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

Holly Douglas<sup>1</sup>, Jennifer Kingston<sup>1</sup>, Hanna Leek<sup>2</sup>, Amber Balazs<sup>3</sup>, Nichola Davies<sup>1</sup>, Linda Thunberg<sup>2</sup>, Yamin Htet<sup>3</sup>, Jonathan Furbey-Taylor<sup>4</sup>, Kranthi K. Nandyala<sup>4</sup>, Richard Andersson<sup>4</sup>, Sviatoslav Blokhin<sup>4</sup>, Johan Ulander<sup>5</sup>

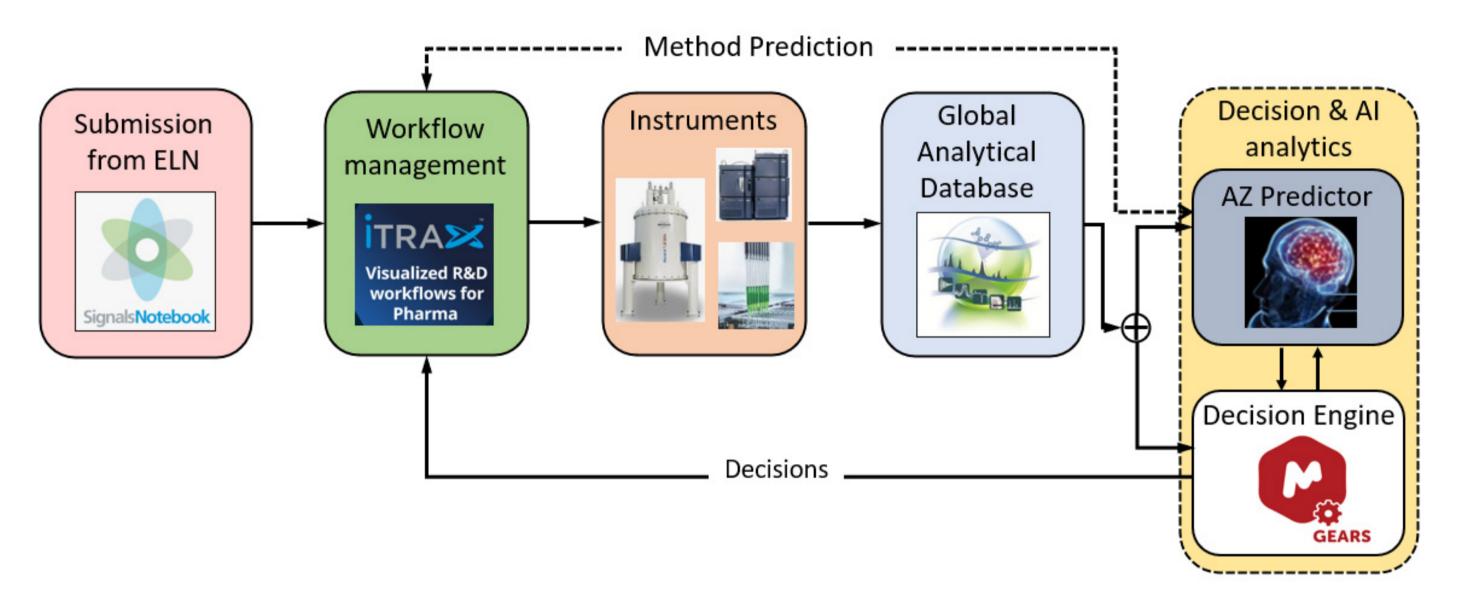
1.Oncology R&D, AstraZeneca, Cambridge, United Kingdom, 2. BioPharmaceuticals R&D, AstraZeneca, Gothenburg, Sweden, 3.Oncology R&D, AstraZeneca, GHP, US, 4.R&D IT, 5. Data Science & Modeling, PharmSci, Gothenburg

