

Petroleomics: Past, present and future

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Advances in mass spectrometry enable identification of tens of thousands of species in petroleum and environmental samples at the molecular level (elemental composition assignment). Current ionization methods amplify the utility of such detailed compositional information through the selective ionization of basic, acidic and aromatic species (\pm ESI and APPI). The ability to fingerprint, identify and track compositional changes in complex natural mixtures spawned the field of 'Petroleomics'. Although the past and current applications are largely limited to high resolution Fourier transform ion cyclotron resonance mass spectrometry, the future of 'Petroleomics' lies in the expansion and method development on the latest instruments in all areas of analytical chemistry.

Here we present an overview of the birth and development of Petroleomics and highlight the latest developments in our 'petroleomic' research efforts with an emphasis on the diversification of analytical workflows to maximize attainable compositional information. Specifically, microdistillation, 2-D HPLC, GC x GC, LC-TOF, preparative scale LC and FT-ICR MS will be discussed. Geochemical, oil production and refinery applications that include down-hole, deposits, offshore platform, terrestrial production and distillate samples reveal the need for a diversified analytical approach combined with high field FT-ICR mass spectrometry for problem solving and advances in the fundamental knowledge of the composition and behavior of petroleum derived materials.

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High-frequency climate cycles in the Westernmost Mediterranean during the last 20,000 yrs

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High-sedimentation rates in the westernmost Mediterranean (Alboran Sea basin) allow excellent resolution for paleoclimate reconstructions at millennial- to centennial-scales. Here, a novel cyclostratigraphic analysis has been conducted on a marine record, revealing major and secondary peaks related to climate cycles during the last 20,000 yrs. Spectral analysis on time-series corresponds to several multi-proxy groups, including detrital, redox, paleoproductivity, and paleotemperature-paleosalinity, which reveals cycles of different confidence level at particular periodicities. Main periodicities at 1,300, 1,515, 2,000, and 5,000 yrs plus secondary harmonics at 650, 1,087, and 3,000 yrs derive from diverse climate forcing mechanisms. Thus, the 1,300 yr cycle appear to be principally influenced by North Atlantic freshwater inflow. The 1,515 yr cycle, equivalence to the Bond cycle in the North Atlantic, is linked to the North Atlantic thermohaline circulation and changes in the intensity and position of the North Atlantic Oscillation (NAO) and the Inter-Tropical Convergence Zone migrations (ITCZ). Although the 2,000 yr cycle is only punctually registered, it supports a global connection with records distributed at high-, mid-, and low-latitudes, pointing to variations in solar activity as main climate forcing mechanism. In contrast, the cycle at 5,000 yrs is well-registered and presents a direct relationship with orbital forcing responses, also accompanied by monsoonal variations and NAO oscillations. Thus, the obtained spectral periodicities reinforce the evidence on the strong connection between Mediterranean and North Atlantic climates, being climate oscillations mainly forced by solar variations, the NAO and the ITCZ migrations.

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