

Supplemental Information

Emerging contaminants: A One Health perspective

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Table S1. Some examples of advanced methods for the detection and analysis of emerging contaminants

Techniques	Detectors	Target analytes	Sample matrix	Sample pretreatment	Identification	Quantification	References
GC-QTOF	HRMS	N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD)	Tire tread wear particle leachates	Fractionation	✓		(Tian et al., 2021)
		Organophosphate flame retardants	Air particulates	Pressurized liquid extraction	✓		(Liu et al., 2021)
LC-QTOF/ LC-Orbitrap	HRMS	6PPD-quinone	Diluted extracts of roadway runoff and	Fractionation	✓	✓	(Tian et al., 2021)

			receiving water samples			
Endocrine- disrupting chemicals		Source and drinking water sampled from major rivers	Solid-phase extraction	✓		(Li et al., 2023)
Thiol DBPs	reactive	Waters treated using both chemical disinfection and advanced	<i>Solid-phase extraction, glutathione (GSH) incubation</i>	✓		(Yeung et al., 2023)

		oxidation processes				
IM-QTOF	HRMS	Bisphenols, alternative plasticizers, organophosphate flame retardants, perfluoroalkyl substances	Urine samples	Dilute-and-shoot	✓	(Belova et al., 2021)
LC-IM-QTOF	HRMS	Per- and polyfluoroalkyl substances	Aqueous film-forming foams	Dilute-and-shoot	✓	(Luo et al., 2020)
FT-ICR-MS	UHRMS	Unknown DBPs	Chlorinated and	Ultrafiltration, XAD	✓	(Dong et al., 2023)

			chloraminat ed drinking water	Resin Extraction			
SFC- QTOF	HRMS	Halogenated sulfonic acids	Water samples from drinking water production, tap water, and swimming pool	Freeze- drying	✓	✓	(Nihemai ti et al., 2023)
Pyr-GC- MS	MS	Pyrolysis products of MP	Sea water, beach sand, sediment,	Filtering, density separation,	✓	✓	(Zhang et al., 2023)

				air, rice, solvent-based seafood, human blood					
spICP-MS	MS	MPs	Consumer products	Filtration and dilution	✓				(Laborda et al., 2021)
	HRMS	MPs	Aqueous suspensions	Dilute-and-shoot	✓				(Hendriks and Mitrano, 2023)
NMR	Various nuclei (^1H , ^{13}C , ^{15}N , ^{19}F , ^{31}P)	Metals and organic compounds	Solution, solid and gels	Various, depending on the sample type	✓	✓			(Simpson and Simpson, 2014)

Antibody	Electrochemical	-	PAHs	Oysters interstitial fluid	Filtration	✓	✓	(Prossner et al., 2022)
	Electrochemical	Metallic nanoparticles	Cocaine	Urine, sweat, saliva, serum	-	✓	✓	(Sanli et al., 2020)
Aptamer	UV-Vis absorption spectrum	Cage Au@Au nanoparticles	Chloramphenicol	Honey	Dissolve in ultrapure water	✓	✓	(Zhou et al., 2022)
	Electrochemical	Graphene@black phosphorus nanocomposites	Bisphenol A	Wastewater	Filtration	✓	✓	(Gao et al., 2022)

Electrochemical	Poly (propylene imine) dendrimer-carbon nanofiber nanocomposite	Bisphenol A	Water	Dilution with Tris-HCl buffer	✓	✓	(Tsekeli et al., 2021)	
Photo-electrochemical	Au/Bi ₂₄ O ₃₁ Br ₁₀	Enrofloxacin	Sewage river water	-	✓	✓	(Dong et al., 2022)	
Algae	Luminescence device	Microfluidic	Pesticides	Tap water	-	✓	✓	(Tahirbegi et al., 2017)
Luminescence	Porous silicone	Herbicides	Aquatic samples	-	✓	✓	(Haigh-Flórez et al., 2014)	

The table provides a selection of advanced methods for detecting and analyzing emerging contaminants, but it's important to recognize that there are numerous other methods available for this purpose. While the table illustrates specific examples or groups of contaminants analyzed by each method, it's essential to understand that one method can be utilized to analyze multiple emerging contaminants.

Belova, L., Caballero-Casero, N., van Nuijs, A.L., and Covaci, A. (2021). Ion mobility-high-resolution mass spectrometry (IM-HRMS) for the analysis of contaminants of emerging concern (CECs): database compilation and application to urine samples. *Analytical Chemistry* 93, 6428-6436.

Dong, H., Cuthbertson, A.A., Plewa, M.J., Weisbrod, C.R., McKenna, A.M., and Richardson, S.D. (2023). Unravelling High-Molecular-Weight DBP Toxicity Drivers in Chlorinated and Chloraminated Drinking Water: Effect-Directed Analysis of Molecular Weight Fractions. *Environmental science & technology* 57, 18788-18800.

Dong, J., Xu, L., Dang, S., Sun, S., Zhou, Y., Yan, P., Yan, Y., and Li, H. (2022). A sensitive photoelectrochemical aptasensor for enrofloxacin detection based on plasmon-sensitized bismuth-rich bismuth oxyhalide. *Talanta* 246, 123515.

