

Supplementary materials for

In-Vitro and In-Vivo Human Body Odor Analysis Method using GO;PANI/ZNRs/ZIF-8 adsorbent followed by GC/MS

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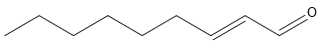
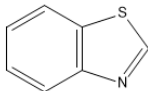
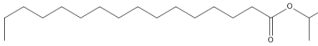
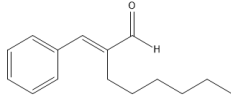
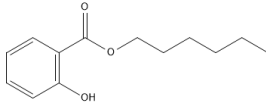
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S1. Experimental

Chemicals and Instrumentation

Sulfuric acid (Samchun, Seoul, Korea, 95.0%), sodium nitrate (Sigma-Aldrich, St. Louis, Missouri, USA, >99.0%), potassium permanganate (Samchun, Seoul, Korea, 99.3%), hydrogen peroxide (Daejung, Gyeonggi-do, Korea, 30%), hydrochloric acid (Samchun, Seoul, Korea, 35.0 ~ 37.0%) were used to oxidize natural graphite powder (30 μ m, 99.9%) from US Research Nanomaterials, Inc (Houston, USA). Aniline (>99.5%), zinc nitrate hexahydrate (98%), hexamethylenetetramine (99%), 2-methyl imidazole (99%), and N,N-dimethylformamide (>99.8%) were purchased from Sigma-Aldrich (St. Louis, Missouri, USA) to make GO;PANI/ZNRs/ZIF-8 coating layer on stainless steel wire

Table S1. Physicochemical properties of target compounds

Compound	Structure	Molecular weight (g/mol)	Boiling point (°C)	logP _{o/w}
<i>trans</i> -2-Nonenal		140.23	188~190	3.06
Benzothiazole		135.19	227~228	2.01
Isopropyl palmitate		298.5	160	7.17
α -Hexyl cinnamaldehyde		216.32	174~176	4.70
Hexyl salicylate		222.28	290	5.06

Optimization using response surface methodology (RSM)

Table S2. Experimental design matrix for optimization of reactants concentration in fabrication of adsorbent

Run	Coded factor		
	GO	Aniline	2-MI
1	-1	0	1
2	0	0	1
3	1	0	1
4	-1	-1	1
5	-1	1	1
6	-1	1	-1
7	-1	0	0
8	-1	1	-1
9	-1	1	-1
10	-1	1	-1
11	-1	1	-1
12	1	0	1
13	0	0	0
14	0	1	1
15	-1	-1	-1
16	1	1	-1
17	-1	-1	0

Table S3. Experimental design matrix for optimization of HS-INME condition

Run	Coded factor		
	Extraction temp.	Adsorption time	Desorption time
1	-1	0	1
2	0	0	1
3	1	0	1
4	-1	-1	1
5	-1	1	1
6	-1	1	-1
7	-1	0	0
8	-1	1	-1
9	-1	1	-1
10	-1	1	-1
11	-1	1	-1
12	1	0	1
13	0	0	0
14	0	1	1
15	-1	-1	-1
16	1	1	-1
17	-1	-1	0

