The Methods Database Project

Method Transfer Between Chromatographic Data Systems And Across Instruments Through the Methods Database

Key information:

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The Pistoia Alliance Methods Hub is envisioned to be a *platform* where semantically *interoperable analytical methods* and supportive tools are available to the Pharmaceutical Industry.

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Sponsors/partners:

Business Benefits

- Conceptional separation of the application from the underlying standard will allow more than one software company to adopt the Methods Db standard
- Improved method exchange capability from one instrument to another irrespective of vendor and CDS creates higher flexibility, efficiency, and reproducibility
- Improved data quality and integrity through linking Method, instrument status and result data
- Leveraging the ADF framework beyond result data management reduces the number of system interfaces and enhances value of this framework

Call for participation

For the next phase of the project we would like to engage more members from CROs, software providers and pharma companies to show ROI and work on new use cases.

The project

The Pistoia Alliance has successfully completed a pilot on the digital transfer of analytical High Performance Liquid Chromatography (HPLC) methods and results between chromatography data systems (CDS) in the cloud using a common, machine-readable data format. Method and associated data sharing within a company or between collaborators often employs semi-templated documents with inconsistent terminology in different proprietary platforms. Unavoidably, these practices lead to human interpretation errors, create time-intensive implementations, and reduces the reproducibility and efficiency of methods exchange or transfers. Therefore, the Methods Database project set out to develop a consistent, digital representation of analytical methods that can be broadly applied to research and development as reliable, machine-readable instructions to instrument control software.

Having standardized the terminology with the Methods Db LC-UV data model, the pilot study constructed Allotrope Data Format (ADF) converters to enable digital transfer of HPLC-UV execution parameters between chromatographic instruments and CDS across vendors. For an interoperable transfer between Empower™ CDS and OpenLab CDS, ADF adapters were built (Orbis Lab systems and Agilent technologies), Figure 1.

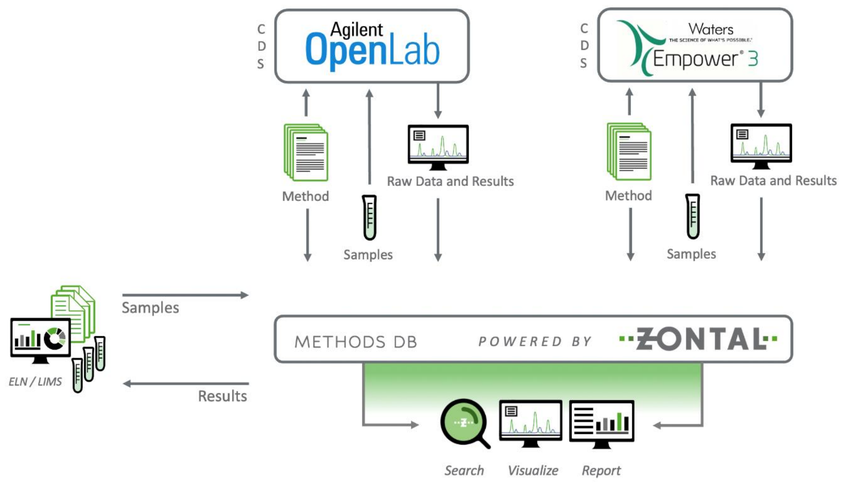


Figure 1. After execution, methods parameters / acquisition parameters in Water Empower CDS is converted from JSON to the ADF representation and exported to the Methods Database in ZONTAL space. The ADF of the desired method can be downloaded and imported though the OpenLab CDS interface where the ADF adapters convert the acquisition parameters for automatic execution.

