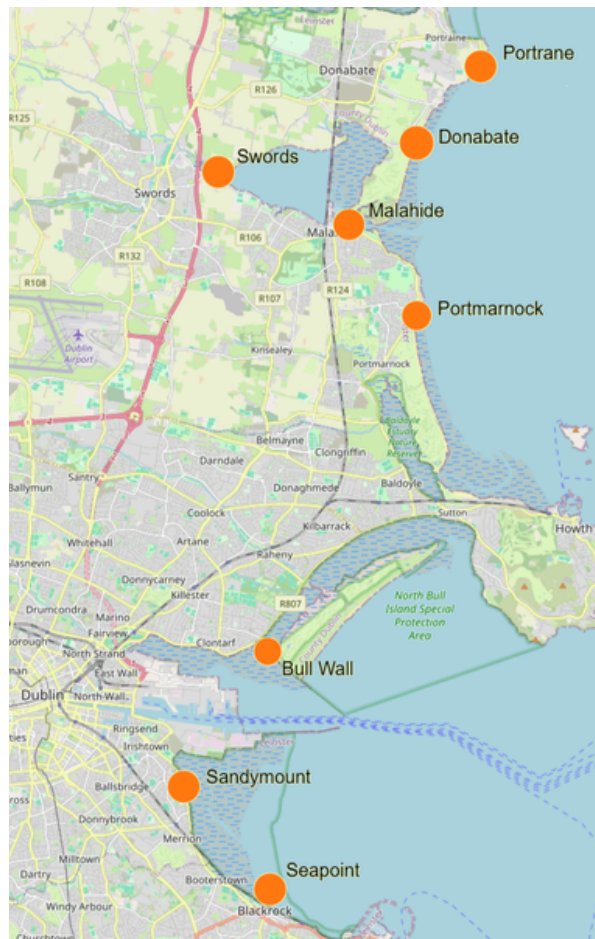


## Objectives of This Study

Contaminants of emerging concern (CECs) are a complex group of chemicals that make their way into the environment through various means.<sup>1</sup> Coastal hubs such as Dublin Bay become a hotspot for these contaminants to gather, given the saturation of human activity in the area. Pesticides from agricultural land use and urban pest control enter the environment through run-off or seep into groundwater sources. Wastewater treatment plants release effluent that may not successfully remove trace quantities of pharmaceuticals or personal care products. Recreational areas introduce the presence of sunscreen agents such as UV filters into the coastal environment.<sup>2</sup> These contaminants possess a wide range of physicochemical properties; some stay in solution in seawater, while others have the ability to precipitate out and accumulate in the sediment. Dangers of bioaccumulation in benthic organisms can have adverse effects on the food chain, potentially affecting human health as well. These potential hazards give rise to the needed importance of monitoring coastal sediments for the presence of these CECs.

## Sampling Location - Dublin Bay



Samples of seawater (1 L in amber glass bottles) and sediment (in 250 mL amber glass bottles) were collected around the Dublin Bay area (Figure 1). Anthropogenic activity was taken into consideration for site selection. All samples were transported back to the lab on ice.

Figure 1. Map of sampling locations around Dublin Bay

## Analytical Methods

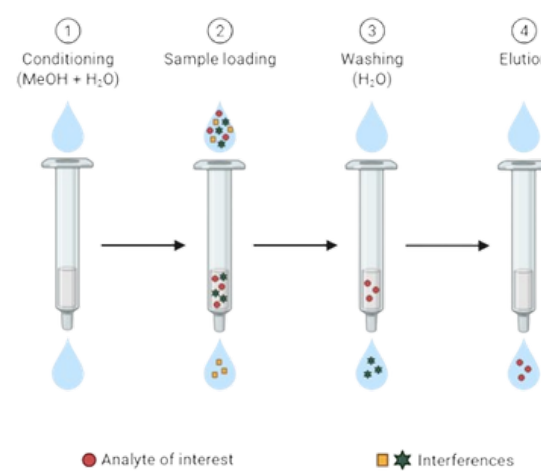


Figure 2. Solid phase extraction method for water samples

**Sediment samples** were freeze-dried, homogenised, and sieved to remove debris (Figure 3). A fraction of <2 mm was selected for extraction. The sample (2 g) was extracted with a methanol-acetone (95:5) mixture by ultrasonication. The sample was centrifuged and the supernatant collected. The extract was dried down under nitrogen and reconstituted in 1 mL LC-MS mobile phase.

