

International Conference on

BIOCHEMISTRY, PROTEOMICS & BIOINFORMATICS

May 16-17, 2018 Singapore

**Jong Shin Yoo***Korea Basic Science Institute, Republic of Korea*

Automatic identification of site-specific glycosylation in proteomics using mass spectrometry and bioinformatics

Protein glycosylation, one of the most prevalent posttranslational modifications in proteins, plays important roles in biological systems via various processes, such as adhesion, signaling through cellular recognition, and response to abnormal biological states. However, due to the complexity and heterogeneity of a glycoprotein, current analyses focus mainly on the identification of either glycosites or the released glycans only. In this study, we have developed MS-based high throughput method for intact N-glycopeptides analysis, named GlycoProteomeAnalyzer (GPA) for analysis of N- and O-glycosylation in proteomics, which combines tandem Mass Spectrometry (MS) with a database search and algorithmic suite. We created novel scoring algorithms for confident identification of N- and O-glycosylation of proteins with calculation of False Discovery Rate (FDR). In our approach, all amino acid sequence as well as glycosylation site information were obtained from the Uniprot database. From the Swiss-Prot accession number of human protein, our GPA program automatically construct tryptic N- and O-glycopeptide database for the proteins in human plasma sample. It allows automatic identification of site-specific N- and O-glycopeptides of protein mixtures using HCD, CID, and ETD MS/MS spectra with GPA-DB from Uniprot with estimated $FDR \leq 1\%$. GPA has been designed to easily handle high-throughput glycoproteomic data with a graphical user interface and demonstrated on website (<https://www.igpa.kr/>). It can also be integrated with cloud computing service that eliminates the need for local clusters and increases throughput of data analysis.

Biography

Jong Shin Yoo has completed his PhD in 1992 from Michigan State University and Postdoctoral studies from Harvard School of Public Health in 1993. He is the Principal Investigator of Biomedical Omics Group at Korea Basic Science Institute. He has published more than 100 papers in proteomics-related journals and has been serving as an Editorial Board Member of *Proteome Science*.

jongshinyoo@gmail.com

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