

MathSpec Rational Numbers™ on the Sun™ Grid Compute Utility

Meet Tight Project Deadlines



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. However, this brute force computational approach is best suited to scientists who have vast computational power at their fingertips.

Highlights

- Is much less time-consuming than traditional manual interpretation. This helps mass spectrometrists meet tight project deadlines without constantly working overtime.
- Keeps mass spectral identification work from being a bottleneck in the overall research and development process.
- Sun Grid gives you on-demand access to a supercomputer with no long-term contracts and at a predictable \$1 per CPU-hour.

Save time for other tasks

MathSpec, Inc., has teamed up with Sun Microsystems to deliver *Rational Numbers*™ on the Sun™ Grid Compute Utility. For a mere U.S. \$1/CPU-hour¹, mass spectrometrists can analyze their mass spectral data on the Sun Grid Compute Utility. The Sun Grid can now do much of the tedious work, freeing mass spectrometrists to spend more time on higher level tasks.

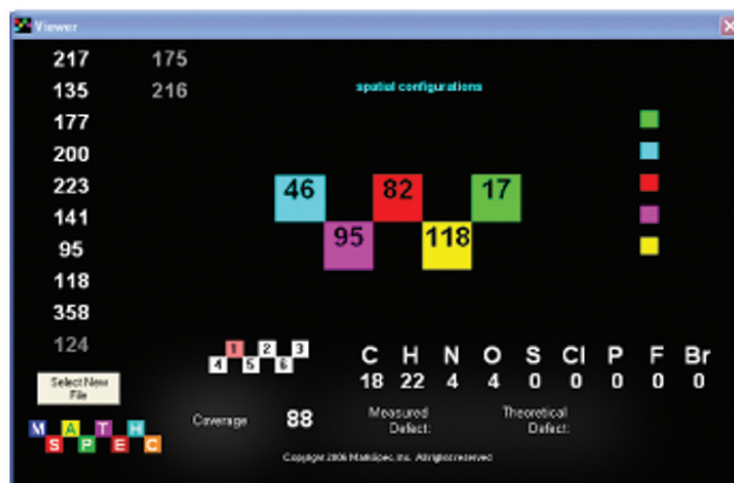
See the *Rational Numbers* difference

Completely complementary to traditional interpretation and spectral library searching, *Rational Numbers* software is designed to assist scientists in identifying small organic compounds from mass spectral data. The overall objective is to draw a rough picture of molecules that could yield a particular set of

numbers, and, where applicable, to search through molecular structure databases to find matching compounds.

Rational Numbers software treats small molecules as mathematical partitions and then summarizes the mass spectral data in a visual format (subfragments and modular structures). The program has the unique capability of combining up to eight spectral files from different types of mass spectrometers in both positive and negative ion mode, using both accurate-mass data and integral-mass data, and analyzing all of the data from one compound as a single data set. The software strategy is not based on fragmentation mechanisms, but rather on the numbers derived from the mass spectra, atomic properties, and logic tables.

1. License fees also usually apply.



This software tool can do three tasks. If the compound of interest is known, *Rational Numbers* software can assign fragment ions in its spectrum (Assign). If the compound is unknown but previously reported, the program can search accurate-mass fragmentation data directly against molecular structure databases (Search); traditional mass spectral libraries, therefore, are no longer needed. If the compound is novel, the program can compute and generate modular structures that closely approximate the molecular structure (Partition).

The Sun Grid Compute Utility

Pressure to meet tight project deadlines can cause strain for scientific teams. Frustrations increase as outside factors, such as limits on compute resources, add delays. The Sun Grid Compute Utility gives enterprises the ability to quickly augment in-house processing by providing affordable, on-demand access to compute power—with no long-term contracts, no hidden fees, and no reservations required. Using a secure network connection, organizations can easily harness hundreds of CPUs within the Sun Grid Compute Utility at the predictable price of U.S. \$1/CPU-hour.

The Sun Grid Compute Utility solution is built using Sun and industry-best practices and includes comprehensive security for user jobs. Enabled by Sun Fire™ x64 servers, the Solaris™ 10 Operating System, Solaris Containers technology, and Sun N1™ Grid Engine software, the Sun Grid Compute Utility delivers secure, high-performance execution of 32-bit and 64-bit batch workloads.

An unbeatable combination

Rational Numbers software is one of the first commercial scientific applications offered on the Sun Grid Compute Utility. For MathSpec and its customers, running *Rational Numbers* on the Sun Grid offers two major advantages.

First, the Sun Grid offers the ability to run CPU-intensive algorithms, such as Search, in parallel. This means that the mass spectrometrists can get results faster, while paying for the same amount of CPU time. In fact, some tedious tasks that could take up to four hours to complete manually can be done in about ten minutes—with the Sun Grid doing all the work for half that time. Plus, each customer has virtually unlimited computer capacity when large numbers of datasets need to be processed.

Secondly, a local software implementation requires that someone periodically perform software and database updates. By offering *Rational Numbers* on the Sun Grid, MathSpec can update its software and databases without inconveniencing its customers. So mass spectrometrists can focus on doing what they do best—mass spectrometry.

Learn More

For more information about *Rational Numbers* on the Sun Grid Compute Utility, visit Network.com, mathspec.com, or talk to your local Sun representative.