Statistically Significant Differences in Composition of Petroleum Crude Oils Revealed by Volcano Plots Generated from Ultrahigh Resolution Fourier Transform Ion Cyclotron Resonance Mass Spectra

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Results and Discussion

A "volcano" plot provides a visual means for identifying statistically significant differences between two populations. Here, we introduce the volcano plot as a means for simple, visual identification and statistical ranking of compositional differences between petroleum crude oils.

Ultrahigh-resolution Fourier transform ion cyclotron resonance mass spectrometry yields the relative abundances of ions in each spectrum that contains up to tens of thousands of elemental compositions (CcHhNnOoSs). From data acquired with the NHMFL ICR Program 9.4 tesla Fourier transform ion cyclotron resonance mass spectrometer, a volcano plot may be generated by plotting statistical significance (p-value, obtained from t-test) versus log2(relative abundance ratio). The volcano plot data may be color-coded to highlight differences in heteroatom class (NnOoSs) (see Fig. 1), double bond equivalents (DBE = number of rings plus double bonds to carbon), and/or carbon number. The volcano plot may be used either directly, or as a "filter" for including only the most statistically significant differences for data entered into more conventional analyses based on DBE vs. carbon number, van Krevelen diagram, and Kendrick mass defect plots. In each case, the volcano plot provides statistically significant criteria, rather than visual grouping.

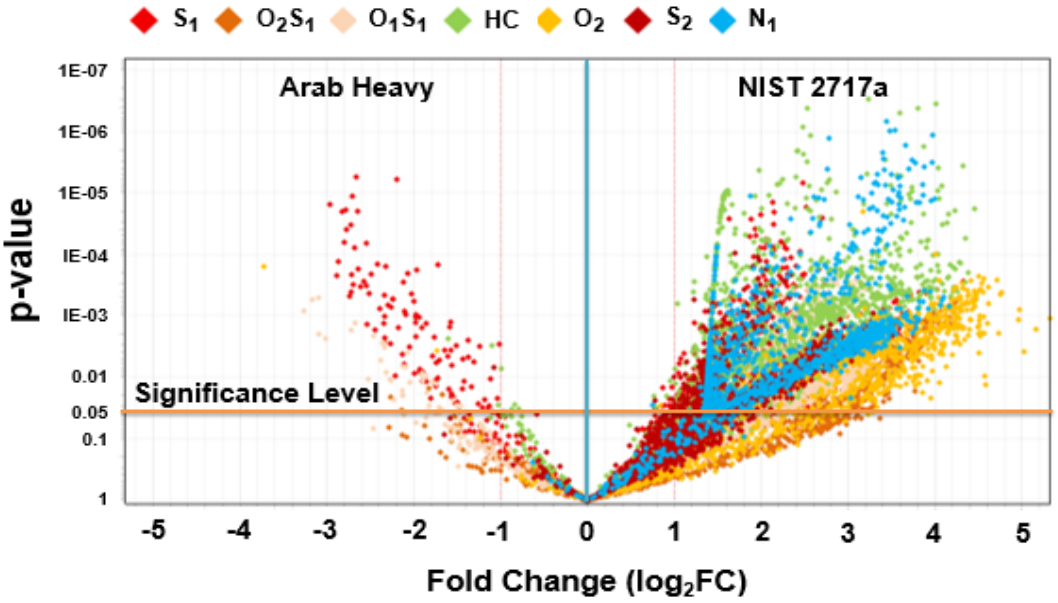

Fig. 1. Volcano plot of p-value (log2 scale) vs. fold change (positive if peak magnitude is higher for NIST 2717a than for Arab Heavy) generated for members of seven major heteroatom classes in ultrahigh-resolution positive APPI 9.4 T FT-ICR mass spectra of Arab Heavy and NIST 2717a crude oils. Each dot represents an elemental composition and each heteroatom class is color-coded.

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References

[1[Hur, M.; *et al.*, Energy & Fuels, **32**, 1206-1212 (2018).