Mnova Gears

Overview

Mestrelab Research

chemistry software solutions

Mnova Gears

Automate your analytical workflows

Automate data processes, from databasing analytical raw data to reporting complex results, with this modular and flexible solution

Mnova Gears is a software suite to build automation workflows for your analytical data, including NMR, MS and others. Using Mnova features and advanced plugins as the starting "bricks", you can replicate Standard Operating Procedures or those boring, repetitive tasks we humans hate so much!
Until now our team has used Mnova Gears to create custom-tailored automated procedures in the pharmaceutical industry. We look forward hearing about your own automatizations. Here are a few examples of where it can be beneficial, to get your ideas running:

Applications Field

- ✓ Quality Control (NMR, Mass Spectrometry, etc)
- ✓ Natural Product Dereplication by NMR
- ✓ Targeted mixtures analysis
- ✓ Multi-technique reporting
- ✓ Protein-ligand Interaction
- ✓ Product ID confirmation
- ✓ Structure verification
- ✓ Reaction Monitoring
- ✓ Quantitative NMR
- ✓ DNA Profiling
- ✓ Screening

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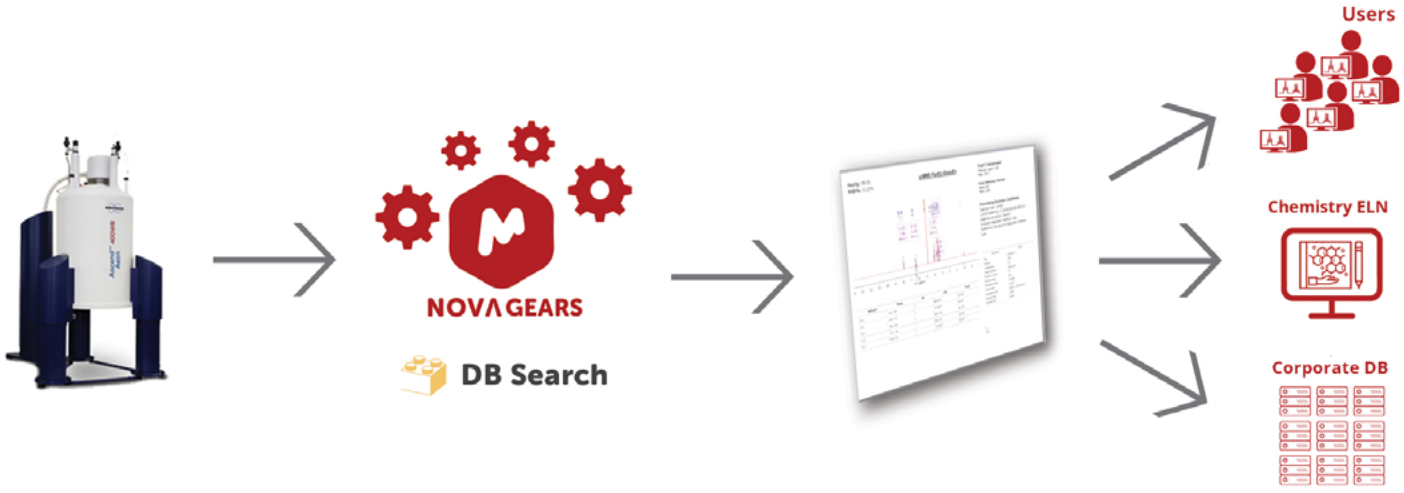
Highlights

Mnova Gears makes automation simpler and faster by given you full control over the design and testing of your workflows

- ✓ New generation of automated solutions that give you full control
- ✓ Faster product support and development, with all your automation analysis in one single software suite
- ✓ The power of Mnova tools for processing, analysis and reporting
- ✓ Customize your automated solutions taking advantage of the scripting nature of this product
- ✓ Real time databasing of experiment results once completed
- ✓ Save specialist time by automating routine processes and workflows
- ✓ Accepts multiple inputs, like NMR, MS, IR and UV spectra from different vendors, historic or at the point of acquisition
- ✓ Produces several types of outputs, from complex pdf reports to a simple Pass/Fail answer

