Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

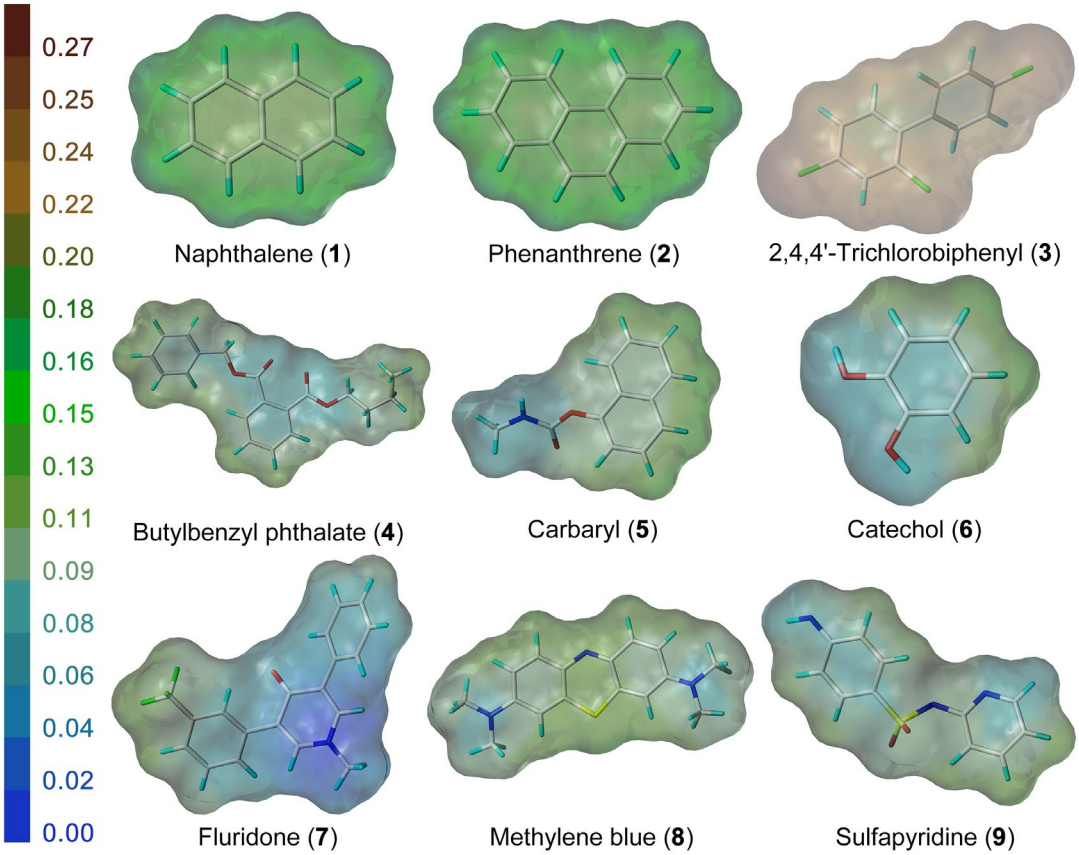

Figure S1 Lipophilic solid surfaces for the investigated compounds. Warm colors indicate lipophilic features, and cold colors indicate hydrophilic features.

