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TOOLbox
PROMPT for comparisons

After identifying proteins by MS, researchers often want to know whether the list includes proteins with certain functions. To perform this analysis, they must integrate sequence and annotation data from many sources that may not be compatible. So, Dmitrij Frishman and Thorsten Schmidt at the Munich University of Technology have developed a software system called protein mapping and comparison tool (PROMPT). The tool uses sequence information to match protein entries with different accession numbers. Protein properties, such as pI or functional categories, are compared, and statistical analyses are conducted. For example, researchers used PROMPT to examine the structural differences between two sets of *E. coli* proteins. Results are visualized as plots or spreadsheets and can be exported in many formats. Academic users can access PROMPT for free at http://webclu.bio.wzw.tum.de/prompt. (*BMC Bioinformatics* **2006**, *7*, 331)

msInspect

Martin McIntosh and co-workers at LabKey Software, the Fred Hutchinson Cancer Research Center, and the University of Washington have developed a bioinformatics software platform for the visualization and quantitation of LC/MS data that is called MS in silico peptide characterization tool (msInspect). With the new platform, data from experiments involving isotope labeling or label-free methods can be analyzed and compared.

The graphical interface allows users to view their LC/MS data as a heat map, with retention time on the x axis and $m>/z$ on the y axis. The brightness of the color on the heat map indicates the signal intensity. Users can zoom in and out of the map and view 1D cross-sectional slices of the data. The researchers applied the algorithms to the quantitative analyses of human serum samples that were labeled with the isotope-coded affinity tag (known as ICAT) method or that were unlabeled. In addition, the programs in the msInspect platform (available at http://proteomics.fhcrc.org) were used to distinguish two bacterial strains. (*Bioinformatics* **2006**, *22*, 1902–1909)

Rapid peptide identifications

Most peptide identification algorithms search experimentally obtained mass spectra against large databases that contain theoretical spectra. Because these searches can take hours, the throughput of proteomics experiments is limited. Databases that include theoretical spectra of posttranslationally modified proteins can take even longer to search with conventional algorithms. Therefore, Smriti Ramakrishnan and colleagues at the University of Texas, Austin, have developed a filtering method that speeds peptide identifications. The method includes a fast coarse-filtering step in which all true positives and some false positives are obtained. In the second step, a fine filter ranks these data by a significance score. The highest-ranked candidate for each spectrum should be the correct match.

The researchers tested the method with spectra from various protein mixtures and databases containing theoretical *E. coli* and/or human spectra. In every test, the new method correctly identified the proteins in the mixture. According to the researchers, the speed of the new method should allow users to automatically search for mutations and modifications in a high-throughput mode. (*Bioinformatics* **2006**, *22*, 1524–1531)

MeMo for metabolomics data

Irena Spasić, Douglas Kell, and co-workers at the University of Manchester and the University of Wales (both in the U.K.) have developed MeMo, a model for the representation of metabolomics data and associated metadata. The model includes an administrative module for procedural information, such as protocols and a listing of the instruments that were used. The "wet experiments" components include biological and chemical information about the sample as well as the data generated by analytical instruments. The "dry experiments" module includes the processing and analysis of experimental results. The background knowledge component stores information from external sources in addition to the experimental data, to facilitate the integration of these data sets. MeMo is available at http://dbkgroup.org/memo. (*BMC Bioinformatics* **2006**, *7*, 281)