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Mass Spectral Library Searching - Without Libraries

The relative ease of obtaining accurate-mass fragmentation data on modern LCMS instruments; faster computers; and the availability of large molecular structure databases have recently made it possible to change the “art” of interpreting mass spectral data into a systematic computational process. MathSpec, Inc. has teamed up with Elsevier MDL and Sun Microsystems™ to deliver *Rational Numbers*™ FragSearch on the Sun™ Grid Compute Utility.

See the Rational Numbers difference

Completely complementary to traditional interpretation and spectral library searching, *Rational Numbers* FragSearch software is designed to assist scientists in identifying small organic compounds from accurate-mass fragmentation data (MS/MS or CID-MS). The overall objective is to draw a rough picture of molecules that could yield a particular set of numbers, and then to search through an index of the MDL® Available Chemicals Directory to find matching compounds. Using the Available Chemicals Directory¹, the leading database of commercially available compounds, matching compounds can then be viewed and conveniently ordered from suppliers.

How Rational Numbers FragSearch Works

Rational Numbers software treats small molecules as mathematical partitions and then summarizes the mass spectral data in a modular format. These "modular structures" have a great deal of structural information, and MathSpec has developed software for searching chemical databases for compounds matching these modular structures. For this purpose, most of the small organic compounds in the Available Chemicals Directory have been sorted by the exact mass at which they would be perceived using ESI LCMS. (e.g. D-(+)-2-PHOSPHOGLYCERIC ACID SODIUM HYDRATE, MFCD00150613, has been indexed with a molecular weight of 185.993, excluding the water of crystallization and replacing the two sodiums with hydrogens.)

The Sun Grid Compute Utility

The Sun Grid Compute Utility² solution is built using Sun and industry-best practices and includes comprehensive security for user jobs. For our customers, the Sun Grid has two big advantages. Each user has virtually unlimited computer capacity when multiple datasets need to be processed. Second, by offering our software on the Sun Grid, MathSpec can update the software and database index without involving you. So you can focus on doing what you do best — mass spectrometry.

1) The MDL Available Chemicals Directory is not included. See www.mdl.com/products/experiment/available_chem_dir, and www.discoverygate.com for a no-fee evaluation. 2) For information about obtaining your account on the Sun Grid Compute Utility, see www.network.com.

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