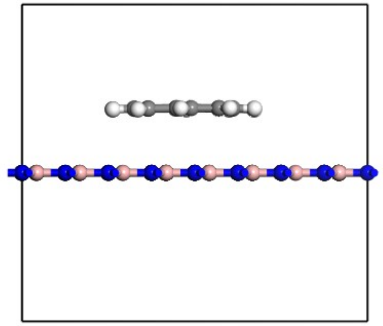
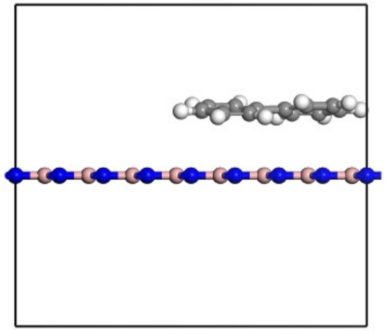
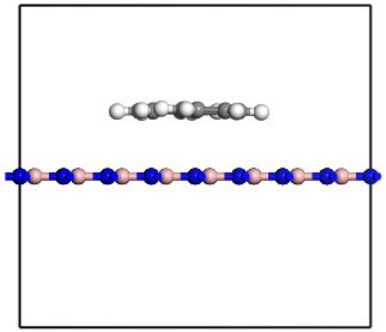
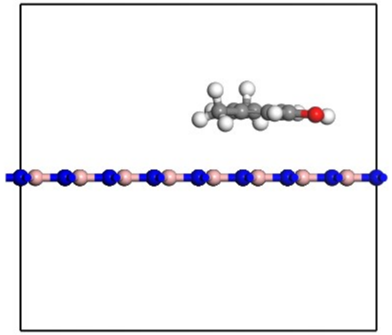
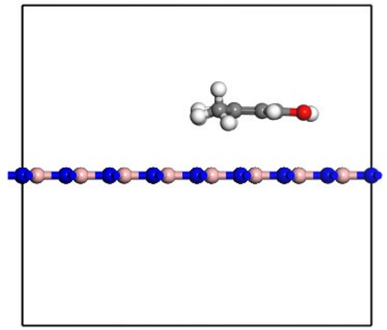
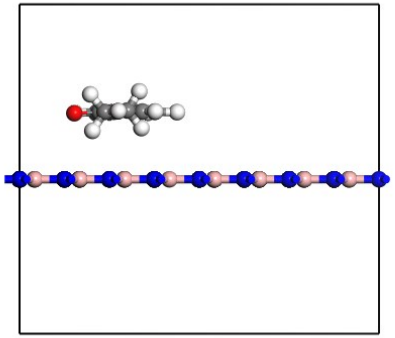
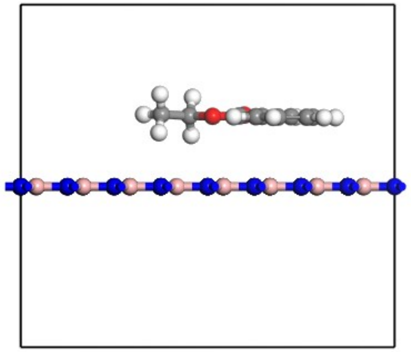
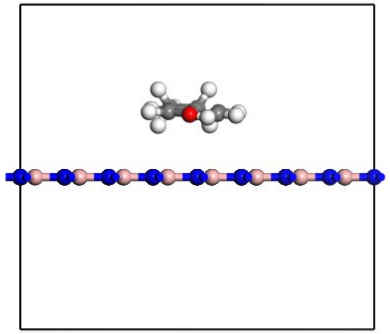
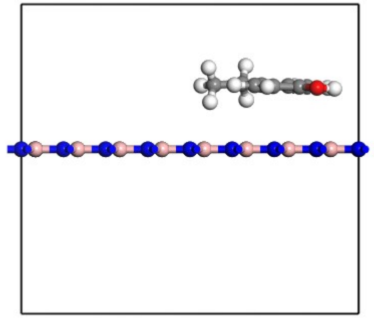
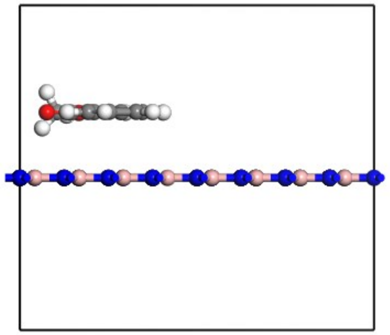
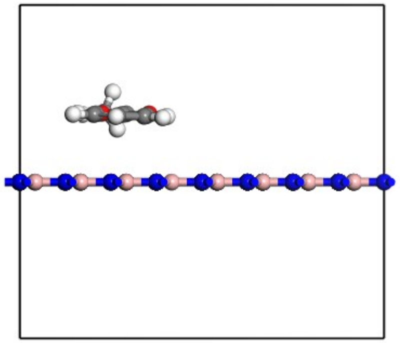
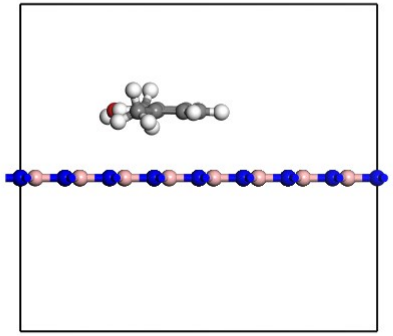
