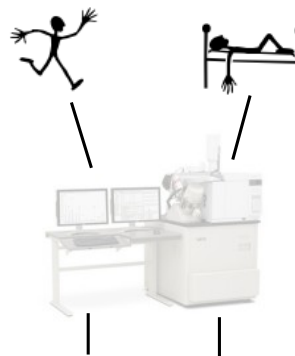
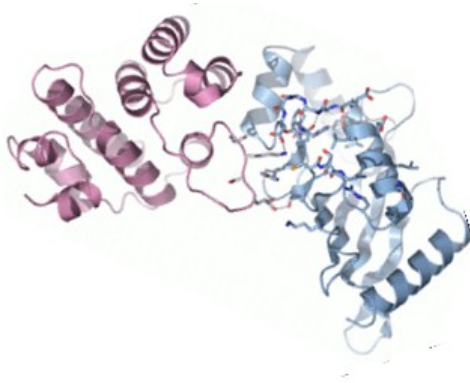


Differential PTM Detection using deltaMasses

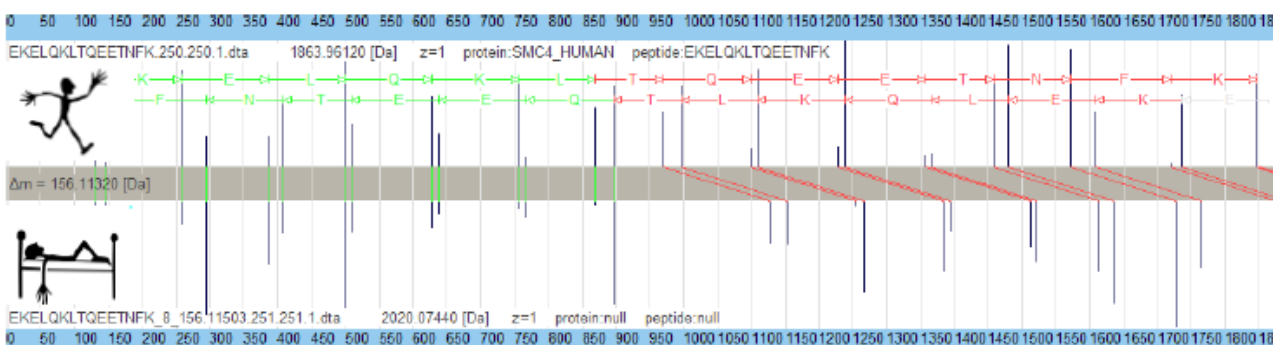
A Quantum Leap in Protein Research



deltaMasses

- Software package
- Discovers protein modifications
- No changes to laboratory equipment
- Compares all MS/MS spectra against each other
- Tool for protein modification based biomarker discovery
- 367 installations in 185 laboratories, 30 countries

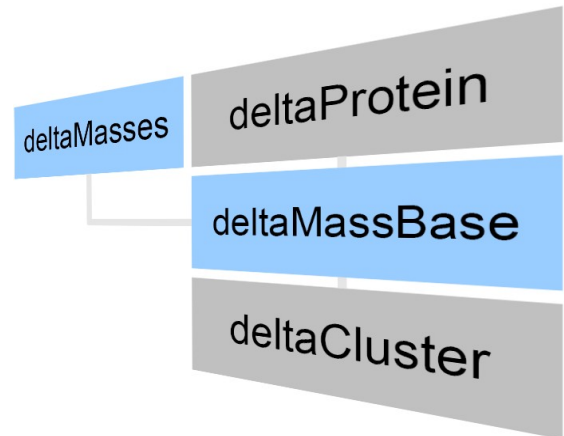
How it works: When you fragment a peptide, a certain fragmentation spectrum will result. Imagine the same peptide, but now with a modified residue. The spectrum will be very similar; the signals now separate into two sets: the first set consists of fragments without the modification; the second consists of fragments containing the modified residue. This can be visualized by „green“ and „red“ channels, respectively. deltaMasses automatically detects such fragmentation spectra showing "paired" characteristics.



Green channel = no modification; mass unchanged. Red channel = fragment contains modification.

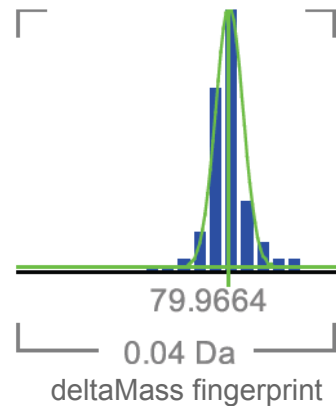
deltaMasses consists of four parts

- PTM detection module
- deltaProtein, the visualization platform
- deltaMassBase, the database system
- deltaCluster, the supercomputing extension



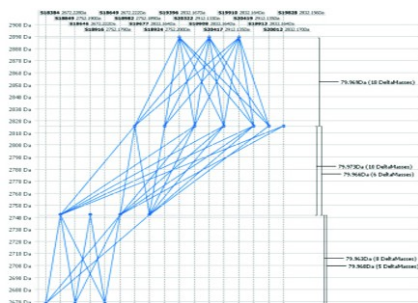
deltaMasses

- The main PTM detection tool
- Easily installed and used
- Runs on Windows 64 bit (Windows 7 or 8)¹
- Implements the deltaMass Fingerprint
- Connects to Mascot Servers



deltaProtein

- The PTM analysis and display system
- Spectrum identification by correlation
- You need to have a Discovery Edition
- Needs deltaMassBase installed
- Detects multiply-modified peptides
- Improved protein characterization