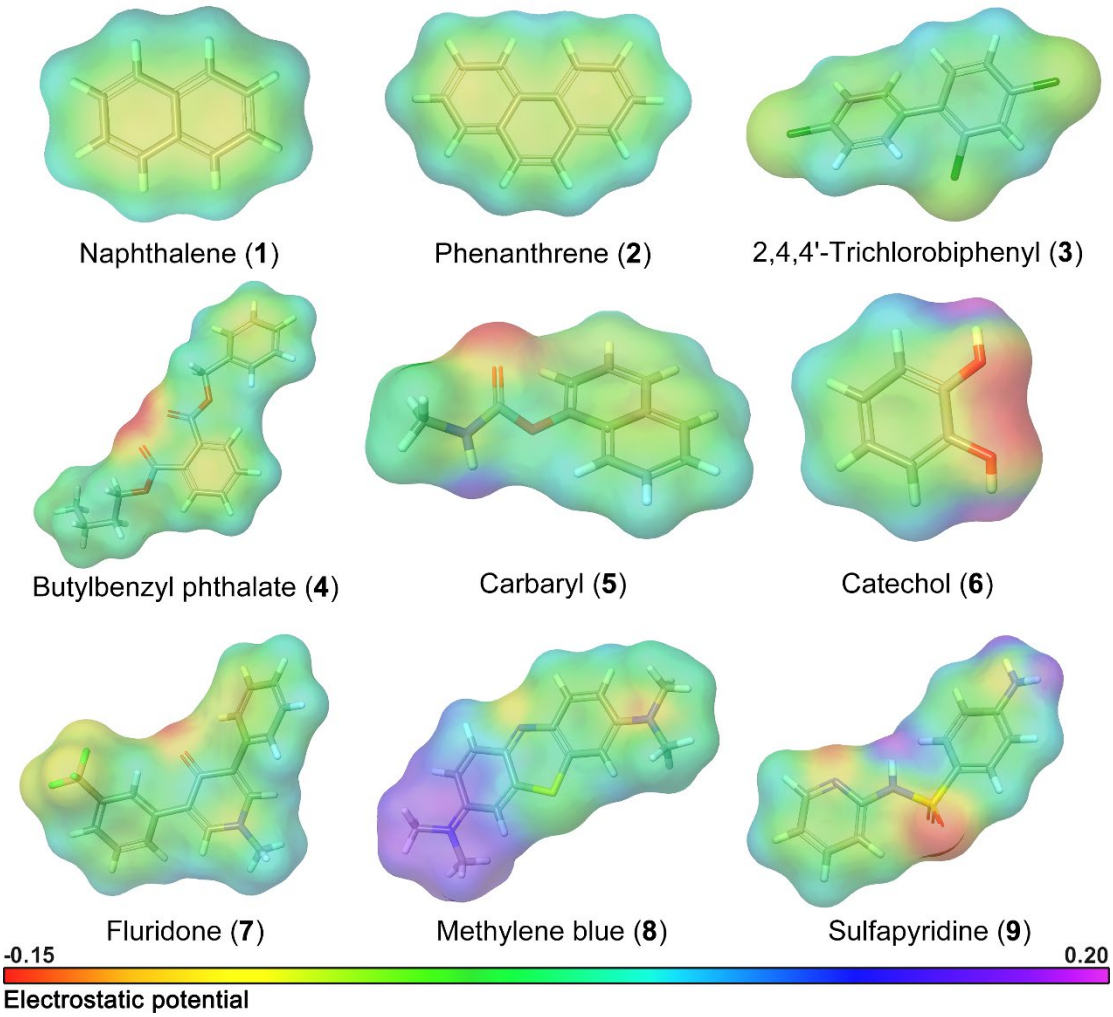

Figure S2 Electrostatic potentials for the investigated compounds. Warm colors indicate negative electrostatic potentials, and cold colors indicate positive electrostatic potentials.

