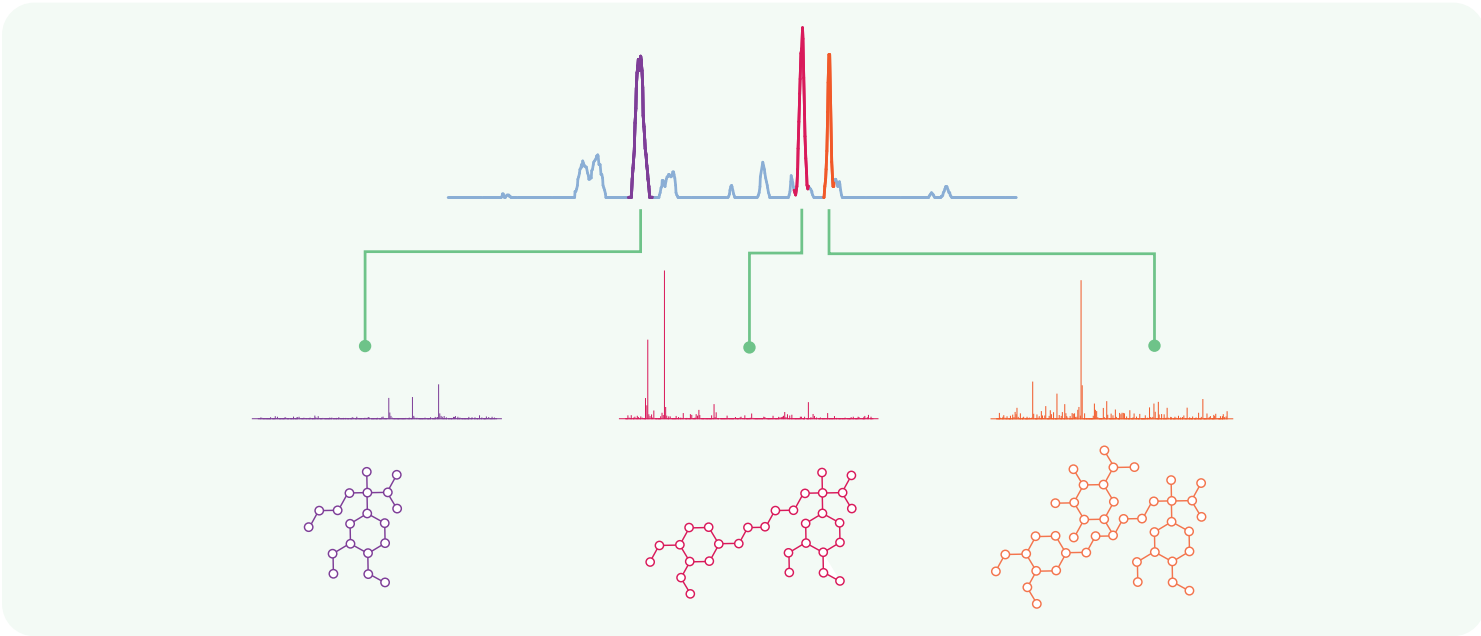
Spectral Interpretation and Component Characterization