An example



Automatic *Custom*

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5-Step Set Up

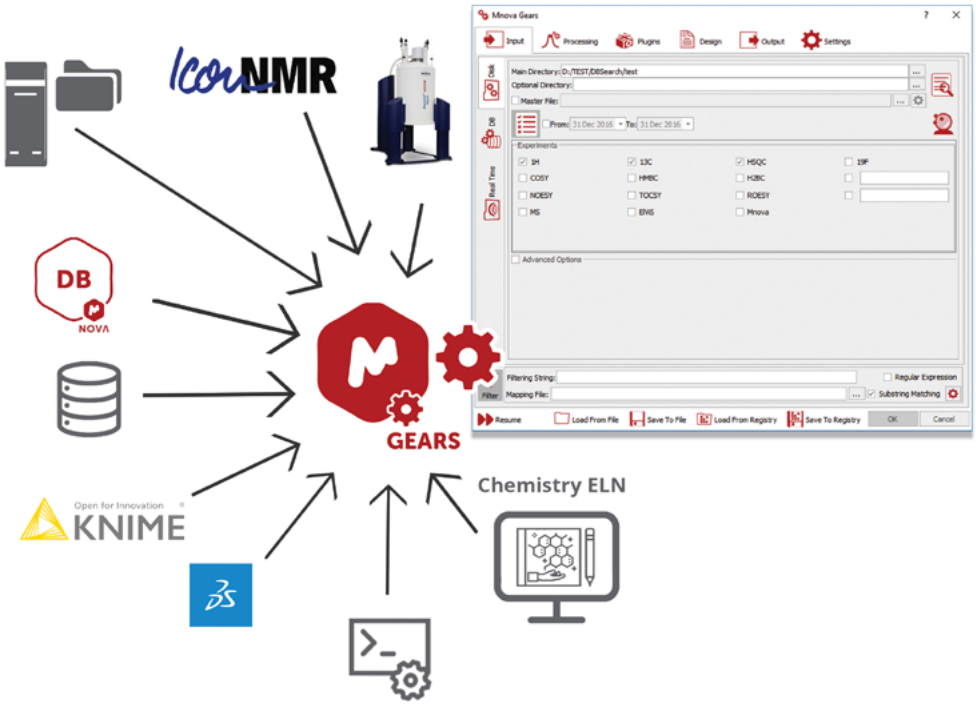
Mnova Gears has been split into five well-defined steps to automatized workflows, each one allowing full customization

1. Input	2. Processing	3. Analysis	4. Reporting	5. Output
Use several sources, filter inputs by different fields	Advised Based on templates Customized	Use the power of Mnova and our bespoke automa-tion plugins	Full control of layour, information included, format, etc	Data and results archived to repository of choice

1-Input

Multi-technique & multi-vendor analytical data added to your automatizations from one single software suite

- ✓ Collect data from different instrument folders you are only talking about input methods
- ✓ Import your data from different environments such as Disk location for Batch and Real Time modes, Databases, Command lines, Pipes, Instruments, GUI, Consoles
- ✓ Simple selection of experiments by type or by applying more advanced filtering (data range, text files, etc.)



