

UniDec

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Chapter 1

Main Page

[UniDec](#) is a Bayesian deconvolution program for deconvolution of mass spectra and ion mobility-mass spectra.

It was originally published in: M. T. Marty, A. J. Baldwin, E. G. Marklund, G. K. A. Hochberg, J. L. P. Benesch, C. V. Robinson, *Anal. Chem.* 2015, 87, 4370–4376.

Detailed descriptions of the algorithm are provided in the paper. Please cite us if you use [UniDec](#) in your research.

[UniDec](#) may be downloaded from unidec.chem.ox.ac.uk.

Please contact michael.marty@chem.ox.ac.uk for questions, suggestions, or with any bugs.

Installing

Python

There are several python libraries that [UniDec](#) will depend on.

matplotlib numpy scipy wxpython natsort twython pymzml networkx

With the exception of wxpython, which can be installed from the [web](#), all of these can be installed from the command line with (for example):

```
pip install natsort
```

Note: I would highly recommend setting up 64-bit Python as the default. MS data works fine with 32-bit, but IM-MS data is prone to crash the memory. If you are getting memory errors, the first thing to try is to upgrade the bit level to 64.

Downloading the Binaries

As described below, the Python code presented here relies on two critical binaries, UniDec.exe and UniDecIM.exe.

These binaries are available for download at unidec.chem.ox.ac.uk.

These binaries should be deposited in the /unidec_bin directory once downloaded.

If you want to convert Waters .Raw files, you will also need to add cdt.dll (for IM-MS) and MassLynxRaw.dll (for MS) to the same directory. These files can be found [here](#) with support numbers DWNL134825112 and DWN-L134815627. See below for more specifics.

I have binaries built for Mac and Linux as well. They are a bit slower than the Windows version because they are compiled with gcc rather than the Intel C Compiler, but they are perfectly functional and still pretty darn fast. I can send these to you on request.

Compatible File Types

[UniDec](#) is built to open .txt files using `numpy.loadtxt`.

For MS data, it opens a two-column either a tab or space delimited list of m/z and intensity values.

For IM-MS, it will open a three-column tab or space delminated list of m/z, arrival time (or bin), and intensity values. Sparse matrices are fine for IM-MS.

Recent versions are compatible with a text header at the beginning of the file. It will skip lines until it reaches the start of the data.

For Water's .raw files, [UniDec](#) is bundled with converters (CDCReader.exe and rawreader.exe) to convert the data to .txt. It will compress the retention time dimension into a single spectrum. A single file can be opened directly, or multiple files can be converted using Tools > Simple Batch Process Raw to Txt. For a fancier conversion such as extracting specific functions or scans, try Tools > Raw to Txt Conversion Wizard.

Water's converters will need `MassLynxRaw.dll` (32-bit, for MS) and/or `cdt.dll` (64-bit, for IM-MS) in the same directory as the converter executables (the unidec_bin folder or the top directory).

For Thermo .raw files, we do not currently have the conversion libraries built in (an enterprising developer should take this on...). The best way to load these files is to convert to mzML using [Proteowizard](#). [UniDec](#) will open mzML file as if they are a text file. We utilize `pymzML` for this. Cite them at: *Bald, T., Barth, J., Niehues, A., Specht, M., Hippler, M., and Fufezan, C. (2012) pymzML - Python module for high throughput bioinformatics on mass spectrometry data, Bioinformatics, doi: 10.1093/bioinformatics/bts066*.

[UniDec](#) Documentation

This documentation is for the Python engine and GUI.

My goal is that this documentation will allow you to utilize the power of the [UniDec](#) python engine for scripting data analysis routines and performing custom analysis. Also, it will allow you to add new modules to the [UniDec](#) GUI.

I'm still working on documenting some of the windows and extensions, but the core features should be here.

The C code is proprietary and not open source. The copyright is owned by the University of Oxford. If you are interested in the C source code, please contact me. It should be possible to share with appropriate licensing or research agreements.

[UniDec](#) Architecture

[UniDec](#) is bilingual. The core of the algorithm is written in C and compiled as a binary. It can be run independently as a command line program fed by a configuration file.

The Python engine and GUI serve as a very extensive wrapper for the C core.

The engine (`unidec.py`) can be operated by independently of the GUI. This allows scripting of [UniDec](#) analysis for more complex and high-throughput analysis than is possible with the GUI. The engine contains three major subclasses, a config, data, and peaks object.

The GUI is organized with a Model-Presenter-View architecture. The main App is the presenter (`GUniDec.py`). The presenter contains a model (the [UniDec](#) engine at `unidec.py`) and a view (`mainwindow.py`). The presenter coordinates transfer between the GUI and the engine.

Getting Started

Here is some sample code for how to use the engine.

```
import unidec

file_name="test.txt"
folder="C:\\\\data"
```

```
eng=unidec.UniDec()
eng.open_file(file_name, folder)
eng.process_data()
eng.run_unidec(silent=True)
eng.pick_peaks()
```

In reading the documentation, it is perhaps best to start with the `unidec.UniDec` class. The main GUI class is `GUniDec.UniDecApp`.