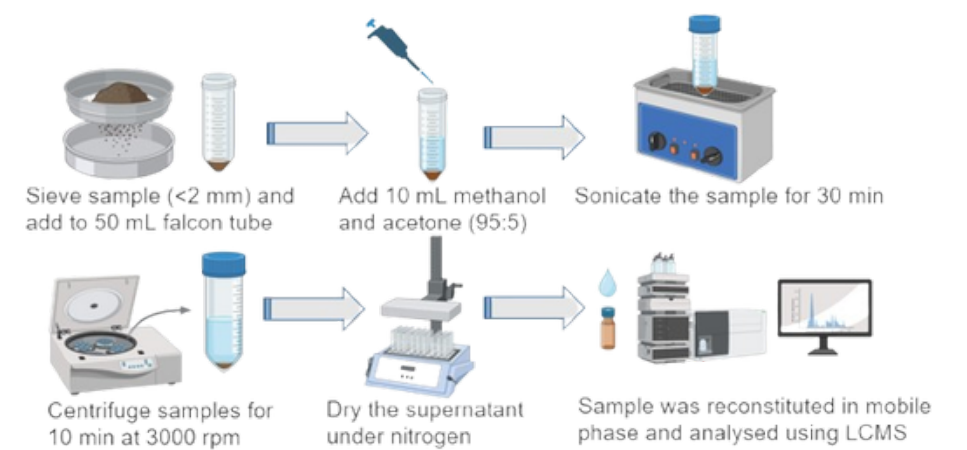


Figure 3. Methanolic extraction method for sediment samples

## Contaminant Detection in Seawater and Sediment Samples

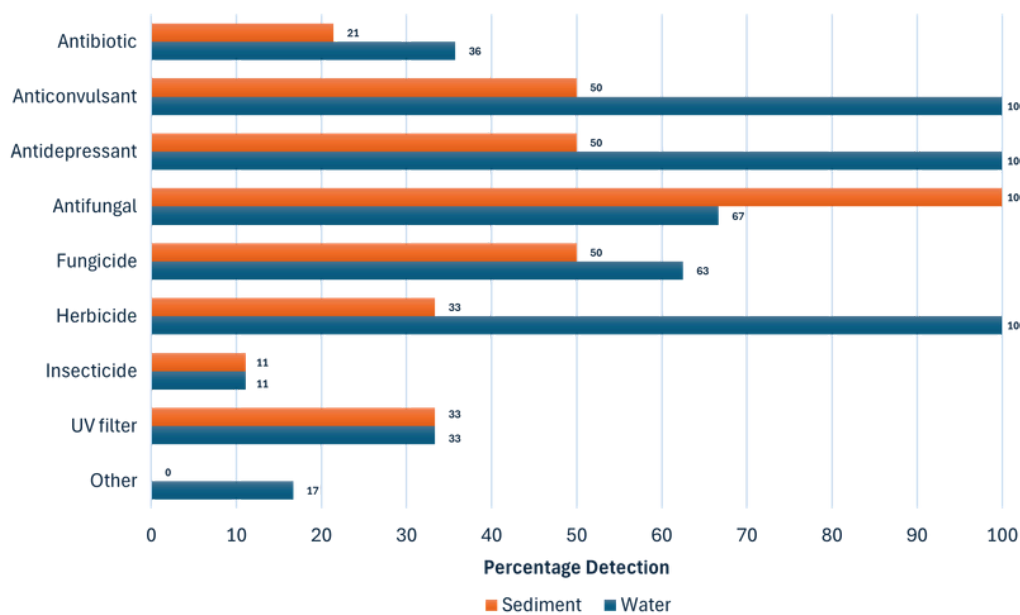


Figure 4. Percentage detection of contaminant classes in water and composite sediment samples (all 11 sites).

