Mnova solutions for LC/GC-MS analyses

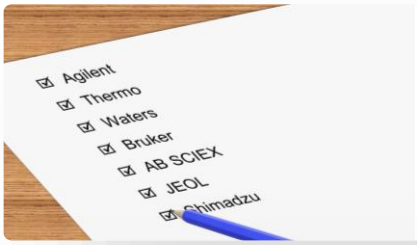
Mestrelab Research

chemistry software solutions

A unique software suite for all your LC/GC-MS-based analyses

High-throughput LC/GC-MS applications have become highly popular, indeed essential, for the daily activities in the majority of analytical laboratories, ranging in use from R&D, to manufacturing, to quality control. These techniques produce large volumes of analytical data that often require significant time and effort to manually process and interpret. We have developed a new range of Mnova solutions to support multiple LC/GC-MS analyses and streamline end-to-end workflows that require minimal human intervention, enable quick decision making, and promote operational agility.

Our software suite provides …



Vendor-independent data processing and analysis

Flexibility to process, analyze and report your LC/GC-MS data from most spectrometer vendors

Unique interface for all your analyses and results

Increase your lab efficiency and simplify data management by running multiple LC/GC-MS analyses (in addition to NMR and electronic and vibrational spectroscopies*), with the ability to view all your results in the same user interface

Workflow automation

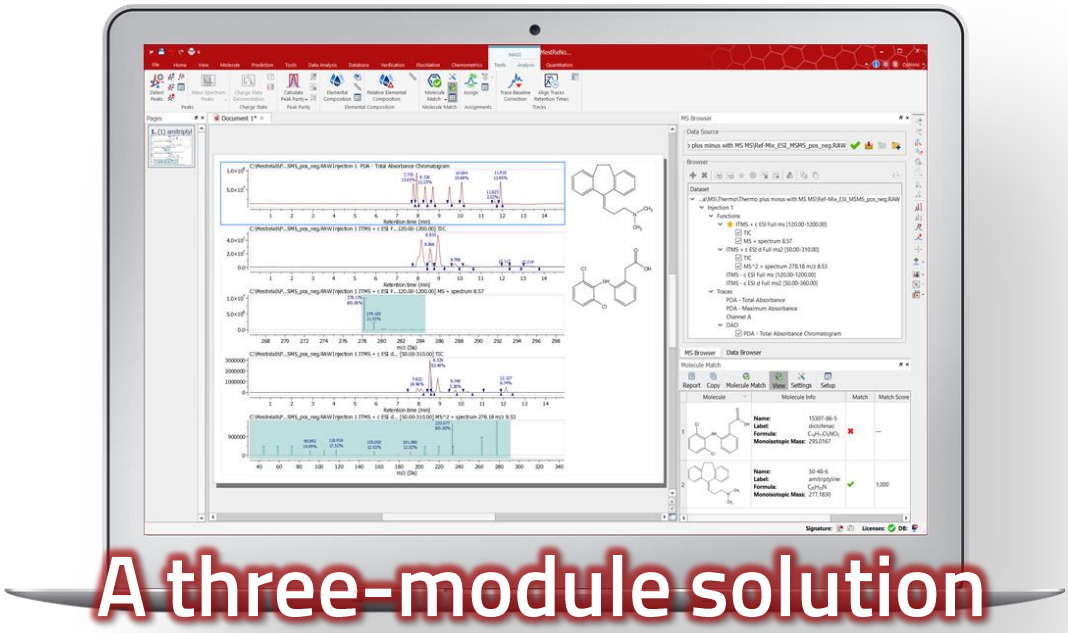
Streamline LC/GC-MS workflows on large datasets in batch or real-time modes by automating data pick up, processing, analysis, and results reporting, archiving and databasing.

**Additional licenses for Mnova NMR and ElVis are required to process NMR and IR/UV/Vis data, etc.*

Leverage the highly flexible and adaptable Mnova architecture to easily integrate fully automated data workflows into your lab environment!

