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SIgN Immunology Seminar

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Challenges in Database Development for Clinical Metabolomics

Host
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Date
Wednesday 10 December 2014

Time
11am – 12pm

Venue
SIgN Seminar Room
Immunos Building
Level 4
Biopolis

Currently, the field of quantitative metabolomics using liquid chromatography tandem mass spectrometry is presented with several challenges including quality of data and a general lack of computational tools and methods for metabolite identification and quantitative data analysis. Additionally, there are a limited number of compound databases and tandem mass spectra libraries that provide a general snapshot of the total metabolome for a given organism, disease process or tissue type. As such, a first logical step in the discipline of un-targeted metabolomics is to produce as complete a search space as possible through curation of data collected from real specimens. In this talk, I will describe a pipeline for curation of data from mass spectrometry experiments designed for custom search space development including MS compound and MSMS spectrum library development while considering compound classes such as lipids. I will also describe development of informatics methods for determining the theoretical probability of ion identification in both MS and MSMS given the theoretical size of the databases. Considered in these approaches are the reliability of detection of an ion, influence of species (eg. Human versus bacteria) on the database size, and the utility of these methods in determining which metabolic pathway might be observed in any given experiment. How these methods have helped us in our approach to clinical metabolomics will also be presented.