Developing Modular Galaxy Workflows for High-Resolution Mass Spectrometry Exposomics Data Processing

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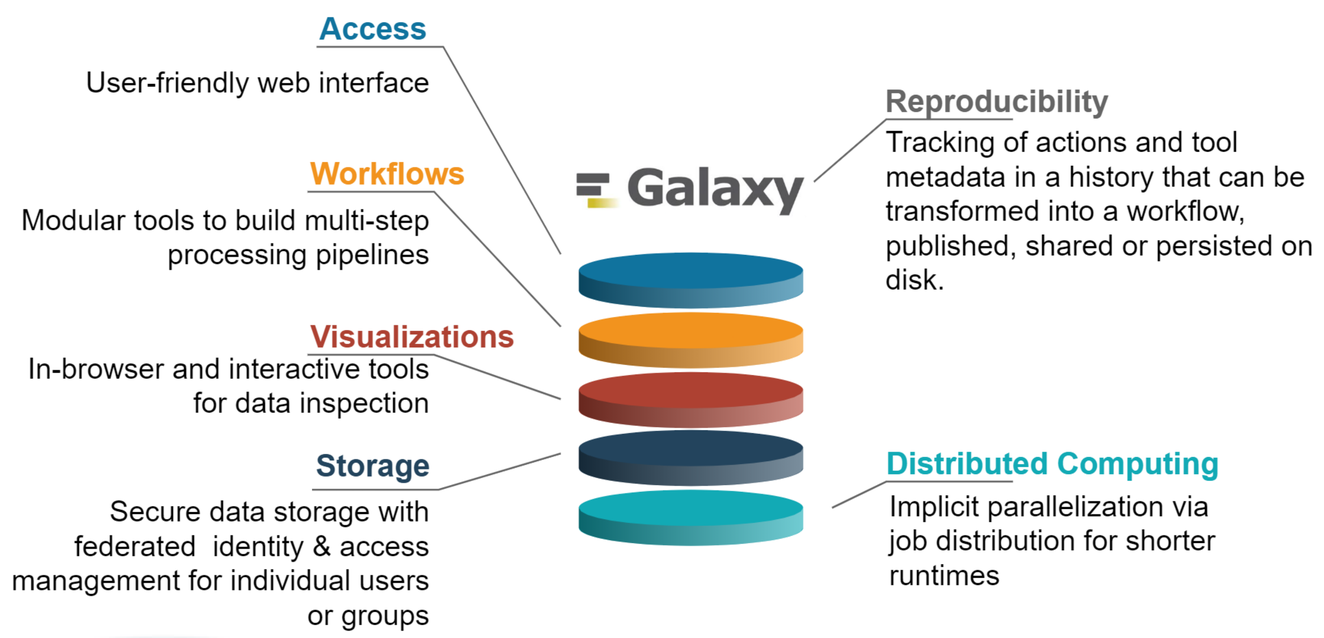
Introduction

Galaxy is an **open-source web based** platform making fully reproducible bioinformatic analysis simpler for scientists [1, 2]. Current **Galaxy tools** to process mass spectrometry of small molecules data are limited [3, 4]. An **Exposome toolbox** for Galaxy is being developed to ease **analysis of high-resolution mass spectrometry (HRMS)** datasets, tailored towards measures of environmentally-derived chemicals.



