

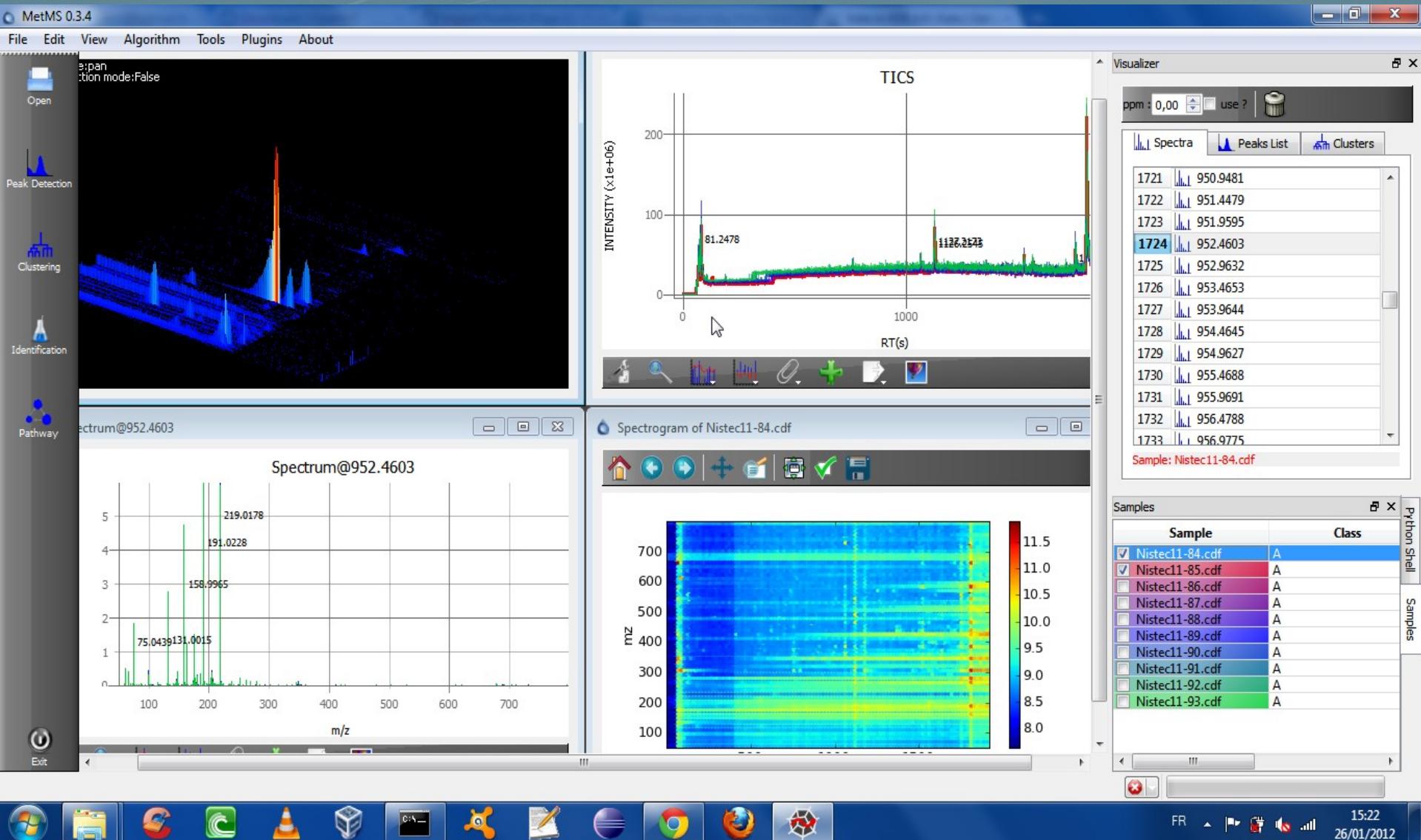
MetMS

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Aim of the project

- Treat **MRM data** :
 - **detection and integration** of features
 - **Alignment**
 - « **Clustering** » : remove fragments/ adducts, isotopic cluster
 - **Identification** (based on the « *Seven Golden Rules for heuristic filtering of molecular formulas obtained by accurate mass spectrometry* »
O.Fiehn, 2006)
- Then, treat **High Resolution data** (Orbitrap)

