

TOOLbox

XCMS for metabolite profiling

Gary Siuzdak and colleagues at the Scripps Research Institute have developed an approach to preprocess LC/MS metabolite data. The method, called various forms of chromatography MS (XCMS; the X represents various forms), includes three algorithms. The peak-detection algorithm identifies relevant peaks from low- or high-resolution data. The peak-matching algorithm matches the peaks across multiple samples by using chromatographic retention and mass data to place the peaks into bins for analysis. The retention-time-alignment algorithm corrects the retention times of the samples in a single step. No standard target sample is required for the alignment. XCMS also provides superimposed, aligned extracted ion chromatograms for selected peaks from several samples. A link to the Metlin Metabolite Database is provided in XCMS to help identify the metabolites. The software for XCMS is freely available at <http://metlin.scripps.edu/download>. (*Anal. Chem.* **2006**, *78*, 779–787)