Analytical Data Handling and Structure Confirmation for Synthetic Chemists
ACD/Spectrus Processor is an all-in-one, multi-technique data processing and chemical characterization tool for medicinal, synthetic and process chemists, and the gateway to the ACD/Spectrus analytical and chemical knowledge management platform.

Spectrus Processor helps synthetic chemists by speeding up the routine characterization of new molecular entities, and confirmation of known and expected chemical structures.

Working with analytical experts, organizations use Spectrus Processor to enable complete systems for fast analytical data interpretation and structure confirmation.

Did I make what I think I made?

Structure verification using NMR and LC/UV/MS data can help quickly confirm the consistency of chemical structures with experimental spectra. Simply drag-and-drop or copy and paste a chemical structure to receive immediate feedback on the consistency between structure and data.

For LC/UV/MS data, add a structure, formula, or mass data to the Table of Components to automatically extract a relevant mass chromatogram, or assign a peak to generate a mass spectrum.

Corporate Knowledge Management

Spectrus Processor is the gateway to the ACD/Spectrus platform which provides chemical and analytical knowledge management. Within an organization, data is collected by different groups for different purposes and traditionally sits in discrete data silos. With Spectrus Processor, knowledge—be it predicted or experimental results, metabolite identification information complete with associated analytical data, open access, or any other—can be accessed by colleagues throughout the organization, or permissions granted based on project, division, or location.

Process or Access data directly from the instrument, open access system or database, and re-process data when required

Analyze and Review spectral assignments and interpretations

Confirm proposed chemical structures with help from automated structure verification

Search corporate, third-party, and commercial databases to investigate mysterious or unexpected signals

Report the most important elements of your analysis to include in a paper or electronic notebook, or to create a report.

Color-coded MS match factor indicates consistency of monoisotopic and isotope peaks.
Uniform Processing
ACD/Spectrus Processor provides synthetic chemists with a toolset to handle NMR, LC/MS, chromatography, optical (including IR, UV/Vis, and Raman), and other analytical techniques in one interface. This intuitive and easy-to-use software package:

- Provides a consistent and intuitive interface for work-up of data across different analytical techniques
- Speeds up analytical review
- Automates routine processing tasks at import including peak-picking, integration, and structure attachment

Multi-vendor, Multi-technique Support
Work with NMR, LC/UV/MS, chromatography, IR, UV/Vis, Raman, TGA, DSC, XRPD, EELS, and other analytical data. Our continuing collaboration with instrument vendors ensures that data can be taken from instruments and treated uniformly for standardized handling of analytical data and ease of use.

In the case of NMR data, the software compares experimental and predicted 1D or 2D spectra, auto-assigns experimental spectra, and provides a match factor indicating consistency.

Knowledge-Sharing Tool for Analytical Specialists
Through database viewing and searching Spectrus Processor provides a powerful knowledge-sharing tool that can help to reduce the burden on analytical specialists. Furthermore, ACD/Labs software advances such as fully automatic verification using NMR, high throughput compound library management, rapid chromatographic method development, and others can form a comprehensive solution to eliminate tedious tasks and bottlenecks in the analytical and separations laboratory.

Database records are searchable by a variety of structural, spectral, and text-based parameters. In Spectrus Processor, spectral search results are automatically overlaid on the query spectrum with color highlighting of matching signals for easy interpretation.
Spend more time on synthesis and less time processing and interpreting your analytical data.

With the increasing demands for productivity, ACD/Spectrus Processor helps the synthetic chemist to make quick work of routine analytical data processing and interpretation. Equipped with unique chemical intelligence and interpretation algorithms, it speeds up structure confirmation. With an intuitive interface and consistency across multiple analytical techniques, the software provides a unified platform for handling of NMR, LC/UV/MS, optical, and other analytical data. Furthermore, access to proprietary and commercial databases offers users a powerful tool for investigating unexpected products, and a platform for collaborative science.

Learn more about ACD/Spectrus Processor at

www.acdlabs.com/spectrusprocessor