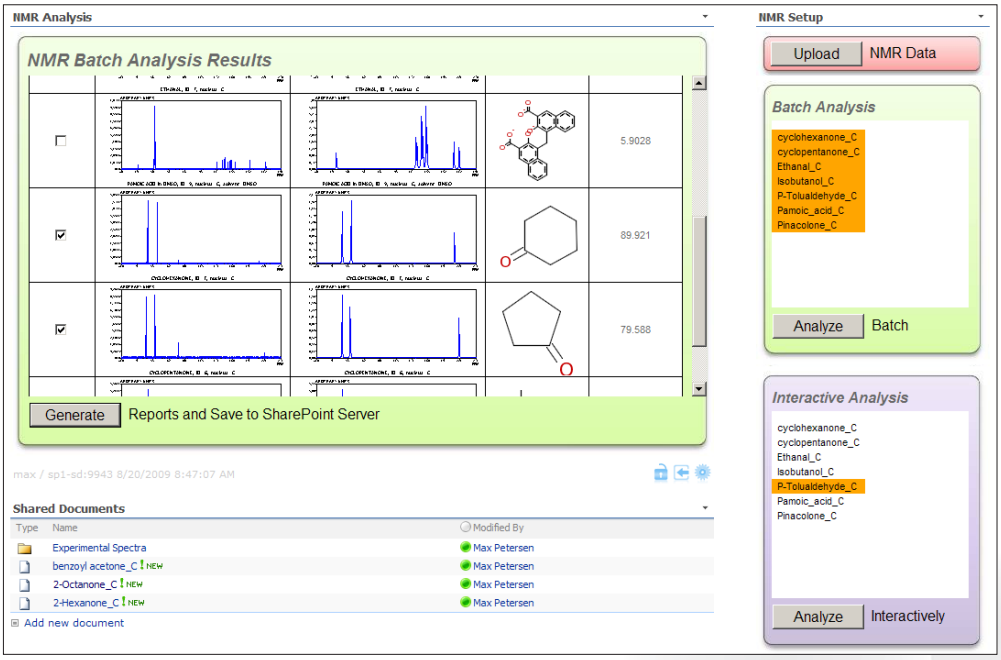
DATASHEET

ANALYTICAL INSTRUMENTATION COLLECTION

The Analytical Instrumentation Collection enables Pipeline Pilot to access, process and share data generated in your analytical lab. With this collection you can streamline the processing of analytical data, generate reports and share results more easily with other departments.

WITH THE ANALYTICAL INSTRUMENTATION COLLECTION YOU CAN:

- Share analytical characterization results more effectively within your organization
- Capture best practices for analyzing your analytical data
- Streamline repetitive data processing and analysis tasks
- Reduce efforts by creating automatic reports that can easily be customized to meet the varying needs of end users
- Integrate otherwise isolated data silos and create collaborative research environments



Simplified interfaces to process NMR data can be deployed in web based portal environments such Microsoft SharePoint. Main benefits include higher turnaround times due to faster processing of data and easy sharing of data using via integration with document repository systems.

THE ANALYTICAL INSTRUMENTATION COMPONENTS

Readers and Writers: The collection supports open standards such as JCAMP-DX, SPC, RheoML and AnIML. In addition, you can read instrument specific data formats such as Bruker and Varian NMR formats. You can store spectra in JCAMP-DX or in XML based formats.

Calculators and Manipulators: The collection supports common data processing operations:

- Peak Identification
- Peak Integration
- Line width analysis
- Background detection and removal
- Interpolation, truncation, scaling and smoothing of spectra
- Subtraction of spectra
- General purpose Fourier transform

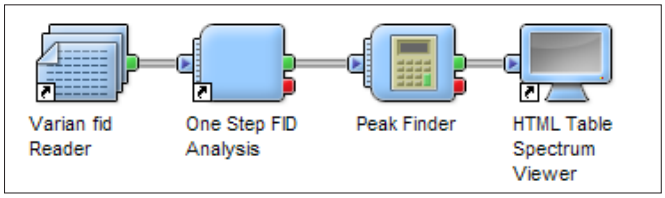
NMR specific functionality includes:

- One-step FID analysis to convert FID's to chemical shifts. This component performs Fourier transformation, dephasing and referencing steps.
- Generating NMR spectra from chemical structures (C13 and proton shifts supported) via out-of-the box integration with Modgraph NMRPredict.

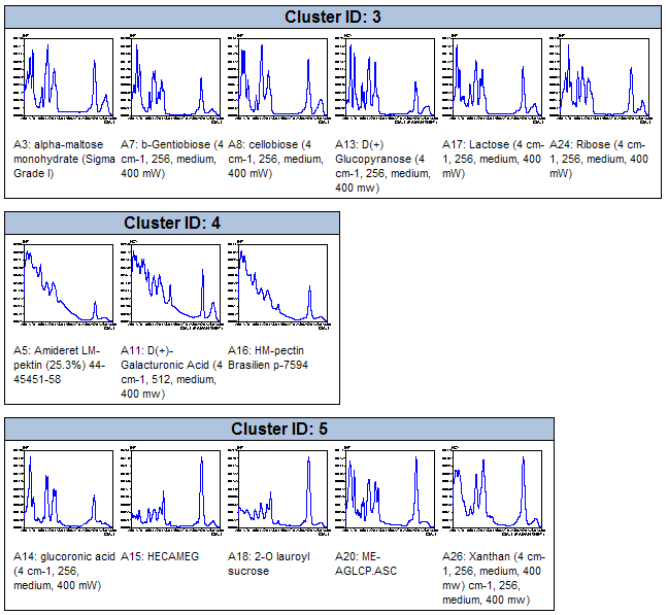
Search and Similarity: The collection allows calculating spectra similarity based on weighted cross-correlation, Spearman's rank order coefficient or Pearson's r factor. This functionality can generate correlation matrixes to support clustering applications or rank the similarity of a single spectrum to a series of spectra, which supports applications such as database matching.

Viewers and Reporting capabilities: With this collection, you can easily display spectra in reports, including axis modifications, peak display and labeling, and scale conversions. Other data such as peak tables are equally easy to generate and include into reports.

To learn more about Pipeline Pilot, go to
accelrys.com/pipeline-pilot



Pipeline Pilot protocol that performs a typical NMR analysis sequence: First, raw Varian instrument data are read. Next, raw data are converted to chemical shifts via Fourier transformation, dephasing and referencing steps. Finally, peaks are detected and reported.



With the Analytical Instrumentation Collection you can perform similarity analyses such as clustering and pattern matching operations.