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Structural studies of proteins using chemical crosslinking and tandem mass spectrometry

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Macromolecular complexes are involved in almost every cellular process, and they are important targets for structural and functional analyses in diverse areas such as structural genomics, drug development, and cell signaling. Such complexes, however, are often not amenable to high-resolution structural techniques such as NMR or X-ray crystallography, either because they exceed the size threshold (> 100kDa) for analysis by NMR or because they possess multiple covalent modification sites and/or flexible structural features that hinder crystal formation. Chemical crosslinking, on the other hand, is amenable to the analysis of large protein complexes with the above features. The coupling of crosslinking with the increasingly sensitive mass spectrometric (MS) methods has successfully provided structural information for interacting proteins. Despite the value of this approach, its full development has been hindered by thelack of an efficient bioinformatics framework that allows researchers to confidently assign crosslinking targets. During this talk, I will present Xlink-Identifier 2.0, a webbased software package that has been developed for meeting this need. Built upon its predecessor Xlink-Identifier 1.0, the new version is significantly faster and takes much less memory, allowing it to search against the entire proteome of many organisms with hundreds of proteins. In addition, Xlink-Identifier 2.0 is equipped with the capability that display annotated MS/MS spectra and matching details. In particular, the matching details are presented in a sortable and searchable table, allowing researchers to quickly identify matched ions of interest. This capability drastically speeds up visual examination of identifications of crosslinked peptides.

Biography

Xiuxia Du obtained her Ph.D. from Washington University in St. Louis in 2005. She then did her postdoctoral research on computational proteomics with Dr. Richard Smith at the Pacific Northwest National Laboratory. In 2008, she joined the Department of Bioinformatics & Genomics, University of North Carolina at Charlotte as an Assistant Professor. Her lab focuses on developing novel computational algorithms for mass spectrometry-based proteomics and metabolomics studies.

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