Medicinal Chemistry

SmartPeak Automates Metabolomics, Fluxomic, and Lipidomic Data Processing

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Abstract

Technological advances in high-resolution mass spectrometry (MS) vastly increased the number of samples that can be processed in a life science experiment, as well as volume and complexity of the generated data. To address the bottleneck of high-throughput data processing, we present SmartPeak (https://github.com/AutoFlowResearch/SmartPeak), an application that encapsulates advanced algorithms to enable fast, accurate, and automated processing of capillary electrophoresis–, gas chromatography–, and liquid chromatography (LC)–MS(/MS) data and high-pressure LC data for metabolomics, lipidomics, and fuxomics experiments. The application allows for an approximate 100-fold reduction in the data processing time compared to manual processing while enhancing quality and reproducibility of the results.

Biography

Douglas McCloskey obtained his PhD in 2017 in bioengineering in the lab of Bernhard O. Palsson at the University of California, San Diego. During his studies, he was awarded the prestigious Siebel's Scholars Foundation grant. Douglas McCloskey is currently a group leader at the NNF Center for Biosustainability (CfB) at the Technical University of Denmark. At the CfB, He is leading a group of automation engineers, software engineers, and analytical chemists to develop Big –Omics data generation workfows and leading a group of PhDs and Postdocs to develop advanced machine learning and biochemical modeling algorithms to learn from Big –Omics data.

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