

## Association of Biomolecular Resource Facilities

Proteome Informatics Research Group (iPRG)

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## Re: iPRG-2012: Proteome Informatics Research Group Study: Detecting modified peptides in a complex mixture

## Dear Potential Study Participant,

Nature uses a wide variety of protein post-translational modifications to regulate protein structure and activity and tandem mass spectrometry has emerged as the most powerful analytical approach to detect these moieties. However, modified peptides present special challenges for characterization. First, they are generally present at sub-stoichiometric levels, meaning that without enrichment strategies samples are dominated by unmodified peptides, so finding the modified peptides may be a challenge. Secondly, the modifications may have unique fragmentation behaviors in collision-induced dissociation (CID), which may need to be considered by database search engines. Finally, if there are multiple residues within a given peptide that could bear a particular modification type, then it is necessary to identify fragment ions that frame either side of the modification site in order to be able to localize the exact site of modification within the peptide.

The Proteome Informatics Research Group (iPRG) of the Association of Biomolecular Resource Facilities (ABRF) invites you to participate in a collaborative data analysis study to enable proteomics laboratories to evaluate their ability to find a variety of post-translationally modified peptides within a complex peptide mixture background. The dataset consists of nearly twenty thousand high resolution and high mass accuracy tandem mass spectra. Within the sample there are peptides with a range of different natural and chemical modifications. This study will enable participants to evaluate their data analysis capabilities and approaches relative to others in analyzing a common data set, with a particular emphasis on their ability to detect and characterize peptides with modifications of potential biological significance.

Participants will be supplied with data in a range of formats and a template for reporting results. Upon completion, the participant will also be asked to complete a web-based questionnaire summarizing the methods they used. Results submission is anonymous, so whether you are experienced in this type of analysis or not, we encourage you to take part.

This study will be launched on January 5<sup>th</sup> 2012 and results must be returned by February 3<sup>rd</sup> 2012 in order to enable sufficient time to analyze the results for presentation at the 2012 ABRF Meeting (March 17<sup>th</sup>-20<sup>th</sup> 2012 in Orlando, FL). If you would like to take part or get more information, please download the study participation instructions from the ABRF iPRG web site: http://www.abrf.org/index.cfm/group.show/ProteomicsInformaticsResearchGroup.53.htm

This study is open to both ABRF members and non-members. However, we do strongly encourage non-members to join, and thus help support ABRF (for more information visit <a href="http://www.abrf.org">http://www.abrf.org</a>). A summary of the results of this study will be presented orally and as a poster at the ABRF 2012 meeting, subsequently posted on the ABRF website, and published in a peer reviewed journal.

We thank you for your support of the ABRF and look forward to your participation in this year's study.

Sincerely,

The ABRF Proteome Informatics Research Group (iPRG)

Robert Chalkley – UCSF (Chair)

Nuno Bandeira - UCSD

Matt Chambers – Vanderbilt University

Karl Clauser - Broad Institute of MIT and Harvard

John Cottrell – Matrix Science Ltd

Eric Deutsch - Institute for Systems Biology

Eugene A. Kapp - WEHI

Henry Lam - Hong Kong University of Science and Technology

W. Hayes McDonald - Vanderbilt University

Ruixang Sun – Chinese Academy of Sciences

Thomas Neubert (EB Liaison) - New York University