Standing on The Shoulders of Giants: Metabolomics Made Easy for Non-Experts By Adopting Community Best Practices with Intelligent Automation

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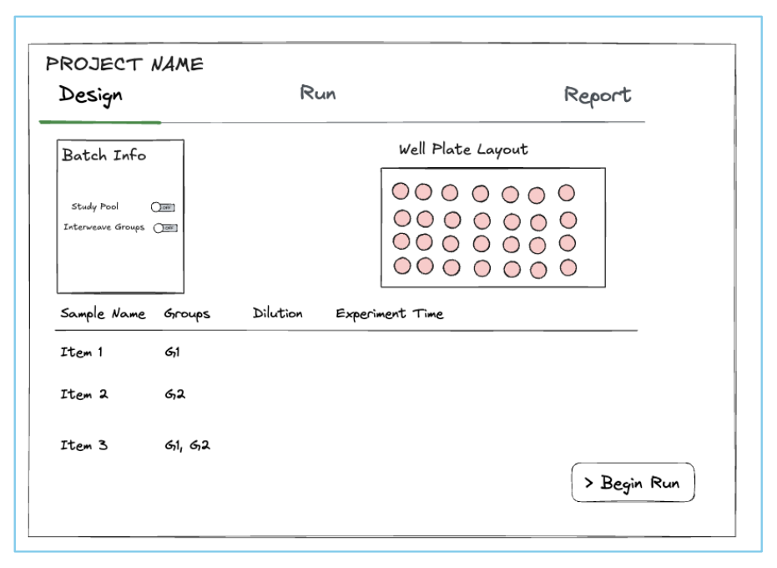
Introduction

Democratizing access to quantitative metabolite measurements is key to expanding metabolomics into new fields and gaining new users. Currently, most non-experts access metabolomics through service models due to steep learning curves across sample prep, method development, data collection, and analysis. This poster presents an end-to-end workflow using CE-MS, consumables, and intuitive software—all aligned with community best practices—to make hands-on metabolomics accessible to non-experts.

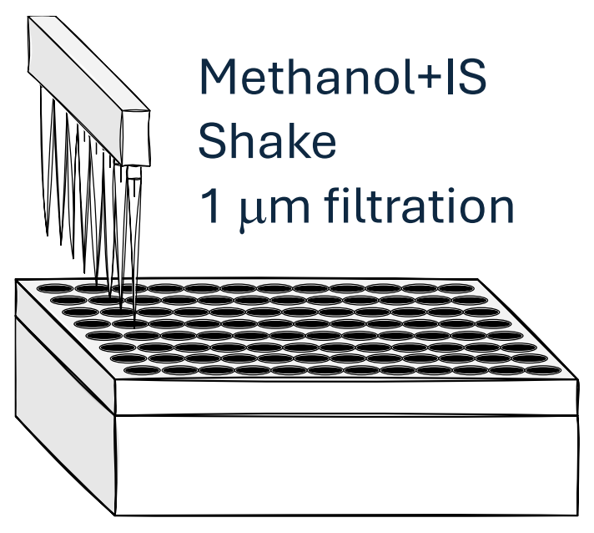
The pillars of an accessible metabolomics workflow are outlined below. The workflow is being sold as MoveKit^{TM} CE.