A threefold phosphorylated peptide displayed by deltaProtein

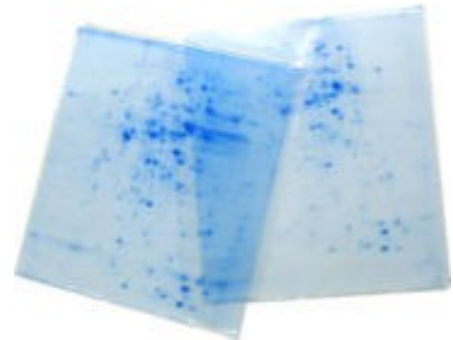
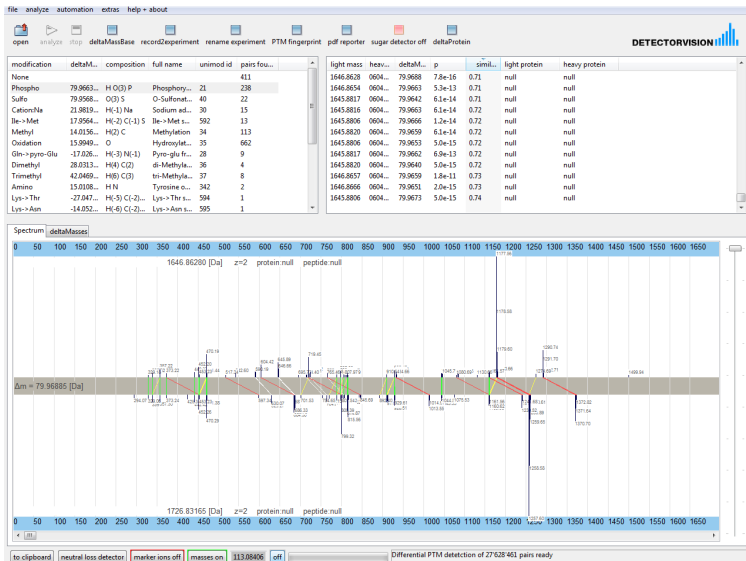


deltaMassBase report: Wed Mar 28 09:26:18 CEST

Gaussian fits to deltaMassBase signals			
deltaMass	pairs	height	sigma
15.996540	1229	219.0	0.0045
132.079034	384	238.6	0.0013
88.052590	331	189.5	0.0014
176.105243	255	135.7	0.0015
14.015334	171	104.2	0.0013
79.966320	247	63.3	0.0031
275.133336	215	41.9	0.0041
17.026619	143	58.5	0.0020
44.026686	69	47.0	0.0012
128.095364	117	35.9	0.0026

pdf reports provided

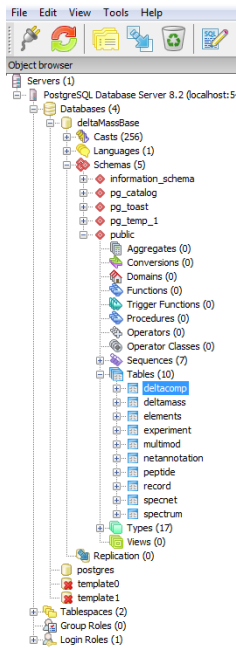
¹ Minimum system recommendations: 8 Gigabyte RAM, Display 1680*1050 pixels. Multicore processor recommended (best buy: Intel I7 2600 K)



deltaMasses can be used for LC-workflows and 2D-gels after high-accuracy mass spectrometry

deltaMasses PTM Discovery Workstation. Screenshot. Learn more from MS/MS data you already acquired and identify previously unexplained spectra

deltaMassBase

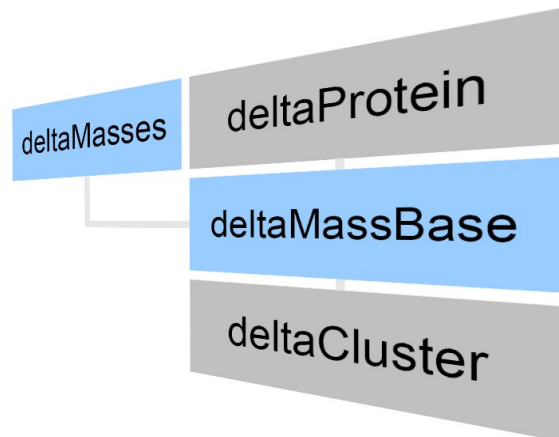


- The database system
- Runs the free of charge postgresQL system
- Keeps track of up to a million spectra
- Included in Discovery and Personal Edition
- Required to use deltaProtein or deltaCluster
- Hub for protein modification based biomarker discovery



deltaCluster

- The multicore / supercomputing extension
- Ideal for Windows Quadcore+ Systems
- Needs deltaMassBase installed
- Compares spectra across runs



Example: deltaCluster on an HP xw8600



On an HP xw8600 double quadcore desktop, comparing 500'000 spectra against each other runs about 7 times faster than on a comparable single core CPU. This example deltaCluster computation consists of 125 billion MSMS comparisons and is done in less than a day.

References

- Database independent detection of isotopically labeled MS/MS spectrum pairs
<http://dx.doi.org/10.1016/j.jchromb.2004.12.009>
- The Mass Distance Fingerprint: A statistical framework for *de novo* detection of predominant modifications using high-accuracy mass spectrometry
<http://dx.doi.org/10.1016/j.jchromb.2007.04.0>
- Protein identification by spectral networks analysis
<http://www.pnas.org/cgi/content/abstract/104/15/6140>
- Modificomb, a new proteomic tool for mapping substoichiometric PTMs, ...
<http://www.mcponline.org/cgi/content/abstract/5/5/935>

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