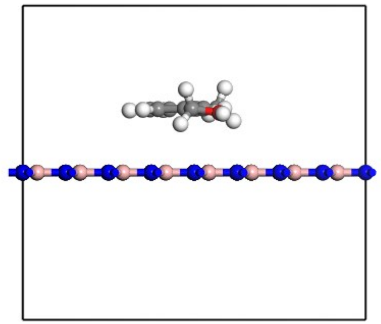
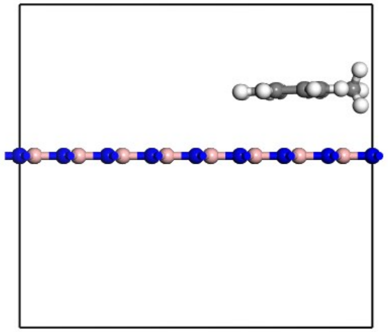
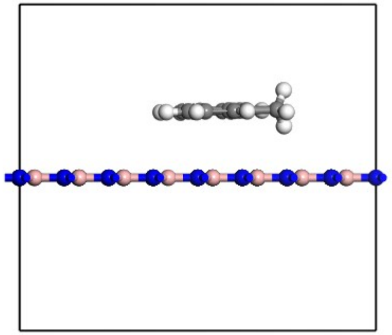
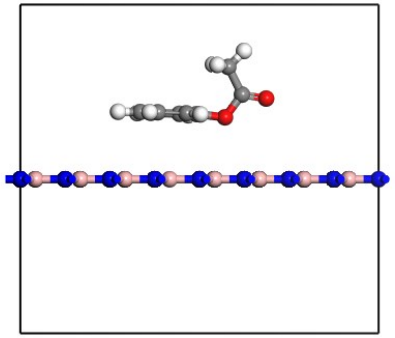
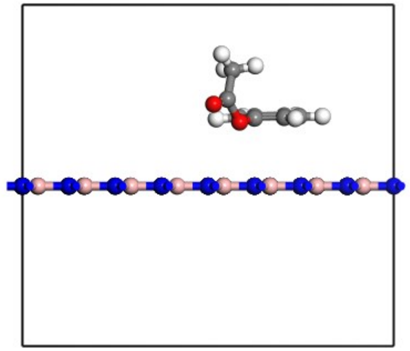
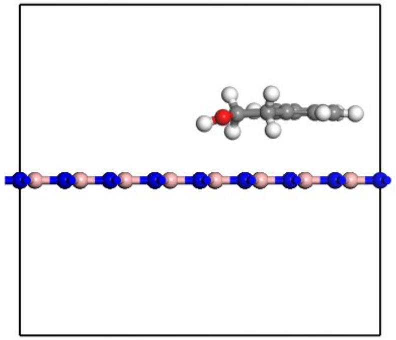
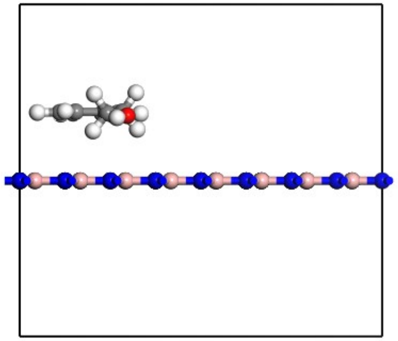
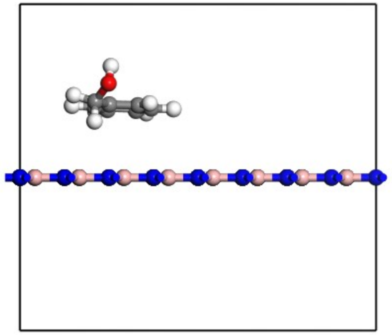
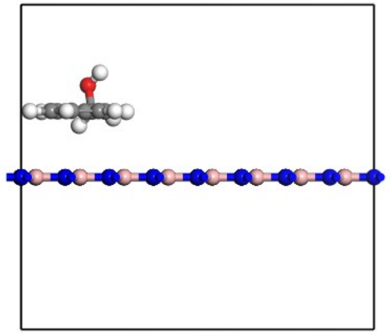
Table S1. Adsorption equilibrium configuration for the 28 organic compounds on boron nitride nanosheet

