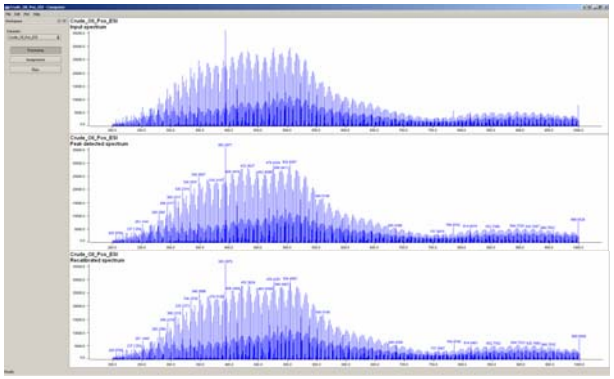
Composer

Sierra Analytics' **Composer** software is a state of the art processing and visualization system for assignment of chemical composition to FT-ICR-MS spectra of complex hydrocarbon mixtures.

Developed in collaboration with researchers at the National High Field FT-ICR Spectrometry Facility at Florida State University's National High Magnetic Field Laboratory, **Composer** embodies the analysis and presentation methods developed over years of research and documented in dozens of publications.

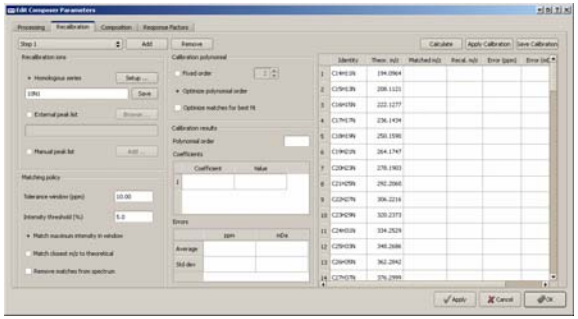


DATA IMPORT

Composer reads raw data directly from major FT-ICR data system formats, including:

- ThermoScientific Xcalibur
- Bruker Compass
- NHMFL MIDAS (with FFT)

with co-addition of multi-scan datasets if desired. Support for certain formats may require licenses obtained separately from the respective owners.



DATA PROCESSING

Composer works directly with raw, profile (continuum) mode mass spectral data and applies its own algorithms to reduce it for composition assignment:

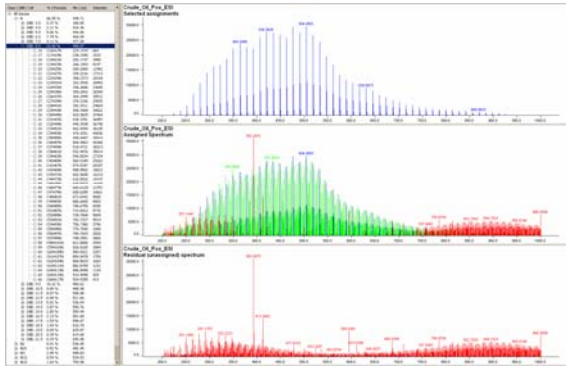
Peak detection: Centroid calculation from profile spectra, taking into account scan law and resolution, to yield peak height or peak area intensities.

Multi-level recalibration: Nth-order polynomial based recalibration using multiple stages, including external calibrants, internal series, or manually-selected peaks. Each stage is independently parameterized and optimized for best fit and polynomial order.

Composition assignment: Assignment of chemical formulas is based on the techniques perfected at the NHMFL FT-ICR facility. The set of constraints applied by the assignment algorithm is large and flexible, to fine-tune the process to the sample type and experimental protocol and prevent spurious assignments.

Response factors: To assist in quantitative estimation of composition, response factors can be assigned by chemical class. These response factors will be applied to adjust relative fractional abundances displayed in tables and visualizations.

Molecular weight distributions: For each chemical class and each double bond equivalence group within classes, **Composer** computes molecular weight averages, distributions, and relative abundances.

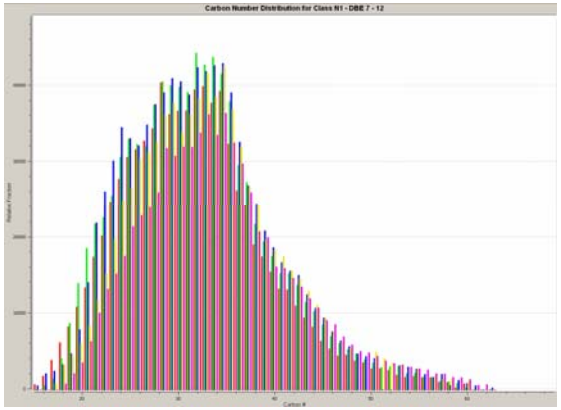


COMPOSITION BROWSER

Composer's composition browser provides a multi-level, tree-structured view into the assigned compositions. At the topmost level, assignments are grouped by chemical class, and within that by double bond equivalent, and finally by carbon number.

Selecting an item at any level of the tree displays the spectral features assigned to all of the compositions at that level, independently and color-coded within the

entire spectrum. This spectrum also color-codes peaks that are unassigned, below or above the m/z limits, or below the intensity threshold.



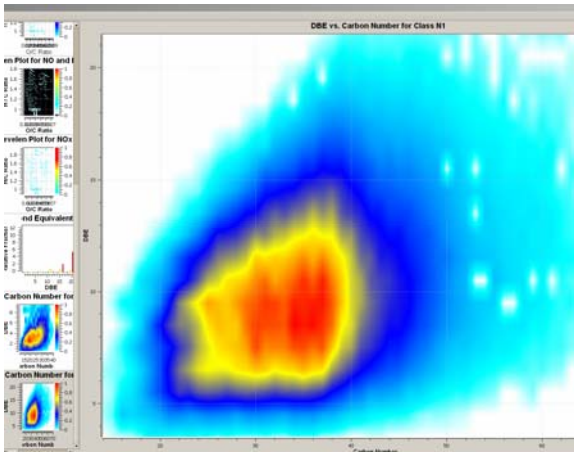
VISUALIZATION

Composer's graphical displays turn the lists of thousands of chemical compositions assigned in a typical analysis into useful information.

Results from single or multiple analyses can be transformed into chemically significant images that display the overall composition in a single picture.

Plots include bar charts and images of:

- Class distribution in multiple samples
- DBE distribution
- Carbon number distribution
- van Krevelen element ratios
- DBE vs. carbon number
- Kendrick mass defect vs. Kendrick nominal mass



RESULT EXPORT

Complete results are saved in human-readable XML format, including all compositions, spectral assignments, and distributions.

An XSLT processor is provided, along with sample XSL scripts, to extract and convert these results into tabular form for import in Microsoft Excel or other programs.

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SIERRA ANALYTICS

COMPOSER

State of the art software for

Petroleomics

Mass spectral processing and visualization for compositional analysis of complex hydrocarbon mixtures