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Environmental Forensics: Molecular Insight into Oil Spill Weathering Helps Advance High Magnetic Field FT-ICR Mass Spectrometry¹

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The depletion of terrestrial global oil reserves has shifted oil exploration into offshore and ultra-deep water (> 5000 ft) oil reserves to meet global energy demands. Deep water reservoirs are currently in production in many parts of the world. including the Gulf of Mexico, but production is complicated by the water depth and thick salt caps that challenge reservoir characterization / production. The explosion aboard the Deepwater Horizon in April 2010 resulted in an estimated total release of ~ 5 million barrels (BP claims that they collected ~ 1 M barrels, for a net release of 4 M) of light, sweet crude oil into the Gulf of Mexico and shifted attention toward the environmental risks associated with offshore oil production. The growing emphasis on deep water and ultra-deep water oil production poses a significant environmental threat, and increased regulations require that oil companies minimize environmental impact to prevent oil spills, and mitigate environmental damage when spills occur. Every oil spill is unique. The molecular transformations that occur to petroleum after contact with seawater depend on the physical and chemical properties of the spilled oil, environmental conditions, and deposition environment. Molecular-level knowledge of the composition, distribution, and total mass of released hydrocarbons is essential to disentangle photo- and bio-degradation, source identification, and long-term environmental impact of hydrocarbons released into the environment. Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is unsurpassed in its ability to characterize complex mixtures at the level of elemental composition assignment. Only FT-ICR mass spectrometry can routinely achieve the required minimum resolving power necessary to elucidate molecular-level characterization of crude oil. Conversely, the spectral complexity of petroleum facilitates identification of systematic errors in the accumulation, transfer, excitation, and detection events in the FT-ICR experiment. For example, the high density of peaks at each nominal mass unit provides unprecedented insight into how excitation conditions affect ion motion during detection. Aggregated oil (i.e., tar balls, tar mats) that reached the surface exhibits a more than two-fold increase in the total number of detected species, with an increased number of oxygenated species. Principal component analysis (PCA) applied to two possible source oils (contained within the same ship) and weathered samples provide the first application of FT-ICR MS for source identification. Molecular formulae from parent and weathered oil indicate that the lightest petroleum fractions (saturated hydrocarbons) are the most readily oxidized components, and can serve as a template to determine chemical transformations that occur throughout the water column. The ability to differentiate and catalogue compositional changes that occur to oil after its release into the environment relies heavily on gains achieved in nearly all steps in the FT-ICR mass spectral experiment required to accommodate larger ion populations inherent to heavily weathered crude oil. Here, we present the requirement for FT-ICR MS for comprehensive oil spill characterization, and highlight advances made to FT-ICR MS experimental conditions developed from petroleum characterization.