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NATIONAL LABORATORY

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Metabolite Profiling for Synthetic Biology using Ion Mobility-Mass Spectrometry and Data-Independent Acquisition with Improved Targeted Data Extraction Software

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Skyline User Group Meeting Online

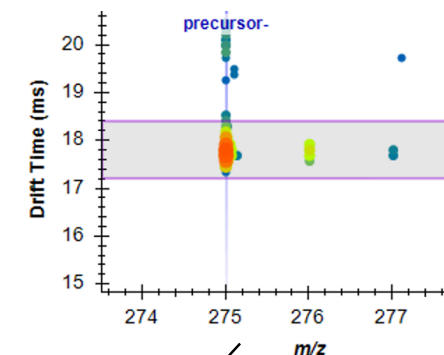
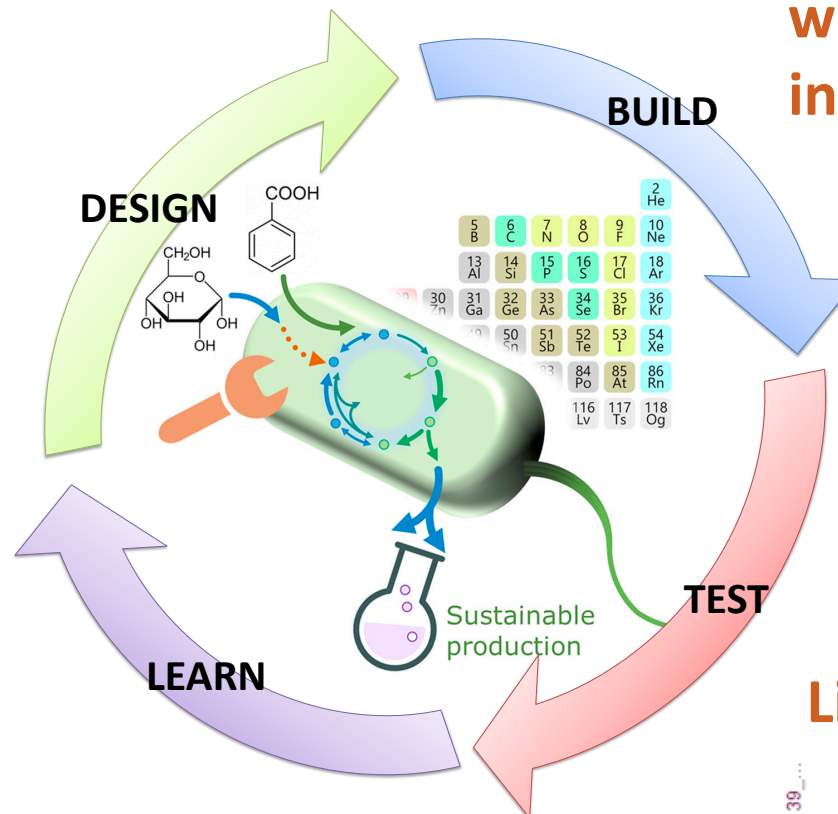
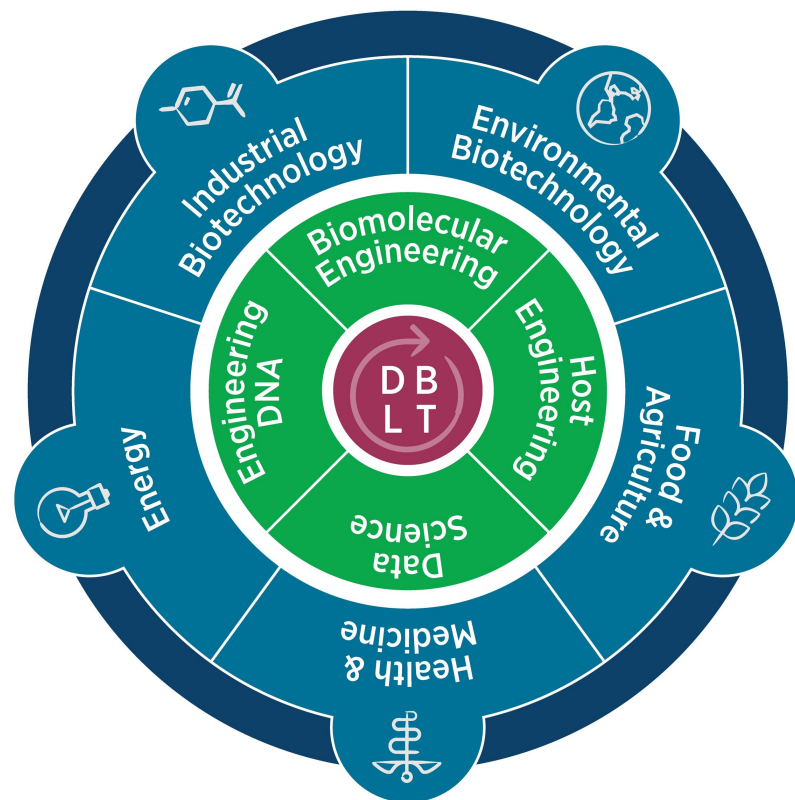
May 27, 2020

