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Bioinformatics tools toward GC-MS and LC-MS data analysis, management and visualization

Zeeshan Ahmed
University of Massachusetts Medical School, USA

In metabolomics studies, analyzing mass spectrometric data is one of the complex tasks as it requires massive data handling and implementation of biostatistics. Nowadays, based on the concepts of computations biology several bioinformatics tools have been developed towards the fields of biochemistry and pharmaceutical biology which are heavily contributing in spectral data analysis. Based on the some of the previously reported achievements and our own newly proposed developmental approach i.e., Butterfly, we have produced three different Bioinformatics tools: LS-MIDA, Isotopo and Lipid-Pro. These solutions have been developed to analyze the Gas chromatography-Mass spectrometry (GC-MS) and Liquid chromatography–Mass spectrometry (LC-MS or alternatively HPLC-MS) data. LS-MIDA and Isotopo are two new scientific applications, implement (fully & partially) Brauman's least squares approach to analyze the isotopic data and estimate the abundance and absolute enrichment values. However, Lipid-Pro is a new solution towards lipdomics data interpretation. These all three tools efficiently help in complex spectral data analysis, management and visualization.

zeeshan.ahmed@umassmed.edu

Systems pharmacology augments drug safety surveillance

Tatonetti Nicholas P
Columbia University, USA

Small molecule drugs are the foundation of modern medical practice yet their use is limited by the onset of unexpected and severe adverse events (AEs). Regulatory agencies rely on post-marketing surveillance to monitor safety once drugs are approved for clinical use. Despite advances in pharmacovigilance methods that address issues of confounding bias, clinical data of AEs are inherently noisy. Systems pharmacology the integration of systems biology and chemical genomics can illuminate drug mechanisms of action. We hypothesize that these data can improve drug safety surveillance by highlighting drugs with a mechanistic connection to the target phenotype (enriching true positives) and filtering those that do not (depleting false positives). We present an algorithm, the modular assembly of drug safety subnetworks (MADSS), to combine systems pharmacology and pharmacovigilance data and significantly improve drug safety monitoring for four clinically relevant adverse drug reactions.

npt2105@cumc.columbia.edu

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