Reducing Human Variability in Quantitative Metabolomics through Automated, Reproducible Workflows

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Poster 13.07

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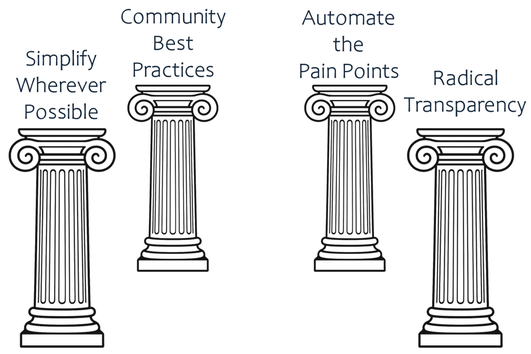
Introduction

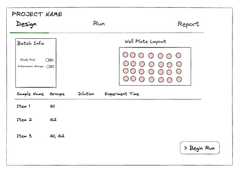
Motivation. Quantitative metabolomics is often constrained by manual steps and subjective decisions. Differences in sample handling, setup, and data analysis or interpretation can lead to inconsistent results and reduce precision in downstream analyses. The integration of metabolomics in ML models holds great promise for advancing process development, precision medicine, and other fields, but variability in data quality could limit the reliability of the models and of the predictions made using them.



Technical pillars for making metabolomics easy.

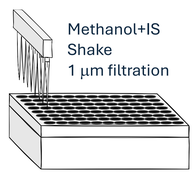
Approach. We describe a metabolomics methodology using capillary-electrophoresis mass spectrometry that combines robust analytical frameworks—such as internal standards, calibration materials, and validated mass spectrometry methods—with software automation to minimize human bias across sample preparation, experimental design, and quantitative processing. The goal is to produce metabolomics workflows which are deployable by non-experts but yield expert-level data quality. The approach we use is generalizable to LC-MS workflows as well.

Design → Prep → Run → Report



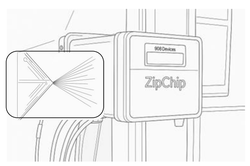
5 mins

Intuitive UI / Design
Assign Key Parameters
Export



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

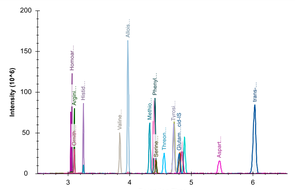
Go/No Go SST
Automated Data Check
Quantitative Output

MoveKit™ CE Consumables

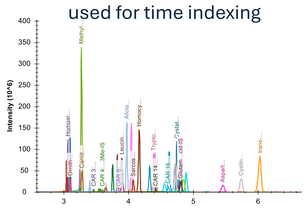
What's Included:
Extraction filter and collection 96-well plates
Extraction and Focusing Reagent
Internal standards (50 SIL, custom from CIL)
SST, Blank, Calibration, and QC Samples

Protocol
20 uL 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



17 internal standards used for time indexing



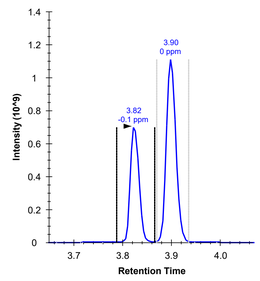
Full complement of internal standards used in the MoveKit CE method

Materials and Methods

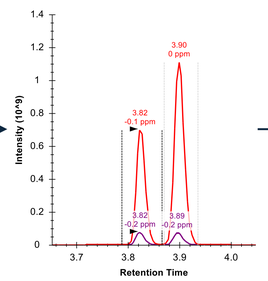
Metabolites were extracted from 20 µL sample using the MoveKit™ CE kit (Move Analytical), which includes reagents, plates, stable-isotope internal standards (Cambridge Isotope Labs), calibration standards, and QCs. Cell culture media is diluted 10x in PBS prior to sample preparation. The protocol (protein 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 MoveApp software guided users through experimental setup, QC, and data visualization. The MoveApp™ software package was written using Electron, React, Python, and FastAPI.

Technical Pillars for Fundamental Improvements

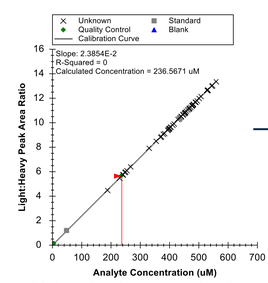
Simplify Wherever Possible. Small-molecule MS quantification doesn't need reinvention: we use stable-isotope labeled internal standards and value-assigned reference materials based on biological matrices. AI and automation target real pain points—data quality, correct peak assignment, integration boundaries, and automated QC.



