SUPPORTING INFORMATION

Paraben Adsorption on Carbon-based 2D Nanomaterials: Molecular Mechanisms and Implications for Environmental Pollutant Detection

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Dedicated to Professor G. Narahari Sastry on the occasion of his 60th birthday, honoring his outstanding contributions to the field of noncovalent interactions.

Table S1: AIM-derived electron densities (a.u.) at the bond critical points for the graphane-paraben complexes

S.No	GA-Paraben	GA-Methyl Paraben	GA-Ethyl Paraben	GA-Propyl Paraben
1	0.004	0.004	0.004	0.004
2	0.007	0.006	0.006	0.007
3	0.004	0.007	0.006	0.006
4	0.007	0.005	0.005	0.005
5	0.007	0.006	0.006	0.006
6	0.006	0.008	0.009	0.009
7	0.007	0.006	0.006	0.006
8	0.006	0.006	0.007	0.007
9	0.007	0.007	0.007	0.007
10	0.007	0.006	0.006	0.006
11	0.006	0.006	0.006	0.004
12	0.007	0.007	0.006	0.007
13	0.006	0.006	0.006	0.006
14	0.006	0.008	0.004	0.006
15	0.006	0.006	0.008	0.007
16	0.006	0.005	0.007	0.004
17			0.007	0.006
18			0.005	0.008
19				0.005
20				0.006

Table S2: AIM-derived electron densities (a.u.) at the bond critical points for the graphene-paraben complexes

S.No	GE-Paraben	GE-Methyl Paraben	GE-Ethyl Paraben	GE-Propyl Paraben
1	0.006	0.006	0.005	0.006
2	0.006	0.007	0.007	0.007
3	0.008	0.008	0.008	0.008
4	0.008	0.008	0.008	0.008
5	0.008	0.008	0.008	0.008
6	0.008	0.008	0.007	0.007
7	0.006	0.009	0.008	0.006
8	0.006		0.007	0.007
9				0.006
10				0.008

Table S3: HOMO-LUMO energy gap (in eV) of paraben adsorption on Graphane (GA) and Graphene (GE)

	HOMO	LUMO	Energy gap
GA	-7.59	2.28	9.87
GA-Paraben	-7.51	-0.32	7.19
GA-Methyl Paraben	-7.52	-0.30	7.23
GA-Ethyl Paraben	-7.52	-0.27	7.25
GA-Propyl Paraben	-7.52	-0.26	7.26
GE	-5.77	-1.73	4.04
GE-Paraben	-5.82	-1.78	4.03
GE-Methyl Paraben	-5.79	-1.75	4.04
GE-Ethyl Paraben	-5.80	-1.76	4.04
GE-Propyl Paraben	-5.80	-1.77	4.03