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Computational methods in top-down proteomics to address challenges in proteoform analysis

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Top-Down Proteomics (TDP) has emerged as the dominant method for elucidating the intricacies of proteoform diversity, providing insights crucial for understanding biological processes. With development ranging from sample preparation to instrumentation, there has been a notable increase in research endeavors adopting and developing different TDP protocols that suit the objectives of the studies. Moreover, the information density within TDP data sets have grown dramatically, and more TDP data sets are being deposited in the public repository like PRIDE.

Fully realizing the potential of TDP for proteoform resolved analysis requires robust, flexible, and reproducible computational methods capable of handling the complexity of analytes (proteoforms) and data (spectra), while also accommodating the different requirements inherent in each experimental protocol. Due to distinct characteristics (e.g., complexity of ion signals), the computational tools used in the well-established field of bottom-up proteomics (BUP) cannot be readily adopted for TDP; dedicated methods are still demanded for the data analysis, data acquisition, and signal processing.

In this talk, I will introduce our contribution to the field of computational TDP, which include various computational methods such as deconvolution and quantification. I will provide a concise overview of the main concepts and core results of each method, and outline the future directions our group intends to pursue. Finally, the current project for the proteoform identification and characterization method that push the boundaries of the existing search engines will be discussed.

User consent

yes

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