Workshop 4 Tuesday, 18th September, 17:15-19:15 (Room D)

Mass++ and MassBank: Tools for Data Processing and Database on PC

Organizers: Satoshi Tanaka (Shimadzu, Japan), Takaaki Nishioka (NAIST, Japan)

Topics 1:

"Mass++: A Visualization and Analysis Tool for Mass Spectrometry"

Satoshi Tanaka (Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation, 1, Nishinokyo-Kuwabaracho Nakagyo-ku, Kyoto 604-8511, Japan)

Abstract: Mass++ (mass plus plus) is freeware for viewing and manipulating various types of mass spectrometric data. Its primary objectives are: 1. To provide essential functionality for proteomics and metabolomics analysis. 2. To support a wide range of vendors' data file formats. 3. To be easily extendible using plug-in technology.

This year we have released a new version of Mass++ (Mass++ 2.1.0), which contains new functionality such as AXIMA file reading, Batch Processing, De novo sequencing, a new peak detection algorithm, statistical analysis, and overlapping trace settings. The new version of Mass++ also makes it easy to identify substances with search engines such as Mascot and MassBank. Previously, MassBank could be used directly from Mass++, but Mascot could not; to use Mascot search, users had to extract peak data and search databases using other software, which was very time-consuming. In the latest version of Mass++, users can easily perform Mascot search on raw data. Mass++ can be downloaded from http://www.first-ms3d.jp/english/achievement/software.

Topics 2:

"Constructing MassBank Database on Laboratory PCs"

Takaaki Nishioka (Nara Institute of Science and Technology, Ikoma, Nara 630-0192, Japan)

Abstract: MassBank (http://www.massbank.jp) is a public repository for sharing mass spectra among research community. Data shared on MassBank are not placed on the MassBank site, but distributed on the contributor's data servers. Currently 24 research groups contribute from nine data servers. Contributors prepare their mass spectral data in "MassBank Record Format", provide PCs as data servers, and manage their data on their own data servers. Users are able to access to all the distributed MassBank data from the access point, "www.massbank.jp". Thus MassBank project has provided various user's tools to search the data and to prepare and manage MassBank records on their data servers. Recently we transferred these technologies to "In-House MassBank" on Windows PCs. Users are able to build their in-house MassBank databases by depositing their own mass spectral data and the copied MassBank data from the MassBank download site. One of the applications of in-house database is to search user's in-house database with a large set of query data that LC-MS output. Mass++ imports and submits the query data to the spectral search against the in-house database by using MassBank batch SOAP-API. This relieves users from tedious, repeated manual works for the identification of the small molecules detected by LC-MS.

Scope of Session: Mass++ (mass plus plus) is freeware for viewing and manipulating various types of mass spectrometric data. Mass++ 2.1.0, which was released recently, is easy to use as search engines such as Mascot and MassBank. MassBank is a public repository for sharing mass spectra of small molecules among research community. A bottleneck in metabolomics is to submit a large amount of mass spectra from LC-MS as the queries to database searches manually. Mass++ and MassBank projects have collaboratively developed a tool that relieves the users from the repeated manual works. Two projects will give tutorials of their tools.

Key words: Freeware, Proteomics, Metabolomics, Multi-vendor, Chemical identification