mzScope: fast MS data visualization and exploration tool based on the mzDB file format

Christophe Bruley[1*], Véronique Dupierris[1*], Anne-Marie Hesse[1*], David Bouyssié[2*]

[1] Laboratoire Biologie à Grande Echelle, U1038 INSERM/CEA/UGA, BIG, CEA Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9
[2] Institut de Pharmacologie et de Biologie Structurale, CNRS UMR5089, Université de Toulouse, 205, route de Narbonne, 31077 Toulouse
* ProFi, Proteomic French Infrastructure

mzScope is a visualization and exploration tool written in Java allowing users to visualize scans and chromatograms extracted from mzDB file. Thanks to the mzDB format, chromatogram extraction is usually performed in few hundred of milliseconds over a 2 or 3h gradient time range. Since mzDB format support DIA MS data, mzScope also provides MS2 chromatogram extraction within a selected isolation window that can be performed on user supplied m/z values or from ion fragment masses imported from a spectral library. Those features combined with the efficiency of the mzDB format make mzScope a suitable tool for MS data visualization and exploration or for raw MS signal comparison.

Chromatograms Extraction

MS1 chromatogram extraction from a user's specified mass over charge ratio (m/z) value or from a mass range selected from an MS scan or from a list of precursor's m/z values

Fragmentation events matching to the extracted m/z can also be overlaid.
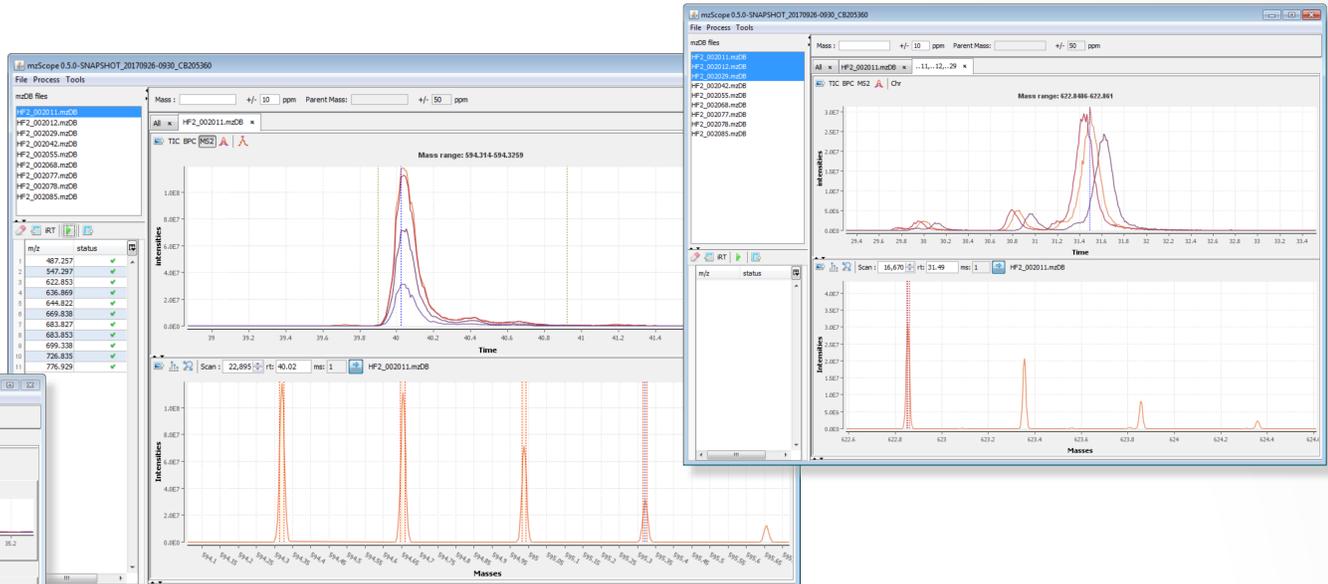
Multiple Extraction

extraction can be applied to a single mzDB file or to a set of MS files simultaneously. The extracted chromatograms can be visualized through multiple synchronized views or stacked in a single view to be easily compared.

