Software R and D

Custom software solutions are being designed to provide enhanced data processing and statistical analysis for screening and metabolomics analysis.

Custom NMR software developed by Christian Ludwig and Ulrich Günther for NMR data processing and post-processing include NMRLab and MetaboLab, which offer algorithms for scaling, alignment, glog-transform, de-noising PCA, PLS(-DA).

Data Links to the SESAME LIMS system, the CCPNMR package, andcommercial and non-commercial metabolite spectral databases (Chenomx, AMIX; Madison Metabolomics Consortium Database (MMCD), HMDB: the Human Metabolome (Edmonton, Canada) are being explored.

Micelle docking: Felician Dancea and Michael Overduin developed a fast protein-micelle docking methodology that yields 3D structures of proteins inserted into micelles. The docking restraints can be derived from any technique that detects insertion of protein residues into a membrane, and can be applied to virtually any peripheral membrane protein or membrane-like structure (published in Biophys J, 2007).

© University of Birmingham 2015