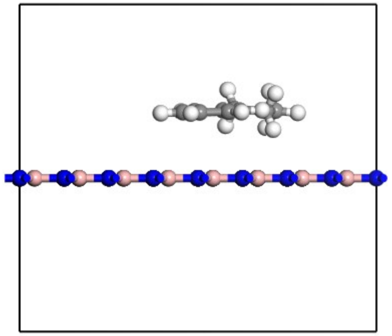
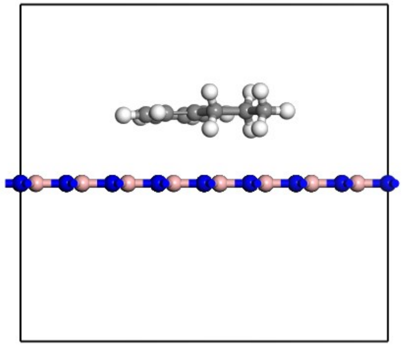
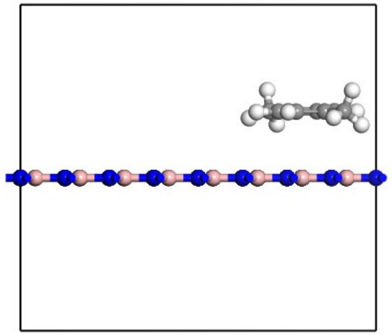
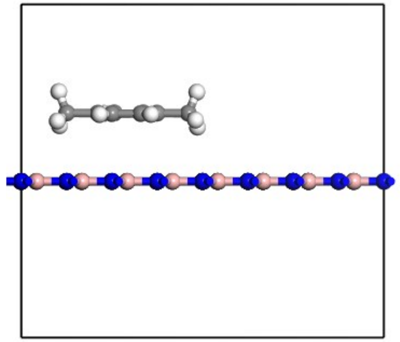
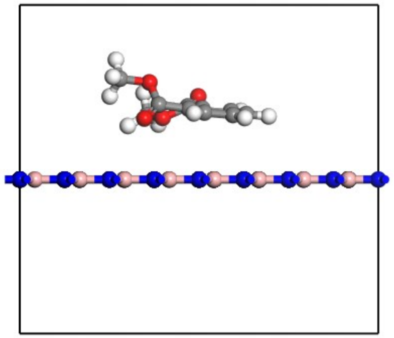
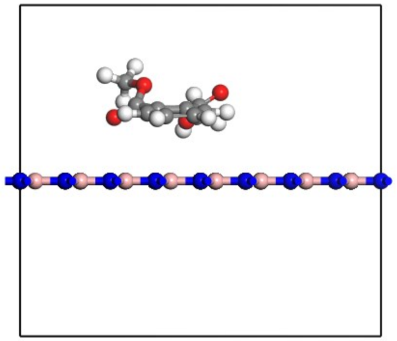
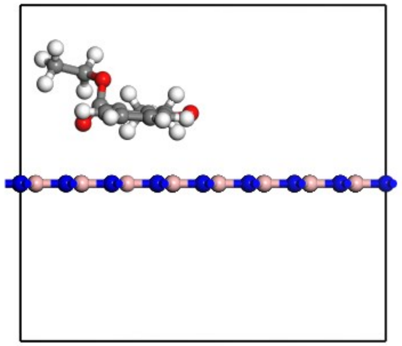
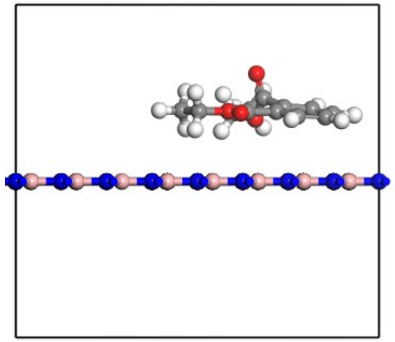
Gaseous phase	Aqueous phase	Gaseous phase	Aqueous phase
 d = 3.376 Å benzene	 d = 3.408 Å benzene	 d = 3.200 Å nitrobenzene	 d = 3.200 Å nitrobenzene
 d = 3.504 Å toluene	 d = 3.296 Å toluene	 d = 3.200 Å phenol	 d = 3.392 Å phenol

