

MsXelerator IPeaks v2.9



SILAC Quantitation and Isotope Recognition Software

MsXelerator: an advanced LC/MS data processing platform providing both label-free and SILAC based quantitation

The IPeaks module offers different modes and algorithms to recognize and quantify SILAC™ isotopic peak pairs:

- Search Isotopic Patterns directly in the raw LC/MS data
- Run quantitation based on Mascot result files
- Run quantitation based on user supplied Excel files

Software Features:

Raw Data - Isotope Pattern Search

Directly search your raw LC/MS data files for the presence of peaks having specific isotopic signatures. MsXelerator contains powerful peak picking algorithms to convert detected features into monoisotopic peaks, automatically determine charge states and start quantitation/recognition based on user defined labeling patterns.

Mascot Result Files

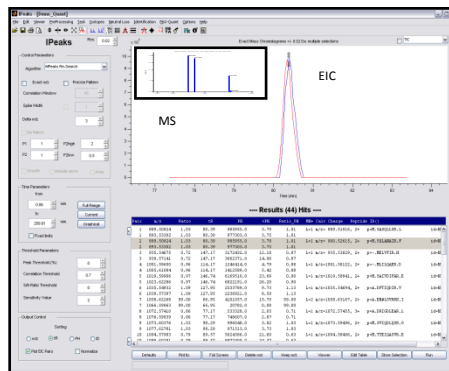
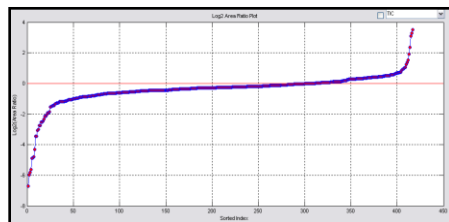
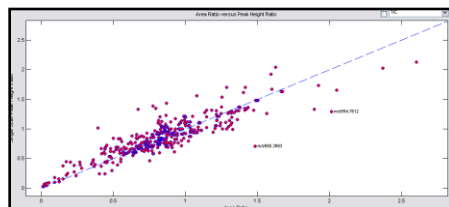
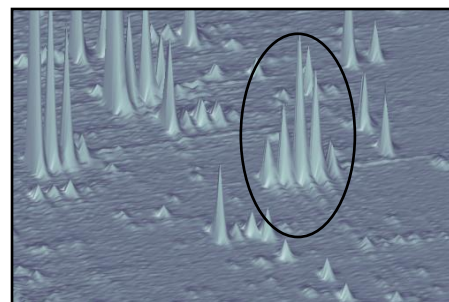
Import Mascot result files. Recalculate, extract and view extracted ion currents and MS data. Use pre-processing filters to remove redundant MSMS scans or peptides having low scores. Quantitation is based on peptide sequence and user specified labeling patterns, including $^{14}\text{N}/^{15}\text{N}$ labeling. Quantitation can be based on accurate EIC peak areas or peak heights (mono- and full isotopic range). Automatically validate your results based on peak shape analysis algorithms.

Excel Source Files

Import user created Excel files containing specified list of ions to be used for quantitation. Operates on raw and deconvoluted data sets. Automatically determine the number of labels in a peptide using loop-processing in case that no sequence information is available. Clear output and graphics for viewing and validation of results. Also works for non co-eluting light and heavy labeled peptides.

Data Import

Support of all major vendors: Thermo, Waters, Sciex, Bruker and Agilent.



No.	Sequence ID	m/z L	m/z H	Charge	L (p/du/z)	M (p/du/z)	# Labels	# Peaks	Ratio A	Ratio B
1	W. AKAQGLAEMR001	899.502	899.513	-1.16	-0.26	89.391	3	1	0.13	0.21
2	M. DQALALIMR002	899.502	899.533	-1.03	-0.36	89.391	3	1	1.09	1.01
3	L. AELTITQIMR003	899.540	899.574	-0.24	-0.47	247.177	2	1	0.72	0.25
4	L. IELIGALIMR004	1001.896	1009.411	4.77	-0.24	214.149	3	1	0.06	0.88
5	M. AELTITQIMR005	1019.899	1023.928	3.04	-1.27	146.788	3	1	0.87	0.39
6	A. DFTIQIMR006	1039.899	1039.574	-0.39	-0.43	137.394	3	1	1.09	1.13

MsXelerator: *Accelerating Data Analysis in LC-MS*

- Drug Metabolite Profiling
- Differential Analysis
- Proteomics
- Biomarker Discovery
- GC-MS Data Processing

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