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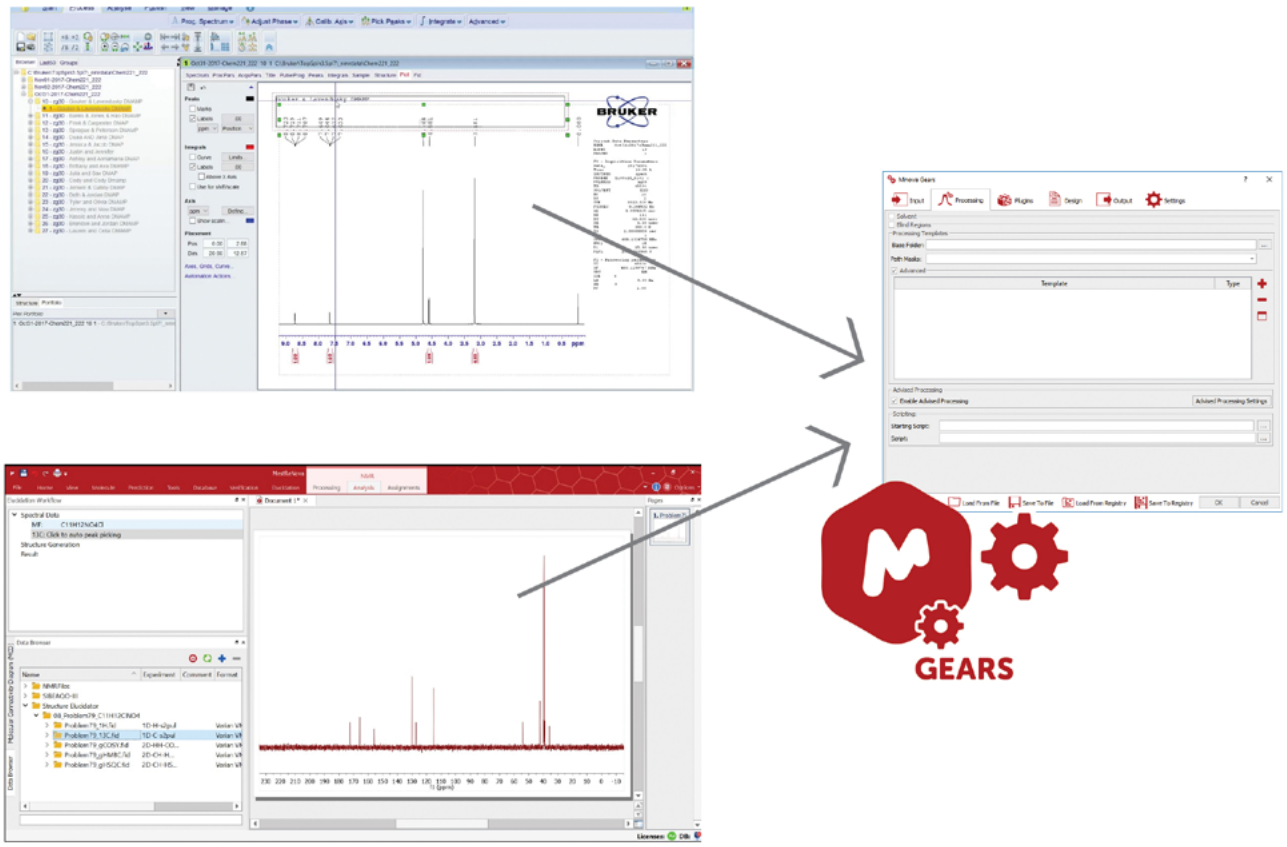
2-Processing

Tired of repeating simple, routine processing steps?

Free your time for some true NMR analysis by letting Mnova do the repetitive work in the background. You can choose to use our 'Advised processing', create your own processing templates, or you can ask our help to implement ad hoc processing (customized).
Would you not prefer a machine to do some of these for you?

- ✓ Baseline correction
- ✓ Apodization
- ✓ Zero filling
- ✓ Phase Correction
- ✓ Referencing



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3-Customized Analysis

Create your own routine analyses and automate them

Free your time for some true NMR analysis by letting Mnova do the work in the background.

Mnova Gears starts with the standard, common features: data retrieval, basic processing and analysis, reporting, and saving. To this basic work flow you can now include additional, specialized analyses. These are based on familiar Mnova add-ins, and we call them “bricks” in this context. You could, for example, use this framework to introduce fully automated qNMR and/or verification.

Would you not prefer a machine to do some of these for you?

- ✓ **Customizable:** Every step of workflow automation can be adapted to your specific needs, whether processing settings, advanced analysis algorithms or the design of your reports
- ✓ **Scalable:** The number of bricks you can use is not limited, you can start with easy workflows and build complexity
- ✓ **Example workflows:** We make it easy by loading some plugins with pre-sets. You can use them as such, or customize adapt them to better suit your own work