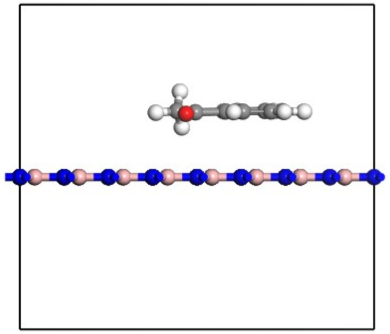
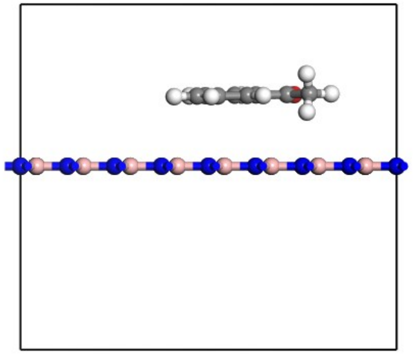
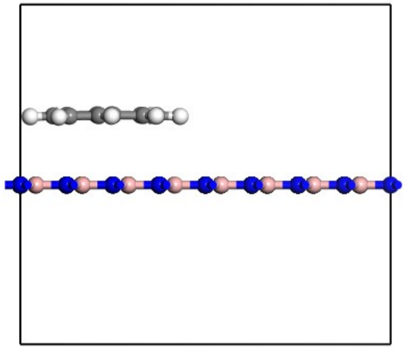
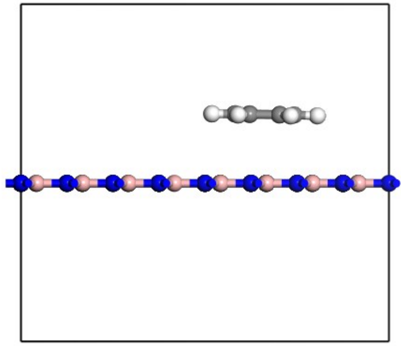
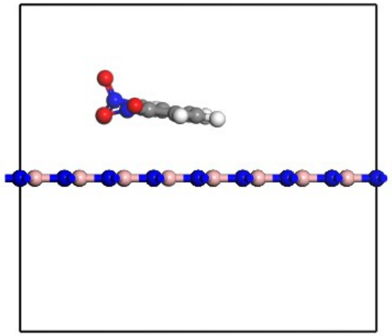
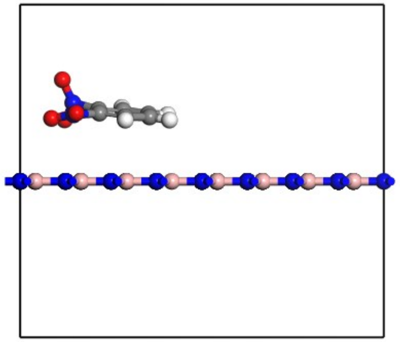
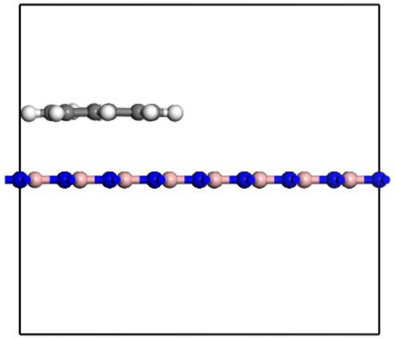
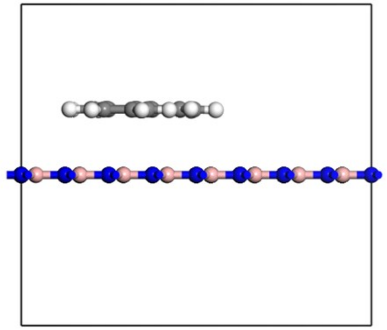
Gaseous phase	**Aqueous phase**	**Gaseous phase**	**Aqueous phase**
 d = 3.200 Å aniline	 d = 3.248 Å aniline	 d = 3.232 Å 1,3-dinitrobenzene	 d = 3.248 Å 1,3-dinitrobenzene
 d = 3.216 Å 4-nitrotoluene	 d = 3.216 Å 4-nitrotoluene	 d = 3.168 Å 2, 4-dinitrotoluene	 d = 3.216 Å 2, 4-dinitrotoluene

