

Isotope Distribution Calculator

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The 64 bit version requires a compatible processor and a 64 bit version of Windows.

This is a Windows console application for calculating isotope distributions for molecules. It is designed to work with both small molecules and proteins. The element definitions are provided in a separate file, which can easily be edited to allow for isotopically labelled compounds. The output is to the console by default, but can be redirected to a file, and consists of pairs of mass and abundance values.

To install the software, simply extract the files from the zip archive (right click the icon, then select `Extract All...` from the menu). To uninstall, just delete the files.

To run, start up the windows command prompt (under accessories on the Start Menu on XP, or type `cmd` in the search box on later versions), then `cd` to the directory where you unpacked the files. Then type:

```
isotopes formula
```

where formula is the molecular formula of interest. It currently understands "standard" elements, but not any other chemical abbreviations. Valid formulae could include $C_{25}H_{37}N_6O_7S_6$ for insulin and C_2H_6O for ethanol. CH_3CH_2OH will work too. Parentheses are not yet supported.

There are various other options:

```
isotopes formula filename.txt
```

The optional filename specifies that the program should use a different atom definition file. The file format is straightforward, and contains the element symbol, followed by atomic number and then pairs of mass and abundance values (tab separated) for each isotope.

-n Normalizes the most intense peak to 100%, as is conventional for mass spectra
 -f *filt* Normalizes and discards peaks of intensity < *filt*
 -t *thr* Specifies a probability threshold *thr*, defaults to 0.001. Lower thresholds will find more peaks (and take longer to calculate)
 -p *prec* Specifies the output precision *prec*, default is 8
 -c Outputs a comma separated table. The default is tab
 -r *res* Peaks separated by <*res* will be merged. Defaults to 0.1
 -z *charge* Specifies the charge, defaults to 0
 -mtz *charge* Outputs mass-to-charge ratio and sets charge. By default outputs mass
 Any unrecognised options will simply be ignored. In the event that the program cannot calculate the distribution an error message will result.

Examples:

`isotopes C254H377N65O75S6` Calculates isotope distribution for insulin (bovine) using default settings.

`isotopes C254H377N65O75S6 -f 1` Calculates isotope distribution for insulin, normalizes and outputs peaks of intensity >=1%.

`isotopes C254H378N65O75S6 -f 1 -mtz 1` Calculates mass-to-charge ratio for protonated singly charged insulin, normalizes and outputs peaks of intensity >=1%.

`isotopes C254H377N65O75S6 -n -p 5 -c > insulin.csv` This calculates the insulin isotope distribution, outputting 5 figures of precision, normalizing the most intense peak to 100%, and sends the results to a comma separated file called `insulin.csv` (which will open in MS Excel if this is installed).

`isotopes C254H377N65O75S6 -t 0.00001` Calculates the distribution, but will consider less likely isotopomers than with the default `thr` setting of 0.001

The algorithm used is based on a published procedure (J. A. Yergey, *Int. J. Mass Spectrom. Ion Phys.* 1983, 52, 337) but is implemented rather differently from the way described in the paper, and will not give numerically identical results.

If specifying a charged molecule with the `-z` or `-mtz` options this adds or subtracts electron(s) only. If you are interested in calculating electrospray or MALDI mass spectra you will need to adjust the number of hydrogens too if the charge on the ion of interest is provided by protonation. The `-z` and `-mtz` options will give the same result when the charge is +1.

The values for masses and abundances in the supplied file `isotopestable.txt` are those given by NIST. Coursey, J.S., Schwab, D.J., Tsai, J.J., and Dragoset, R.A. (2015), Atomic Weights and Isotopic Compositions (version 4.1). [Online] Available: <http://physics.nist.gov/Comp> [2019, 08, 08]. National Institute of Standards and Technology, Gaithersburg, MD.