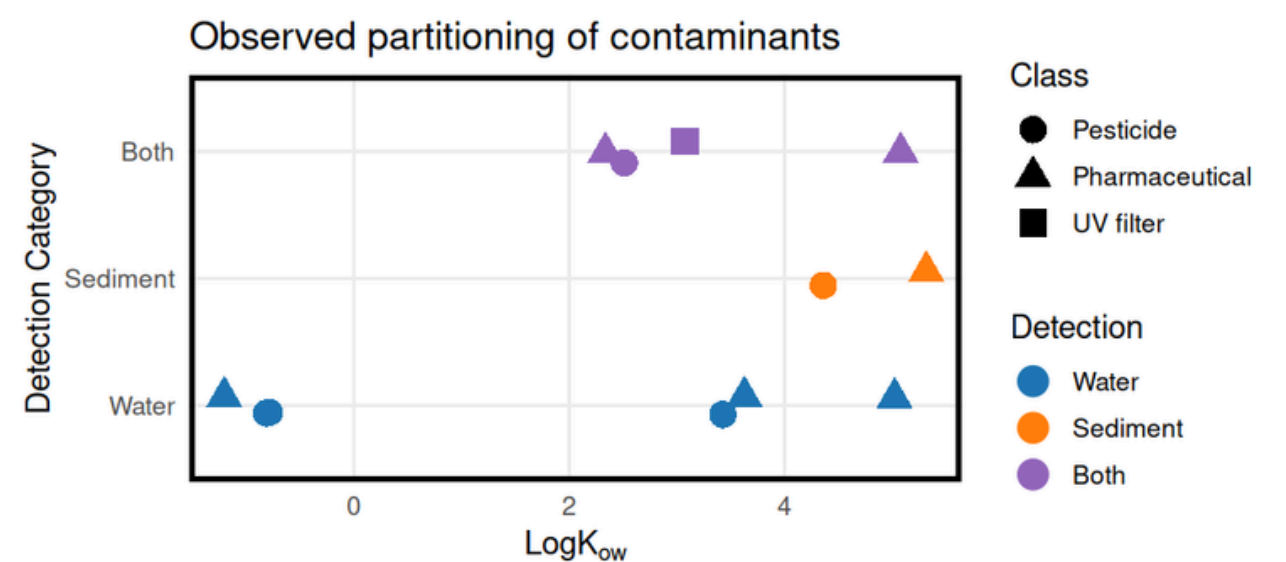


Figure 5. Scatter plot of contaminant  $\text{LogK}_{ow}$  grouped by their presence in seawater, sediment, or both matrices.

## Discussion

Figure 4 illustrates the occurrence of contaminants in water and sediment as a function of class. This shows that certain contaminants, such as anticonvulsants, antidepressants, and herbicides, which are primarily detected in water, are highly mobile, continuing to distribute into the environment. Anthropogenic activity, such as wastewater treatment plant effluent or agricultural runoff, contributes to the presence of these CECs in the environment. While some classes are detected frequently, others are not. This highlights the rapid degradative nature of certain CECs.<sup>3</sup> Figure 5 shows the partitioning of select contaminants across all sites based on their partitioning coefficients. Compounds with low partitioning coefficients (gabapentin and 2,4-D) were detected only in seawater samples. A transitional zone was seen with compounds that were detected across both matrices (benzophenone and carbamazepine). While some contaminants follow the expected trend of only being detected in water samples or sediment samples due to their low or high  $\text{LogK}_{ow}$  values, respectively, some contaminants do not follow this trend (azithromycin and prochloraz). The work conducted by León et al., demonstrates the importance of detecting CECs in not just seawater samples but also sediments and the potential effect they pose to inhabiting organisms.<sup>4</sup>

## Conclusion

This study highlights the importance of marine sediment monitoring. Due to the wide range of physicochemical properties at play, various parameters like  $\text{LogK}_{ow}$  play a role in determining individual contaminant partitioning between seawater and sediment. This study aims to influence legislative bodies in developing monitoring strategies that can identify and mitigate the effects of these pollutants on the marine environment.

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