1. A popular desktop application for processing

Mnova MSChrom offers intuitive, easy-to-use tools to visualize, analyze, and report LC/GC-MS data from various vendors. It automates a range of functionalities such as data import and display, integration, background subtraction, display of extracted mass chromatograms, molecule match, enumeration of molecular formulae, etc. It is ideal for processing data interactively, usually one dataset at a time.



2. A backbone automation engine

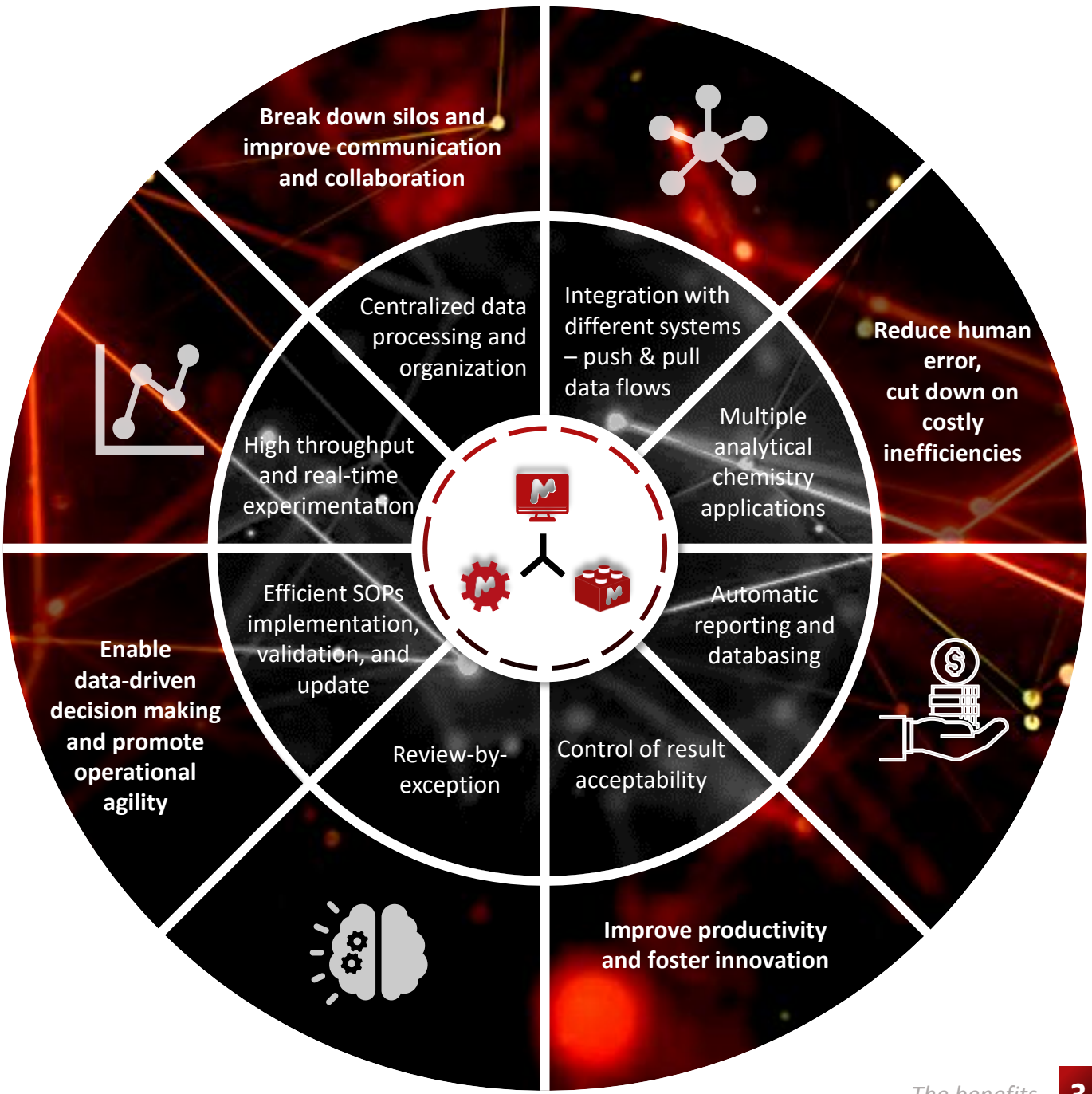
Mnova Gears provides the backbone for any automated workflow. It handles data detection and pickup for processing and matching datafiles with corresponding information provided in .txt, .csv, or .sdf files, applies default or custom-made processing and design templates, and saves reports to predefined disk directories or databases. The engine can also connect to and communicate with other external systems.