Overview



Languages: Python, C, C++, R

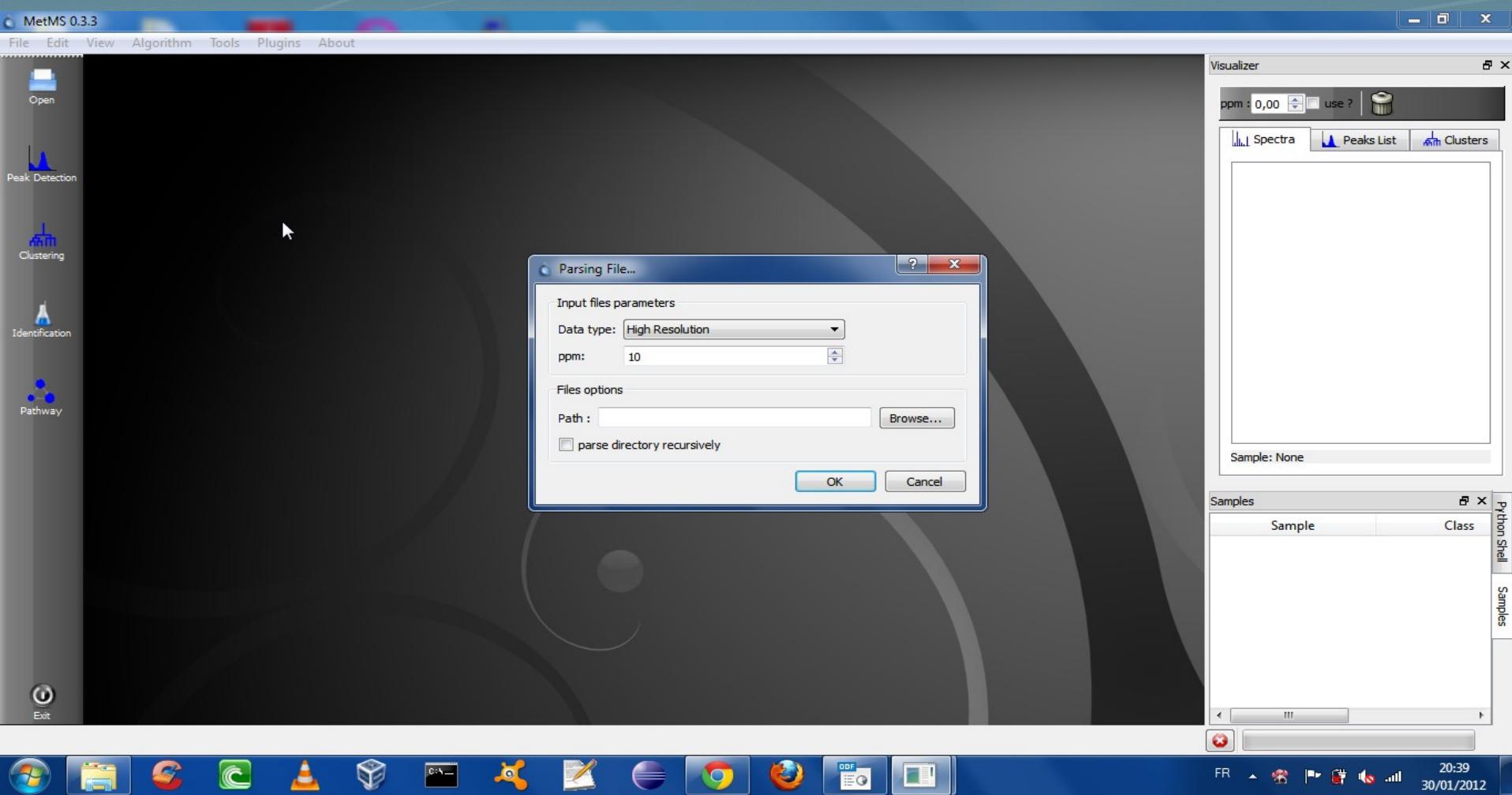
Platforms: Linux, Windows

Graphics: Qt GraphicsScene/View Framework, backend OpenGL



FR 15:22
26/01/2012

Import Function

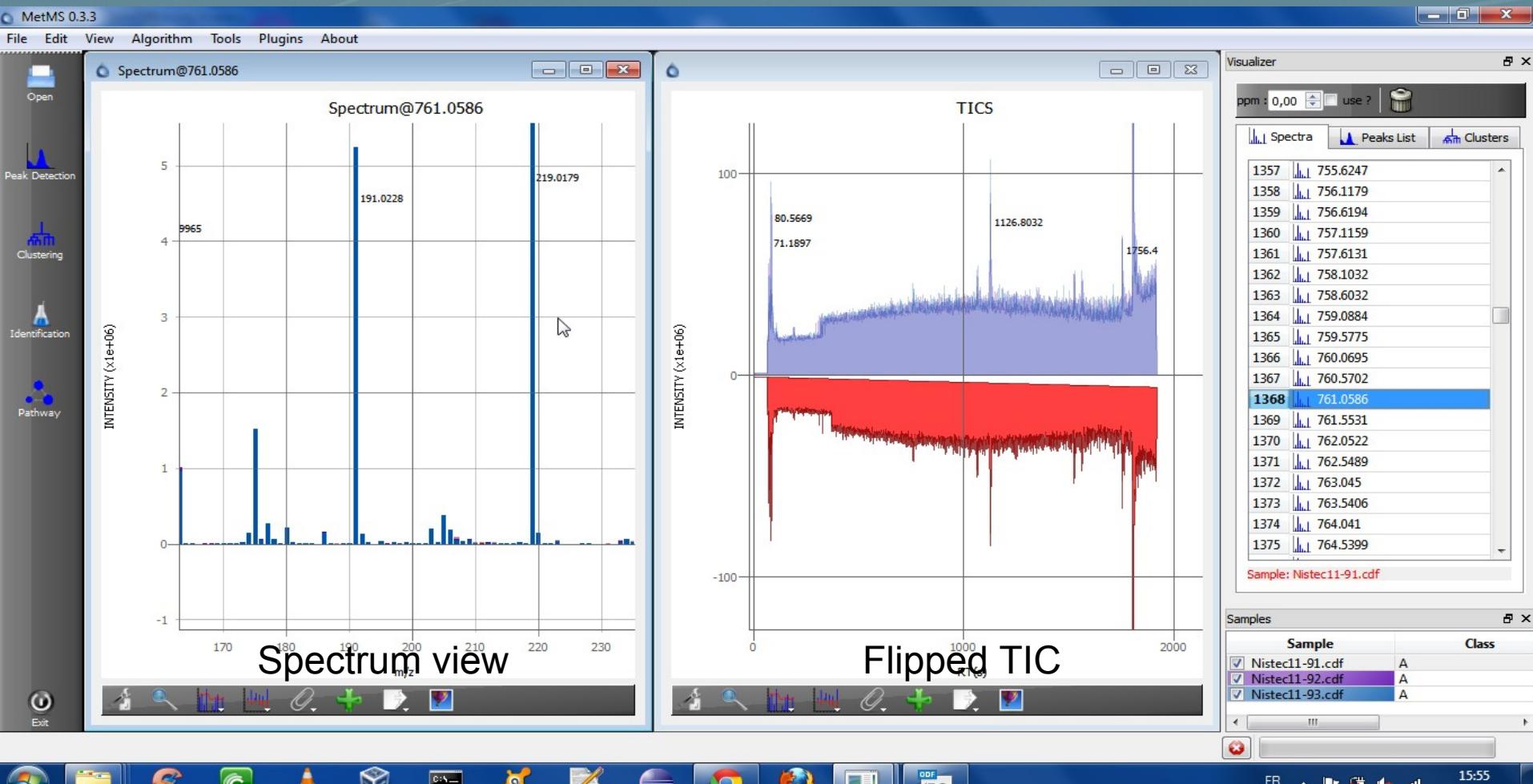


Resolutions : **unitary** (initially designed for MRM), **High Resolution**

File formats: **mzXML(MSn)**, **netCDF(MS1)**

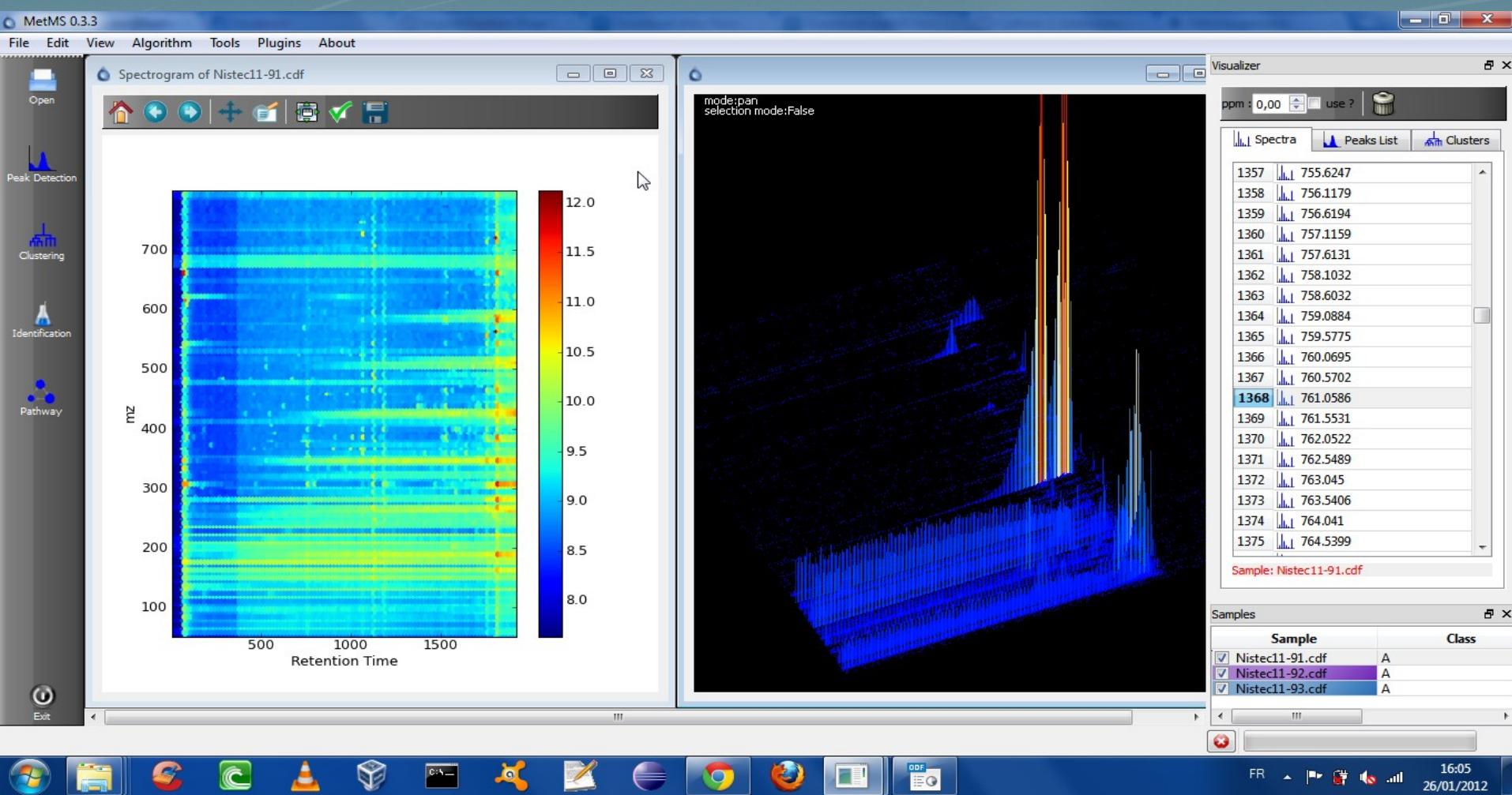
Multiple import

Visualization tools



- Efficient zooming and panning
- Smoothing
- Flip
- Annotation
- Save to .png, .svg

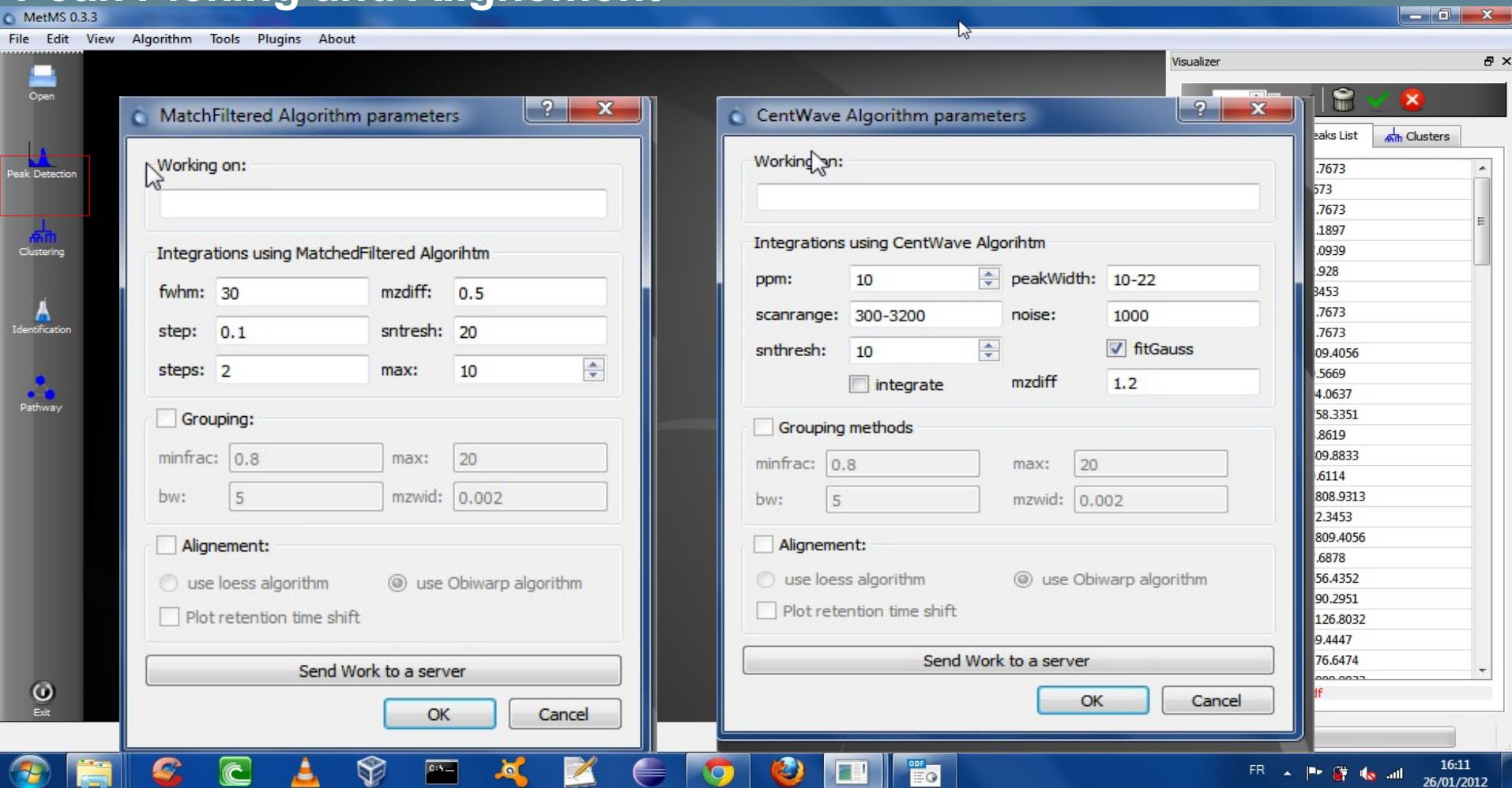
Visualization tools



Spectrogram view(2D view)

3D view (first designed to MRM sample)

Peak Picking and Alignment



- XCMS detection and integration algorithms (**matchFiltered, Centwave algorithms**)
- XCMS Alignement (**ObiWarp**)
- Home made alignment (**polynomial fitting, timeWarping**)

By default **parallel computing** on all the cores of the computer

Peak Picking and Alignment

MetMS 0.3.3

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Open



Peak Detection



Clustering



Identification



Pathway



Exit

42		195.0728/1186.7861
43		195.0873/66.4457
44		200.2014/1565.2544
45		201.2043/1564.7598
46		205.0858/1126.7368
47		209.0917/170.2458
48		212.1181/557.8409
49		222.1833/1564.7598
50		223.0959/1126.7368
51		224.0996/1126.7368
52		231.0437/83.5743
53		245.0784/1126.7368
54		246.0815/1126.7368
55		247.2416/1809.8178
56		249.0741/1186.7861

