JASON
JEOL Analytical Software Network

New version: JASON 6.0

- **A new machine-learning based pick picking engine for 1D NMR spectra is available in the algorithm options**
- **The MAGRES plugin is updated to version 3.1 bringing improved user control for building the molecular crystal and finding accurate bonds**
- **EDS and MS users can now use layout rules which complements the introduction of new tables; Peak Tables for EDS and MS and Centroid Tables for MS**
- **It is now possible to exclude points from the fitting analysis**
- **Swap Item Position functionality has been introduced to allow you to swap the position of two items on the canvas**
- **A new curved annotation has been added to the annotation options**

See how JASON version 6.0 can help you.

NMR Analysis:

- **A machine-learning based engine now powers a new peak-picking algorithm for 1D NMR spectra**
- We've also improved classical 1D peak picking, so fewer peaks are missed.

SMILEQ and qNMR:

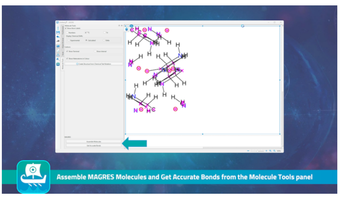
- External standard SMILEQ can be run via command line, this extends the large-scale automation capabilities of SMILEQ
- There are also several improvements to the SMILEQ Reference Integral. Highlight the references that are not present in the Reference Editor. The reference integral's number of nuclei is correctly displayed. Existing integrals can be used for the Reference with the "use existing integral" option
- Quantitative analysis templates now include PULCON preferences

AffinityScreen

- We have further improved the user interface, thank you to the beta-testers for their feedback

MAGRES is updated to 3.1:

- The options of building molecular crystals and finding accurate bonds from MAGRES structures are separated to user-accessible commands. These are available on the Molecular Tools panel, instead of being applied automatically during the MAGRES import. This gives more flexibility and control over to the user

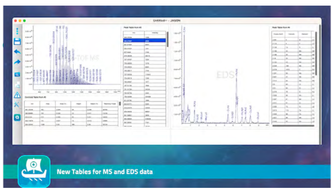


SolidSpin:

- A SIMPSON script is added which simulates two independent quadrupolar sites with variable intensities.

MS and EDS data:

- **Peak Tables can be created from EDS and MS data. Centroid Table can be created from MS data as well**



- Layout Rules are now supported for MS and EDS data and can be applied automatically while loading the data

NMR file formats support:

- **Support for 1D and 2D NMRPipe file formats**
- Improved support for SPINit data, offering better handling of 2D and pseudo-2D formats, such as relaxation measurements

Fitting Tools:

- **Sometimes it is necessary to exclude points from a fitting analysis. This is now possible by clicking (toggling) the points in the Fitting dialog chart. It is possible to interactively zoom on charts (similar to spectrum zooming) this makes clicking on individual points to exclude them much easier**

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User Programming:

- Users can implement a function for External Command processing steps that reports what changes were applied on the NMR spectrum to other processing commands. This enables External Command processing steps to be better integrated into the processing chain
- MOL-file representations of molecular structures are available in JJH5 files (read-only)
- A new, compact, format is available for NMR processing lists

User experience and GUI enhancements:

- We have simplified canvas browsing when scrolling using, for example, the mouse wheel. Now, scrolling to change the spectrum zoom will not apply if no spectrum is selected, even if the mouse is hovering over the spectrum. This reduces unintentional modifications when navigating the canvas
- **We've made some improvements to the titles of stacked spectra. These changes enable the use of symbols (such as Greek characters) and allow independent control of the text formatting**
- **To speed up re-organization of your canvas, you can now "Swap Item Positions" of two items on the canvas**

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Finder order, helping you keep track of your files

- **We've added to our family of annotations, the new simple curved annotation adds to the rectangle, text, straight line, triangle and ellipse that are currently available.**

We also performance-tuned our software and fixed a few bugs.

TRY IT NOW!

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SMILEQ
Spectral Management Interface
Launching Engine for Q-NMR