

## Special Issue on Computational Mass Spectrometry

### Call for Papers

Galloping technological advances in mass spectrometry (MS) continue to advance existing analytical capabilities towards a unified understanding of the dynamic complement of the cell.

As was recognized by the 2002 Nobel Prize in chemistry, mass spectrometry is nowadays the major technique for the analysis of proteins, metabolites, carbohydrates, and lipids. More than 13,000 articles from the life sciences that are related to MS have been published in the year 2010. MS is also an indispensable tool for studies in chemistry, biochemistry, pharmacy, or medicine.

Computers and computer programs have supported MS experts in the interpretation of mass spectra since at least the 1960's. With a more formal treatment of problems and methods, computational mass spectrometry became a mainstream technique in the mid-1990s and has since become an indispensable tool for the automated analysis of MS data. Questions of interest include the identification of peptides, proteins, metabolites, and glycans, as well as quantitative proteomics and metabolomics. As mass spectrometry is rapidly evolving, questions and paradigms for the computational analysis perpetually change.

We invite researchers to submit new original research and review articles spanning the whole field of computational mass spectrometry. Potential topics include, but are not limited to:

- Raw data analysis and peak picking
- Advanced methods for database searching
- Computational analysis of quantitative data
- *De novo* sequencing of peptides and proteins
- Identifying and localizing posttranslational modifications
- Combining peptide identifications into protein identifications
- Proteogenomics matching of spectra to six-frame translations of genomes
- Spectral library searches
- *De novo* interpretation of metabolite MS data
- Identifying the unknowns: characterizing metabolites not in any database
- Glycan *de novo* sequencing

- Interpreting glycan MS data

Before submission authors should carefully read over the journal's Author Guidelines, which are located at <http://www.hindawi.com/journals/abi/guidelines/>. Prospective authors should submit an electronic copy of their complete manuscript through the journal Manuscript Tracking System at <http://mts.hindawi.com/> according to the following timetable:

Manuscript Due	August 1, 2011
First Round of Reviews	November 1, 2011
Publication Date	February 1, 2012

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