3. Task-specialized analysis bricks

A **Gears brick** takes care of all aspects specific to a defined application. It allows the configuration of the analysis method in line with any standard operating procedures and facilitates the sharing and ad-hoc use of the so-called method by both experts and non-experts who need to run LC/GC-MS. A Gears brick can be used as standalone tool or combined with other bricks to run multi-step workflows.

Our focus has always been to improve scientists' productivity in order to accelerate research, enable faster, more robust decisions, and free up scientists' time for the highly complex and creative activities where most of their value is generated. When looking at the high volumes of data that LC/GC-MS instruments are able to generate, and at the labor-intensive and monotonous review processes, the automation of the analyses performed with these techniques represents an obvious opportunity to leverage the very flexible and adaptable automation environment we have developed with Mnova Gears

Santi Dominguez, CEO - Mestrelab Research



Organic synthesis optimization and quality control

Chrom Reaction Optimization GEARS

With **Chrom Reaction Optimization** you can automate LC/GC-MS data processes to quickly find the safest, most efficient, cost-effective synthetic schemes for your chemical reactions. The tool will track a defined set of chemicals (Starting Materials, Products, Impurities, and By-products) across multiple parallel reactions to compare their quantities and conclude on the best experimental conditions to employ. >> Read more

Chrom Cal GEARS

You can run **Chrom Cal** before your Chrom Reaction Optimization analysis to generate calibration curves for your reaction's components and use the output files to achieve absolute quantification.

Chrom Cal will allow you to obtain well-defined calibration curves for all your compounds at once, saving you the pain of plotting your curves manually and risking transcription and calculation errors. >> Read more

Preparative chromatography and compound purification workflow

What are the best separation conditions for my compound?

With **Chrom Best Method** you can seamlessly screen and compare several chromatographic methods to identify the one that is more likely to yield a pure compound. This plugin will automate LC-MS data processing, target and impurities identification, method scoring, and report generation, to provide you with quick and robust answers. >> Read more

Should I pool the fractions collected for my sample during the chromatography run or not?

Fraction Analysis will help you answer this question quickly by automating the analysis of the collected fractions and suggesting the most adequate action to undertake. The tool will evaluate the number and size of the peaks present in each fraction, match and assign your target peak, calculate its purity, then score and report the results automatically. >> Read more

Is the sample obtained pure enough?

Once your analyte is dried and bottled, **Chrom QC** will allow you to perform the last quality control check to confirm your compound's identity and assess its purity before releasing it to downstream processes or to the market. Chrom QC will provide a molecule match score, a percentage purity, and a concentration if calibration information is provided.

>> Read more

Combine and adapt these solutions to your standard procedures to reap even more benefits to your organization.

High-throughput quality control for your compound libraries

Fully automate qualitative and quantitative analyses on your synthesized and purchased compounds to confirm elemental composition and purity before compound registration and use in biological assays or chemical reactions.

