Allotrope, the silent enabler of deep integration between Mnova and ZONTAL
Why do we collect analytical data?

“I want my data to be readily accessible in tools that do the things I need to get answers about my experiments”

“I need the data to be secure and retrievable / readable in the future”

“I want data from all sources in a standard format so I can mine it”
Why do we collect analytical data?

It is hard to meet all their needs
Mestrelab and ZONTAL

Why collaborate?

- Mestrelab is strong in providing user focused tools that give scientists the answers they need from analytical data
- Mestrelab supports NMR, LC and GC MS, UV, IR and other optical spectroscopy techniques
- Mestrelab has worked with Allotrope members to convert and archive proprietary NMR data into a common format stored in ADF
- ZONTAL provides a FAIR Data Hub supporting the Allotrope Data Format natively
A synergy can be achieved
Orchestration of Laboratory Workflows

- Buffer & Mobile phase preparation
- Standard Preparation
- Sample Preparation
- Instrument Set up and execution
- Data Acceptance and submission

Analytical Data Hub

- Balances
- Analyzer Devices
- CDS Systems
- MNova
- ELN/LIMS
Mnova Solution Architecture

Ad hoc user processing

Spectroscopic searches

Test Request

Automated processing

Analytical Data Hub

.ZONTAL SPACE
What data can I use with Mnova?

- NMR data
- LC and GC MS
- UV, IR and other optical spectroscopies

We can process the data in ways that give scientists answers.
How we apply the Allotrope Framework

- For LCMS we use a model aligned to LCUV, using additional elements from the PSI ontology
- For NMR we use a proposed Allotrope Data Model, developed in collaboration with allotrope members
- For Processed Data we use the ADF container and a model based on Allotrope Design Patterns.
Open access Chemistry Use Case

Demo

This use case uses a ZONTAL configured sample interface to load proposed structure (.mol file) via request.

Mass spec samples will be generated and placed in ZONTAL Space. The data will then automatically be converted to ADF and pushed to Mestrelab for structure verification. The results will then be ingested back into ZONTAL Space. This includes the .mnova file, a json file, and a printed pdf.

The integration highlights ZONTAL’s ability to ingest files in the required time for the chemists and how automated processing of the data can be executed by Mestrelab.
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Open access Chemistry Use Case

- Processed Data
- Metadata
- PDF Report
- Thumbnail
Summary

- Mestrelab and ZONTAL products are fully integrated
  - Benefits all users who interact with analytical data
  - Gives access to all content in the ZONTAL Analytical Data Hub directly from within an analytical data client
- Integration enables the following automated capabilities
  - Automated data processing, indexing, and archiving on ingestion into ZONTAL
  - Automated structure verification on the fly – confirm that the putative structure is consistent with the data supplied
  - Automated report generation
  - Automated transfer of reports and analyzed data to ZONTAL
- Huge benefits saving chemist time processing and analyzing routine analytical data
  - Reproducible and standard processes minimize human errors and
- Integration allows access to the complete set of Mnova analytical data tools
  - Enables access to tools for working manually with all types of analytical data
  - Enables access to tools for on-demand structure verification
  - Enables access to workflows for analysts involved with structure elucidation
  - Enables access to archived data for spectroscopically and chemically meaningful searches