S2. Optimization of body odor adsorbent fabrication conditions using RSM

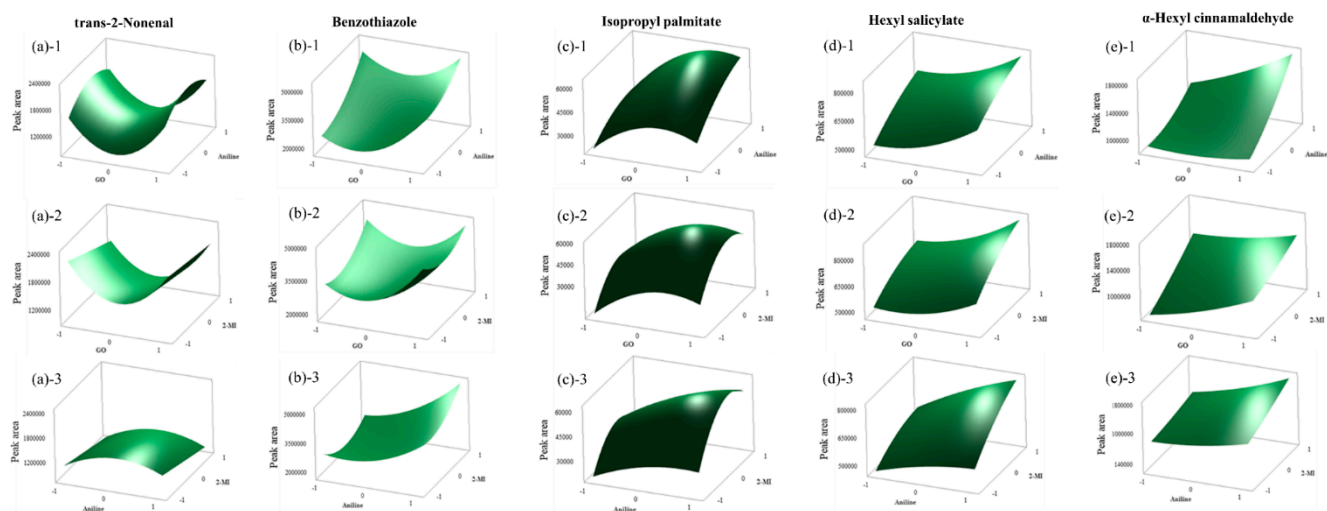


Figure S1. Response surface diagrams of target compounds by factors; (a) *trans*-2-nonenal, (b) benzothiazole, (c) isopropyl palmitate, (d) hexyl salicylate, (e) α -hexyl cinnamaldehyde, and correlation between 1: amount of GO and amount of aniline, 2: amount of GO and amount of 2-MI, and 3: amount of aniline and amount of 2-MI.

S3. Optimization of INME extraction conditions using RSM

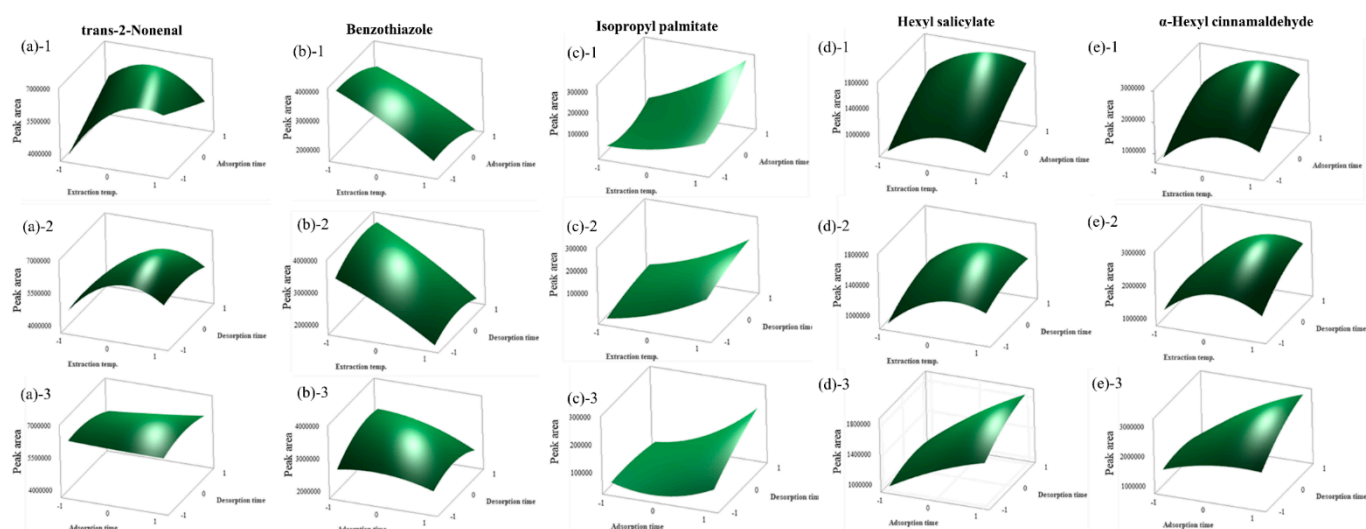


Figure S2. Response surface diagrams of target compounds by factors; (a) *trans*-2-nonenal, (b) benzothiazole, (c) isopropyl palmitate, (d) hexyl salicylate, (e) α -hexyl cinnamaldehyde and correlation between 1: extraction temp. and adsorption time, 2: extraction temp. and desorption time, and 3: adsorption time and desorption time.