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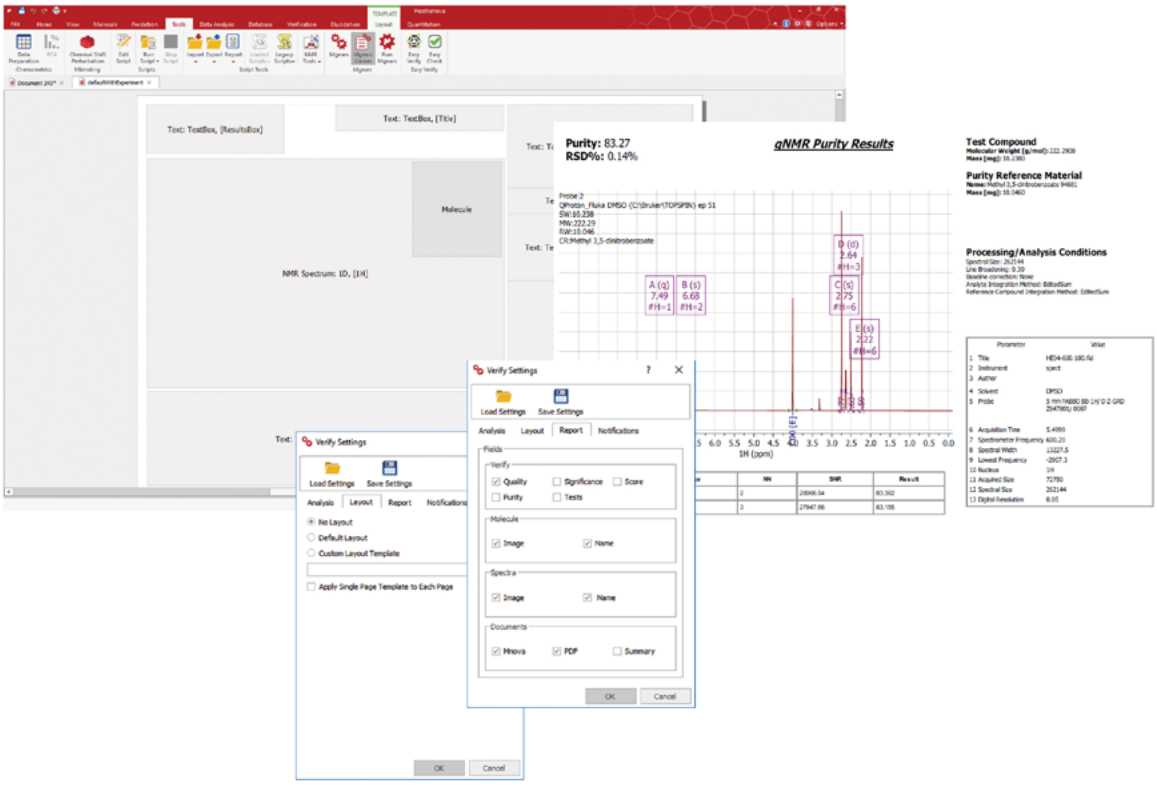
4-Reporting

- ✓ Select bespoke visualization of the results
- ✓ Export results as PDFs, CVS, Mnova documents, etc.
- ✓ Use Mnova layout templates to produce a final report that looks the way you want. Additional customization is possible by using small scripts.
- ✓ Customize your reports to fit corporate standards

Some of the objects you can easily include in reports are:

Spectra	Tables	Other objects
NMR	Peak assignment	Molecular structure
MS	Retention times	Processing & analysis parameters
MS-LC, MS-GC	Screning scores	Bespoke diagrams summarising results
UV	Purity measurements	Metadata from equipment files
IR		
Raman		



