

Automatic Analysis and Purification : Vision, Progress, and Implementation for Early Discovery Compounds



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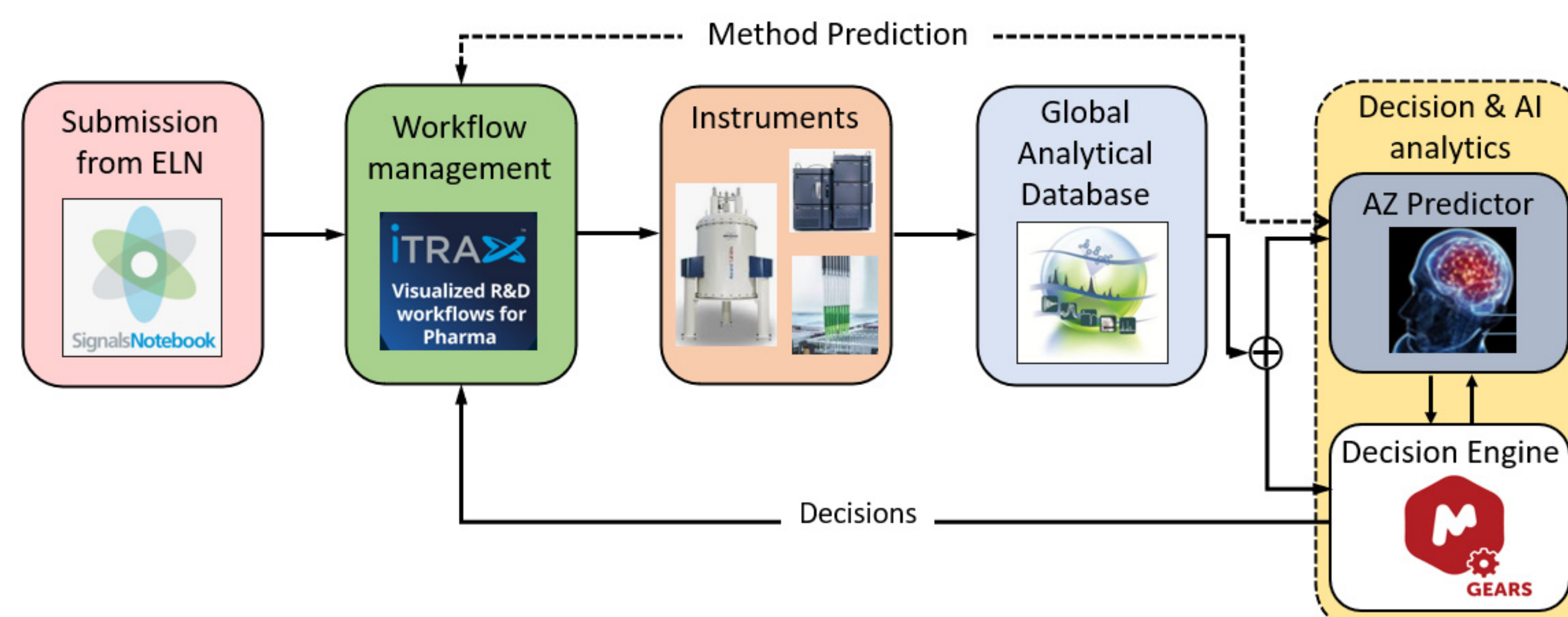
Introduction

A global, team of analytical chemists, IT and data scientists have collaborated across sites to design and deliver a global strategy for automating analytical processes within AstraZeneca. Raw analytical data, acquired on instruments across the globe, is captured in near real-time into a global analytical database (GAD), providing a valuable, central data repository.

Datasets in the GAD can be identified, extracted and processed automatically using software tools which have been successfully integrated into the IT environment. This allows for remote intelligent decision-making and has enabled automated analytical and purification workflows to be developed. These developments lay the foundation for end-to-end automated processes which will allow accelerated cycle times in the discovery process.

Herein we share details of our global vision towards seamless workflows improving efficiency and freeing up our scientists to dedicate more time for scientific pursuits.

Vision for automated purification workflows



Automatic data assessment



Since manually viewing and processing of analytical data is time consuming there is a huge need to automate this process. We have successfully adopted and customized the MGears software to replace multiple manual processes with automated solutions across different analytical workflows. The software is designed to make complex decisions based on the data, removing bottlenecks and enabling streamlined workflows. This includes automated monitoring of instrument performance, enhanced processing and semi-automated analytics to support purification workflows and streamlined reporting.