Design, Build, Test, Learn (DBTL) workflow for biomanufacturing research with cutting edge TEST

Ion mobility and MS/MS with All-Ions data-independent acquisition

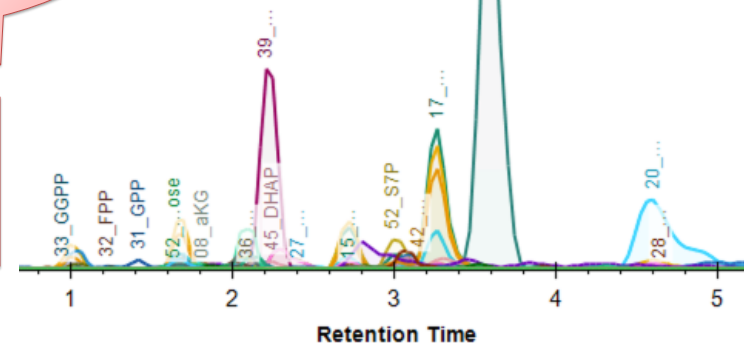
Engineering Biology

A Research Roadmap for the Next-Generation Bioeconomy

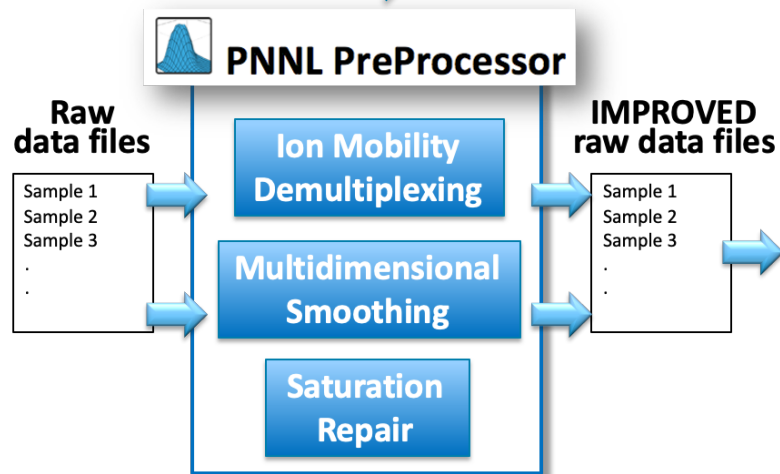
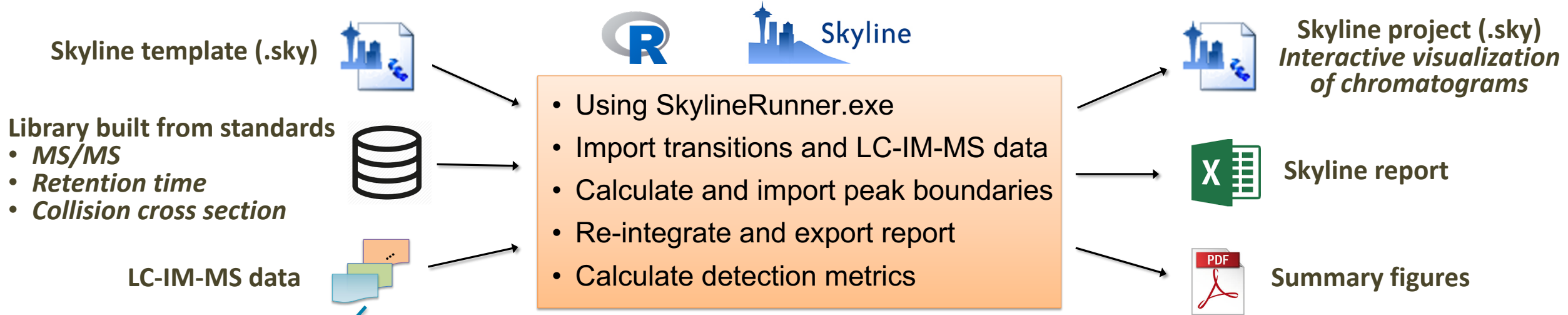


