Supplementary Information

Zirconium-Based Metal–Organic Framework (UiO-66) Anchored on Magnetic Graphene Oxide as a Superior Sorbent for the Determination of Polycyclic Aromatic Hydrocarbons in Water Samples

Maryam Asefi [a], Mahtab Eraghi [b], Amirhassan Amiri*, [a], Mehdi Baghayeri [b]

[a] Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, 9177948974, Mashhad, Iran

[b] Department of Chemistry, Faculty of Science, Hakim Sabzevari University, PO. Box 397, Sabzevar, Iran

***E-mail address: ah.amiri@um.ac.ir**

Table S1. Univariate optimization procedure: summary of parameters optimized, ranges tested, optimal values selected, and constant conditions maintained during each optimization step.

Optimized Parameter	Range Tested	Optimal Value	Parameters Kept Constant During Evaluation
Desorption solvent type	Toluene, dichloromethane, hexane, methanol	Dichloromethane	Sorbent amount (10 mg), desorption solvent volume (1 mL), extraction time (3 min), desorption time (3 min), ionic strength (NaCl 0%), sample volume (20 mL).
Sorbent amount (mg)	5 – 25	15	Desorption solvent (dichloromethane), desorption solvent volume (1 mL), extraction time (3 min), desorption time (3 min), ionic strength (NaCl 0%), sample volume (20 mL).
Desorption solvent volume (mL)	0.5 – 1.5	1.0	Desorption solvent (dichloromethane), sorbent amount (15 mg), extraction time (3 min), desorption time (3 min), ionic strength (NaCl 0%), sample volume (20 mL).
Extraction time (min)	1 – 4	2	Desorption solvent (dichloromethane), sorbent amount (15 mg), desorption solvent volume (1.0 mL), desorption time (3 min), ionic strength (NaCl 0%), sample volume (20 mL).
Desorption time (min)	1 – 4	2	Desorption solvent (dichloromethane), sorbent amount (15 mg), desorption solvent volume (1.0 mL), extraction time (2 min), ionic strength (NaCl 0%), sample volume (20 mL).
Ionic strength (NaCl %, w/v)	0 – 20	10	Desorption solvent (dichloromethane), sorbent amount (15 mg), desorption solvent volume (1.0 mL), extraction time (2 min), desorption time (2 min), sample volume (20 mL).

Table S2. Input data used for the AGREEprep greenness assessment.

AGREEprep Criterion	Input Parameter / Selection	Value / Description
Sample preparation placement	Location of sample preparation	Ex-situ
Hazardous materials	Total amount of hazardous substances	1 mL (DCM)
Sustainability, renewability, and reusability	Origin of materials	Materials are not sustainable or renewable
Waste generation	Total waste volume	1.5 mL
Sample size economy	Sample volume	1 mL
Sample throughput	Number of samples prepared per hour	10 samples h^{-1}
Integration and automation (steps)	Number of steps in procedure	3 steps
Integration and automation (automation level)	Degree of automation	Manual system
Energy consumption	Energy per sample	4 Wh per sample
Post-sample preparation configuration	Instrumentation type	GC with non-MS detection
Operator safety	Number of hazards	1 hazard

Table S3. Evaluation criteria used for the BAGI greenness assessment.

BAGI Criterion	Input Parameter	Value / Description
Type of analysis	Analytical purpose	Quantitative
Multi-/single-element analysis	Number of analytes	Multi-element analysis (2–5 compounds)
Analytical technique	Instrumentation level	Simple instrumentation available in most laboratories
Simultaneous sample preparation	Parallel processing capacity	2–12 samples
Sample preparation	Procedure type	Miniaturized extraction sample preparation
Sample throughput	Samples per hour	2-4 samples h^{-1}
Reagents and materials	Availability	Common commercially available reagents
Preconcentration	Requirement	Preconcentration required (single-step enrichment)
Degree of automation	Operational mode	Manual treatment and analysis
Amount of sample	Sample volume	10-50 mL for environmental samples