The DeconTools Framework: an Application Programming Interface Enabling Flexibility in Accurate Mass and Time Tag Workflows for Proteomics and Metabolomics


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Overview

- A new .NET API geared towards early MS data processing
- DeconTools Framework API enabled use of RAPID, an alternative to Decon2LS' standard THRASH-based algorithm, without extensive modification to the codebase.
- Addition of automated result validation tasks is now possible and expected to provide downstream data processing tools with 'cleaner' MS features.
- Targeted AMT tag workflows are enabled by the framework. Application of these workflows to the extraction of quantification expression ratios will be further examined.

Methods

Before: Decon2LS UI and Engine

- Inserting new modules into traditional workflows
- DeconEngine.dll
- THRASH
- Data smoothing
- RAPID
- Decon2LS
- THRASH-set

Now: DeconTools UI + DeconTools Framework

- DeconTools User Interface
- DeconEngine.dll
- THRASH
- Data smoothing
- RAPID
- Decon2LS
- THRASH-set

New data processing workflows: a targeted AMT tag approach to quantification

Introduction

- Identifying peptides using the high throughput accurate mass and time (AMT) tag proteomics approach involves several data processing steps.
- At the beginning of the data analysis pipeline, the software tool Decon2LS (pronounced "decon tools") extracts raw data, detects peaks, and finds peptide features (e.g., masses, retention times, etc.).
- Until now, Decon2LS users were limited to a single workflow and restricted to using only the algorithms made available by the DeconTools developers, a C# library.
- Addition of new deconvolution algorithms or alternative workflows required cumbersome changes that led to unmanageable ‘spaghetti’ code.
- Here, we wrap the previous DeconEngine in a new .NET framework and provide intuitive data objects and workflow control structures to facilitate easy MS data processing.

Results

Inserting new modules into traditional workflows

1) Alternative Deconvolution using RAPID

- Question: Can we introduce our standard THRASH deconvolutor with AMT?
- Approach: Wrap RAPID with a class that implements from Task and insert into workflow.

Figure 1. Comparison of THRASH and RAPID deisotoping of data from five mouse plasma samples. Deconvolutor data from manual THRASH deconvolution of five mouse plasma samples. Data from THRASH shows lower noise in the total ion chromatogram (TIC) than RAPID, and also shows higher noise in the total ion chromatogram (TIC) than RAPID

2) The ResultValidator

- Question: What percentage of MS features extracted by THRASH and RAPID had monoisotopic peaks correctly selected?
- Approach: Add a ResultValidator module to the workflow, that flags those features which are confirmed to be monoisotopic peaks (see information below)

Figure 2. Example of flagged target feature profile for quality control 5, controls dataset. RAPID data shows using THRASH and RAPID workflows to the extraction of quantification expression ratios will be further examined.

Conclusions and future directions

- DeconTools Framework API enabled use of RAPID, an alternative to Decon2LS' standard THRASH-based algorithm, without extensive modification to the codebase.
- Addition of automated result validation tasks is now possible and expected to provide downstream data processing tools with 'cleaner' MS features.
- Targeted AMT tag workflows are enabled by the framework. Application of these workflows to the extraction of quantification expression ratios will be further examined.

Acknowledgements

This work was supported by the National Cancer Institute (NCI) and the Department of Energy (DOE). We thank Peter Mayampurath and Ying Chen for providing software tools used in this study. We also thank Weijun Qian and Carrie Nicora for providing mouse plasma samples.

References