Liquid chromatography

Fast and reproducible analytical-computational workflow

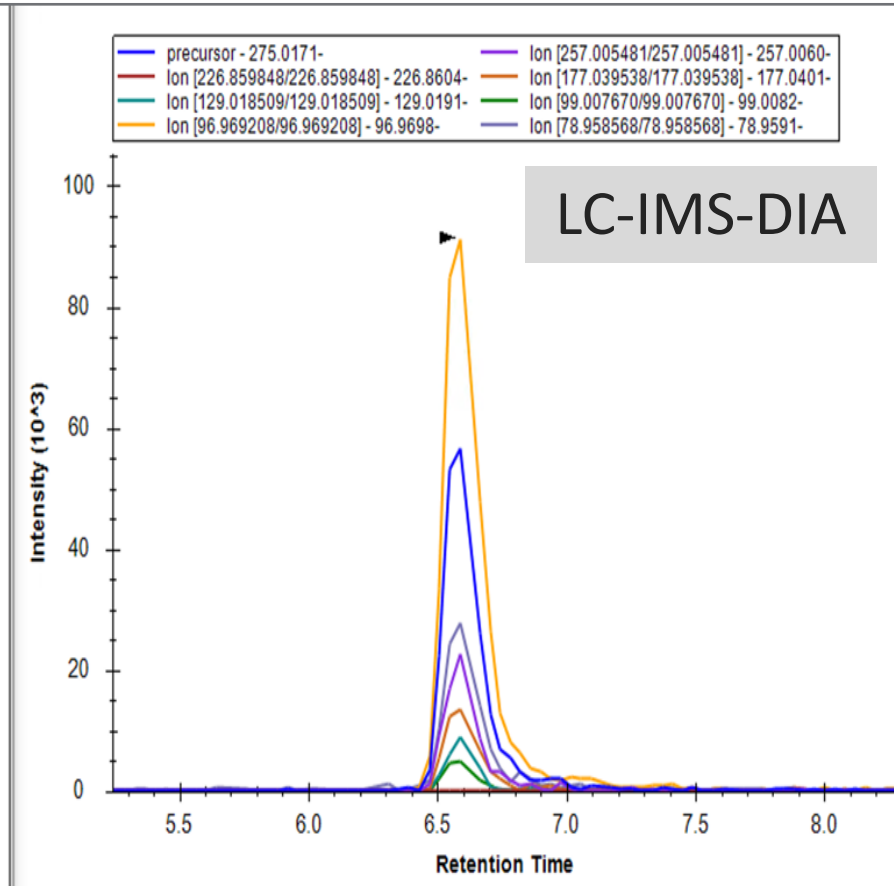
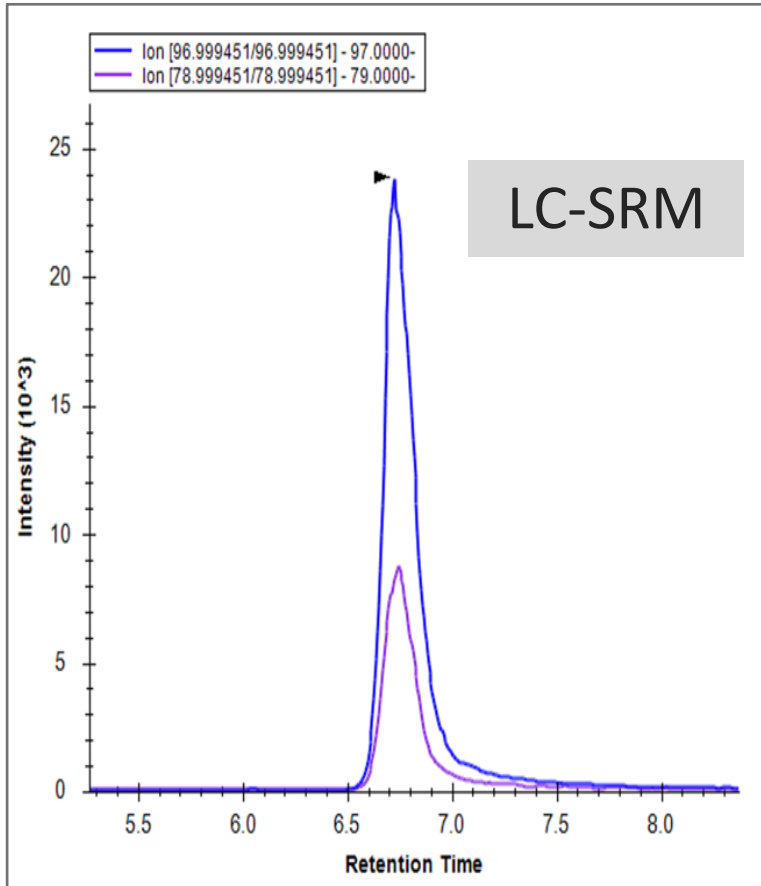