S4. Characterization of the adsorbent

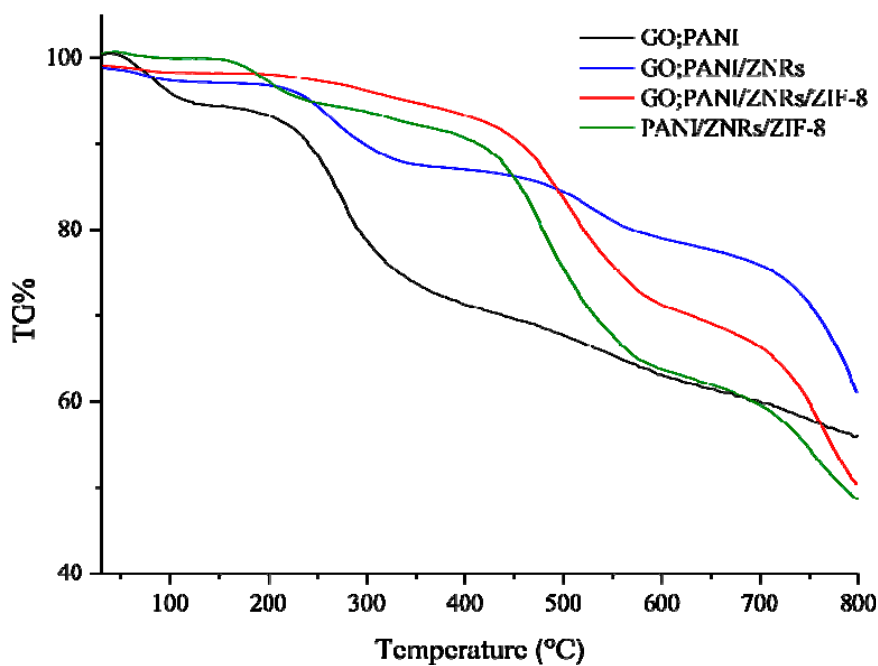


Figure S3. TGA curves of GO;PANI, GO;PANI/ZNRs, GO;PANI/ZNRs/ZIF-8, and PANI/ZNRs/ZIF-8.

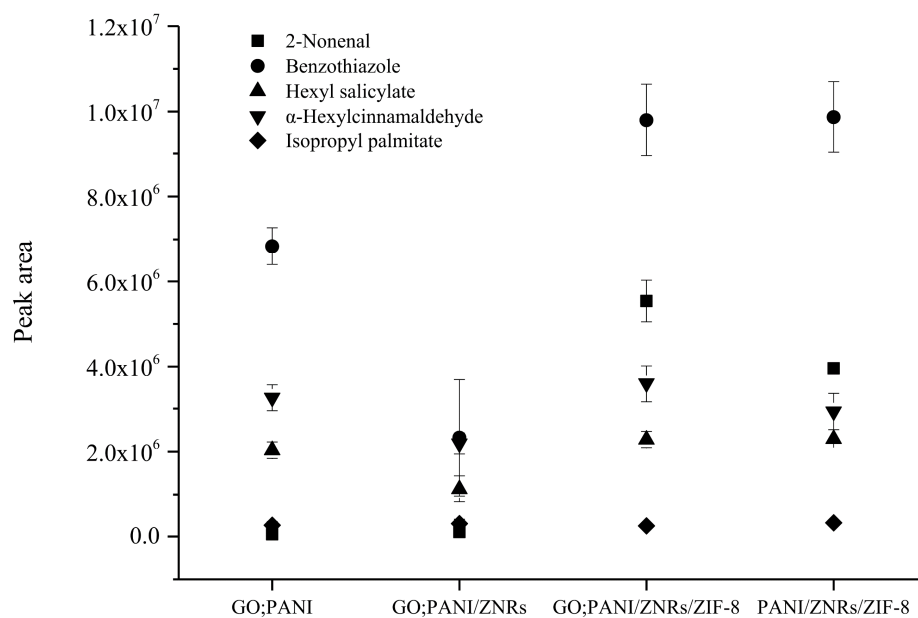


Figure S4. Comparison of adsorption amount of five target compounds according to the adsorbent synthesis steps, and without GO.