For each feature in the peak list

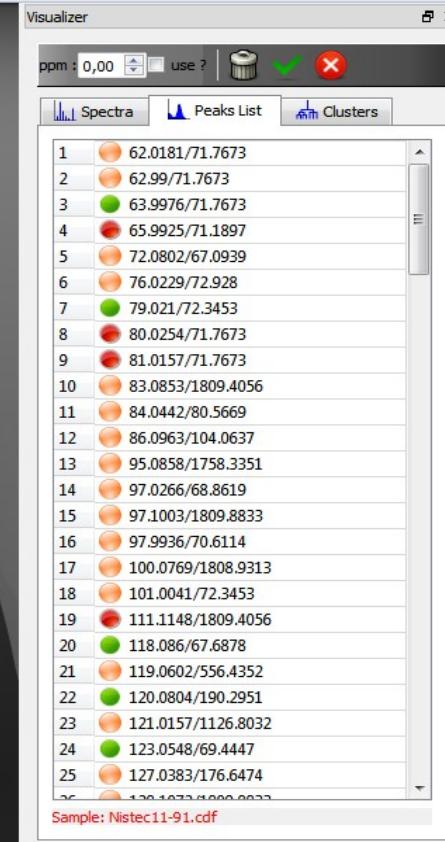
For each spectrum corresponding to this feature

If the mass is not present (red)

If the mass is present

if one of the M+1 is present (green)

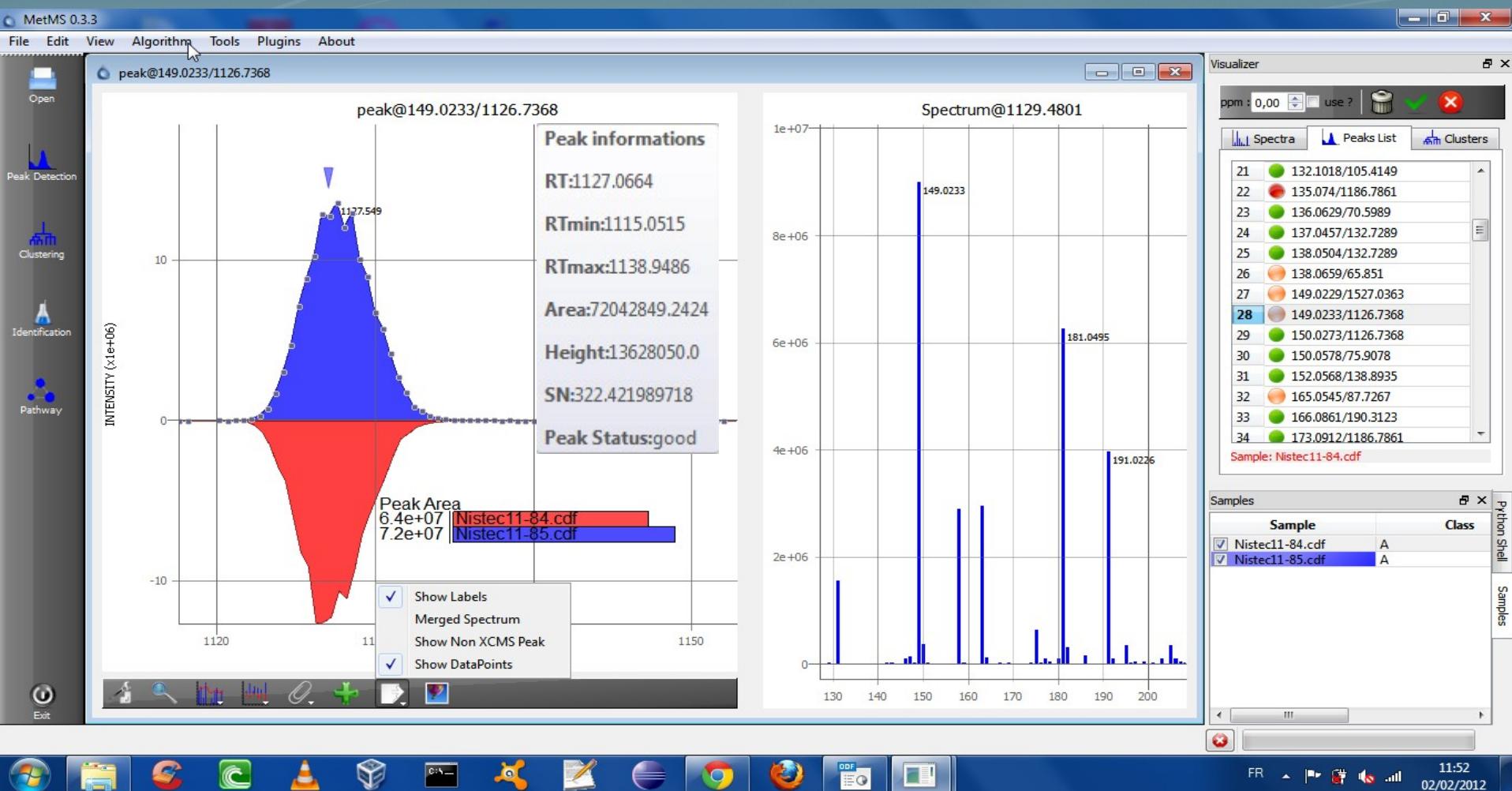
else orange



Automatic detection leads to false positive features :

→ Feature validation based on raw data

Feature Visualization



Peak information tooltip
Compare intensities among samples directly
Summary tables...

101.0062/11.7489	814459.84	0.0
104.0631/74.0886	0.0	730679.29
113.0359/92.528	1911141.62	0.0
118.086/67.6522	3257218.61	5672130.59
119.0602/558.85	2974517.64	0.0
120.0803/190.0776	9402675.12	11515285.98
121.017/1127.0664	0.0	1798509.92
123.055/69.124	5828484.75	6408067.83
128.107/1809.7586	1046810.48	1086626.95

Clustering

The screenshot shows a software interface for mass spectrometry data analysis. The main window has a menu bar with File, Edit, View, Algorithm, Tools, Plugins, and About. On the left is a vertical toolbar with icons for Open, Peak Detection, Clustering, Identification, and Pathway. A status bar at the bottom shows the version 1.0.0.0.