Gaseous phase	**Aqueous phase**	**Gaseous phase**	**Aqueous phase**
 *d* = 3.264 Å anthracene	 *d* = 3.200 Å anthracene	 *d* = 3.280 Å pyrene	 *d* = 3.248 Å pyrene
 *d* = 3.264 Å biphenyl	 *d* = 3.264 Å biphenyl	 *d* = 3.216 Å 3,5-dimethylphenol	 *d* = 3.232Å 3,5-dimethylphenol

Gaseous phase	Aqueous phase	Gaseous phase	Aqueous phase
 d = 3.264 Å ethylbenzoate	 d = 3.280 Å ethylbenzoate	 d = 3.232 Å 4-ethylphenol	 d = 3.280 Å 4-ethylphenol
 d = 3.232 Å methylbenzoate	 d = 3.248 Å methylbenzoate	 d = 3.280 Å (3-methylphenyl)methanol	 d = 3.216 Å (3-methylphenyl)methanol

Gaseous phase	Aqueous phase	Gaseous phase	Aqueous phase
 $d = 3.264$ Å 1-methylnaphthalene	 $d = 3.280$ Å 1-methylnaphthalene	 $d = 3.616$ Å phenylacetate	 $d = 3.600$ Å phenylacetate
 $d = 3.248$ Å 2-phenylethanol	 $d = 3.264$ Å 2-phenylethanol	 $d = 3.648$ Å phenylmethanol	 $d = 3.440$ Å phenylmethanol

Gaseous phase	**Aqueous phase**	**Gaseous phase**	**Aqueous phase**
 d = 3.280 Å propylbenzene	 d = 3.344 Å propylbenzene	 d = 3.264 Å p-xylene	 d = 3.264 Å p-xylene
 d = 3.568 Å DMP	 d = 3.568 Å DMP	 d = 3.680 Å DEP	 d = 3.488 Å DEP

Gaseous phase	**Aqueous phase**	**Gaseous phase**	**Aqueous phase**
 *d* = 3.216 Å acetophenone	 *d* = 3.296 Å acetophenone	 *d* = 3.280 Å naphthalene	 *d* = 3.264 Å naphthalene
 *d* = 3.440 Å 1,2-dinitrobenzene	 *d* = 3.392 Å 1,2-dinitrobenzene	 *d* = 3.280 Å phenanthrene	 *d* = 3.264 Å phenanthrene

d denotes the distance between the center of molecule and that of the boron nitride surface.

