Beyond Petroleomics - Petroleum Geochemistry for the 21st Century

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Petroleum geochemistry was always driven by analytical advances with development of computerized GCMS technologies in the 1970's heralding the practical biomarker technologies and the source rock facies and maturity molecular concepts that we still use today. In the 1970's another analytical development was also taking place, namely that of Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FTICRMS) by Marshal and Comisarow at the University of British Columbia. Four decades later FTICRMS has evolved into a commercially available front line tool capable of analyzing thousands of components in a petroleum mixture at once. It is likely this analytical technology will usher in an equally dramatic revolution in geochemical capability. Already Marshal and Rogers at the High Field Magnetic Lab in Florida have coined the term "Petroleomics" to reflect the molecular resolution and information content available in FTICRMS analysis of petroleum comparable to the information in the human genome. So from the perspective of a practicing petroleum geoscientist what are the challenges and opportunities the FTICRMS revolution brings?

Currently, just as in the early days of routine GCMS, instruments have "personality" and component quantitation and very variable component ionization efficiency is a major issue but these problems will likely be quickly resolved. Data sets are measured in the gigabytes and geochemists are learning the tricks of bioinformaticians and others. Data processing is key to the revolution that is unfolding. Current GCMS based petroleum geochemical protocols quantitatively determine perhaps a few hundred components. FTICRMS potentially can resolve 1000 times this number of components, which when quantitated and with accompanying molecular formulae, opens the door, in principle, to computational routes to fluid property and phase behavior calculations directly from molecular analysis. Interaction of genes, not the genome itself describe biology and so with petroleum, interaction of the multitude of components, not the components themselves control fluid and other properties and it will be definition of this petroleum "interactome" that will be key to unlocking the potential of petroleomics. We describe applications of FTICRMS and advanced data processing to study heavy oil variability, identify some novel biomarkers of potential paleoecological significance and we discuss routes to defining the petroleum "interactome".