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Advancing Next-Generation Proteomics through Computational Research

Computation has become a major factor in high-throughput proteomics, and computational aspects frequently represent the core intellectual contributions of many scientific manuscripts. Yet compared to the opportunities, only a relatively small number of research groups are capable of undertaking such computationally centric research agendas in part due to the combination of technical skills and substantive mass spectrometry knowledge required. There has been an unprecedented improvement in the quality and quantity of commercial proteomics data generation technologies, making data generation more accessible to many researchers. However, more and more discoveries will be led by researchers in command of the skills necessary to mine and extensively interpret the volumes of data. Already the ability to generate data vastly outpaces our ability to interpret it, and the lack of expertise in interpreting data is the current gating factor in the advancement of proteomics sciences. Proteomics scientists with training solely in data generation techniques will be shut out of more and more research opportunities. Likewise, computational scientists lacking any training in analytic or biochemistry techniques will be largely relegated to a support role. Initiatives are needed to bridge the gap between research opportunities and related algorithmic and statistical expertise and to usher in a new generation of computational mass spectrometry researchers. Achieving the full potential of innovative cutting-edge techniques will only be possible if these sibling communities come together at regular open forums designed to promote close interactions and cross-disciplinary training, including training laboratory scientists in computation, but also to encourage more computational researchers to take their rightful role in leading substantive research programs in proteomics.

The RECOMB Satellite Conference on Computational Proteomics (RECOMB-CP) is a yearly conference that aims to bridge this communication gap by directly connecting leaders in the development of new mass spectrometry approaches with scientists with the skills to develop algorithmic and statistical approaches aimed at high-throughput interpretation of mass spectrometry data. The parent RECOMB (Research in COmputational MOlecular BIOlogy) conference is the leading generic bioinformatics conference covering all aspects of computational biology; RECOMB Satellite conferences are usually smaller and more focused conferences aimed at specific areas of bioinformatics with well-defined research communities. The healthy growth of the computational proteomics community and the partnership with the *Journal of Proteome Research* since RECOMB-CP 2010 further underscore the success of RECOMB-CP in directly connecting our community to leaders in the development of new mass spectrometry instruments (e.g., ion mobility and electron dissociation methods), protocols (e.g., post-translational modifications and alternative enzymatic digestions), and applications (e.g., systems biology and protein–protein interactions). Not to be outdone, the computational community responded with novel contributions ranging from traditional (e.g., peptide and protein identification) to emerging (e.g., cross-linking

and peptide/domain interactions) areas of computational research. These were further complemented by a series of tutorials introducing novel computational strategies and lively poster sessions sparking enthusiastic discussions around connecting pressing needs in one field with their potential solutions from the other. Establishing such communication channels between innovative computational advances and deep hands-on knowledge of the critical needs and cutting-edge developments in proteomics mass spectrometry are key to ushering in an era of computationally enabled mass spectrometry discoveries and researchers.

We are committed to continuing the RECOMB-CP forum by inviting your contributions of original manuscripts, poster abstracts, and active participation at its fearless discussions and lively interactions.

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