

Bioanalytical and non-targeted mass spectrometric screening for contaminants of emerging concern in Southern California bight sediments

Alvine C. Mehinto ^{a,*}, Bowen Du ^a, Ellie Wenger ^a, Zhenyu Tian ^b, Edward P. Kolodziej ^{b,c,d}, Dennis Apeti ^e, Keith A. Maruya ^a

^a Southern California Coastal Water Research Project, Costa Mesa, CA, USA

^b Center for Urban Waters, Tacoma, WA, USA

^c Interdisciplinary Arts and Sciences, University of Washington, Tacoma, WA, USA

^d Civil and Environmental Engineering, University of Washington, Seattle, WA, USA

^e NOAA National Centers for Coastal Ocean Science, Silver Spring, MD, USA

ABSTRACT

Assessing the impact of chemical contaminants on aquatic ecosystem health remains challenging due to complex exposure scenarios and the myriad of impact metrics to consider. To expand the breadth of compounds monitored and evaluate the potential hazard of environmental mixtures, cell-based bioassays (estrogen receptor alpha (ER α) and aryl hydrocarbon receptor (AhR)) and non-targeted chemical analyses with high resolution mass spectrometry (NTA-HRMS) were used to assess the quality of ~70 marine sediment samples collected from 5 distinct coastal and offshore habitats of the Southern California Bight. AhR responses (<0.12–4.5 ng TCDD/g dry weight) were more frequently detectable and more variable than for ER α (<0.1–0.5 ng E2/g dry weight). The range of AhR and ER α responses increased by habitat as follows: Channel Islands < Mid-shelf < Marinas < Ports < Estuaries. The narrow range and magnitude of ER α screening response suggested limited potential for estrogenic impacts across sediments from all 5 habitats. The AhR response was positively correlated with total PAH and PCB concentrations and corresponded with a chemical score index representing the severity of metal and organic contamination. NTA-HRMS fingerprints generated in positive electrospray ionization mode were clearly distinguishable among coastal vs. offshore samples, with the greatest chemical complexity (n = 982 features detected) observed in estuarine sediment from a highly urbanized watershed (Los Angeles River). The concordance and complementary nature of bioscreening and NTA-HRMS results indicates their utility as holistic proxies for sediment quality, and when analyzed in conjunction with routine targeted chemical monitoring, show promise in identifying unexpected contaminants and novel toxicants.

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