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Cloud-Based Systems Biology Analyses Guided by Metabolomics

Systems-wide analysis has been implemented into the XCMS cloud-based metabolomic platform (XCMSOnline.scripps.edu) to guide multi-scale omic experiments. This autonomous approach superimposes high accuracy mass spectrometry metabolomic data directly onto metabolic pathways, which is then integrated with genetic and proteomic data. To date, the utility of this platform has been demonstrated on thousands of studies from the platforms 12,000 registered users. Our streamlined systems biology analysis is a one-step approach within XCMS Online that integrates metabolic pathway analysis with proteomic and genomic data to decipher the metabolic network at the systems level. The workflow initially involves the upload of raw mass spectral data files onto XCMS Online, which are processed to extract metabolite features, correct retention time deviations, and align extracted ion chromatograms. This technology then prioritizes metabolic features involved in locally enriched metabolic pathways where the metabolite identities can be further validated using autonomous tandem mass spectrometry data acquisition. We have also reconfigured the traditional analysis workflow described above to allow metabolite mapping and analysis of genomic and proteomic networks simultaneously. Thus, XCMS has been designed to streamline metabolomic-guided systems biology data analysis within our freely available cloud-based resource (XCMSOnline.scripps.edu)