Peak/Feature detection

The software can also perform elution peaks detection by using the algorithm implemented in the Proline software or peak grouping into MS features through the Proline deisotoping algorithm.
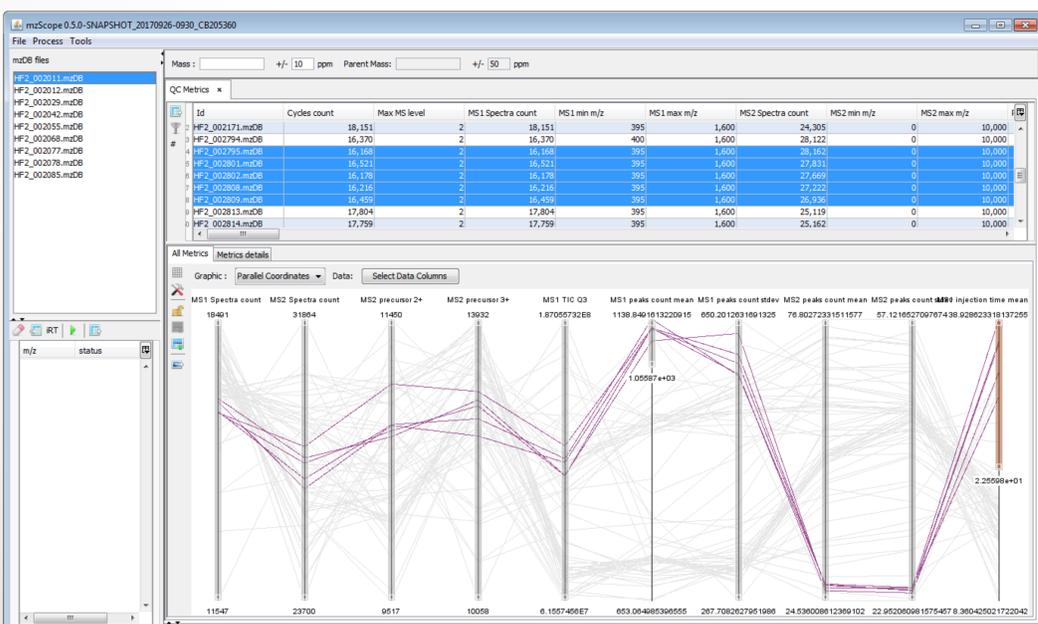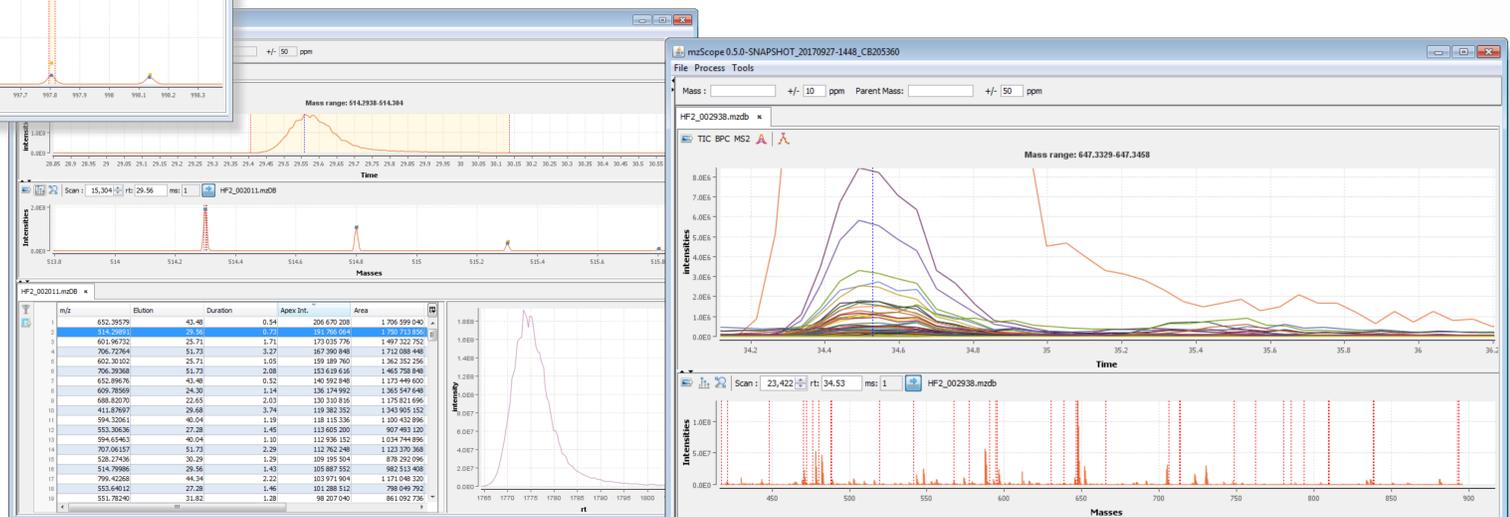
MS/MS fragment chromatograms from DIA run

MS2 chromatogram extraction within a selected isolation window that can be performed on user supplied m/z values or from ion fragment masses imported from a peaklist or spectral library.

mzScope :
http://proline.profiproteomics.fr

raw2mzdb conversion tool :
https://github.com/mzdb/pwiz-mzdb

ID free Quality Control metrics

mzScope supplies various metrics computed from the MS data that can be used as identification-free quality control of the Liquid Chromatography Mass Spectrometry coupling.