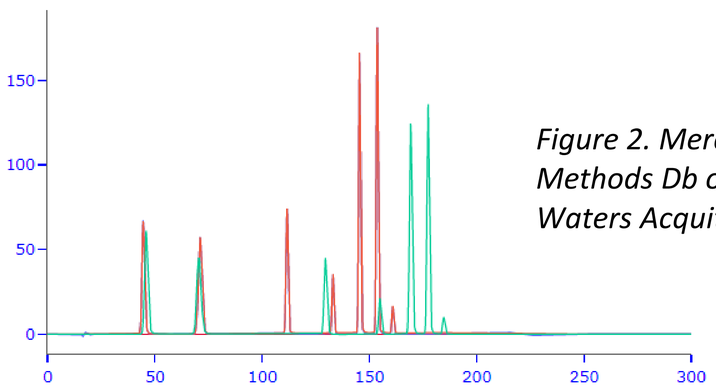
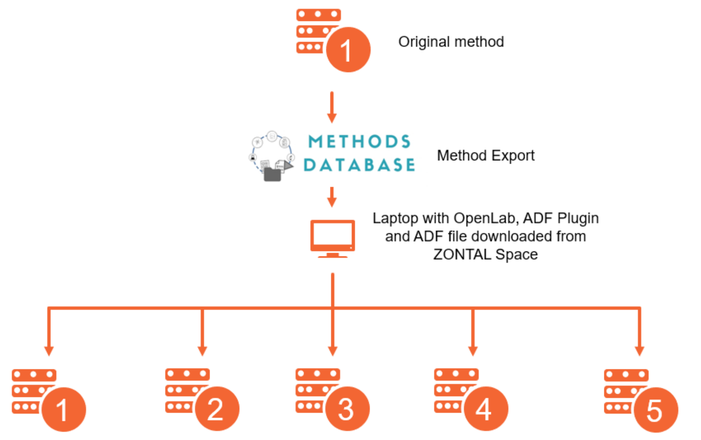


Figure 2. Merck gradient method imported from the Methods Db onto Agilent 1290 (dwell volume 137 µL) and Waters Acquity (dwell volume 357 µL) instruments at GSK.



ADF method files imported onto instruments with different modules stacking

Module	Instrument 1: WU_STV11	Instrument 2: WU_S29	Instrument 3: STV_02	Instrument 4: S56 (Biopharma)	Instrument 5: LC2
Pump	G7120A: 1290 Infinity II Binary Pump	G1312A: 1200 Binary Pump	G7120A: 1290 Infinity II Binary Pump	G7111B: 1260 Infinity II Quaternary Pump	G1312B: 1260 Infinity Binary Pump
Injector	G7167B: 1290 Infinity II Multisampler	G1329A: 1100 Autosampler	G7167B: 1290 Infinity II Multisampler	G7167A: 1260 Infinity II Multisampler	G7167A: 1260 Infinity II Multisampler
Column Compartment	G7116B: 1290 Multicolumn Thermostats	G1316A: 1200 Thermostatted Column Compartment	G7116B: 1290 Multicolumn Thermostats	G7116B: 1290 Multicolumn Thermostats	G1316C: 1200 Thermostatted Column Compartment
Detector	G7117B: 1290 Infinity II Diode Array Detector	G1314B: 1200 Infinity Variable Wavelength Detector	G7117A: 1290 Infinity II Diode Array Detector	G7115A: 1260 Infinity II Diode Array Detector Wide Range (WR)	G4212B: 1260 Infinity Diode Array Detector

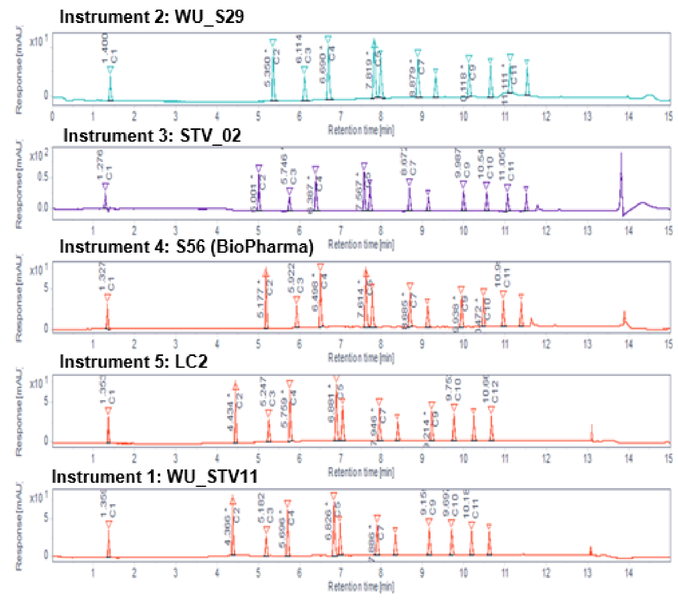


Figure 3. The pilot reimagine method exchange and transfer, validate the possibility of centralized methods storage as executable instructions as methods are automatically recapitulated instead of being recreated. Here, a method is imported and executed on 5 different instruments.

Figure 2 and 3 confirms the successful transfer of instrument method between instruments and CDS software. The availability of chromatograms and meta data around method parameters and instrument configurations at one place allowed the scientist to conduct instantaneous data analytics.

Conclusion

The Methods Db now allows for a significant streamlining of method related workflows. A digital workflow reduces documentation effort and the chance of human transcription errors when method parameters are transferred across different instruments and CDS software.