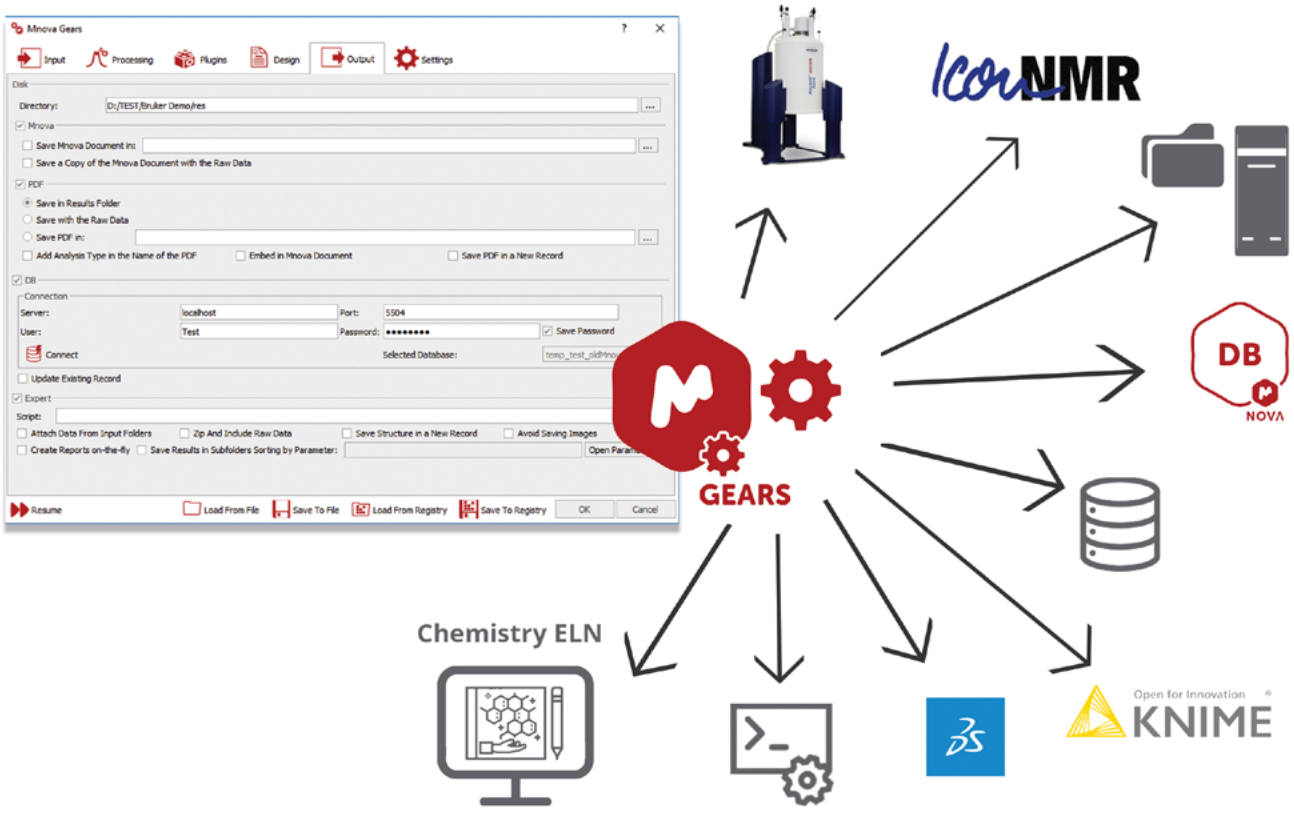
5-Output

Create automatic workflows to archive data and results

Need to import your multiplet reports as CSV files? Got it!

Your team may have decided to follow a new data standard. You can specify the requirements in the standard in your output options, so all new data will be archived correctly. You could also create a workflow to automatically save your historic data to the new standard, harmonizing your formats across years and sites.

Mestrelab is always keen to add new import/export formats to its existing coverage, so do contact our support team if you have a specific request.



