Annoucing the official release of PEAKS with timsTOF Pro data support

- Built-in support for raw data loading from timsTOF instruments using PASEF acquisition
- Interactive data visualization tools to view data projected on m/z-rt or m/z-1/k0 dimensions
- 4D feature detection & feature separation based on ion mobility
- Analyze IMS-MS data using PEAKS de novo, identification and quantification workflows
- Export IMS-MS results as visual reports, text, and/or Skyline/Scaffold supported file formats

Waterloo, ON: May 10, 2018 - Bioinformatics Solutions Inc. was happy to collaborate with Bruker Daltonik GmbH over this past year to support ion mobility data from their timsTOF Pro instruments using PASEF acquisition.

Ion Mobility Spectroscopy - Mass Spectrometry (IMS-MS) provides a compelling analytical workflow for complex biological and chemical mixtures by adding an additional dimension of ion separation. With IMS-MS, ions are separated based on their mobility through a buffer gas, which provides the capability to differentiate ions based on their size, shape, charge and mass mobilities. Thus, it is possible to resolve ions that may be indistinguishable by traditional mass spectrometry. One type of IMS-MS is trapped ion mobility spectroscopy (TIMS), where all precursor ions are accumulated in parallel and released sequentially as a function of their ion mobility. This method overcomes the limitation posed by data dependent analyses where precursors are fragmented one at a time and the others are discarded entirely, even though many precursors elute from the column simultaneously.

Utilizing TIMS technology, Bruker's timsTOF front-end TIMS analyzer optimizes higher-speed shotgun proteomics with smaller sample amounts, while maintaining outstanding identification performance. Its unique dual TIMS geometry allows ions to be accumulated in parallel in the first TIMS section, and after an additional TIMS separation step in real time, the ions are released from the second TIMS section for MS/MS fragmentation. This results in nearly 100% duty cycle, giving this parallel accumulation and serial fragmentation (PASEF) technique unprecedented performance for reproducible nanoflow LC-MS analysis of enzymatically digested protein mixtures.

To enhance this technology further, Bioinformatics Solutions Inc. has officially released PEAKS with timsTOF data support. PEAKS provides a unique de novo assisted data analysis workflow. The combination of de novo sequencing with traditional database searches ensures a complete interpretation of raw spectral data to embrace the complexity and sensitivity of mass spectrometry which offers advanced solutions for proteomic and therapeutic protein discovery as provided through peptide/protein identification and quantification, peptide mapping, post-translational modifications and sequence variants.