

Share analytical characterization results with your entire organization

Generate automated reports that fulfill the needs of your end users

Streamline and automate the processing and analysis of your instrument data

## 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

The screenshot displays the 'NMR Analysis' web interface. The main window is titled 'NMR Batch Analysis Results' and contains a grid of four rows. Each row shows a checked checkbox, a 1D NMR spectrum, a 2D NMR spectrum, a chemical structure, and a numerical value (79.427, 96.629, 5.9028, and 79.000). Below the grid is a 'Generate Reports and Save to SharePoint Server' button. To the right, there are two panels: 'NMR Setup' with an 'Upload NMR Data' button, and 'Batch Analysis' with a list of compounds (2-Octanone\_C, cyclopentanone\_C, isobutano\_C, P-Tolualdehyde\_C, Pamoic\_acid\_C) and 'Analyze Batch' buttons. Below that is an 'Interactive Analysis' panel with the same list of compounds and 'Analyze Interactively' buttons. At the bottom, there is a 'Shared Documents' table and an 'Add new document' button.

Type	Name	Modified By
Folder	Experimental Spectra	Max Petersen
File	Pinacolone_C ↓ NEW	Max Petersen
File	cyclohexanone_C ↓ NEW	Max Petersen
File	benzoyl acetone_C ↓ NEW	Max Petersen
File	2-Hexanone_C ↓ NEW	Max Petersen

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

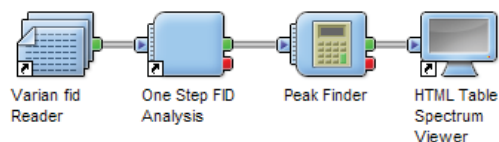
NMR specific functionality includes:

- 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.

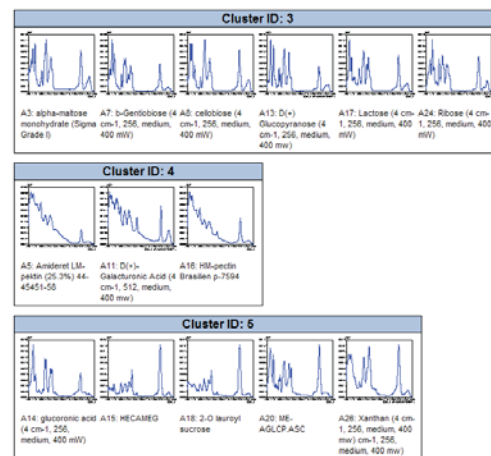
**Search and Similarity:** The collection allows calculating spectra similarity based on weighted cross-correlation, Spearman's rank order coefficient or Pearson's r factor. This functionality

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.



*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.*