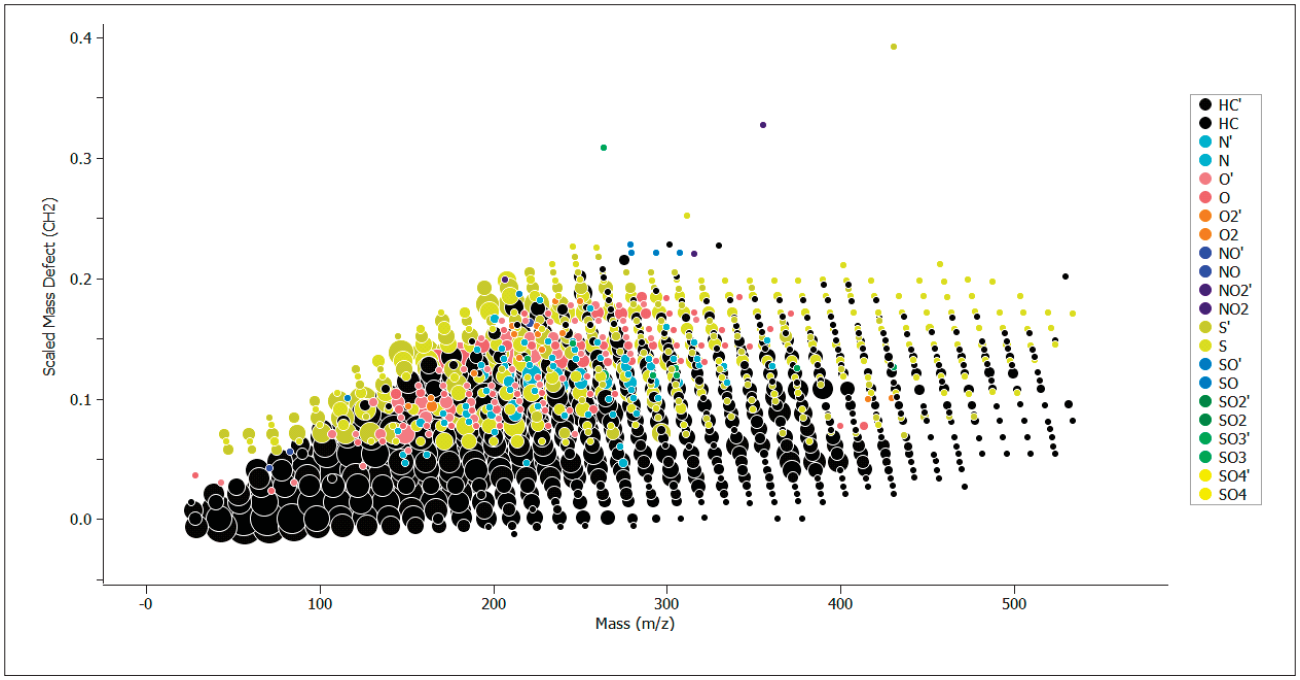
Spectral Analysis Tools (SAT)

Option for Pegasus® GC-HRT+

Harness the power of accurate mass and high resolution mass spectrometry with SAT. This innovative toolkit, paired with ChromaTOF® brand software, is designed to streamline identification and relative quantitation of heteroatomics species in either GC or GCxGC data sets.

Particularly useful in Petroleomics and Environmental workflows, SAT provides extensive functionality built on top of standard mass defect plots, as well as new van Krevelen and Degree of Unsaturation (RDBE versus C#) plots.



Kendrick's scaled Mass Defect Plot of Crude Oil Sample with heteroatomic species classified by color (see legend, note ' indicates odd electron ion).

