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# Software **MassFeatGen**

## Calculation of numerical features from low resolution mass spectra for use in multivariate data analyses and spectra similarity searches

**Input**      A file containing  $n$  low resolution mass spectra in JCAMP format.  
A text file with feature definitions.

**Output**     A text file with the computed spectral features  
containing  $n$  rows and  $m$  columns (for  $m$  user-defined features).  
This file can be easily imported into other software.

### Spectral features

A spectral feature is a number that can be automatically computed from a spectrum. For mass spectra has been shown that appropriate features are closer related to molecular structures than the original mass/intensity data. Spectral features are usually obtained by nonlinear transformations of peak/intensity data considering spectroscopic and mathematical aspects.

Demuth W., Karlovits M., Varmuza K.: *Anal. Chim. Acta*, **126**, 75-85 (2004).

Werther W., Demuth W., Krueger F. R., Kissel J., Schmid E. R., Varmuza K.:  
*J. Chemom.*, **16**, 99-110 (2002).

Varmuza K.: *Anal. Sci.*, **17** [suppl.], i467-i470 (2001).

### User-defined spectral features

The features have to be defined in a text file. For instance the widely applied *modulo-14* features are created by the simple code **MD 14 31 800** (31 and 800 define the used mass interval). Codes for already successfully used features of electron impact mass spectra are provided together with the software.

**Implemented feature groups** Modulo-14 summation,  
Autocorrelation,  
Logarithmic intensity ratios,  
Intensities at selected masses,  
Averaged intensities of selected mass ranges,  
Spectra type characterization,  
Presence of defined peak groups,  
Presence of defined peak intensity patterns.

**Operating modes**

- **Interactive** (Windows user interface).
- **Remote/batch** (fully controlled from another software - for instance from a Matlab or C++ program). Filenames and parameters are transferred via a command file in text format; status information can be optionally transferred by semaphore files.

**Platform** Microsoft Windows 2000/XT

**Example** 1000 mass spectra and 500 features typically require  
1 s computation time (Pentium 4, 2.6 GHz).

**Free download** User Guide for Full Version (42 pages),  
Demo Version of MassFeatGen including demo data,  
[www.lcm.tuwien.ac.at](http://www.lcm.tuwien.ac.at) (software)

**Full version** Introductory price EURO 100.  
Orders by email welcome to [kvarmuza@email.tuwien.ac.at](mailto:kvarmuza@email.tuwien.ac.at).

**Authors** W. Demuth [wilhelm.demuth@meduniwien.ac.at](mailto:wilhelm.demuth@meduniwien.ac.at)  
K. Varmuza [kvarmuza@email.tuwien.ac.at](mailto:kvarmuza@email.tuwien.ac.at)

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**Laboratory for ChemoMetrics**



[www.lcm.tuwien.ac.at](http://www.lcm.tuwien.ac.at)

Kurt VARMUZA

Vienna University of Technology  
Institute of Chemical Engineering  
Getreidemarkt 9/166-2, A-1060 Vienna, Austria

[kvarmuza@email.tuwien.ac.at](mailto:kvarmuza@email.tuwien.ac.at)

Fax: +43-1-58801-16091

Voice: +43-1-58801-16060