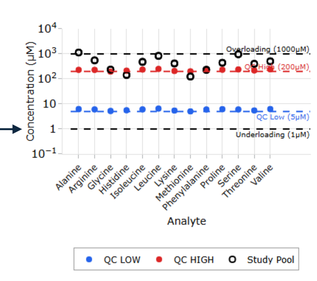
Peak (re)assignment



Ratio to SIL Internal Standard

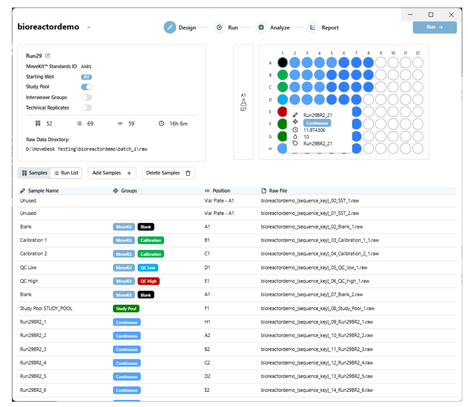


Value Assignment Against Reference Material



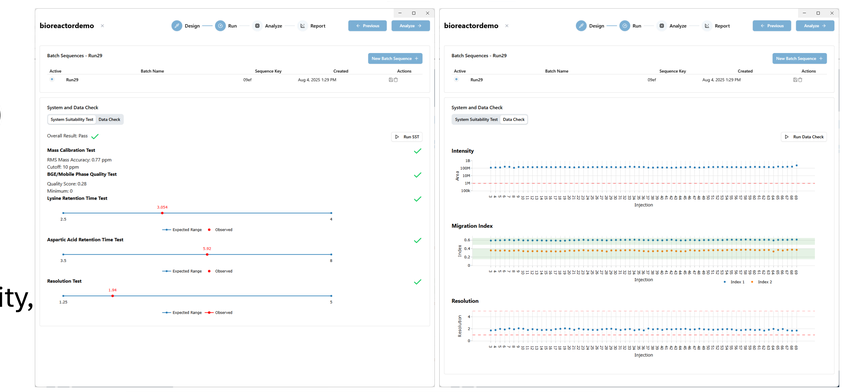
Validation at Batch Level

Radical Transparency. We save a Skyline document for transparent quantification and to allow manual tuning if desired, but as a user you are not required to use Skyline. The process shown above is completed automatically, under the hood.

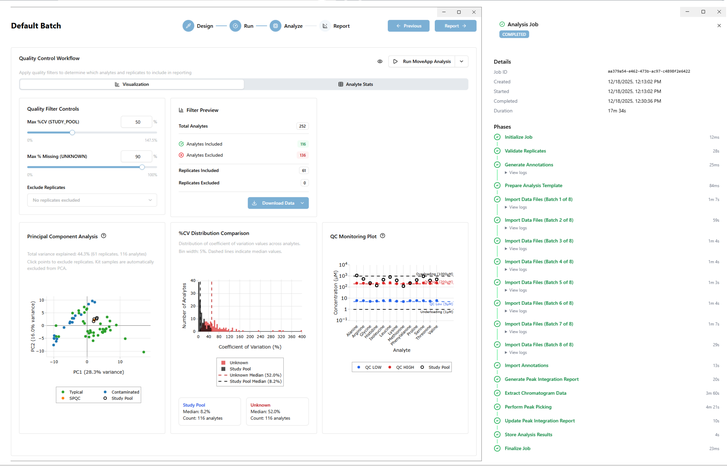


Adopt Community Best Practices for Quality Control
Users import a sample list and define key study design elements (study pool, replicates, start position, randomization). Setup takes ~30 seconds.

Automate the Pain Points – SST and Data Check
System Suitability Tests (SST) are generated automatically with GO/NO-GO criteria per metric. During acquisition, Data Check provides real-time feedback on intensity, migration index, and critical pair resolution.



Automate the Pain Points – Eliminate Subjectivity
A novel peak-assignment model incorporates elution order, peak height, predicted RT, mass accuracy, and replicate consistency. Hands-on time is reduced >90% (17.5 min vs. 4 hr manual), reproducing expert curation with unparalleled accuracy. PCA, variance metrics, and QC plots are generated automatically.



Acknowledgements and Conflicts

All authors are cofounders and own interest in Move Analytical. We gratefully acknowledge our continued collaborations with Cambridge Isotope Laboratories, Repligen corporation, Thermofisher Scientific, UNC MAP Core, and Astrazeneca.

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