Design ⟶ Prep ⟶ Run ⟶ Report



5 mins

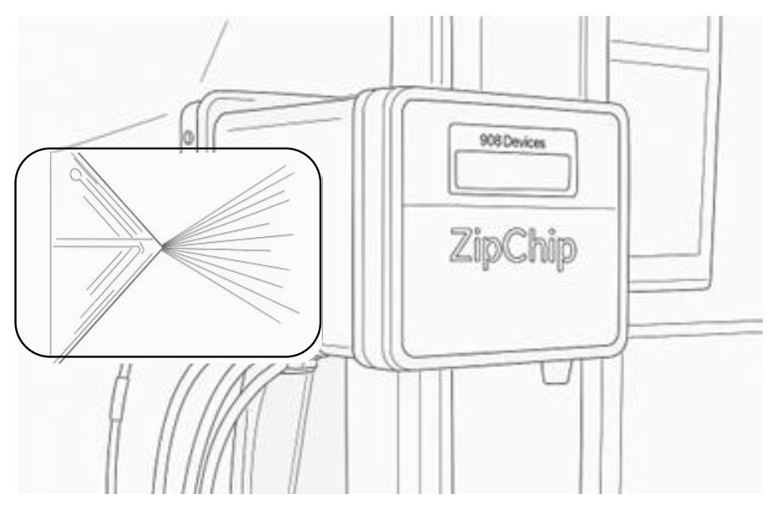
Intuitive UI / Design
Assign Key Parameters
Export



Methanol+IS
Shake
1 µm filtration

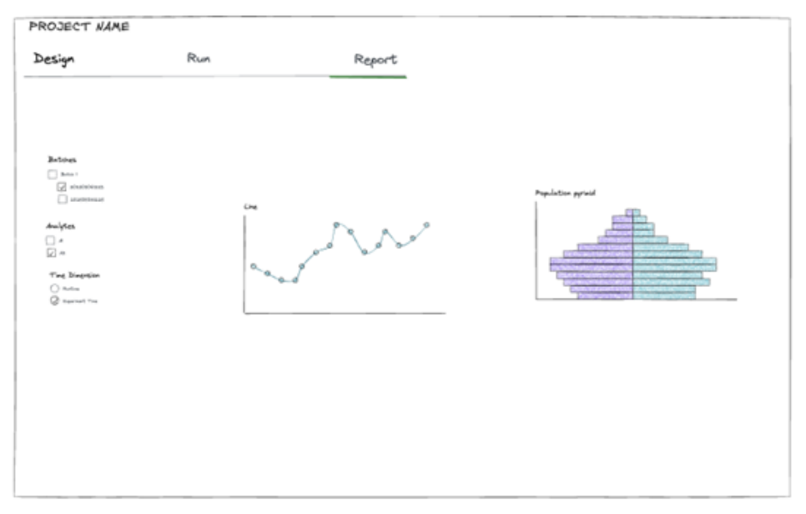
30 mins/plate

No derivatization
Manual or automated
Everything included



12 mins/sample

Push-button
Microchip CE-MS
Low matrix effects
High sensitivity



10 mins/plate

Go/No Go SST
Automated Data Check
Quantitative Output

These pillars can be expanded to other LC-MS based workflows.

Consumables for Rapid Method Deployment

Reduce Decision and Training Fatigue.

Automate the Pain Points.

Unlock Data Exploration.

What's Included:
Extraction and collection 96-well plates
Extraction and Focusing Reagent
Internal standards (36 SIL)
SST, Blank, Calibration, and QCs
Software

Protocol
20 µL sample (10:1 diluted for media)
180 uL of extraction+focusing reagent
Shake (15 min)
Filter (spin or vacuum manifold)