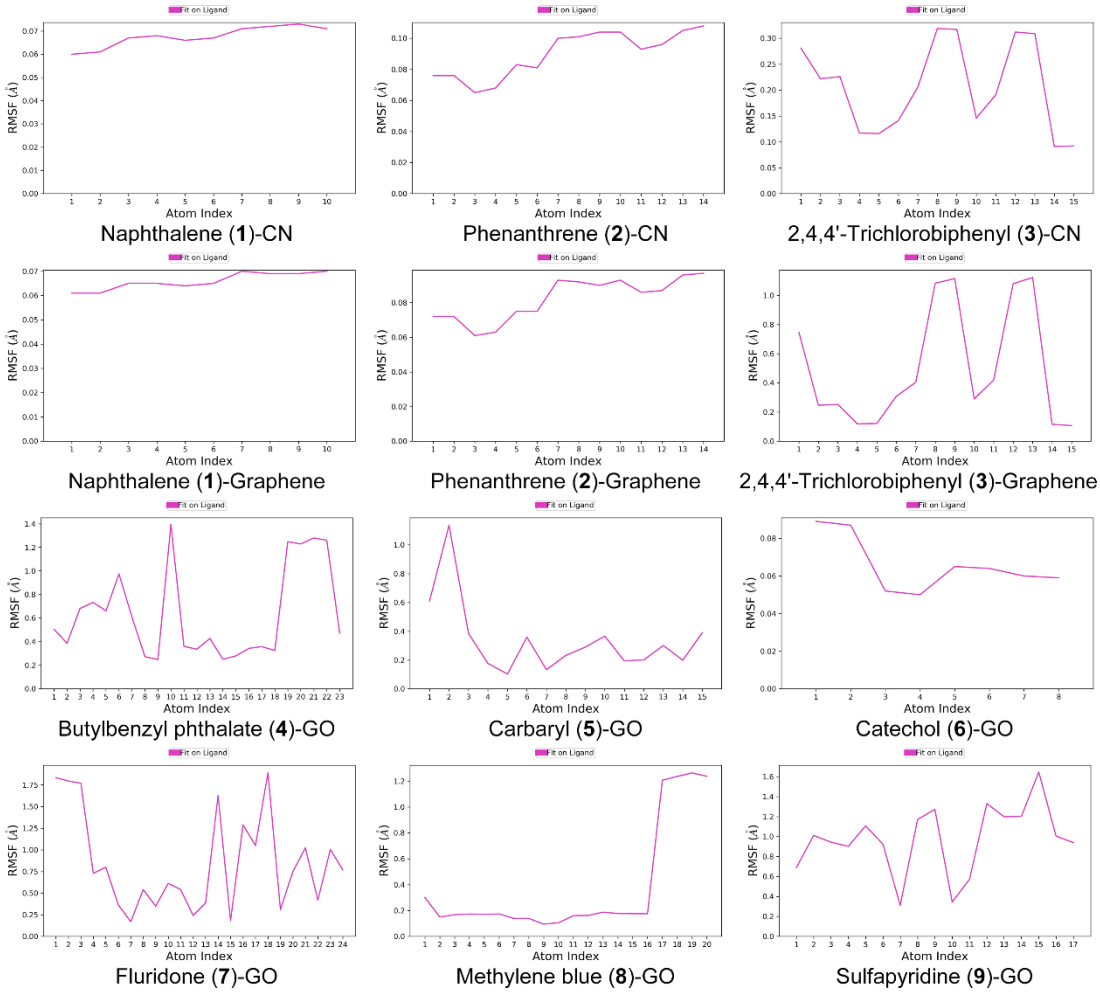

Figure S3. RMSF for the investigated environmental contaminants interacting with biochar nanocomposites during MD simulations.

Table S1 Summary of organic and microbial contaminants sorbed on various biochars and their removal mechanisms.

Organic contaminants	**SMILES**	**Proposed sorption mechanisms**	**PubChem CID**
1-Naphthol	c1cccc(c12)cccc2O	Partitioning and surface adsorption	7005
2,4-Dichlorophenoxyacetic acid	O=C(O)COc1c(Cl)cc(Cl)cc1	Surface adsorption	1486
2,4,4'-Trichlorobiphenyl	c1cc(Cl)cc(Cl)c1-c2ccc(Cl)cc2	π-π EDA interactions, H-bonding.	23448
Atrazine	CC(C)Nc1nc(nc(n1)Cl)NCC	Partitioning	2256
Bisphenol A	c1cc(O)ccc1C(C)(C)c2ccc(O)cc2	π-π EDA interaction and pore filling mechanism	6623
Butylbenzyl phthalate	CCCCOC(=O)c1c(cccc1)C(=O)OCc2ccccc2	H-bonding	2347
Carbamazepine	c1cccc(c12)N(C(=O)N)c3c(C=C2)cccc3	Hydrophobic adsorption	2554
Carbaryl	CNC(=O)Oc1cccc(c12)cccc2	Hydrophobic and π-π EDA interactions.	6129
Catechol	Oc1c(O)cccc1	Pore-filling and diffusion	289
Diazinon	CC(C)c1nc(C)cc(n1)OP(=S)(OCC)OCC	H-bonding with polar groups	3017
Dibutyl phthalate	CCCCOC(=O)c1c(cccc1)C(=O)OCCCC	H-bonding	3026