Automated and improved data analysis workflow

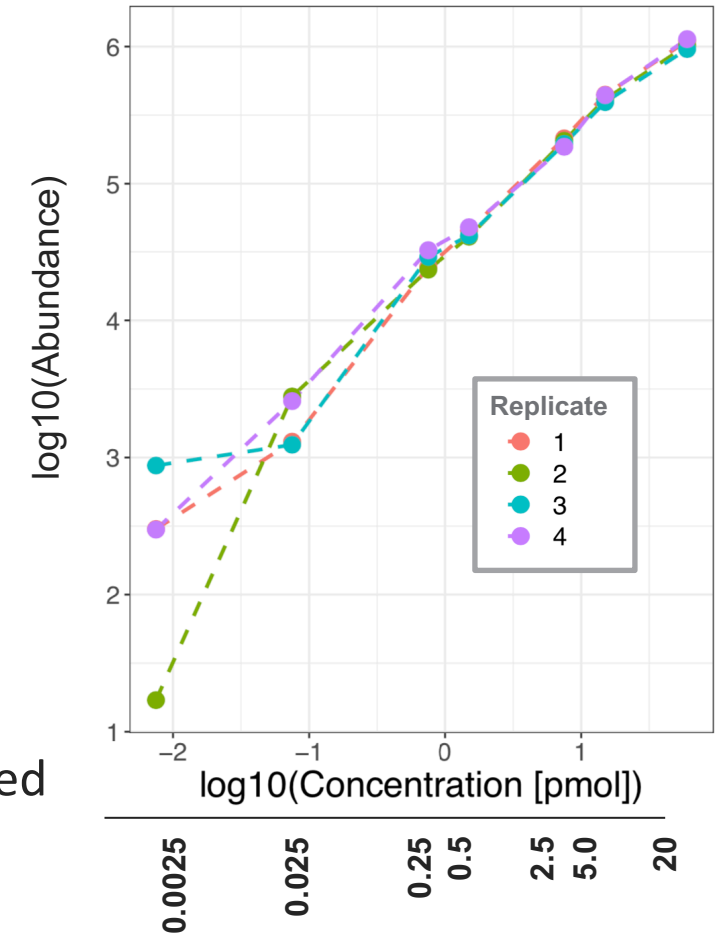
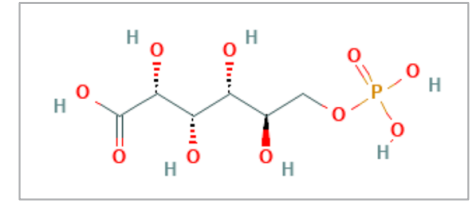


- Enhanced raw data quality for better results
- Faster downstream processing
- Developed in collaboration with Agilent Technologies (John Fjeldsted)
- Free download: <https://omics.pnl.gov/software/pnnl-preprocessor>