MS Workbook Suite



The Complete Software Solution for Mass Spectrometrists

Quickly detect, distinguish, identify, characterize, and quantitate components

Automatically annotate peaks & better understand your spectra

Increase confidence in your structure assignment

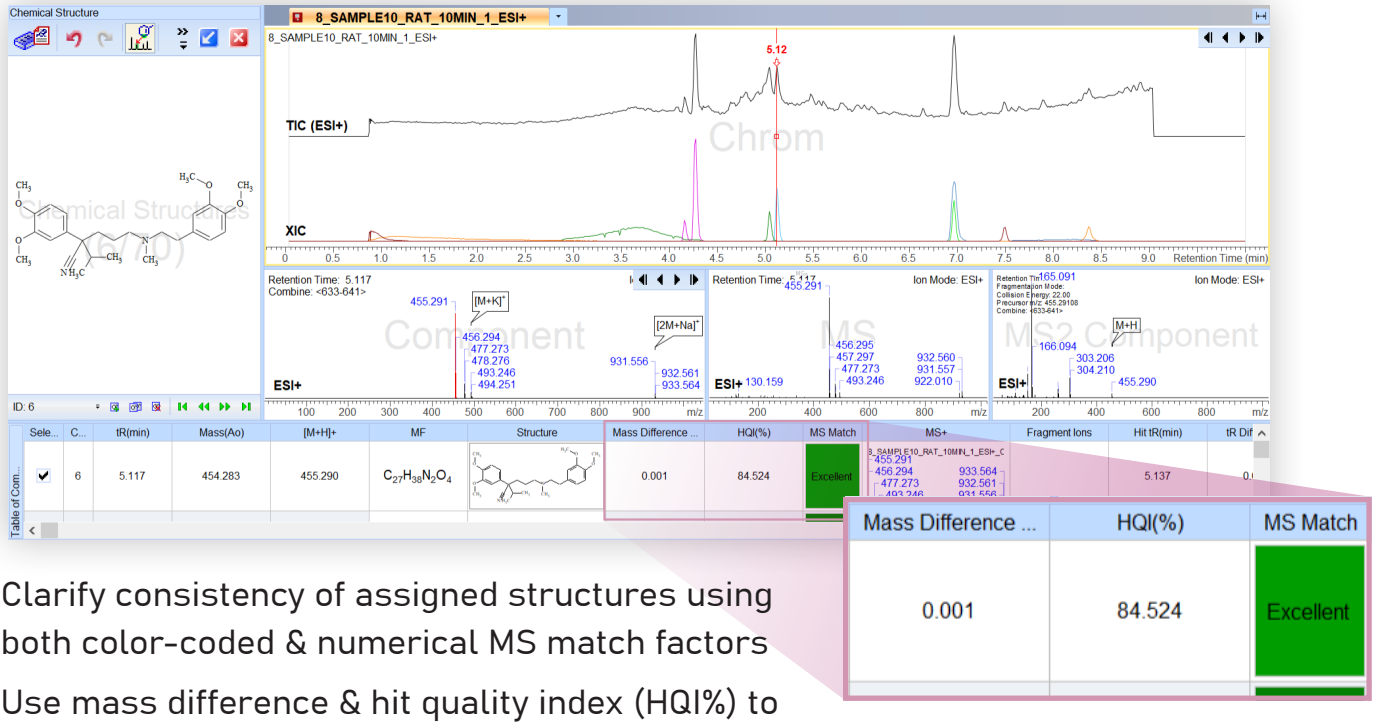
Connect peaks to structures, to immediately know what you are looking at

Store your results in a searchable database, to find all relevant information

ACD/Labs®

Quickly Identify and Characterize Components

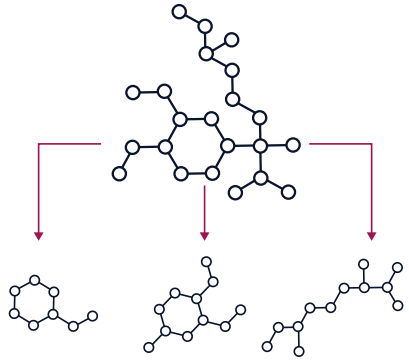
- Visualize all GC/MS and LC/MS data together in one interface
- Assign chemical structures to chromatographic peaks and automatically annotate component mass spectra
- Select integrated chromatographic components to view associated MSn data and generate a pure component mass spectra.



- Clarify consistency of assigned structures using both color-coded & numerical MS match factors
- Use mass difference & hit quality index (HQI%) to further evaluate structure assignments

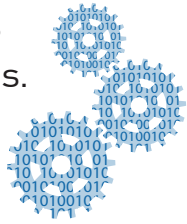
Easily Predict Fragmentation

View mass fragmentation of target structures using a rule-based approach and derive fragment formulae from the original input structure.