Table S2. Charge transfer between the compound and the boron nitride nanosheet from the adsorption complex

No.	Compound	Charge transfer (e)*		No.	Compound	Charge transfer (e)*	
		Gaseous phase	Aqueous phase			Gaseous phase	Aqueous phase
1	benzene	0.009	0.011	15	methylbenzoate	-0.024	-0.024
2	nitrobenzene	-0.003	-0.006	16	(3-methylphenyl)methanol	-0.054	-0.029
3	toluene	-0.010	-0.017	17	1-methylnaphthalene	-0.017	-0.018
4	phenol	0.004	0.013	18	phenylacetate	0.008	0.016
5	aniline	-0.018	-0.015	19	2-phenylethanol	-0.049	-0.029
6	1,3-dinitrobenzene	-0.016	-0.014	20	phenylmethanol	-0.016	-0.032
7	4-nitrotoluene	-0.021	-0.019	21	propylbenzene	-0.064	-0.063
8	2, 4-dinitrotoluene	-0.027	-0.051	22	p-xylene	-0.045	-0.046
9	anthracene	0.011	0.023	23	dimethyl phthalate (DMP)	-0.022	-0.018
10	pyrene	0.016	0.016	24	diethyl phthalate (DEP)	-0.030	-0.096
11	biphenyl	0.009	0.006	25	acetophenone	-0.035	-0.029
12	3,5-dimethylphenol	-0.035	-0.039	26	naphthalene	0.006	0.005
13	ethylbenzoate	-0.053	-0.048	27	1,2-dinitrobenzene	-0.010	0.003
14	4-ethylphenol	-0.022	-0.033	28	phenanthrene	0.010	0.009

*Charge transfer: the positive value represents that the electron transfers from the compound to the boron nitride nanosheet, while the negative value means that the electron transfers from the boron nitride nanosheet to the compound.

Table S3. Estimated logarithm values for adsorption equilibrium coefficient (log$K$) for fluorene from DFT computations and prediction models in the gaseous and aqueous environments

Model	Gaseous		Aqueous	
	log$K$ (DFT)	log$K$ (predicted)	log$K$ (DFT)	log$K$ (predicted)
Eq 9 (pp-LFERs)	14.90	12.25	-	-
Eq 10 (pp-LFERs)	-	-	9.97	10.13
Eq 11 (QSAR)	14.90	11.10	-	-
Eq 12 (QSAR)	-	-	9.97	11.21