Clustering parameters Dialog (Left):

- Working on: Nistec11-168.cdf;Nistec11-165.cdf;Nistec11-166.cdf;Nistec11-167.cdf
- Algorithms parameters:
 - rt drift: 6
 - isocluster length: 6
 - gap: 0
 - positive mode (radio button selected)
- Adducts(name, mass, nmol):
 - 1 [M+H]+, 1.0072277, 1
 - 2 [M+2H]2+, 2.0144553, 1
 - 3 [M+Na]+, 22.98992, 1
- Buttons: UnCheck All

Clustering parameters Dialog (Right):

- Working on: Nistec11-168.cdf;Nistec11-165.cdf;Nistec11-166.cdf;Nistec11-167.cdf
- Algorithms parameters:
 - rt drift: 6
 - isocluster length: 6
 - gap: 0
 - positive mode (radio button selected)
 - Monotonic IC (checkbox checked)
 - idms length: 0-0
 - keep bad peaks (checkbox unchecked)
 - resolve conflicts (checkbox checked)
- Adducts(name, mass, nmol):
 - 1 [M+H]+, 1.0072277, 1
 - 2 [M+2H]2+, 2.0144553, 1
 - 3 [M+Na]+, 22.98992, 1
- Fragments(name, mass, nmol):
 - 1 CH2, 14.0156, 1
 - 2 CH2(C13), 15.019, 1
 - 3 O1, 15.9948, 1
- Buttons: UnCheck All, OK, Cancel

Controller Window:

- ppm: 0.00
- use? (checkbox unchecked)
- Spectra, Peaks List, Clusters tabs (Peaks List tab selected)
- Peak list table:

Mass	Abundance
149.0941	1194.0613
150.0971	1194.0613
151.0907	1194.0613
154.9282	62.8814
156.9252	62.8814
164.0716	191.4038
165.0887	1194.0613

List of known adducts/fragments
In +/- ionization mode

Look for **Isotopic patterns** in peak list
Adducts/fragments
→ Make clusters of related peaks

Clustering

Group features by retention time

For each group

For each featur $M_f(m_f, RT_f)$

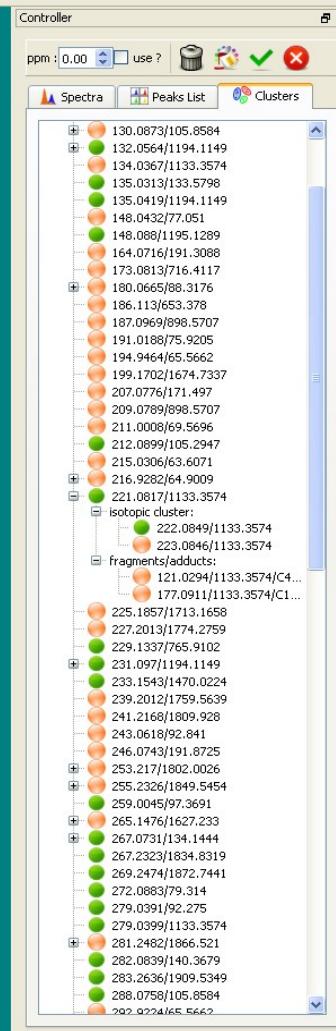
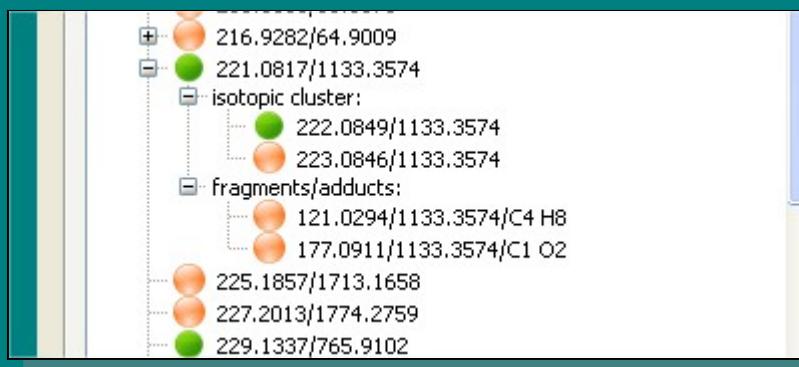
Compute all potential M_0 that can lead, by fragmentation or adduct, to M_f

For each M_0 in **the raw data** (*not in Camera*)

If the M_0 is in the group then attach M_f to M_0 (*not in Camera*)

