Release Notes

Proteograph™ Analysis Suite v2.0
August 3, 2022

- **PAS Proteogenomics Workflow to identify and explore peptides with protein sequence altering genetic variants**
  - **Build a custom peptide database**
    - New feature to build a customized peptide sequence database using user-uploaded custom or sample-specific variant call files (VCF).
      - VCF files are used to annotate genetic variants that may result in amino acid variants (i.e., variant peptides) not captured in the canonical reference database.
    - Variant peptide sequences are combined with the reference database to generate customized peptide sequence databases.
  - **Search for variant peptides**
    - Using the customized peptide sequence database, now users can search their DDA data for variant peptides using MSFragger.
  - **Variant Peptide Browser and Proteogenomics Data Explorer**
    - *Variant Peptide Browser* – Identified variant peptides are summarized in interactive plots and table.
      - Summary table shows all identified variant peptides and can be sorted/filtered by sample, nanoparticle, protein, variant, and allele frequency. Each variant (row) links to a view within the Proteogenomic Data Explorer.
      - The number of variant peptides found across samples, conditions, and nanoparticles are shown. The distribution of variant peptide intensity is stratified by reference and alternative alleles and homozygous/heterozygous alleles across samples, conditions, and nanoparticles.
    - *Proteogenomics Data Explorer* – Interactive tool to explore peptide and variant peptide data maps in genomic space for entire proteins and at nucleic acid/amino acid resolution
      - Gene structure, protein structure, domain information, and functional region information are displayed.
      - Amino acid variants within variant peptides are highlighted, including both reference and alternative alleles.
- **Improvements to analysis protocols**
  - Integration of MSFragger database search engine.
    - Pre-installed MSFragger-based Proteogenomics protocol (DDA, VCF required).
  - Enabled DIA-NN MBR feature[1].
- **Dashboard to monitor PAS account usage**
  - Track the total number of plates added, projects added, completed analyses, and data storage.
  - Added links to most recently added plates, projects, completed analyses, and data storage.
- **Expansion and improvement of analysis visualizations**
  - Added additional background datasets and overlay for multiple samples in waterfall plots.
  - Added ability to interact with sample correlation and similarity plots and visualize plots showing underlying data for each comparison.
  - Added option to view and compare all metrics from plate map grid across all wells and across all plates analyzed.

    - Added option to select order of comparison for differential abundance group analysis.
    - Added new interactivity with differential abundance group analysis volcano plot display.

- **Changes to file and project management**
    - Added feature to multi-select projects when launching analyses.
    - Added feature to collapse Analyses folders by project.
    - Added project filtering capabilities.

- **Improvements to analysis stability and plot visualizations for large-scale study sizes**
    - Stability and browser performance upgrades.
    - Analysis visualization and plot rendering speed improvements.
    - Streamlined analysis summary menu improves navigation between visualizations.

- **Added PAS software end user license agreement (EULA)**

- **Changes to help content**
    - Updated user guide.
    - Updated tooltips.

- **Other general improvements**
    - Sample Description File is now stored in Data Files.
    - Minor bug fixes.

1. Demichev, V., *et al.* DIA-NN: Neural Networks and interference correction enable deep proteome coverage in high throughput. *Nature Methods* **17**, 41–44 (2019).