Verify will run a set of spectra against potential molecular species/structures to confirm sample identity. It relies on powerful algorithms that allow the calculation of a score for each dataset. It also carries out comparisons of experimental and theoretical data for both NMR and MS techniques in commercial off-the-shelf software. >> Read more

Chrom QC will match the LC/GC-MS data with their corresponding molecular structures, formulae, masses, etc., and analyze the spectra to confirm compound identities, and calculate purities and concentrations. Non-compliant samples can be detected at a glance and manually reviewed by experts for ultimate decision making. >> Read more

Determination of physicochemical properties of lead compounds

Solubility and **LogP** are powerful tools that can assist you in early drug discovery, optimization and formulation process, to characterize and validate lead candidates with adequate bioavailability and lipophilicity.

These software tools automate high-throughput LC/GC-MS quantification and the determination of a compound's solubility and lipophilicity properties, respectively. They handle the entire process of sorting raw datafiles, verifying molecules, performing quantitative analysis, and reporting results.

>> Contact us

Analyzing affinity selection mass spectrometry screening experiments

Affinity Screen automates the analysis of multiplexed affinity selection MS experiments, where many potential ligands are pooled and tested at the same time. It handles dataset pickup and grouping, identification of the ligands present in each mixture using the reference data, matching of the peaks found to the free/bound states and the calculation of the associated ratios. For each well, you will get the number of ligands tested, found, and those that are hits.

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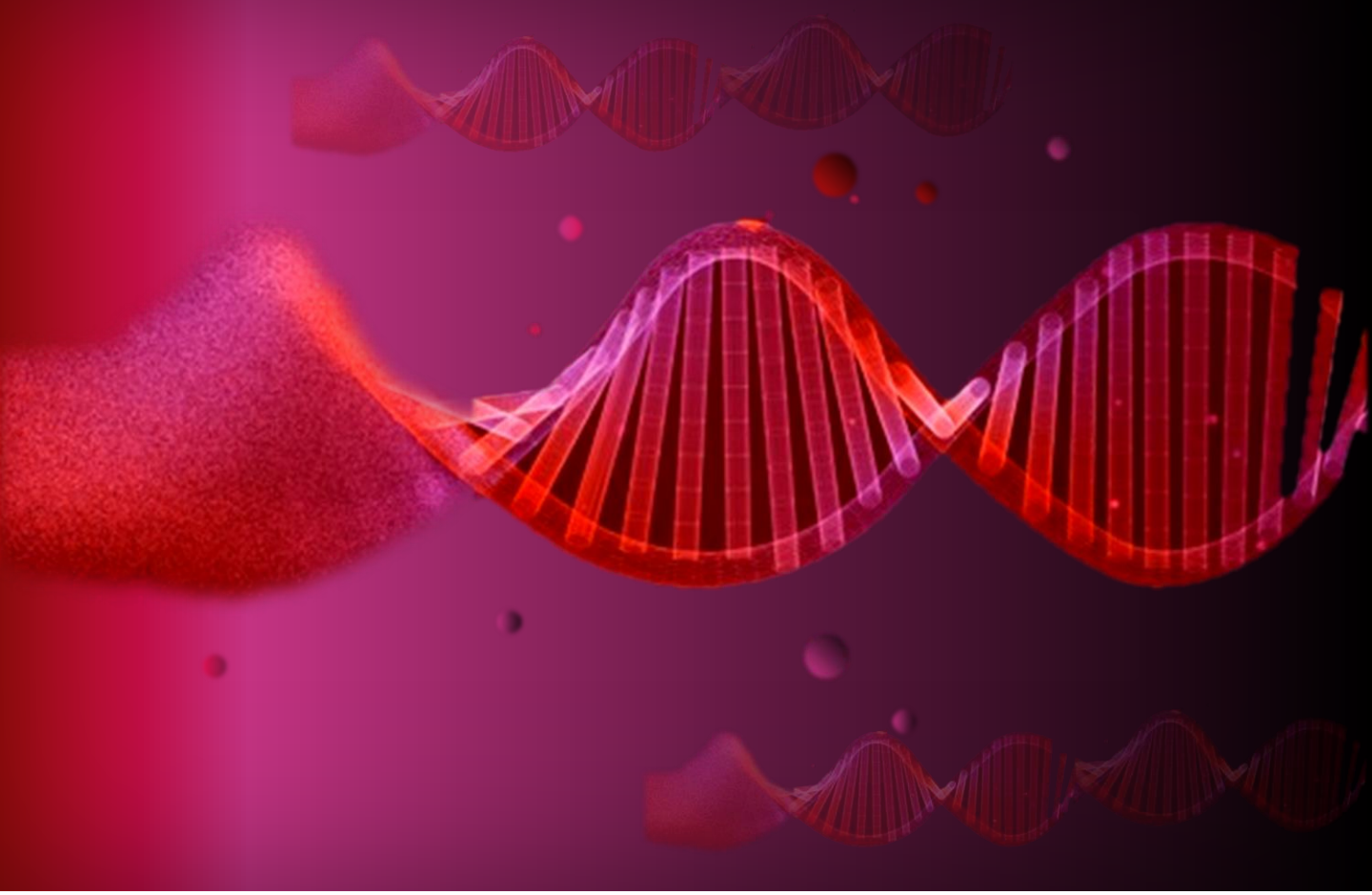