### 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.

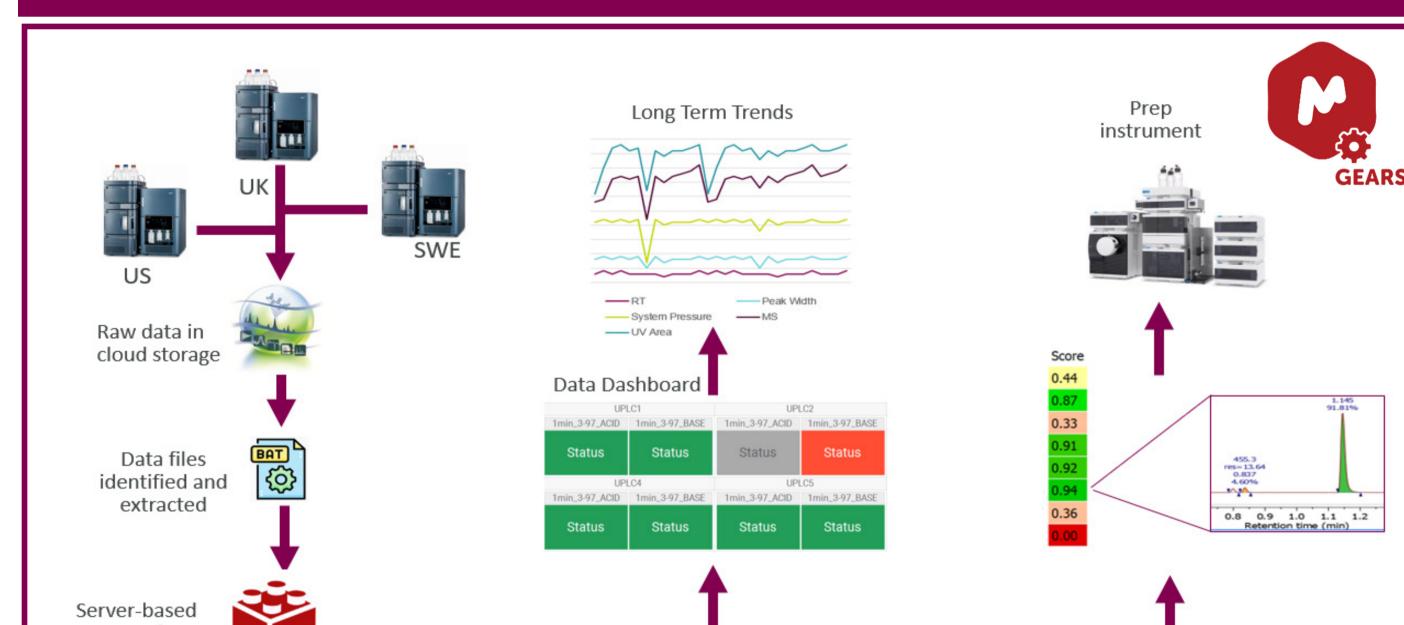
Datasets in the GAD can be identified, extracted and processed automatically using software tools which have been successfully integrated into the IT environment. This allows for remote intelligent decision-making and has enabled automated analytical and purification workflows to be developed. These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

#### Vision for automated purification workflows



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.





# Automatic sample tracking and workflow management

Submitted	Screen	Prep-queue	<b>Prep-active</b>	Dry Down	Reformat	QC	Review
30624: Single Sample PROJECT	30615: Single Sample PROJECT	30608: Single Sample PROJECT	30617: Single Sample PROJECT	30623: Single Sample PROJECT	30376: Single Sample PROJECT	30626: Single Sample PROJECT	30403: Single Sample PROJECT
SAMPLE ID							
R: Requestor							
Amount							
Date							
Final Compound	Final Compound	Intermediate	Intermediate	Final Compound	Intermediate	Final Compound	Final Compound
CA: None	CA: Current Analyst						
3 days	Add Info.	IPA-DEA AD	Add Info.				
30614: Single Sample PROJECT	3 days	a few seconds	IPA-DEA IG	MeOH-NH3 IG	IM MeOH-NH3	MeOH-NH3 IPA-DEA IK	MeOH-NH3 IK
SAMPLE ID	30625: Single Sample PROJECT	30616: Single Sample PROJECT	3 days	3 days	3 days	3 days	a month
R: Requestor	SAMPLE ID	SAMPLE ID	30418: Single Sample PROJECT	30421: Single Sample PROJECT			
Amount	R: Requestor	R: Requestor	SAMPLE ID	SAMPLE ID			
Date	Amount	Amount	R: Requestor	R: Requestor			
Final Compound	Date	Date	Amount	Amount			
CA: None	Final Compound	Intermediate	Date	Date			
3 days	CA: Current Analyst	CA: Current Analyst	Final Compound	Final Compound			
30605: Single Sample PROJECT	Add Info.	MeOH-NH3 IPA-DEA IK	CA:Current Analyst	CA: Current Analyst			
SAMPLE ID	3 days	a few seconds	3 Add Info.	Add Info.			
R: Requestor	30318: Single Sample PROJECT	30415: Single Sample PROJECT	MeOH-NH3 IF IG AD	MeOH-NH3 IPA-DEA IK			
Amount	SAMPLE ID	SAMPLE ID	a month	3 days			
Date	R: Requestor	R: Requestor					
Final Compound	Amount	Amount					
CA: None	Analysed Before	Date					
3 days	Date	Final Compound					
	Final Compound	CA: Current Analyst					
	CA: Current Analyst	2 months					
	Bespoke Method Required No						
	Add Info.	30331: Single Sample PROJECT					
	Cancelled	SAMPLE ID				$  ( \bigcirc )$	
		R: Requestor					