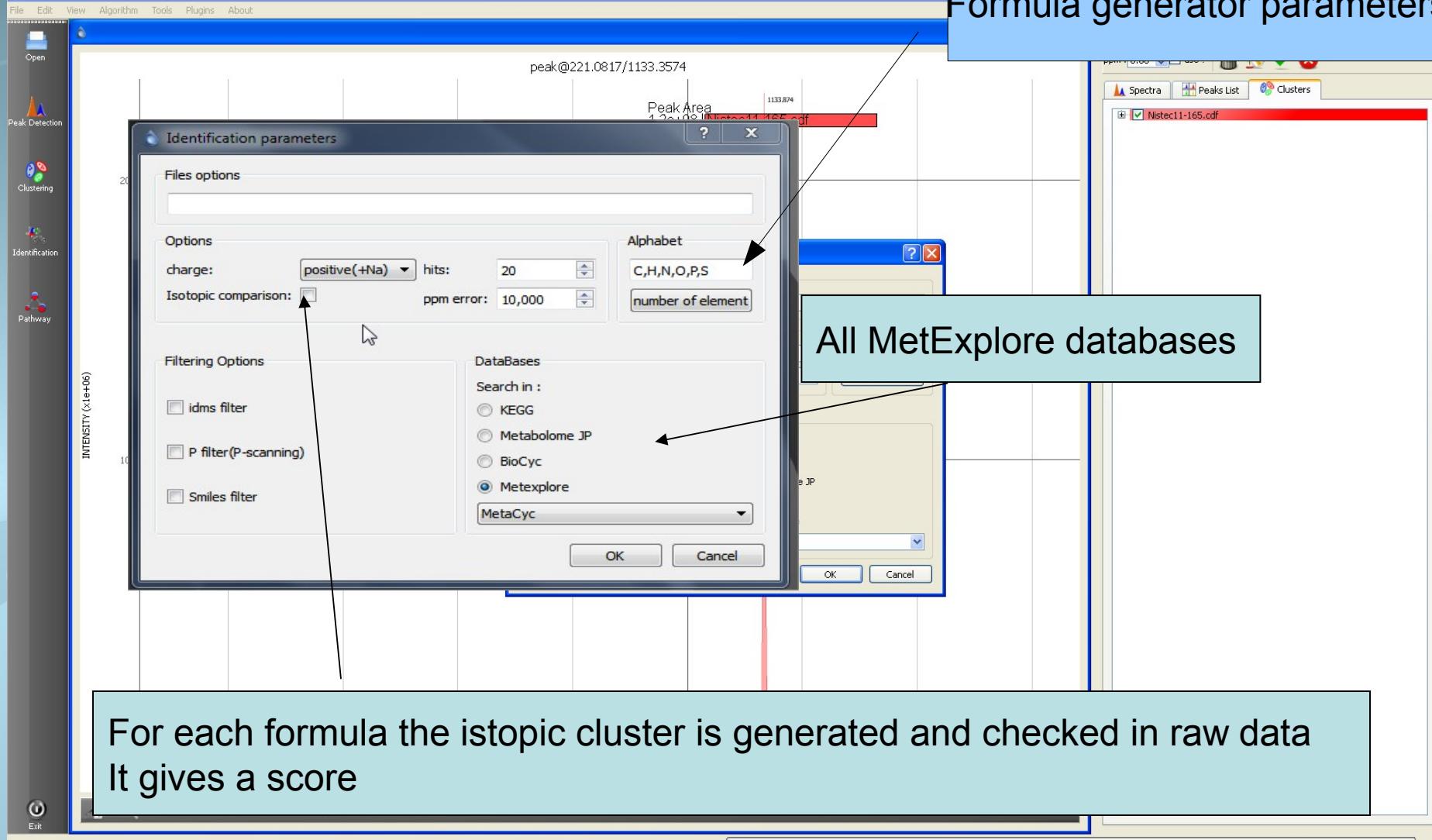
Clustering

File Edit View Algorithm Tools Plugins About



Identification

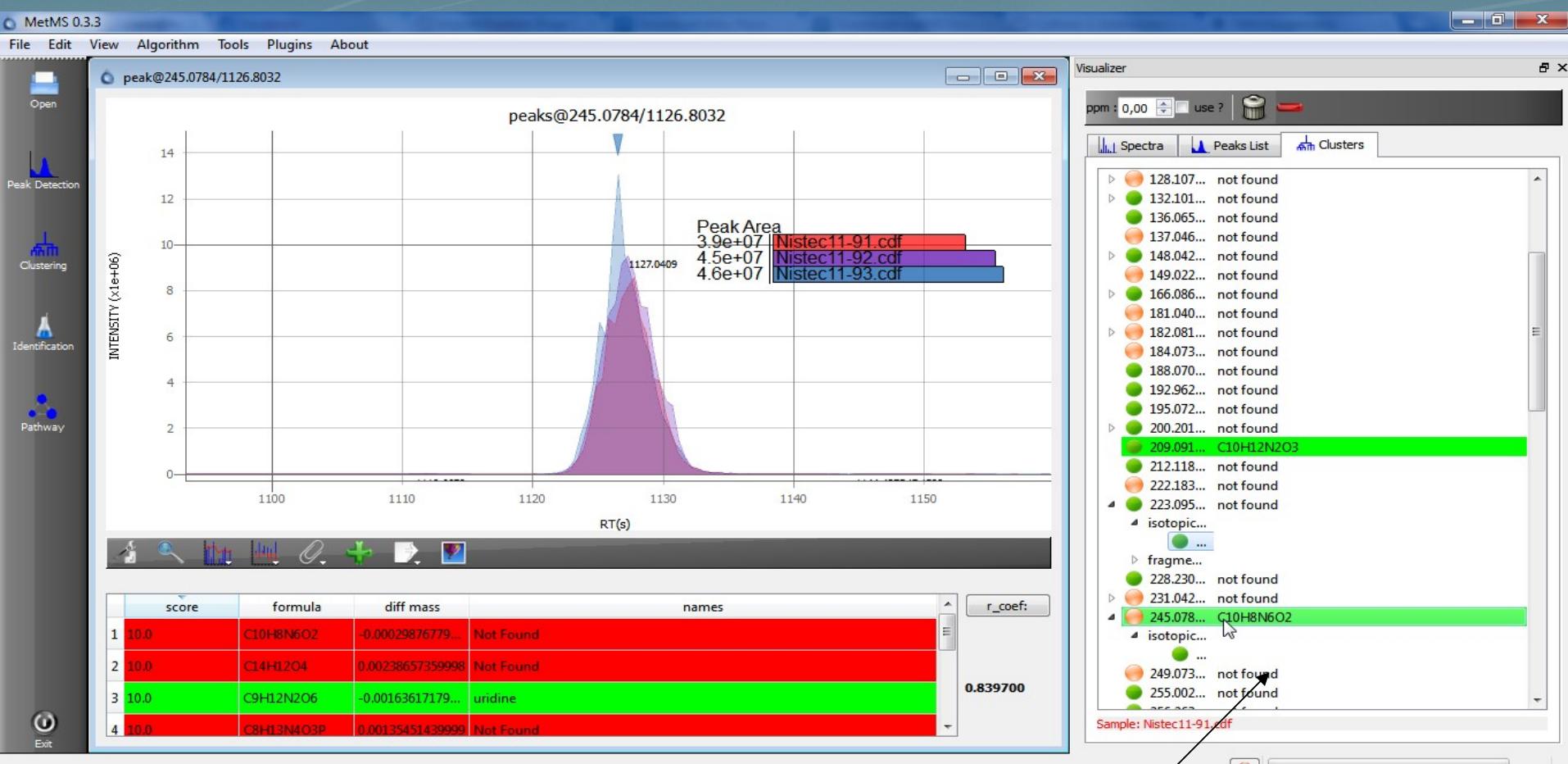
Formula generator parameters



Identification of all M0 found

