

Isotope Calculator

The “isotope calculator” is a java application for the calculation and presentation of isotope clusters of labeled and unlabeled compounds such as peptides, other molecules, averagine. Some of its major features include

- 1) The simulation of isotope distributions.
- 2) The simulation of isotope distributions of labeled compounds.
- 3) The simulation of mixing of labeled and unlabeled compounds.
- 4) The ability to investigate deamidation.

The results are presented in both tabular and graphical modes. The isotope distributions can be plotted at various resolutions including infinite resolutions. Libraries of compounds can be stored to files for later use. Source code and binaries can be downloaded from <https://www.prime-sdms.org/prime/index.htm>.

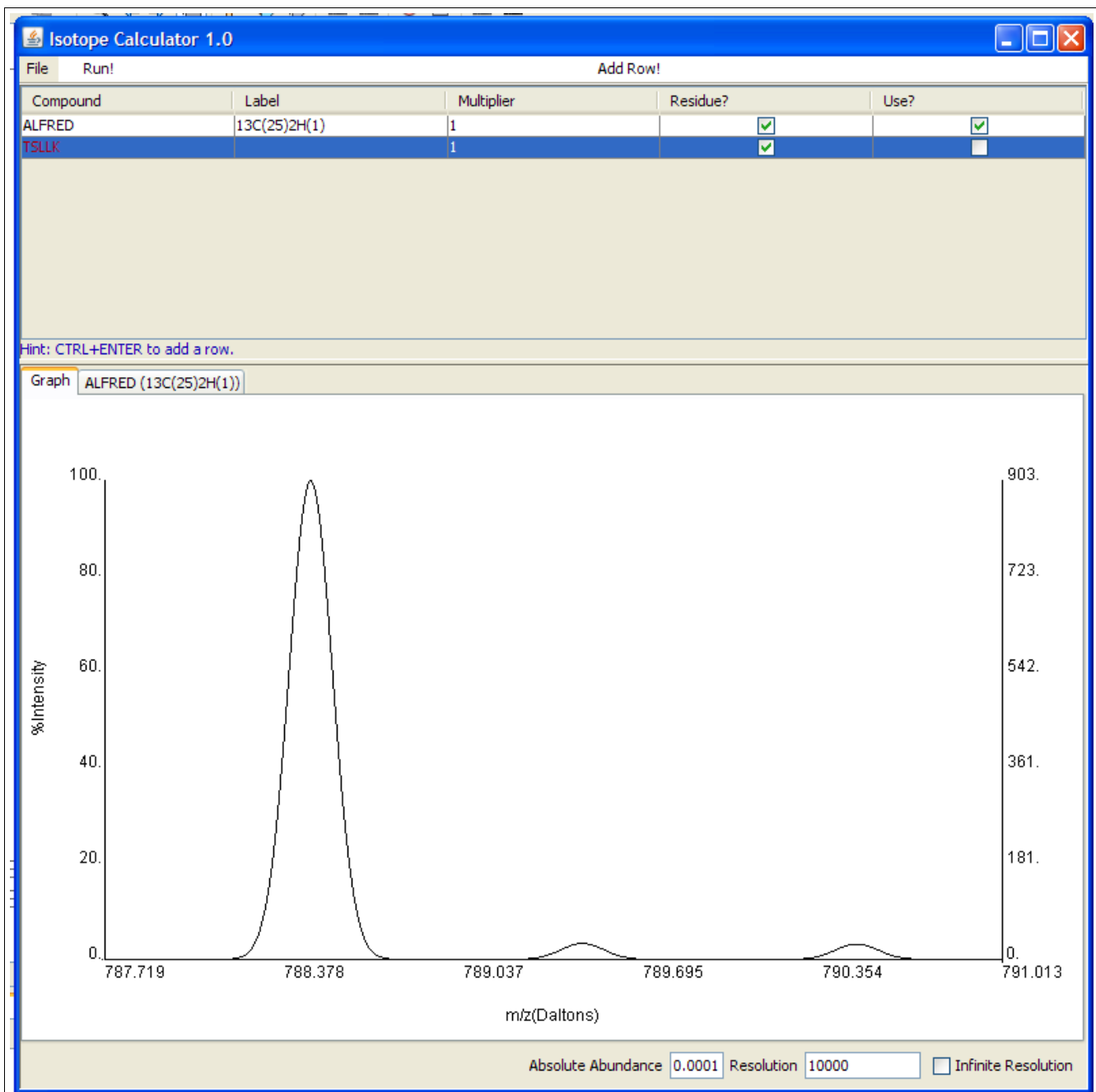


Fig 1. Isotope distribution of labeled peptide ALFRED with $^{13}\text{C}(25)^2\text{H}(1)$ with a resolution of 1000.