Quality control of DNA conjugates or other macromolecules for up to 10 kDa

QC Profiling
GEARS

If you are generating and commercializing DNA encoded libraries (DELs), and spending a lot of time and exhausting resources on data analysis for quality control of the reactions, **QC Profiling** is the tool for you. This brick will process and deconvolute every spectrum and attribute masses, while identifying and excluding unwanted contaminants from analysis (such as non-DNA impurities, and unknown DNA conjugates). It will then quantify the samples' components and label any problematic samples for review.

>> Read more

> *This software easily multiplied our productivity by three, greatly enhancing the reproducibility and drastically reducing the chance of human error*
>
> ***Roberto Martinez, Senior Scientist - Novartis***

Testing the performance state of the LC/GC-MS systems

Chrom SST GEARS

With **Chrom SST** (System Suitability Testing) you can assess the performance of your LC/GC-MS systems before running any valuable samples. The tool will analyze the test spectra and check if parameters such as retention time, limit of detection, peak resolution, instrument pressure, etc., are within acceptable ranges. Such instrument performance testing will provide reasonable assurance that the analytical results obtained with the validated instrument are accurate and reliable.

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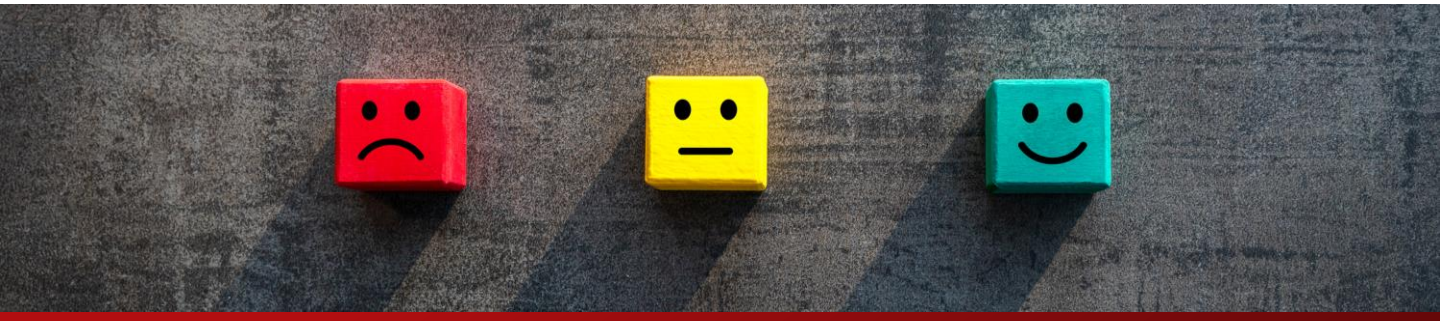

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