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Coon Research Group

Analytical Seminar

Computational Approaches in Mass Spectrometry—Metabolite Identification, Quantitation and Data Visualization

Thursday

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12:15 pm

1315 Chemistry

Gas chromatography/mass spectrometry has emerged as one of the premiere tools for global metabolic profiling. Given that the metabolome is furthest downstream from genotype to phenotype, metabolic profiling has great potential to propel biomedical research and is quickly emerging as a field of interest for both systems biologists and clinical researchers. Currently, mass spectrometry-based metabolomics analyses are limited by the ability to confidently identify measured metabolites. In fact, it is not uncommon that the majority of detected analytes in a given GC/MS metabolomics experiment will remain unidentified. We have developed a combinatorial approach called High-Resolution Filtering (HRF) to determine the plausibility of putative identifications by exploiting accurate mass measurements. This simple method provides orthogonal information to traditional spectral matching and retention indexing. Furthermore, it affords all the benefits of increased MS resolution while simultaneously extending the utility of the expansive unit resolution GC/MS reference libraries currently available.

Beyond these efforts . . . Please attend Nick's seminar to hear the rest of his story.