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Mapping diverse proteome responses with intelligent mass spectrometryDevin K. Schweppe¹¹University of Washington

As experiments sizes and scope grow, inefficiencies in mass spectrometry data acquisition result in instrument bottlenecks. To address this, we and others have been building intelligent data acquisition platforms to adaptively select the best candidate peptide and protein raw data in real time with instrument acquisition. With an eye towards quantitative sample multiplexed analyses, our first iteration of this was the real-time search platform which improved acquisition efficiency by two-fold and enabled quantitation of 8000-9000 proteins across up to 18 samples in just 18 hours.

Taking advantage of the resulting efficiency we profiled the quantitative proteome landscape of aging mice. To do this we profiled 200 anatomical proteomes across age groups to generate a landscape of 10,250 proteins. We found that sex differences in protein abundance aligned closely with previously collected transcriptomics data. However, changes due to aging were more prevalent in proteins and often had no corresponding transcriptional change. We observed protein abundance changes that were both cross-tissue and tissue specific. These changes covered central biological processes that are known effectors of aging pathologies such as immune invasion, metabolic shifts, and proteostasis. We went on to show that protein complex cohesion and potentially activity can be derived from these proteomic alterations with age.

Having built the core platform for intelligent data acquisition we have now begun to expand the tools beyond the initial real-time search schema. To this end we are integrating new modules capable of spectral pre-processing, high-dynamic range tracking of peptides and proteins, and on-the-fly quantitative profiling in the context of sample multiplexing.

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Prosit boosts mass spectrometry-based proteomics one spectrum at a timeMathias Wilhelm¹, Wassim Gabriel¹, Omar Shouman¹, Vitor Sternlicht¹, Ludwig Lautenbacher¹¹Computational Mass Spectrometry, Technical University of Munich, Freising, Germany

The prediction of peptide properties such as fragment ion intensities and retention time has been shown to increase the sensitivity and specificity at which peptides can be identified. Prosit, a deep learning model trained on synthetic peptides generated in the ProteomeTools project, has been used >6 billion times via its various online prediction services to date. Here, we 1) summarize the available models for peptide property prediction, specifically show a single model covering the combination of (non-)tryptic (un-)modified (un-)labeled peptides undergoing HCD or CID fragmentation, 2) give advice on how to use it, and 3) show our current efforts in enabling the community to utilize Prosit via its rich open-source ecosystem, allowing for model training, inference and deployment.

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