Diclofenac	c1cccc(c1CC(=O)O)Nc2c(Cl)cccc2Cl	Hydrophobic adsorption	3033
Diethyl phthalate	CCOC(=O)c1c(C(=O)OCC)cccc1	π-π EDA interactions.	6781
Ethinylestradiol	C#C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)c4c(CC3)cc(O)cc4	Pore-filling	5991
Fluridone	FC(F)(F)c1cc(ccc1)-c2c(=O)c(cn(C)c2)-c3ccccc3	Partitioning on amorphous-C	43079
Ibuprofen	O=C(O)[C@H](C)c1ccc(cc1)CC(C)C	Hydrophobic adsorption and π-π EDA interactions	3672
Methylene blue	CN(C)c(cc1)cc(c12)sc3c(n2)ccc(c3)=[N+](C)C	Electrostatic interaction, diffusion, and π-π EDA interactions	4139
Methylviolet	CNc(cc1)ccc1C(c2ccc(cc2)N(C)C)=C3C=CC(C=C3)=[N+](C)C	Electrostatic interaction	196986
Naphthalene	c1cccc(c12)cccc2	Partitioning on aliphatic-C	931
NDMA	CN(C)N=O	H-bonding and hydrophobic interaction	6124
Nitrobenzene	[O-][N+](=O)c1ccccc1	Pore-filling	7416
Oxamyl	CN(C)C(=O)/C(SC)=N/OC(=O)NC	H-bonding with polar groups	9595287

p-coumaric acid	O=C(O)/C=C/c1ccc(O)cc1	H-bonding	637542
P-nitrotoluene	Cc1ccc([N+]([O-])=O)cc1	Partitioning	7473
Phenanthrene	c1cccc(c1c23)ccc2cccc3	π-π EDA interactions	995
Phenol	Oc1ccccc1	H-bonding	996
Sulfamethazine	Cc1cc(C)nc(n1)NS(=O)(=O)c(cc2)ccc2N	π^{+}-π EDA interactions.	5327
Sulfamethoxazole	Cc1cc(no1)NS(=O)(=O)c(cc2)ccc2N	Pore-filling and hydrophobic interactions	5329
Sulfapyridine	Nc1ccc(cc1)S(=O)(=O)Nc2ccccn2	π-π EDA interactions	5336
t-Cinnamic acid	O=C(O)/C=C/c1ccccc1	H-bonding	444539
Tetracycline	NC(=O)C(=C1O)C(=O)[C@@H](N(C)C)[C@@H]([C@@]12O)C[C@H]3C(C2=O)=C(O)c4c([C@@]3(C)O)cccc4O	π-π EDA interactions.	54675776
Trichloroethylene	ClC(Cl)=CCl	Hydrophobic adsorption	6575

Table S2 Valence energy composed of energies of bond energy,angle energy, torsion energy, inversion energy and valence energy

ligand	receptor	conformation	Valence energy (kcal/mol)	Bond (kcal/mol)	Angle (kcal/mol)	Torsion (kcal/mol)	Inversion (kcal/mol)	Valence energy(cross term) (kcal/mol)
2,4,4'-Trichlorobiphenyl	carbon nanotube	1 of 1	0	0	-0.001	0	0	0
2,4,4'-Trichlorobiphenyl	graphene	1 of 4	0	0.001	0	-0.001	0	0
2,4,4'-Trichlorobiphenyl	graphene	2 of 4	0.001	-0.001	0	0	0	0
2,4,4'-Trichlorobiphenyl	graphene	3 of 4	0	0	0	0	0.001	0
2,4,4'-Trichlorobiphenyl	graphene	4 of 4	0.001	0	-0.001	0	0.001	0
Butyl benzyl phthalate	graphene oxide	1 of 1	0	0	0.001	0	-0.001	0.001

Table S3 Non-bond energy composed of van der Waals and Electrostatic energies

Ligand	**Receptor**	**Conformation**	**Non-bond energy (kcal/mol)**	**Van der Waals (kcal/mol)**	**Electrostatic (kcal/mol)**
2,4,4'-Trichlorobiphenyl	carbon nanotube	1 of 1	-50.02	-46.579	-3.441
2,4,4'-Trichlorobiphenyl	graphene	1 of 4	-28.52	-26.711	-1.809
2,4,4'-Trichlorobiphenyl	graphene	2 of 4	-30.139	-27.278	-2.86
2,4,4'-Trichlorobiphenyl	graphene	3 of 4	-28.731	-25.827	-2.905
2,4,4'-Trichlorobiphenyl	graphene	4 of 4	-29.25	-24.99	-4.26
Butyl benzyl phthalate	graphene oxide	1 of 1	-63.282	-36.938	-26.344