Supporting Information S1:

Title: A Case Study and Methodology for OpenSWATH Parameter Optimization Using the ProCan90 Data Set and 45,810 Computational Analysis Runs

Authors: [1]Sean Peters, [1][2]Peter G Hains, [1]Natasha Lucas, [1]Phillip J Robinson, [1]Brett Tully
[1] ProCan, Children's Medical Research Institute, Faculty of Medicine and Health, University of Sydney, Westmead, NSW 2145, Australia
[2] Cell Signalling Unit, Children's Medical Research Institute, The University of Sydney, Westmead, NSW 2145, Australia

Email: btully@cmri.org.a

Notebooks.zip

- analysis_report.html
  The primary analysis python notebook supporting this work

- analysis_report_with_d_scores.html
  A replication of the analysis_report.ipynb notebook, but with all m_score metrics, plots and rank weighting replaced with d_scores. NOTE: FDR filtering still uses m_scores

- data-description.html
  A short notebook which is used to provide an overview of the result files captured from the large scale AWS Batch run

- manual-chrom-validation.html
  Some example chromatograms and peak groups found by each of the three parameter sets.

- ovarian_analysis.html
  The analysis notebook for the ovarian dataset we used to validate our newly suggested parameter sets

- navarro_plots_and_comments.html
  Comments and plots from our LFQBench run on HYE110 and HYE124 with our newly suggested parameter sets

- comments_plots/
  Some of the plots captured from LFQBench on HYE110 and HYE124 with our newly suggested parameter sets

aws_scripts.zip

The complete set of python scripts used to run our parallel OpenSWATH instances through AWS Batch