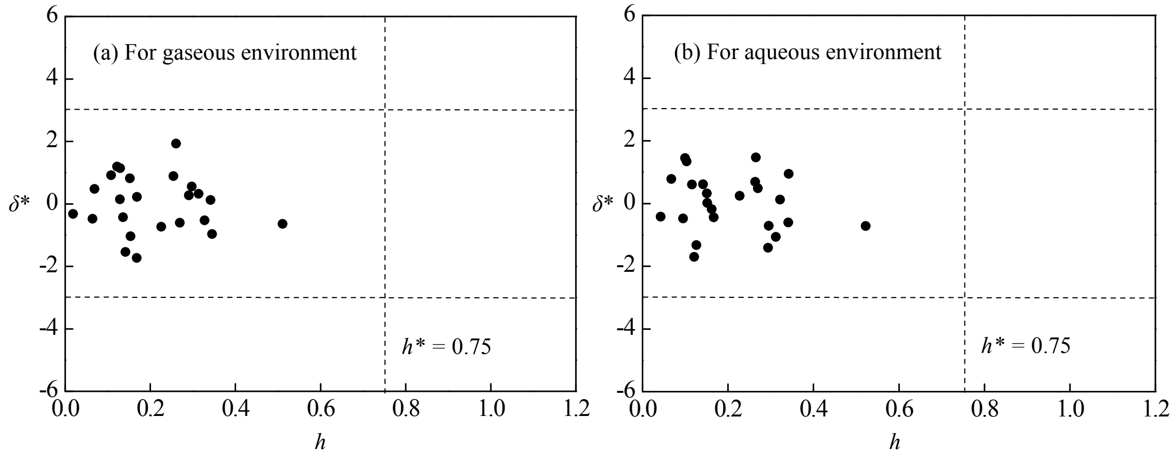


Figure S1. Williams plots of standardized residuals (δ^*) versus leverage values (h) for pp-LFER models (h^* denotes the warning leverage value)

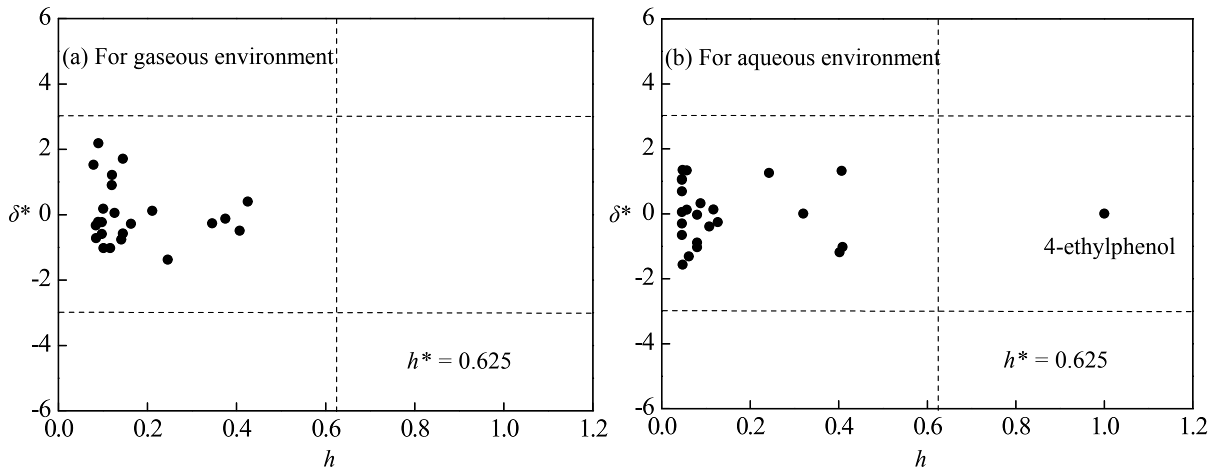


Figure S2. Williams plots of standardized residuals (δ^*) versus leverage values (h) for QSAR models (h^* denotes the warning leverage value)

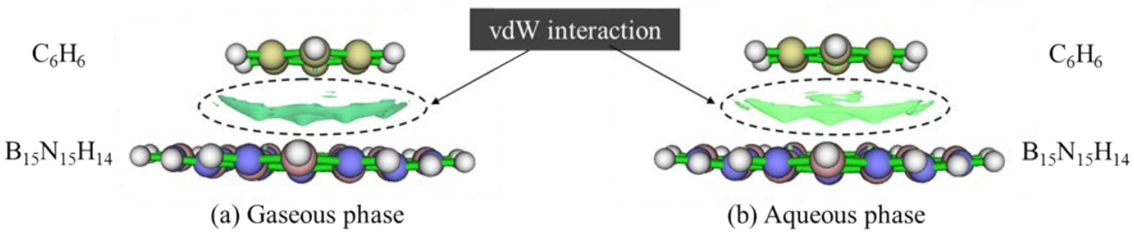


Figure S3. Non-covalent interactions (NCI) analysis for the interactions between C_6H_6 and $B_{15}N_{15}H_{14}$ with the Multiwfn[1] program

REFERENCES

(1) Lu, T. and Chen, F. Multiwfn: A multifunctional wavefunction analyzer. *J. Comput. Chem*. **2012**, *33* (5), 580-592.