Gao, Y., Wang, L., Zhang, X., Shi, C., Ma, L., Zhang, X., and Wang, G. (2022). Similarities and differences among the responses to three chlorinated organophosphate esters in earthworm: Evidences from biomarkers, transcriptomics and metabolomics. *Science of The Total Environment* 815, 152853.

Haigh-Flórez, D., de la Hera, C., Costas, E., and Orellana, G. (2014). Microalgae dual-head biosensors for selective detection of herbicides with fiber-optic luminescent O₂ transduction. *Biosensors and Bioelectronics* 54, 484-491.

Hendriks, L., and Mitrano, D.M. (2023). Direct Measurement of Microplastics by Carbon Detection via Single Particle ICP-TOFMS in Complex Aqueous Suspensions. *Environmental science & technology* 57, 7263-7272.

Laborda, F., Trujillo, C., and Lobinski, R. (2021). Analysis of microplastics in consumer products by single particle-inductively coupled plasma mass spectrometry using the carbon-13 isotope. *Talanta* 221, 121486.

Li, Q., Wang, L., Jia, Y., Yang, M., Zhang, H., and Hu, J. (2023). Nontargeted Analysis Reveals a Broad Range of Bioactive Pollutants in Drinking Water by Estrogen Receptor Affinity–Mass Spectrometry. *Environmental science & technology* 57, 21327-21336.

Liu, Q., Li, L., Zhang, X., Saini, A., Li, W., Hung, H., Hao, C., Li, K., Lee, P., and Wentzell, J.J. (2021). Uncovering global-scale risks from commercial chemicals in air. *Nature* 600, 456-461.

Luo, Y.-S., Aly, N.A., McCord, J., Strynar, M.J., Chiu, W.A., Dodds, J.N., Baker, E.S., and Rusyn, I. (2020). Rapid characterization of emerging per-and polyfluoroalkyl substances in aqueous film-forming foams using ion mobility spectrometry–mass spectrometry. *Environmental science & technology* 54, 15024-15034.

Nihemaiti, M., Icker, M., Seiwert, B., and Reemtsma, T. (2023). Revisiting Disinfection Byproducts with Supercritical Fluid Chromatography-High Resolution-Mass Spectrometry: Identification of Novel Halogenated Sulfonic Acids in Disinfected Drinking Water. *Environmental science & technology* 57, 3527-3537.

Prossner, K.M., Vadas, G.G., Harvey, E., and Unger, M.A. (2022). A novel antibody-based biosensor method for the rapid measurement of PAH contamination in oysters. *Environmental technology & innovation* 28, 102567.

Sanli, S., Moulahoum, H., Ugurlu, O., Ghorbanizamani, F., Gumus, Z.P., Evran, S., Coskunol, H., and Timur, S. (2020). Screen printed electrode-based biosensor functionalized with magnetic cobalt/single-chain antibody fragments for cocaine biosensing in different matrices. *Talanta* 217, 121111.

Simpson, M.J., and Simpson, A.J. (2014). *NMR spectroscopy: a versatile tool for environmental research* (John Wiley & Sons).

Tahirbegi, I.B., Ehgartner, J., Sulzer, P., Zieger, S., Kasjanow, A., Paradiso, M., Strobl, M., Bouwes, D., and Mayr, T. (2017). Fast pesticide detection inside microfluidic device with integrated optical pH, oxygen sensors and algal fluorescence. *Biosensors and Bioelectronics* 88, 188-195.

Tian, Z., Zhao, H., Peter, K.T., Gonzalez, M., Wetzel, J., Wu, C., Hu, X., Prat, J., Mudrock, E., and Hettinger, R. (2021). A ubiquitous tire rubber-derived chemical induces acute mortality in coho salmon. *Science (New York, NY)* 371, 185-189.

Tsekeli, T.R., Sebokolodi, T.I., Sipuka, D.S., Olorundare, F.O., Akanji, S.P., Nkosi, D., and Arotiba, O.A. (2021). A poly (propylene imine) dendrimer-carbon nanofiber based aptasensor for bisphenol A in water. *Journal of Electroanalytical Chemistry* 901, 115783.

Yeung, K., Moore, N., Sun, J., Taylor-Edmonds, L., Andrews, S., Hofmann, R., and Peng, H. (2023). Thiol Reactome: A Nontargeted Strategy to Precisely Identify Thiol Reactive Drinking Water Disinfection Byproducts. *Environmental science & technology*.

Zhang, J., Fu, D., Feng, H., Li, Y., Zhang, S., Peng, C., Wang, Y., Sun, H., and Wang, L. (2023). Mass spectrometry detection of environmental microplastics: Advances and challenges. *TrAC Trends in Analytical Chemistry*, 117472.

Zhou, C., Sun, C., Zou, H., and Li, Y. (2022). Plasma colorimetric aptasensor for the detection of chloramphenicol in honey based on cage Au@AuNPs and cascade hybridization chain reaction. *Food Chemistry* 377, 132031.