

DATE: Day 28 Month 7 Year 2016

SUMMARY of
2015 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, Osaka University

Research Title		Software tools and method for interpreting mass spectrometry experiments and proteomics data
Applicant	Name	Jorge Fernandez de Cossio
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	Present Title	Dr. Mathematical Science, Senior Researcher
Research Collaborator (Host PI)		Prof. Toshifumi Takao
Summary		
<p>A stand along tool were developed for helping browsing the combination of isotopic distribution of mixture signals for phosphorylation analysis and metalocomplex by mass spectrometry. The data of the synthetic peptide treated with a Ser/Thr-kinase were analyzed with IsoMatch web, and subjected to signal separation and relative quantification. By matching the overlapped isotopic distributions of combination of candidate phosphorilated species at the two sites, Ser10 and Thr7, only species modified with a single phosphate group was found. The result showed that the two phosphorylated peptides were successfully separated from each other, even though their relative abundances could not be determined, owing to some contamination of the co-eluting phosphopeptides. The particular results were reported in (Wang et al., 2015).</p> <p>The data obtained with Native MS normally in combination with electrospray ionization was analyzed with the developed tool and IsoMatchWeb for determining the stoichiometry of components by deconvolution of the complex mixtures of isotopic distribution signals in multiple charged mass spectra to reveal the protein complexes and protein interaction with other molecules such as DNA, organic compounds, or metal ions. The particular results were reported in (Ando et al., 2015).</p> <p>The isotopic distribution expose relevant information for de-convoluting quantitatively the structures of complex mass spectra signals. The applications to quantitatively analyze degree of phosphorylation, and protein interaction with metal, are just two example of the diversity of experiments that can be devised to obtain informative data for molecular and macromolecular complex analysis in cellular census. Besides the generality of the applicability of the concept, tailored experiment designs and tools are required for each particular application.</p>		
Research Achievements		
<p>Ando, T., Tannous, E., Fernandez-de-Cossio, J., Tamura, J., Kanaya, S., & Takao, T. (2015). Analysis of a Metalloprotein, Ribonuclease H1 by Native Mass Spectrometry. In The 63th Annual Conference on Mass Spectrometry. Retrieved from http://www.mssj.jp/conf/63_en/program/1B-O2-1800(1P-34).html</p> <p>Wang, Q., Kazuma, I., Ando, T., Femandez-de-cossio, J., Kakimoto, T., & Takao, T. (2015). Identification and quantification of phosphorylation: a synthetic peptide treated with a Ser/Thr-kinase. In <i>The 63th Annual Conference on Mass Spectrometry</i>. Retrieved from http://www.mssj.jp/conf/63_en/program/2P-35.html.</p>		

***Deadline: July 31, 2016**

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