ChromaTOF®

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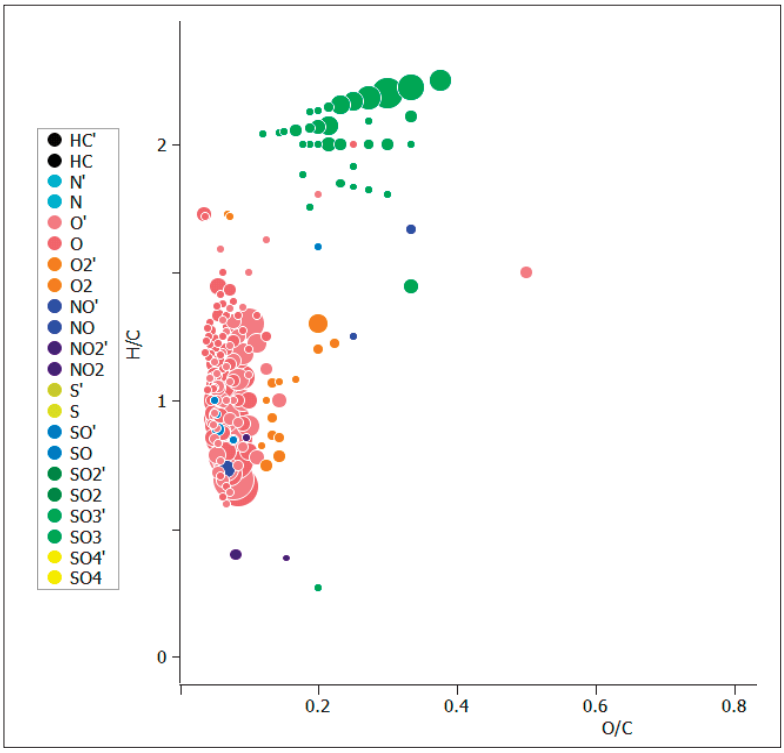
Features

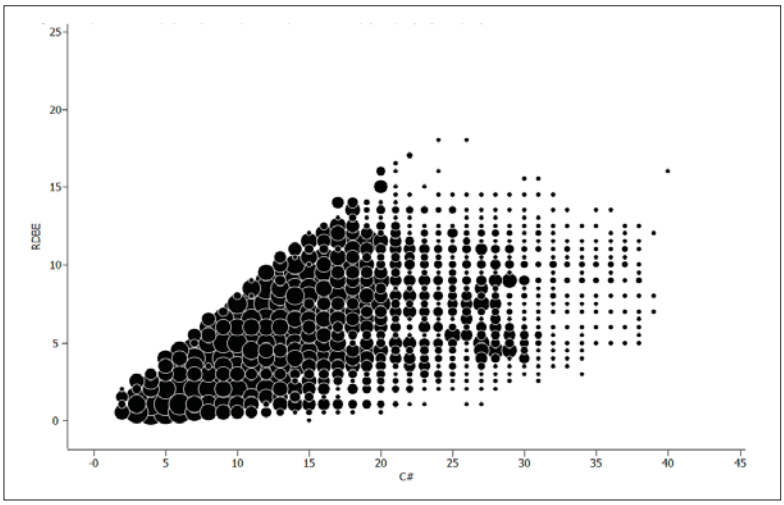
- Automatic formula calculations and identifications linked to Mass Defect Plots are based on the standard iterative formulae.
- Color highlight and relative amounts of identified Heteroatomic species (contain O, N, S, and others) in SAT plots.
- User editable iterative formula tables allow the user to configure the software based on the type of sample. The formula series also can be used to recalibrate mass accuracy.
- Compare Mass Defect Plots from two samples to understand the differences.
- Easily correlate mass classification identity to a chromatogram, and then correlate to spectral confirmation with library search results.
- Enhanced mass filters simplify the interpretation of Mass Defect plots by automatic isotope removal, formula checking, and removal of duplicate information (i.e. from standard neutral losses).
- Van Krevelen Plots indicate the oxidative state of a sample (degree of oxidation or thermal maturity for petroleum applications).
- Degree of Unsaturation plots indicate aromaticity of samples: they are plots of Ring Double Bond Equivalency (RDBE) versus Carbon Number, automatically extracted from the formula calculations.

Part Numbers

709-809-678
709-809-680-B/O



Van Krevelen Plot of Crude Oil Sample shows the shows the ratio of H/C versus O/C for N and O containing species.



RDBE versus Carbon Number Plot of Crude Oil Sample shows the distribution of heavy versus light compounds by class (HC in this case).

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