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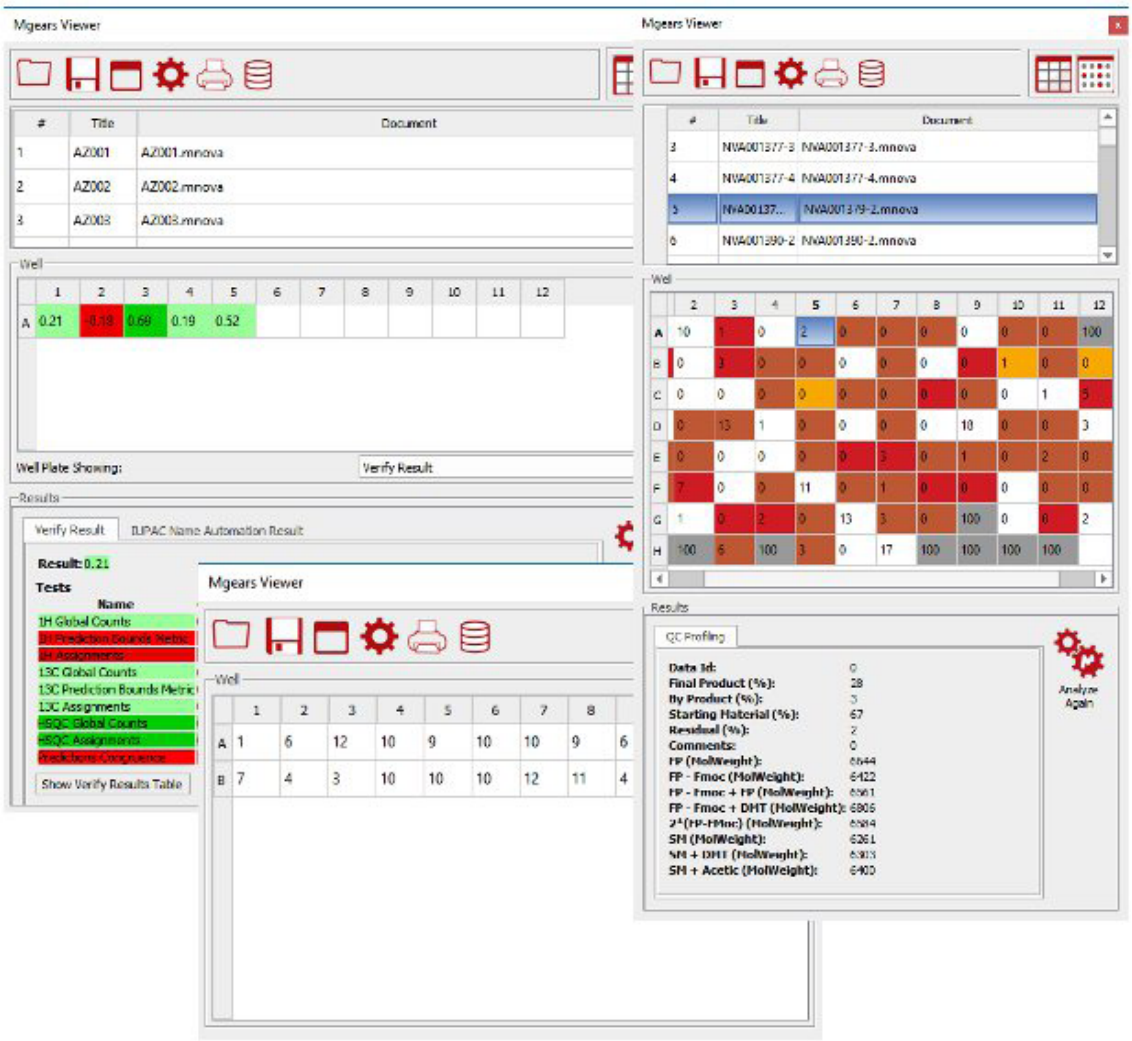
Viewer

Mnova Gears includes Mnova Results Viewer to review & correct results

Experience how easy it is to view results in Mnova with the Results Viewer included in Mnova Gears.
Unconvinced by the results? The Results Viewer is not only pretty, it can also relaunch the evaluation of a selected dataset if the specialist thinks the automation results might need revision.



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Limitless Automations

Not sure how Mnova Gears could be useful to you?
Here are just a few examples of how it could be used[1]:

Drug Discovery

Is your team taking NMR spectra to characterize products or impurities? With Mnova Gears the following steps can be automated, freeing up your precious specialist time!

1. Compare new spectrum with existing databases (internal or provided by third-parties)
2. Identify whether the structure has been analysed in the past, choosing the detailed settings of how the comparison is carried out
3. Find structures with similar 1H and 13C NMR to the current sample, to inform you of potential similar structures that can serve as reference
4. Create a report for the NMR specialist, including the new NMR spectrum, potential matches and similar structures that could be used as references

Purity

Using NMR for quantification? This is how easy it would be to set up your Purity determination experiments:

1. Add the Purity Plugin to your workflow
2. Use a standard analysis "experiment" that you might have validated - an SOP
3. Set your Purity settings or load pre-saved ones, specifying the reference library to be used
4. Generate an automated report, following your own template

Concentration

1. Process and analyze the data
2. Select the multiplets most suitable for quantitation
3. Integrate those multiplets as well as the reference multiplets (or use external reference values)
4. Turn integrals into concentrations (from libraries or at the point of data acquisition)

[1] *Check your licensing conditions to see if you have access to these extra functionality*

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Verify

Evaluates analytical data and makes a judgment as to whether it is compatible with the structure proposed by the user in full automation mode (from libraries or at the point of data acquisition)

Other automations

- ✓ QC Profiling
- ✓ SMA – Mixtures Analysis
- ✓ MS Purity
- ✓ DB Search
- ✓ Multiplet report
- ✓ IUPAC Name
- ✓ Peak Report
- ✓ Spectrum Quality Assessor

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General Enterprise Automation Rapid Solution

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