Application of GCxGC-HRT-MS Petroleomics Based Spectral Analysis of Two Iconic Oil Spills From the Gulf of Mexico for Environmental Forensics

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One overarching tenet of oil-spill science is that the type of spilled oil and its distinct chemical composition are critical to the response, damage assessment, and restoration efforts of impacted areas. Petroleomics based spectral analysis tools were utilized with GC×GC-HRT-MS data in order to gain a detailed inventory of potentially useful petroleum fingerprinting compounds for Ixtoc I and Deepwater Horizon oil spills.

We utilize comprehensive two-dimensional gas chromatography (GC×GC) coupled with time of flight (TOF) and high resolution time of flight (HRT) mass spectrometry in order to gain a more complete understanding of (a) the inventory of compounds spilled into the environment, (b) which compounds persist in the environment and (c) how we can use high-resolution techniques to forensically identify specific petroleum sources.

In order to explore the sulfur-containing compounds in these crude oils in detail, we analyzed each crude using HRT-GC×GC. Accurate mass measurements can be used to determine the elemental composition of an analyte molecule as well as the composition of fragment ions produced by electron ionization or chemical ionization. In addition, we utilized petroleomics based spectral analysis to produce ring double bond equivalents (RDBE) vs carbon number (containing sulfur hetero atoms) to produce a more complete inventory of sulfur-containing species.