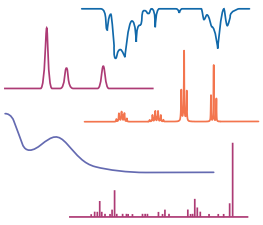
Automate Routine Workflows

Streamline standard processes such as data import and updates. Add scripts and macros for repetitive tasks.



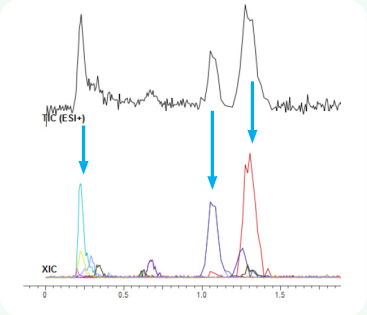
Process All Analytical Data

Use general processing tools for NMR, IR, Raman, and more, to compile all relevant analytical and structural data for a given project together.



Efficiently Extract Chromatograms

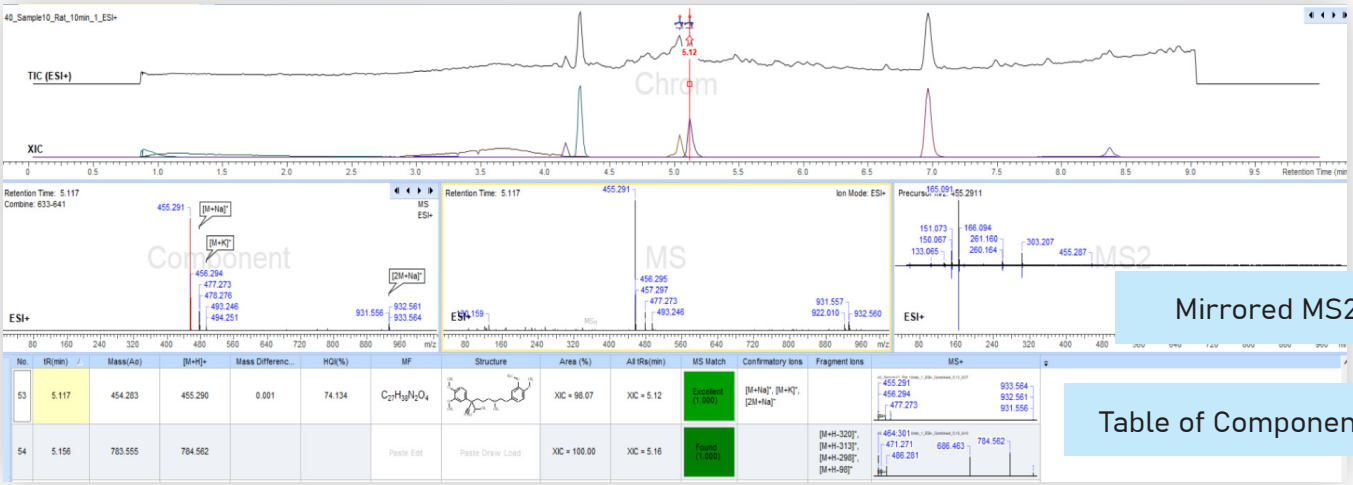
Reduce time for component interpretation



Automated component extraction with the *IntelliXtract* algorithm extracts all known relevant compounds, including co-eluting peaks.

Streamline Structure Identification for Complex MS Datasets

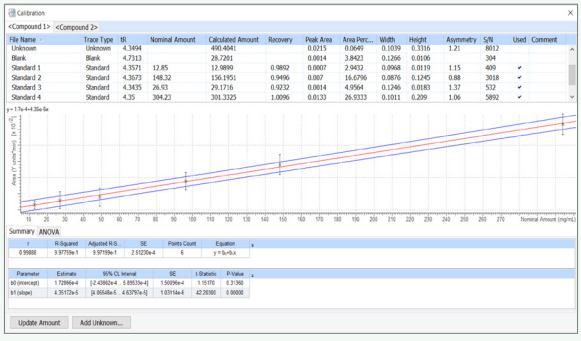
Intelligent Component Recognition (IXCR) – Accelerate identification of unknowns in complex LC/MS and GC/MS datasets through automated spectral searching of MS2 and MS1 databases (respectively).



