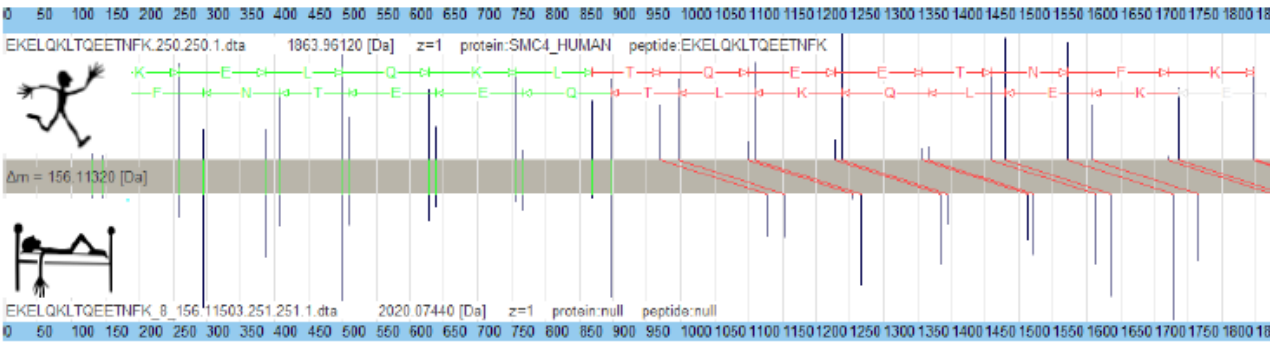
Protein Modification based Biomarker Discovery

The difference in protein content :

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
- 186 installations in 70 laboratories, 20 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 resiude. This can be visualized by „green“ and „red“ channels, respectively. deltaMasses automatically detects such fragmentation spectra showing "paired" characteristics.



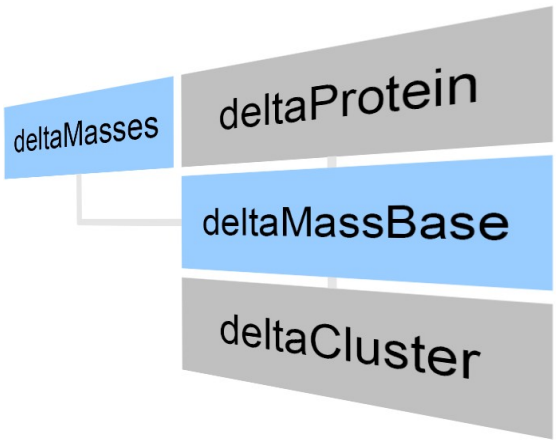
Green channel = no modification; mass unchanged. Red channel = fragment contains modification.

deltaMasses™

DETECTORVISION

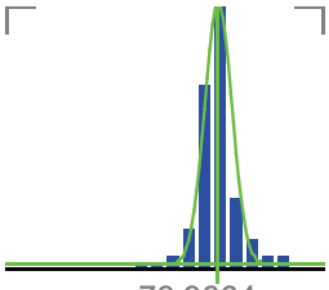
deltaMasses consists of four parts

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



deltaMasses

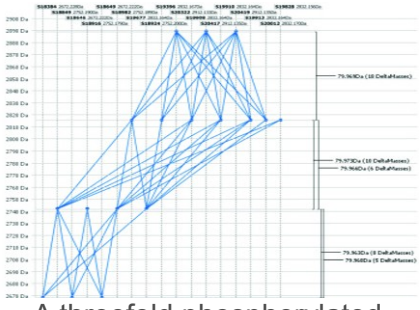
- The main PTM detection tool
- Easily installed and used
- Runs on Windows 2000/XP/Vista
- Implements the deltaMass Fingerprint
- Connects to Mascot Servers