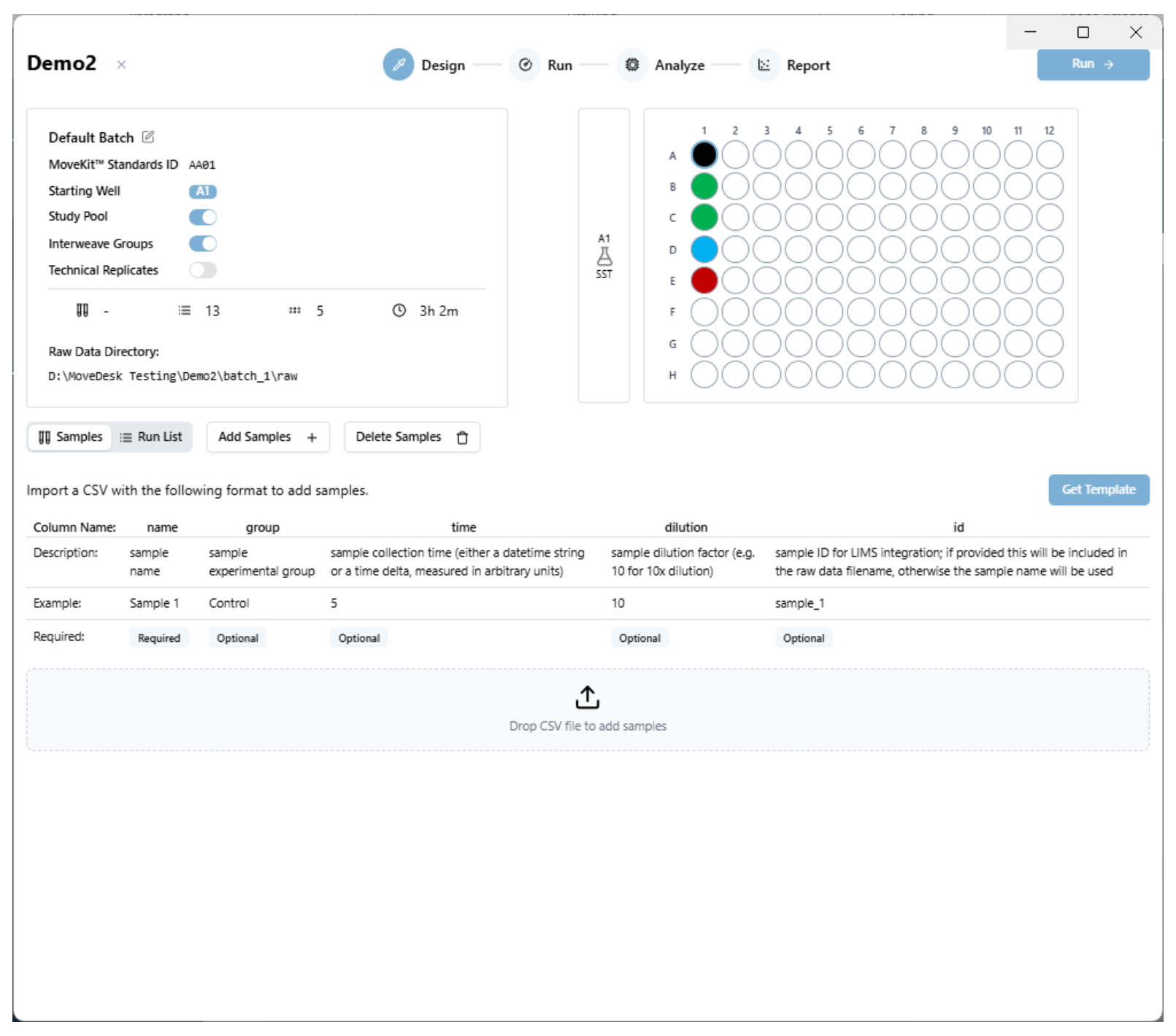
Coverage:
Library of 300+ polar metabolites
14 metabolite classes; no derivatization
Flexibility to add your own compounds to the method!

Materials and Methods

Metabolites were extracted from 20 µL sample using the MoveKit™ CE kit (Move Analytical), which includes reagents, plates, stable-isotope internal standards (Cambridge Isotope Labs), calibration standards, and QCs. The protocol (protein precipitation + filtration) enables 96-well processing in under an hour. Samples were analyzed using Peptides BGE and HR chip on the ZipChip CE system (Repligen) coupled to an Exploris 240 MS (ThermoFisher). The MoveDesk software guided users through experimental setup, QC, and data visualization. Skyline enabled transparent data analysis and quantification. The MoveDesk^{TM} software package was written using Electron, React, Python, and FastAPI.

Software Workflow and Automation

An intuitive UI allows users to make critical experimental design decisions quickly, review the acquisition queue and plate layout, and produce instrument-ready analysis sequences for the batch (below).