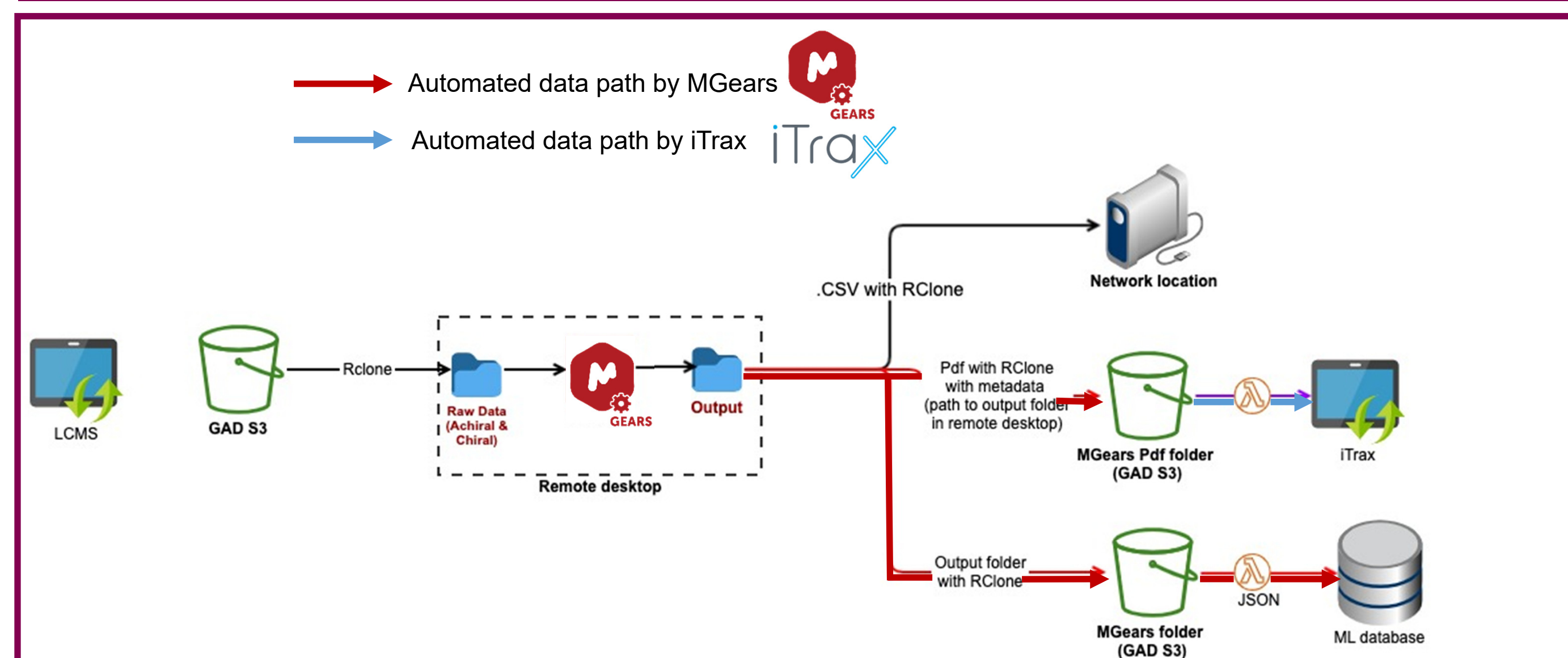
Automatic sample tracking and workflow management



To expedite the project delivery of early discovery compounds, a well-organized global workflow management tool is essential. The sample and workflow management tool, iTrax, facilitates efficient planning of various workflows in a multifaceted team. Advantages of this modern sample tracking software are many; (i) Capability to handle all modalities, (ii) Enables interactive communication between chemists and analysts, (iii) Streamlined workflow management and facilitate automation

In addition, it will also provide a foundation for metrics captured for future planning and improvements.

Developing integrated IT / automation solutions



An important step towards the automatic purification platform was the development of an IT infrastructure that seamlessly integrates both software and hardware components. Here the GAD serves as the foundation, managing the automatic data flow. As instruments collect raw data, they are automatically funneled into GAD. The data can then be consumed by MGears according to our predefined specifications. Output files are then re-integrated into GAD for central storage. Finally, iTrax, our dedicated workflow management tool, can retrieve the processed data from MGears through GAD.

Additionally, the data residing within GAD can also be harnessed for predictive models.

Conclusions and Next Steps

A multi-disciplinary and multi-site team of scientific and IT experts have collaborated successfully to design IT infrastructure to support AstraZeneca's analytical DMT platform. This IT architecture allows analytical raw data to be captured, extracted and automatically processed using optimised software tools. The processed data is captured and can be used to support end-to-end automation of complex analytical and purification workflows.

Furthermore, the platform enables storage of processed data enabling us to interrogate historical information and build future predictive models.

Acknowledgements:

Carolina Sanchez, Katie Proctor, Christoph Bauer, Ali Soltani, Victor Spelling, Marta Passamonti, Nicola Tonge (Mestrelab), Gary Sharman (Mestrelab)