deltaMass fingerprint

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

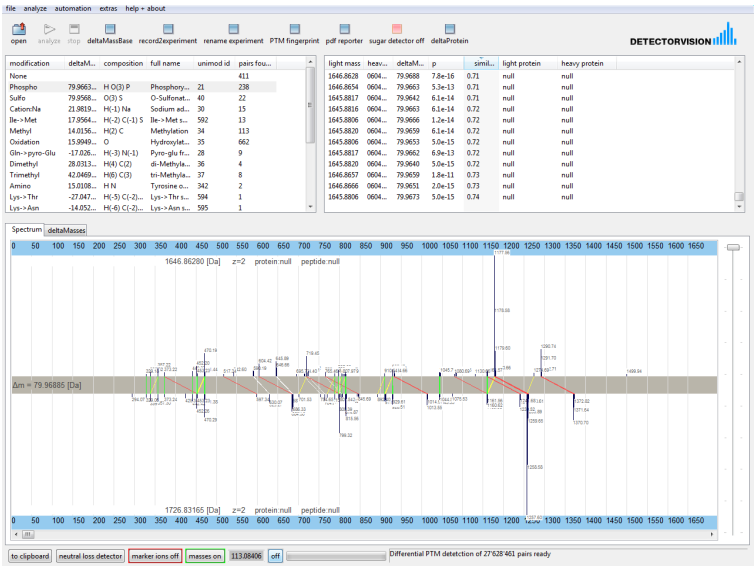
Gaussian fits to deltaMassBase signals

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

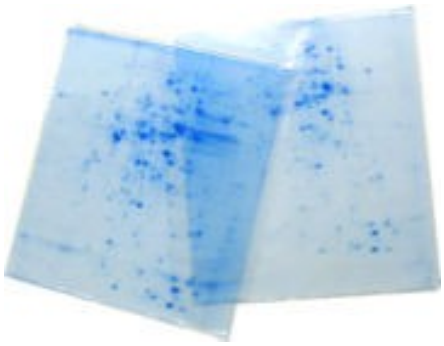
pdf reports provided

deltaMasses™

DETECTORVISION

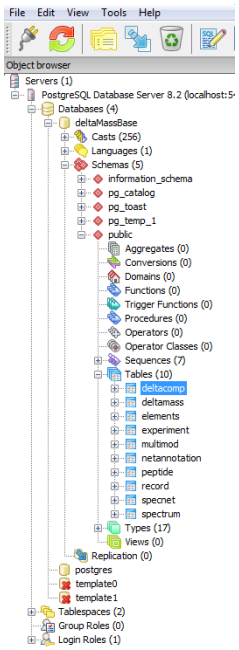


deltaMasses PTM Discovery Workstation. Screenshot. Learn more from MS/MS data you allready aquired and identify previously unexplained spectra



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

deltaMassBase



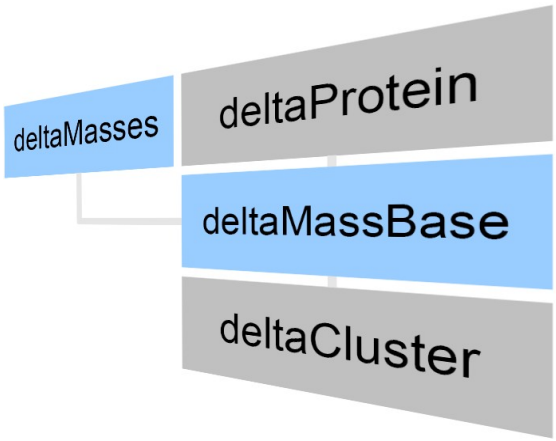
- The database system
- Runs the free of charge postgreSQL system
- Keeps track of up to a million spectra
- Included in Discovery and Personal Edition
- Required to use deltaProtein or deltaCluster
- Hub for protein modification based biomarker discovery

deltaMasses™

DETECTORVISION

deltaCluster

- The multicore / supercomputing extension
- Ideal for Windows Quadcore Systems
- Also on UNIX / LINUX equipment
- Needs deltaMassBase installed
- Compares spectra across runs
- Requires a Discovery Edition



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 on this state-of-the art desktop PC.

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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- Discovery Edition License: 4100.- € [1]
- Includes one year of free updates
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- License requests to info@detectorvision.com
- Available for Windows 2000, XP, Vista
- Discovery Edition Includes deltaCluster and deltaProtein

1 Subject to change at any time. Please ask for a quotation