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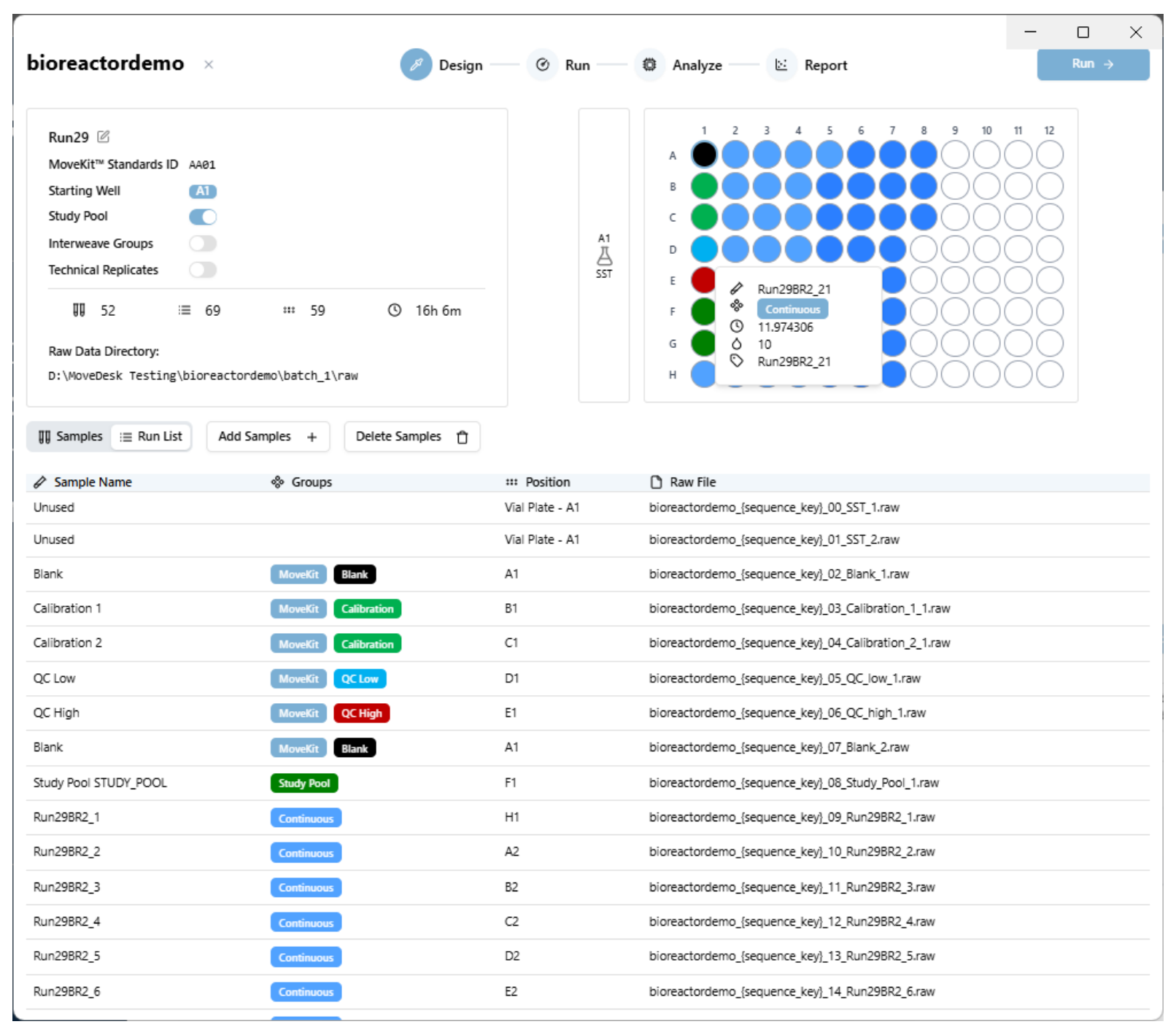
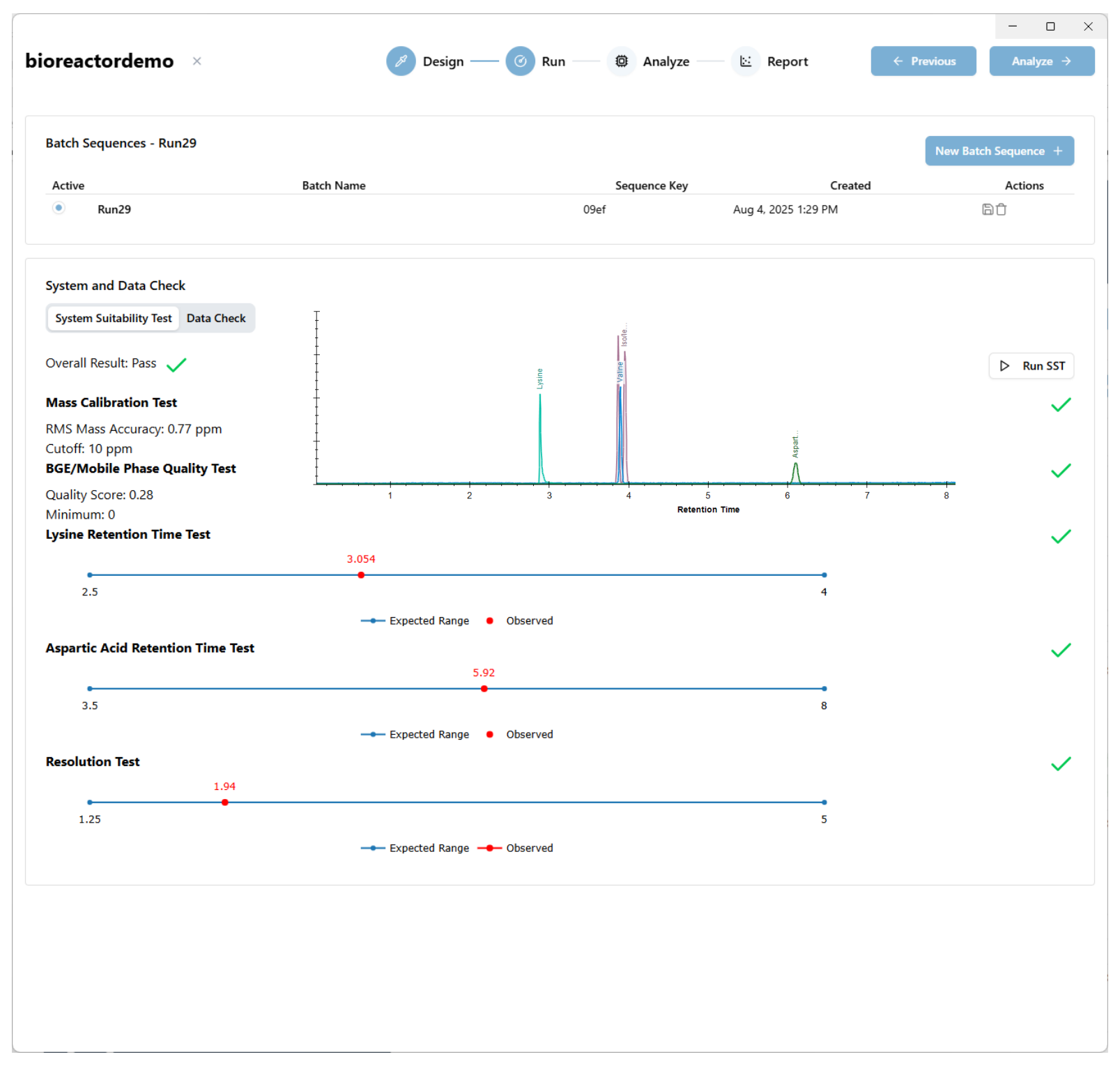


