



Virtual Conference | October 18 - 21

Welcome to MANA 2021

Workshop: A Brief Introduction to Skyline for Small Molecules

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More information (www.skyline.ms)

🗽 Tutorials: /home/software/Skyli 🗙

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https://skyline.ms/wiki/home/software/Skyline/page.view?name=tutorials

Small Molecules











Life Cycle for Metabolomics Studies involving Skyline

A few keys to success:

- Remember that Skyline is a *hypothesis- driven tool*
- It has method export functionality for Agilent, Sciex, Shimadzu, Thermo, and Waters
- Semi-automated method optimization
- Data analysis includes targeted MS/MS, high resolution, and GC-MS
- Quantification can be relative or absolute





The Steps in a Targeted Metabolomics Study

Consultation & Study Design (email and in person)

Platform Selection or Platform Development (if necessary)

Sample Preparation and Data Collection



Data Reporting and Follow-Up Meeting

Publication of Results

Platform Development Cycle (weeks to months)

Define Figures of Merit

Analytical Literature Review

Characterization of Standards by LCMS

Method Dev: Extraction, Calibration, Mini-Validation & Data Analysis





Key Features of Skyline for Small Molecules







Ion Mobility Separations









Automated Method Optimization





Ionization Adducts



Spectral Library Support



Automated Data Import/QC



Making Assays and Results Accessible



Researcher uploads Skyline documents to a folder in their project on PanoramaWeb

Researcher adds experiment annotations (abstract, organism, instrument etc.) to the folder

Researcher creates a **permanent link** to the data on PanoramaWeb

Researcher submits the annotated folder for publication to Panorama Public

PanoramaWeb administrators make a copy of the folder to Panorama Public

Panorama Public Datasets 🗸

Duke - p400HR Ring Trial System Suitability Duke - p400HR Ring Trial System Suitability

Experiment Details

International Ring Trial of a Broad-Spectrum Targeted Metabolomics and Lipidomics Platform for Serum and Plasma Analysis [System Suitability Files]

Link: https://panoramaweb.org/p400HR_SST_RingTrial.url Share

Thompson JW, Adams KJ, Adamski J, Asad Y, Borts D, Bowden JA, Byram G, Dang VD, Dunn WB, Fernandez FM, Fiehn O, Gaul DA, Huhmer A, Kalli A, Koal T, K Mandal R, Meier F, Naser FJ, O'Neil D, Pal A, Patti GJ, Pham-Tuan H, Prehn C, Raynaud FI, Shen T, Southam AD, St. John-Williams L, Sulek K, Vasilopoulou CG, V Winder CL, Wishart DS, Zhang L, Zheng J, Moseley MA. International Ring Trial of a High Resolution Targeted Metabolomics and Lipidomics Platform for Seru Plasma Analysis. Anal Chem [Internet]. 2019 Oct 22; Available from: https://doi.org/10.1021/acs.analchem.9b02908 [Publication]

Organism: Homo sapiens Instrument: Q Exactive HF,Q Exactive Plus,Q Exactive Spikeln: Yes Keywords: p400HR, targeted, metabolomics, Q Exactive, Biocrates Lab head: Will Thompson

Abstract

A significant challenge facing the vision of metabolomics in precision medicine, and the analysis of large human cohorts, is the cross laboratory and longitudinal comparability of quantitative measurements and laboratory protocols used. In this study, 14 laboratories world-wide analyzed various blood specimens using a common experimental protocol provided with Biocrates AbsoluteIDQ p400HR quantify up to 408 metabolites. The specimens included human plasma and serum from male and female d... [Show more]

https://doi.org/10.1021/acs.analchem.9b02908 Thompson JW et al, Anal Chem 2019

Vagisha Sharma

Q Sign In

Resources for Small Molecule Support in Skyline

- Support and feature requests: <u>https://skyline.ms/project/home/support/begin.view</u>
- Brendan MacLean <u>brendanx@proteinms.net</u>
- Small Molecule Development (MRM, PRM, High Res, Spectral Libraries): Brian Pratt <u>bspratt@proteinms.net</u>
- Calibration: Nick Shulman <u>nicksh@proteinms.net</u>
- If you're desperate: Will Thompson <u>wthompson@908devices.com</u>

Where in the world do I go from here?

| Skyline-daily | | | ↔ | - 0 | X |
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Let's dive in and answer that question together!