Developing a global, scalable, modular, and integrated analytical workflow management tool

Yamin Htet[3], Jennifer Kingston[1], Hanna Leek[2], Amber Balazs[3], Holly Douglas[1], Linda Thunberg[2], Jonathan Furbey-Taylor[4], Archana Mann[4], Richard Andersson[4], Sviatoslav Blokhin[4], Martin Harrison[5], Paul Faulder[5], Matt Bardsley[5]

1. Oncology R&D, AstraZeneca, Cambridge, United Kingdom, 2. BioPharmaceuticals R&D, AstraZeneca, Gothenburg, Sweden, 3. Oncology R&D, AstraZeneca, GHP, Waltham, US, 4.R&D IT, 5. Elixir Software Ltd, Macclesfield, United Kingdom

Overview

Developing streamlined analytical workflows and automated processes will enable faster drug discovery cycles. Incorporating automated data workflows saves time, reduces human errors, reduces cost and improves data quality, employee experience and satisfaction.

As part of the AstraZeneca's global automation vision, our aim was to develop an automatic analytical sample management and data tracking software, to include the following capabilities:

(i) Global and versatile solution to support all critical analytical activities in early drug discovery phase

(ii) End-to-end workflow to manage data

(iii) Flexible easy-to-use interface capable of future expansion.

Herein, partnering with Elixir the team, we share details of our newly developed global sample tracking and workflow management tool.

Vision for connected global analytical platform
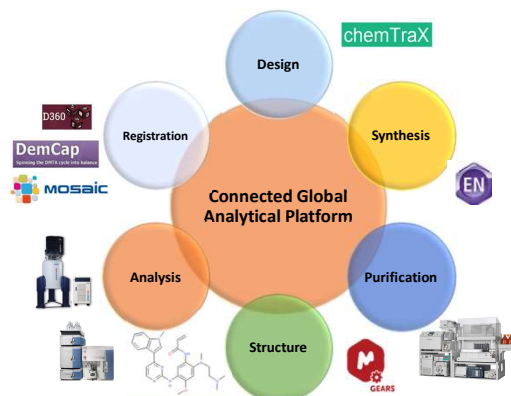
Diverse workflows
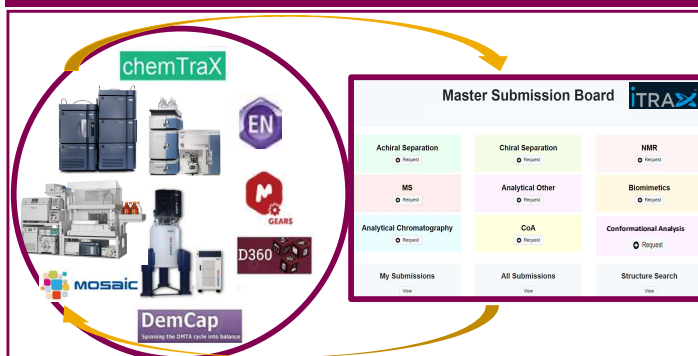
Our new product is designed to meet diverse global needs whilst allowing local flexibility and future expansion. The advantages of this modern sample tracking software has many capabilities:

(i) ability to handle both small molecules, peptides, and oligonucleotides

(ii) streamlined workflow management for a variety of analytical spectroscopic and chromatographic techniques

(iii) interactive communication between chemists and analysts

(iv) standardization among multiple analysts and sites

Automatic sample tracking and workflow management

Our new workflow management tool is based on a simple visual display board showing real-time sample status. The software supports not only sample submissions and tracking but also data management and automatic run-list and report generation, streamlining information flows between analysts and chemists. Advanced features include:

(i) planning and tracking of multi-analyst collaborative input

(ii) agile batching and un-batching of samples in real time

(iii) capturing of processed data

(iv) objective measures of turnover times and metrics

Developing integrated IT / automation solutions
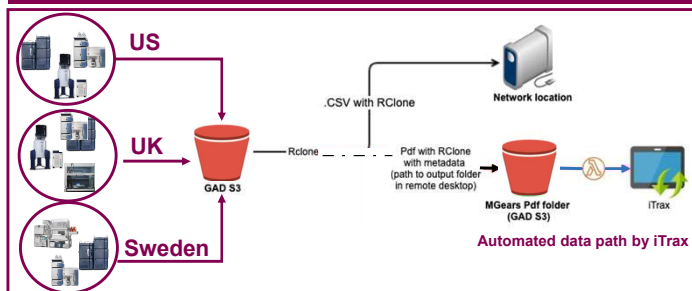
A critical step to enable the automatic sample management software in place is the integration with current IT infrastructure. Here, the in-house global database serves as the foundation, managing the automatic data flow. As instruments collect raw data, they are automatically funneled into the database. The data can then be consumed by an automatic processing software, MGears, according to our predefined specifications. Output files are then re-integrated into the in-house database for central storage. Finally, our dedicated workflow management tool, can retrieve the processed data from MGears through the database. Additionally, the data residing within the database can also be harnessed for predictive models.

Conclusions and future directions

A multi-disciplinary and multi-site team of scientific and IT experts have collaborated with the Elixir team successfully to design a global, scalable and modular sample tracking and workflow management platform with the IT infrastructure to accelerate AstraZeneca's analytical DMTA platform. The newly developed tool meets our global vision, allows local customizations, tracks sample and corresponding processed data, provides real-time sample status, facilitates communication among scientists, and measures metrics objectively. As this project moves into its next phases, of theoretical interest is accurately quantifying the impact of how the sample tracking changes on drug discovery and candidate drug delivery. Methods to measure the impact of this automation tool will be explored for future directions.

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