Better selectivity and sensitivity with IMS-DIA



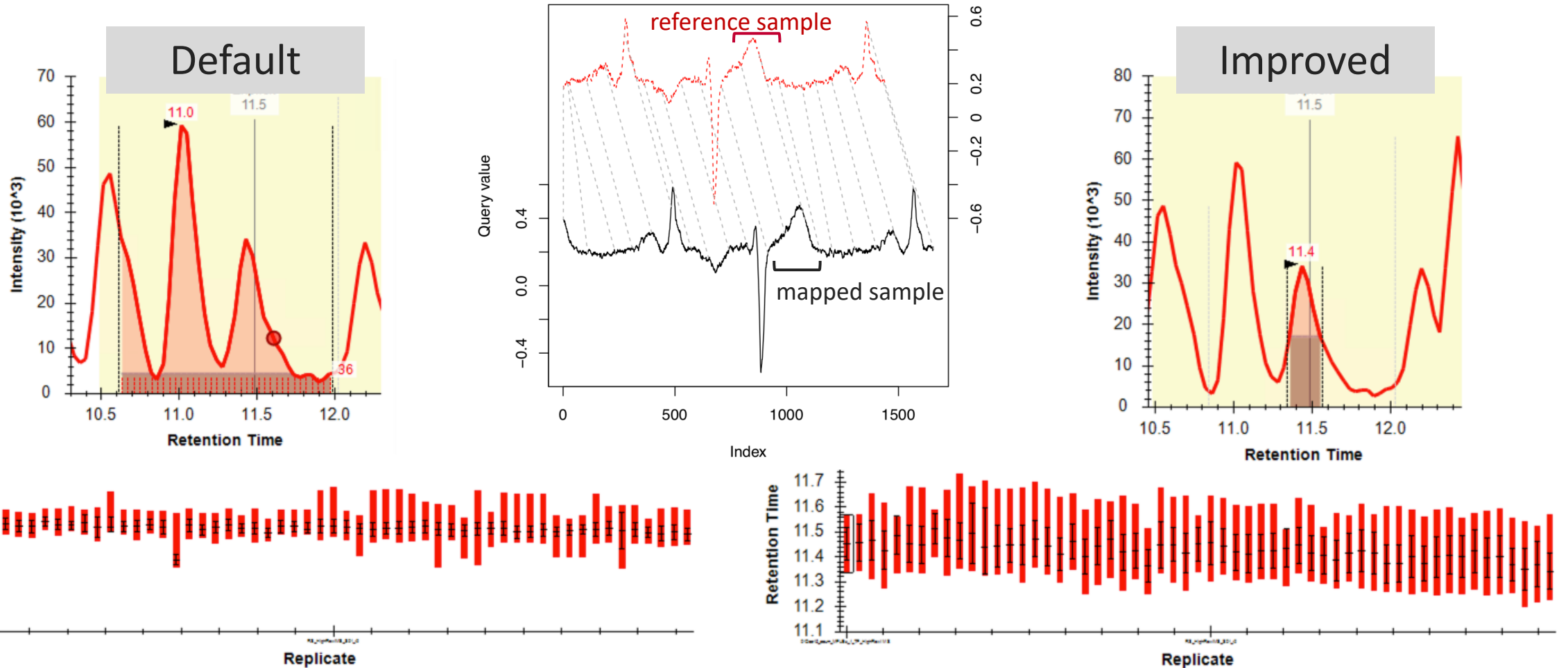
6-Phosphogluconic acid



- For 60% of standards IMS-DIA provided more transitions defined and refined post-acquisition for increased detection confidence
- Good linearity was observed across 4 orders of magnitude (9 out of 12 standards evaluated)
- LC-IMS-MS analyses of real samples in progress

Improved integration boundaries with dynamic chromatogram warping

- Select best peak as reference (from exported chromatograms)
- Define constrained integration boundaries (e.g. FWHM)
- Apply dynamic warping comparing reference peak to the other samples to map integration boundaries



Conclusions

- The advantages of IMS-DIA over SRM are applicable for metabolite profiling
- Having Skyline as the same software suite for analyzing data from the two analytical platforms greatly facilitates comparison
- Both automation and user-friendly visualization are paramount in development of analytical methods and new algorithms for robust and scalable workflows
- More ion mobility metrics could be added to use the separation beyond a signal filter

Acknowledgments



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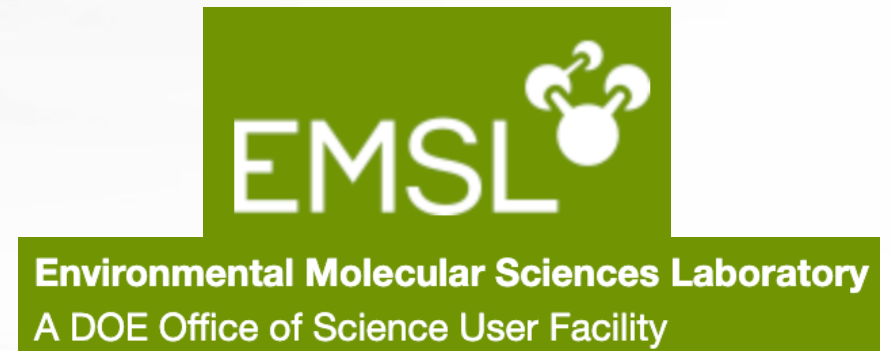


MP 256
INFORMATICS: METABOLOMICS



Agilent Technologies

Alex Apffel



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Thank you very much for your attention!...*