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Tracking decadal changes in complex mixtures of polycyclic aromatic compounds in a sediment core from the inner River Thames estuary, UK, via Fourier transform ion cyclotron resonance mass spectrometry

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Polycyclic aromatic compounds (PACs), which include polycyclic aromatic hydrocarbons (PAHs) and their heteroatom-containing analogues, constitute an important class of environmental contaminant. The 16 priority PAHs proposed by the U.S. Environmental Protection Agency (U.S. EPA) have long been the targets of environmental screening and toxicity studies, although there is growing awareness of the potential for thousands of additional PACs in the environment. Fourier transform mass spectrometry has recently demonstrated utility for the molecular characterization of complex mixtures of PACs, in matrices such as aerosol particulate matter and soil.

In the present study, 8 organic extracts from a Chiswick Ait sediment core (River Thames, London, UK), covering a period of 80-90 years, were analysed using atmospheric pressure photoionization coupled to Fourier transform ion cyclotron resonance mass spectrometry (APPI-FTICR MS). The approach taken represents the untargeted screening of both anthropogenic and natural organic matter in the sediments. The application of complex mixture data analysis techniques, including plots of double bond equivalents against carbon number, and aromaticity index calculations, revealed complex mixtures of PACs in the Chiswick Ait sediment core. Alongside PAHs, PACs with oxygen, sulfur, nitrogen and chlorine heteroatoms were detected, the latter of which represents an emerging contaminant class.

In total, 1538 PAC molecular components were assigned in the core depth corresponding to the 1950s, a decade notable for the coal-induced Great Smog of London event, and a steady decline in numbers of PAC molecular components was observed moving up through the decades to modern times. A case is henceforth presented for an association between these sedimentary PAC trends and the modern history of coal consumption in London. The complex PAC distributions are further related to concentrations of U.S. EPA 16 PAHs, determined for the same sediment core in a recent study by Vane et al. [1]. It is shown that the trends in these U.S. EPA 16 PAH concentrations are indicative of the PAC complex mixture trends.

[1] C.H. Vane, A.W. Kim, R.A. Lopes dos Santos, V. Moss-Hayes, Contrasting sewage, emerging and persistent organic pollutants in sediment cores from the River Thames estuary,