- Identify unknowns through database searching and review results of top search candidates in the Table of Components
- Use mirrored MS2 for direct spectral comparison with database hits

Quantitate LC/UV/MS data

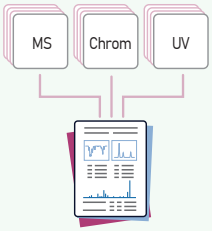
Perform quantitative analysis of LC/UV/MS data based on TIC (mass of compound), DAD (auto-extracted wavelength) or flat chromatogram (specified wavelength) to produce quantitative and reproducible data.



- Create a calibration curve with a line of best fit & error bars
- Quantify several compounds simultaneously & process replicate samples
- Quantify additional unknowns after calibration project has been constructed

Retain & Share Live Knowledge

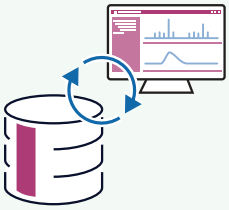
Create comprehensive, searchable databases so you can always find and share all relevant information.



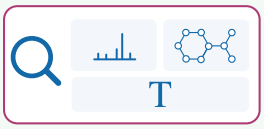
Readily compile MS spectra, chromatograms & UV traces in customizable reports



Quickly export reports to MS Word, Excel, PowerPoint, or PDF



Store live analytical data that is simple to review, reprocess & reinterpret

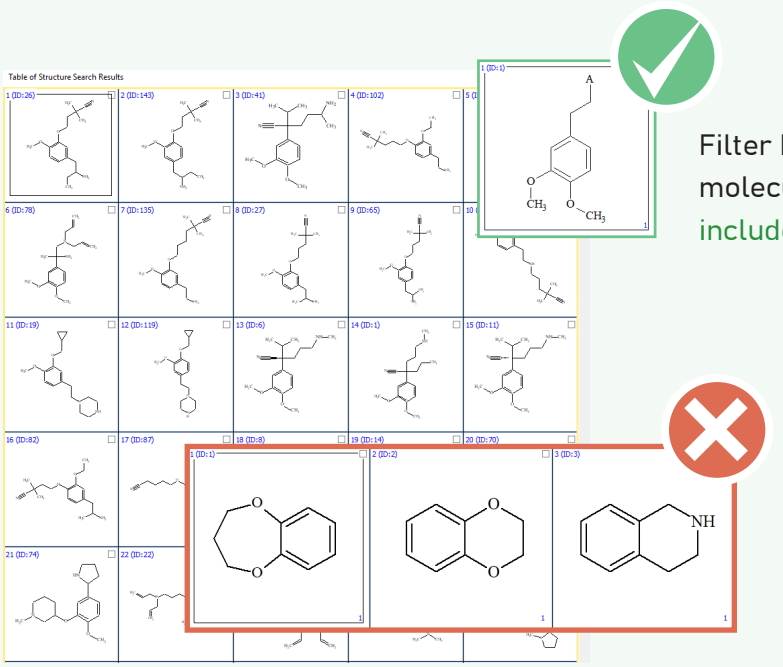


Search databases by structure, spectra, or text parameters

MS Structure ID

Use the MS Workbook Suite add-on to query local databases (PubChem, ChemSpider) for target accurate mass values and molecular formulae.

Search for a target component's accurate mass & predicted molecular formula to generate a ranked structure hit list



Filter hit list by molecular fragment include and exclude lists

To learn more about ACD/MS Structure ID visit www.acdlabs.com/MSWorkbookSuite

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