System Suitability Test (SST) results are produced automatically. During the data collection, the Data Check feature produces real-time feedback on data quality including intensity, migration index, and separation resolution.



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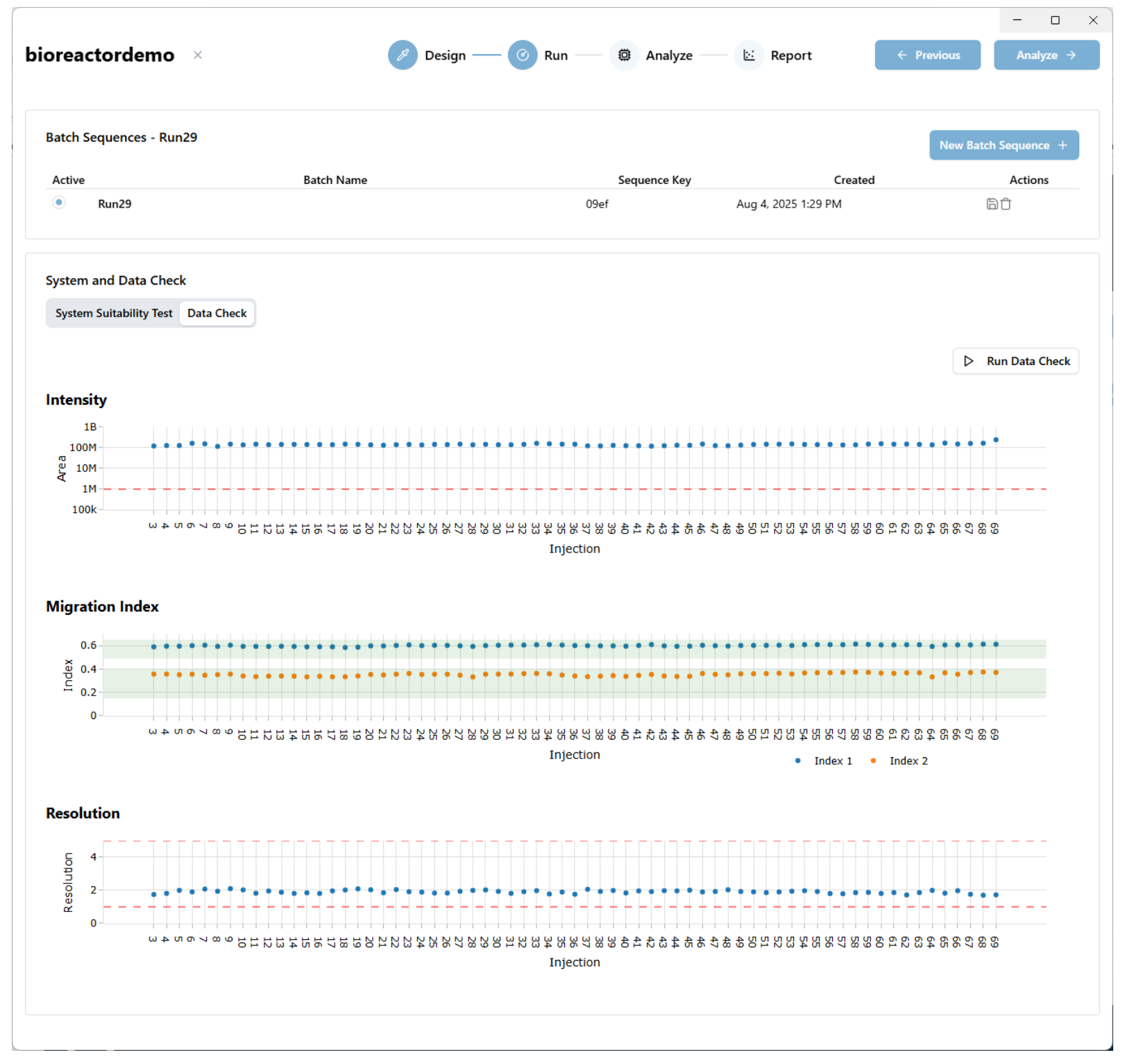
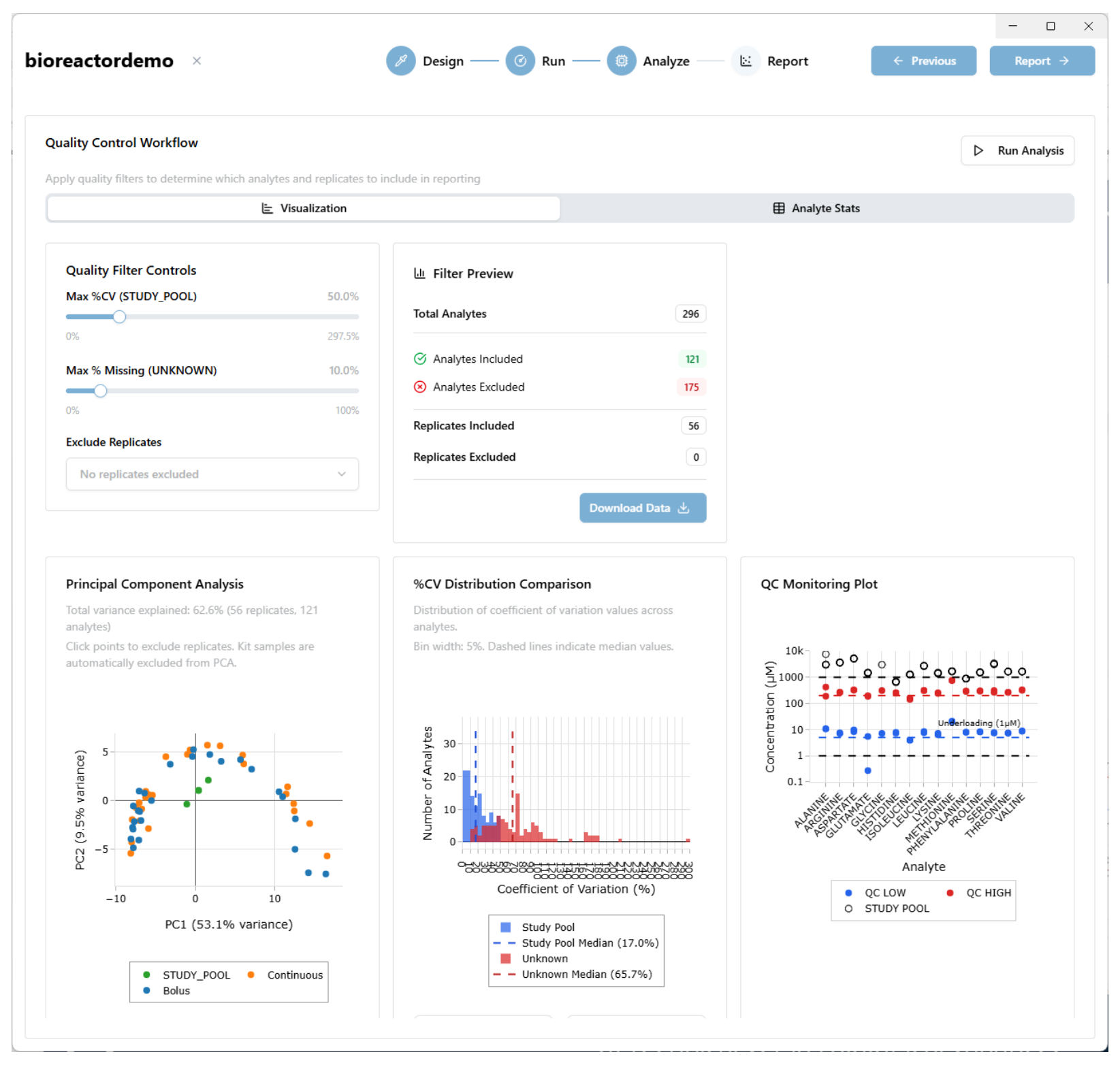