Then Export to .csv to perform statistics

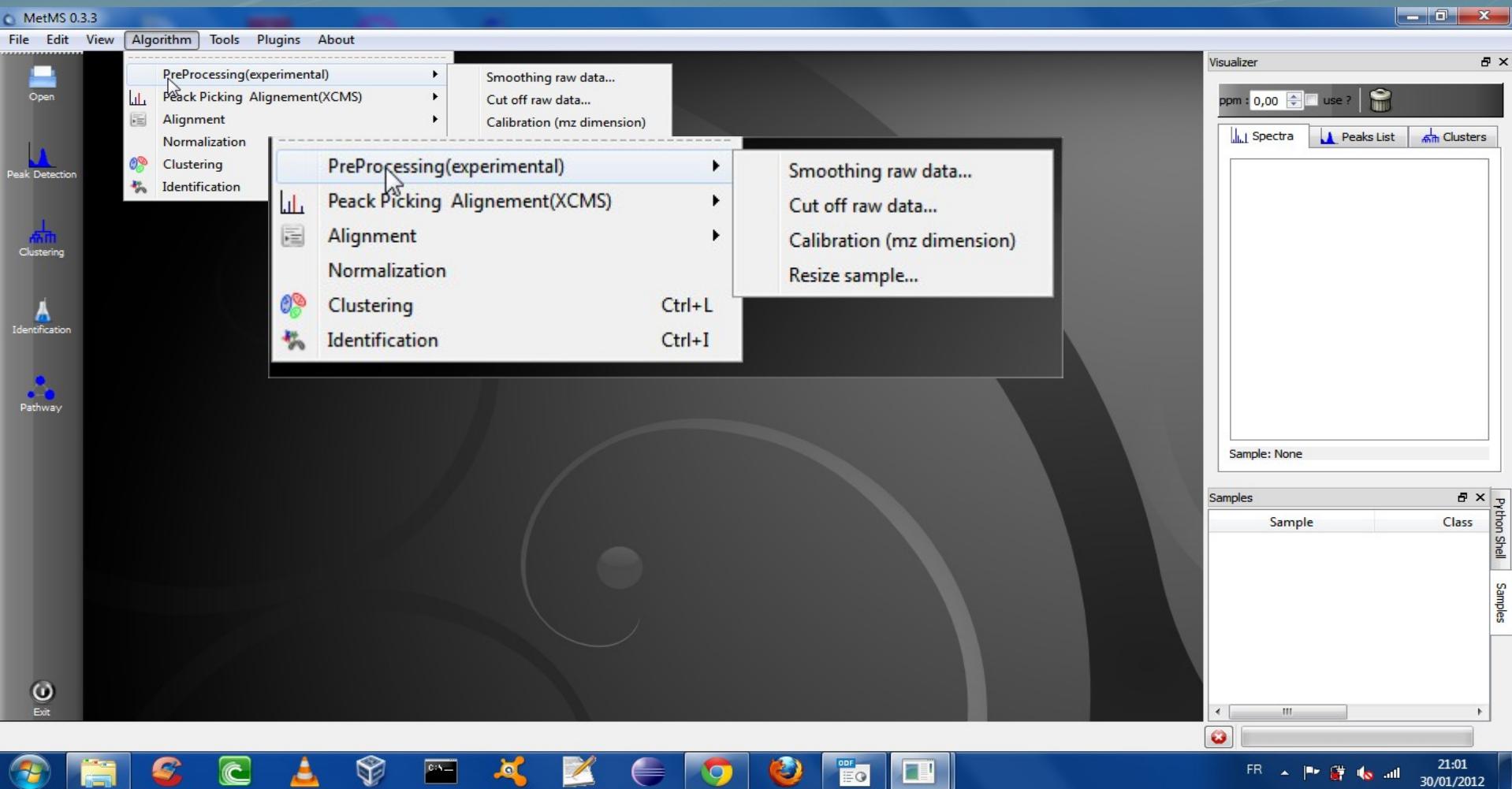
Identification



Identified features (best formula shown)

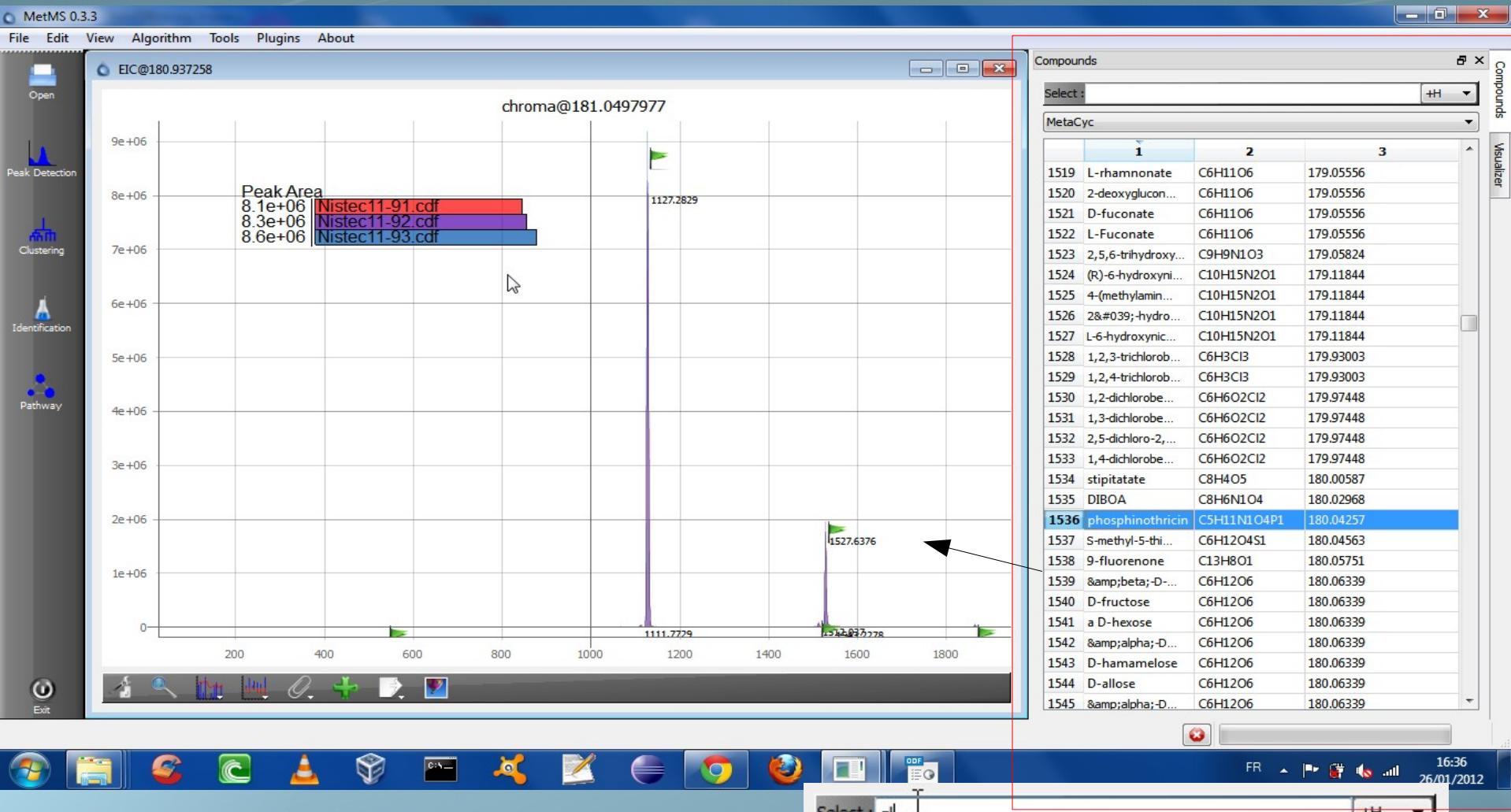
Uridine found in 3th place with good correlation of peak shapes (0,84)