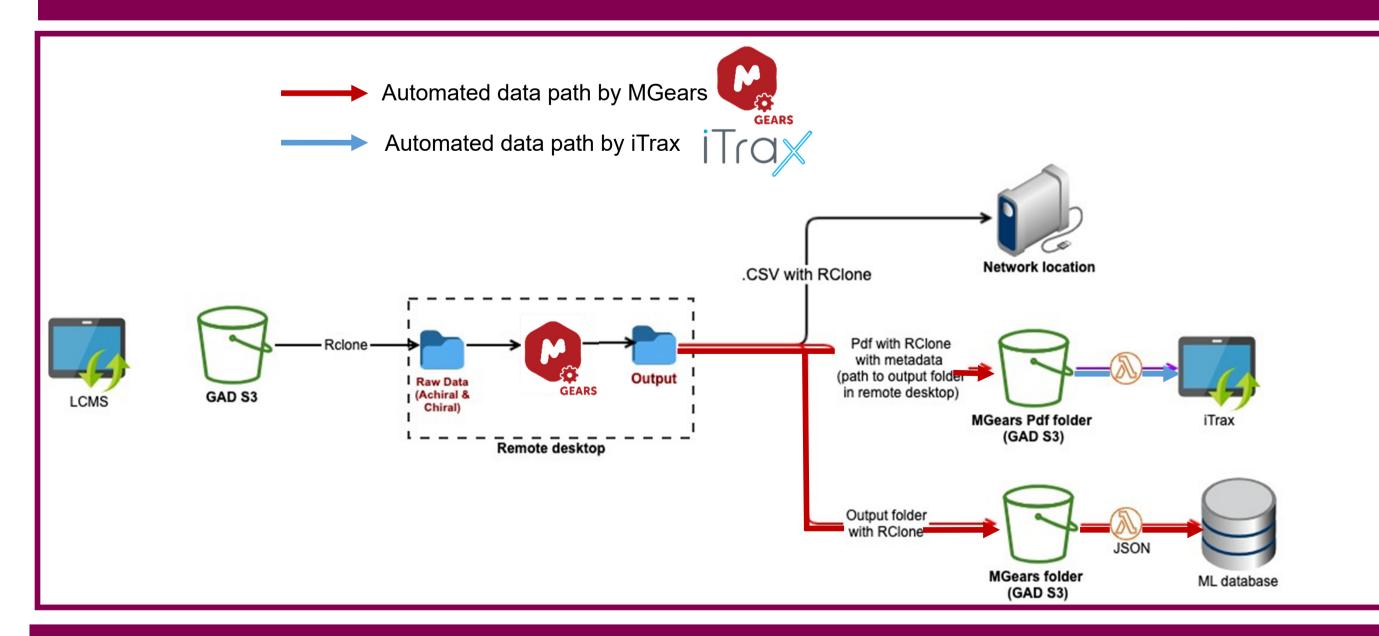


Since manually viewing and processing of analytical data is time consuming there is a huge need to automate this process.

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. To expedite the project delivery of early discovery compounds, a wellorganized 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.

### **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.

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

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