The Analysis uses a Skyline template with automated peak assignment correction. Following quantification, filtering on precision of Study Pool Quality Controls (SPQC), % missing data, and PCA for outlier detection allows only the highest quality measurements to be passed along for statistical comparison or visualization during Reporting.



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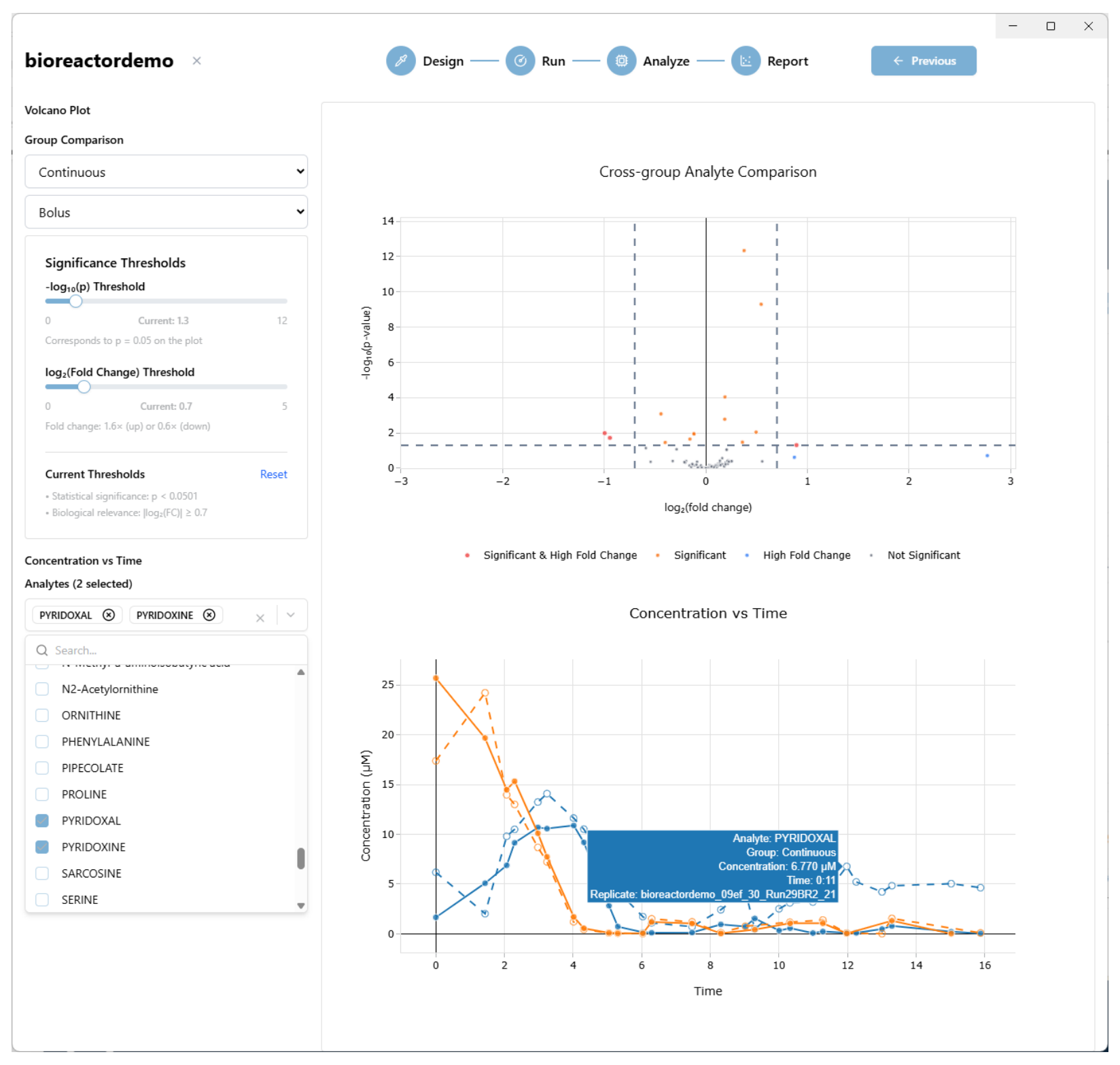

Acknowledgements and Conflicts

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