Other helping functions



Useful preprocessing functions

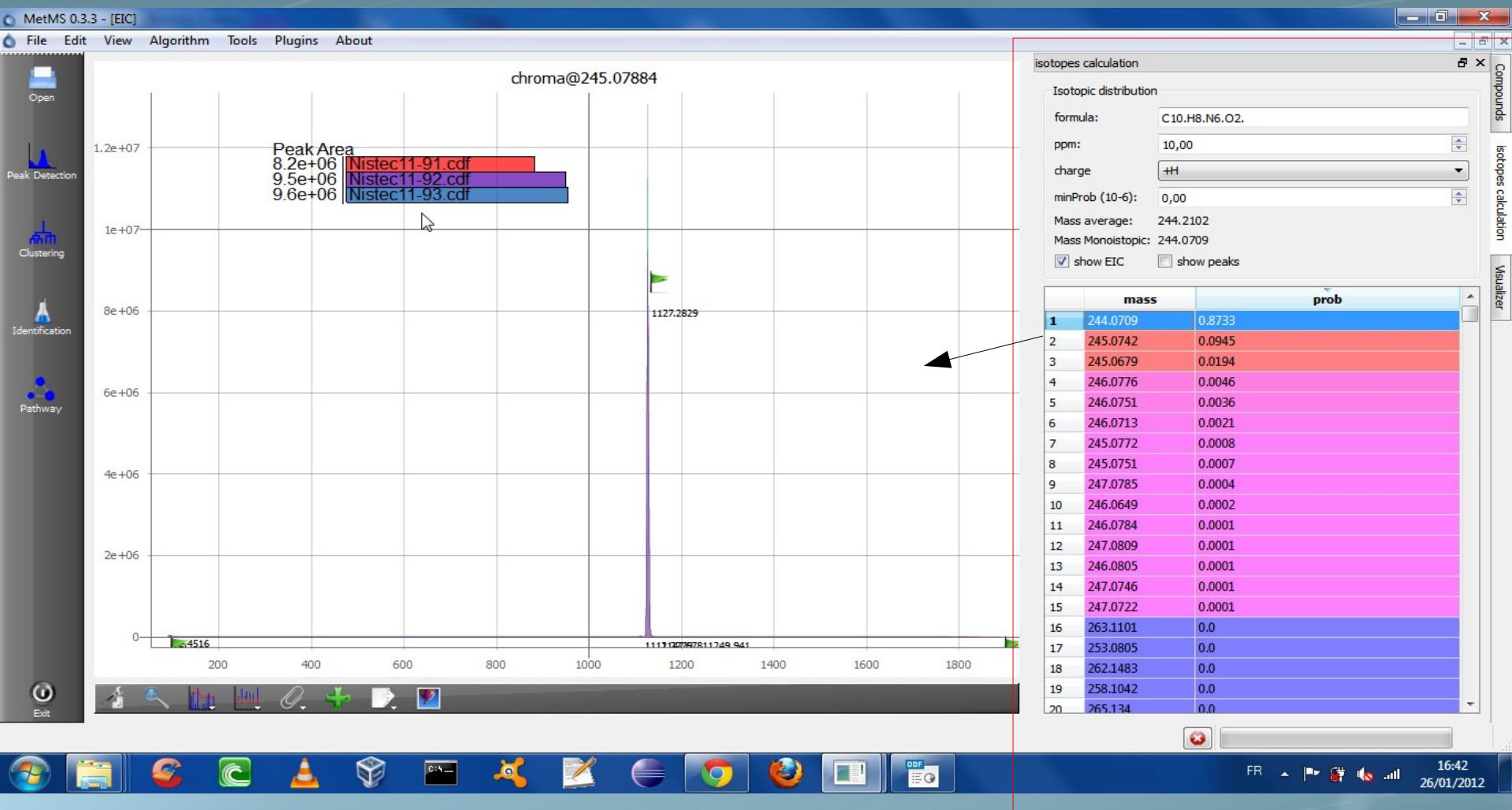
Other helping functions



Compute EIC for well known compounds (based on exact mass)

Home made algorithm for Peak detection and integration

Other helping functions



Isotopic cluster calculation from chemical formula

→ easy to check if the isotopic cluster of one compound is present

Other helping functions

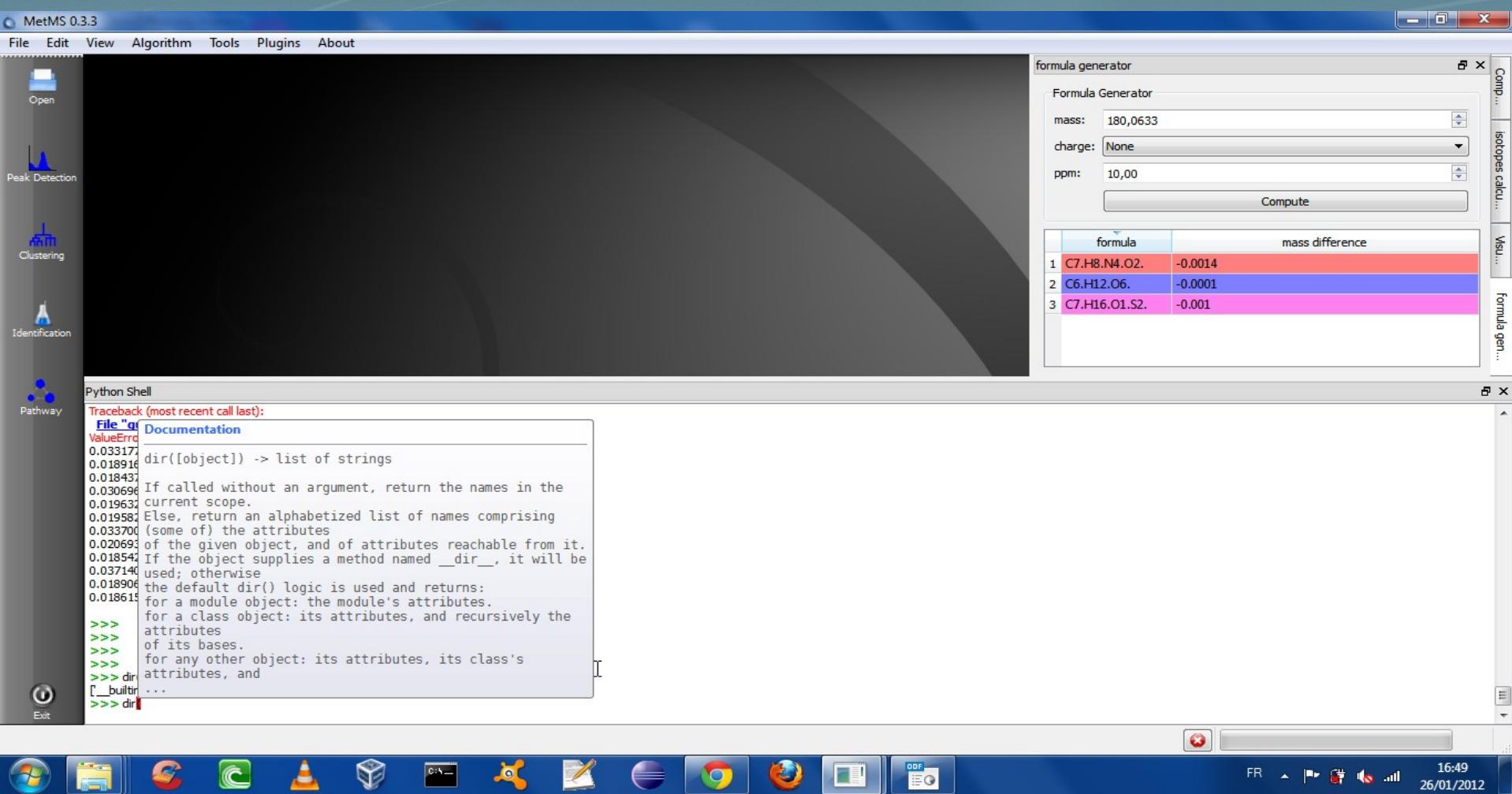
The screenshot shows the MetMS 0.3.3 software interface. The main window has a dark background with a large circular watermark in the center. On the left, there is a vertical toolbar with icons for Open, Peak Detection, Clustering, Identification, Pathway, and Exit. The top menu bar includes File, Edit, View, Algorithm, Tools, Plugins, and About. A floating window titled "formula generator" is open on the right, containing a "Formula Generator" panel with fields for mass (180,0633), charge (None), and ppm (10,00), and a "Compute" button. Below this is a table with three rows:

	formula	mass difference
1	C7.H8.N4.O2.	-0.0014
2	C6.H12.O6.	-0.0001
3	C7.H16.O1.S2.	-0.001

The status bar at the bottom shows various system icons and the date/time: 16:46, 26/01/2012.

Show chemical formulas corresponding to one mass
(check of elementary chemical rules, saturation, lewis, elements ratios...)

Other helping functions



- MetMS embeds a python shell (scriptable)
- Plugin system to extend the application