Methods

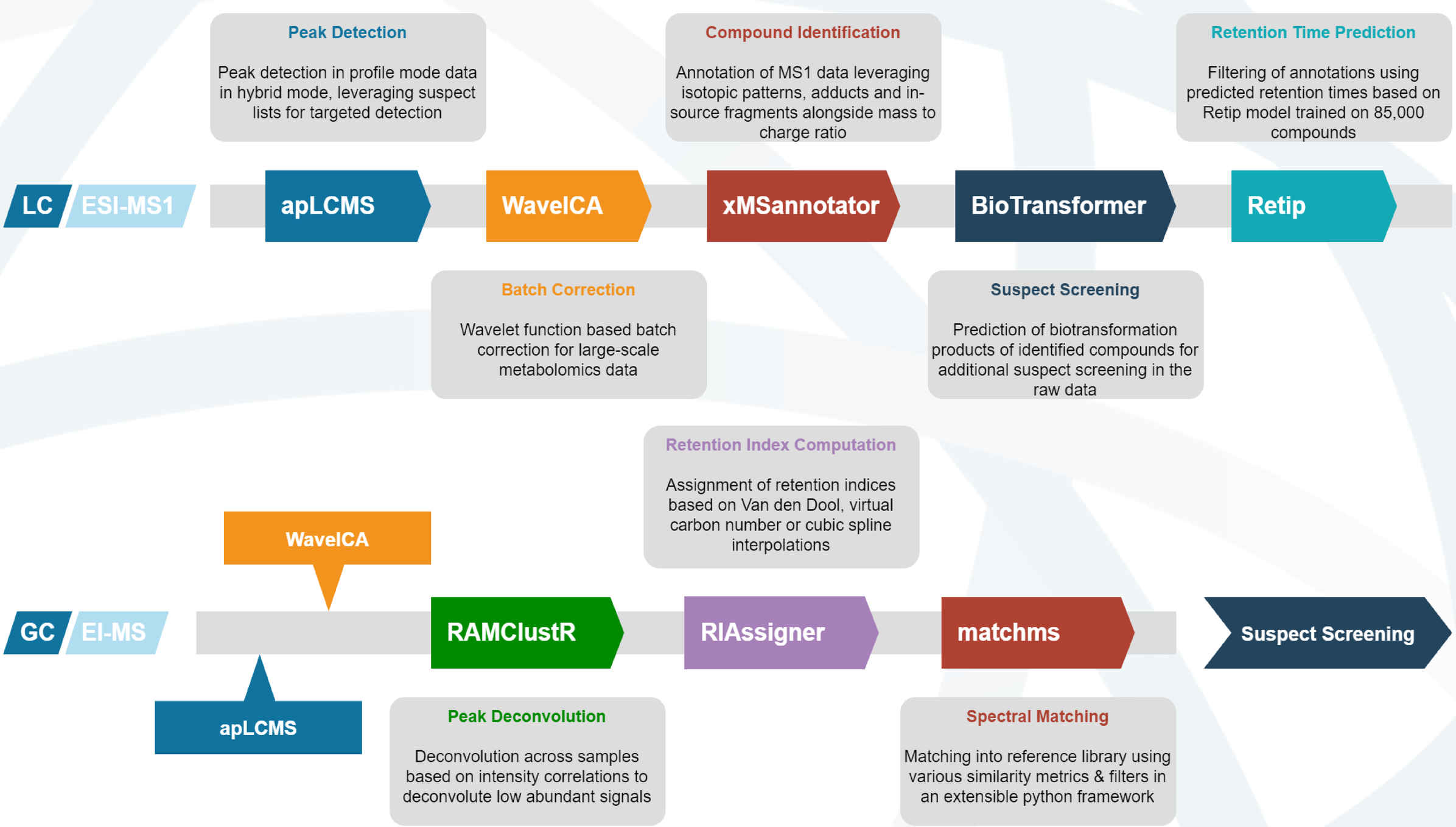
Pipelines were implemented as **modular workflows in Galaxy**. Tools were made available as **Docker containers** or **conda packages** following Galaxy standards and ensuring reproducibility [5]. **Code quality** and maintainability was **improved** with packages partially re-written, **versioned** and **committed to repositories** [6]. Reporting follows the mzTab-M standard [7].

Results

We expanded the available Galaxy resources by several tools and **two novel workflows** for HRMS data analysis. All modifications were carried out following **open-source** and **FAIR data principle**s, in consensus with the original authors. Packages are available on **https://github.com/RECETOX/galaxytools** and tools hosted at **https://umsa.cerit-sc.cz/**.

Future Work

The selected tools form the foundation for future additions and are **complementary to existing Galaxy resources** (e.g Galaxy Europe and Workflow4Metabolomics [8]).
We welcome **contributions** and **collaboration** for ongoing and future developments.



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