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Petroleomics by ESI FT-ICR MS: Monitoring of the Thermal Evolution of Petroleum.

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Introduction and Aim.

Thermal evolution is an important parameter for understanding petroleum maturation in the sedimentary region. It consists of the advancing transformation within the kerogen and petroleum. Thermal evolution can be monitored by a series of geochemical indicators, known as thermal maturation parameters. Despite the accuracy of information provided by the ESI (-) FT-ICR MS on the analysis of petroleum samples with different degrees of thermal evolution, there is a lack of studies to correlate the various classes and series of compounds for use as indicators of petroleum thermal evolution that could be extended to the larger universe of different types of oils. New approaches are pointing to the specific use of thousands of compounds detected and identified by ESI FT-ICR MS.

Materials and Method.

To investigate further this possibility, samples of petroleum (2 mg) were dissolved in 1 mL of toluene. A volume of 0.5 mL of this solution was transferred to a vial of 1 mL and diluted with 0.5 mL of methanol containing 0.1% ammonium hydroxide for analysis in the negative ion mode in a LTQ FT Ultra mass spectrometer (ThermoScientific, Germany). Spectra were converted to txt using the Xcalibur software 2.0 and analyzed by a homemade software for petroleomic data analysis: PetroMS.

Results.

The experimental data of 50 samples were preprocessed using multivariate analysis to remove sources of mathematically undesirable variation. The ESI (-) FT-ICR MS spectra clearly show that the distribution of polar compounds is influenced by the degree of thermal evolution via the narrowing of the polar compounds distribution as a function of thermal evolution with decreased the complexity of ESI FT-ICR MS spectra. The decrease of polar components is reflected mainly in the range of m / z 400-700 Da and can be explained considering the set of chemical reactions which lead to the formation of light hydrocarbons, known to be main products of the thermal induced reactions.

Conclusions.

For the class of carbazoles (N), the ESI(-)FT-ICR MS and too the SIMCA (Soft Independent Modeling of Class Analogy) grading method was applied allowing fast and reliable ratings on the thermal evolution of the petroleum sample.