Licensing

[UniDec](#) is free for noncommercial use under the [UniDec Academic License](#)

Commercial licensing is available. Details are provided at the bottom of the Academic License.

The Python GUI and engine are licensed under the [GNU Public License \(v.3\)](#).

Change Log

v. 1.0.10

Added preset defaults for the **Exactive EMR** under "High-resolution Native". The previous high-resolution preset is now "Isotopic Resolution".

v. 1.0.9

Small change in C code so that the peaks are now multiples of the mass bin size. Will need the updated [binary](#).

Cleaned up single click mass calculations on the raw data plot so that a zoom out is not registered as a click. Control + click will register a click without zooming out.

v. 1.0.8

Fixed Waters IM-MS conversion errors! Thanks to Tim Allison for teaming up to track down the source of these problems. It should now work for any IM-MS file, but it will require 64-bit in everything.

v. 1.0.7

Added a **mass tolerance on matching**. Now, matches that fail to come within a certain tolerance will be ignored.

v. 1.0.6

Added an experimental window for grid deconvolution. This is close to the original implementation of [UniDec](#) back when it was a Nanodisc-only script in Mathematica (see Marty, et. al. JASMS 2014). It has come a long way, but it is still pretty crude.

v. 1.0.5

Added directory name to file names window. Added smarter labeling of plots in data collector. Added ability to specify Variable 1 units in data collector and add this as an axis label. Added support for viridis and other new color maps in matplotlib 1.5.0.

v. 1.0.4

Fixed bugs in parallel processing for Data Collector Utility and Import Wizard.

v. 1.0.3

Added Waters .raw file open and .raw to .txt batch conversion to drag and drop.

v. 1.0.2

Bug fix on KD fit parallel processing.

v. 1.0.1

Added **drag and drop** on the main window. Drag a single file into the plotting area to open it. Drag multiple files to

run them in batch mode.

v. 1.0

Total rewrite of the program to separate the GUI and engine. The engine allows scripting of [UniDec](#) in Python without the GUI. Added documentation and cleaned up code with major refactoring and simplification. Most changes are in the back end and will hopefully be invisible to people using the GUI.

- New Features:
 - Added **automatic peak width** determination with Ctrl + W or Tools > Automatic
 - Added **"Display Mass Differences"** to right click menu in the peak panel. This will display the mass differences between each peak and the selected peak. Very useful (in my humble opinion).
 - Left clicking on two peaks in the m/z spectrum will **solve for the mass from the two m/z values**.
 - To allow left clicking on zoomed region, holding ctrl while clicking will prevent rescaling the axes.
 - Right click on the m/z spectrum will determine the **max and min m/z value from the current zoom on the plot**.
 - Zeroing the zoomed region is now a double right click on the m/z spectrum (useful for eliminating noise spikes).
 - **Middle click** on any plot now opens a **save figure dialog** to allow you to save that specific figure.
 - Sped up autocorrelation, added it directly to the Analysis menu, and added it to the Data Collector.
 - Added "Save Figures as .pdf" as a save figure shortcut.
 - Moved "Get Spectrum from Clipboard" to File menu and added shortcut at Ctrl + G.
 - Moved Integrate/Interpolate option for converting from m/z to mass from the Advanced menu to the Additional Filter/Restraints control window.
- From the last update:
 - Report Center of Mass: Shows the center of mass for the zoomed region in the mass distribution (Plot 2)
 - Plot by Charge: Peak are now charge states rather than mass species. Plot charge state distribution. Plots each charge state as a separate distribution in Plot 4.
 - Plot Charge Offsets: Replot the Mass vs. Charge plot as a Mass vs. Charge Offset. Note: may be slow for large arrays.
 - Auto Match Tools: Basically the same as clicking Oligomer and Mass Tools > Match to Mixed Oligomers > OK. Requires the oligomers to already be defined in the Oligomer and Mass Tools window.
 - Kendrick Mass Analysis: Tools for high-mass mass defect analysis. The paper on this is in press.
 - 2D Grid Extraction: Extract intensity values for predefined mass values in a 1D or 2D grid.
- Experimental Features (Unpublished, untested, and unfinished):
 - Calibration Window: Allows a polynomial calibration to be applied to the m/z data. It will not modify the data file or save the result.
 - FFT Window: Views double FFT for windowed regions of the spectrum. I know this is weird, but this is a sneak peak into something we are working on.
 - Color Plots: Plot specific regions of the spectrum in the color of the peak. This is common for native MS papers, but it can be a mess when there are a lot of overlapping peaks.
 - Get Errors: Working on a automated error determination...

Chapter 2

Namespace Index

2.1 Packages

Here are the packages with brief descriptions (if available):

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Chapter 3

Hierarchical Index

3.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

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C:/Python/UniDec/unidec_modules/tims_import_wizard/ TagTypes.py	434
C:/Python/UniDec/unidec_src/cfunction/ pythonfunctions.c	438

Chapter 6

Namespace Documentation

6.1 UniDec Namespace Reference

Namespaces

- `datacollector`
- `GUUniDec`
- `import_wizard`
- `test_UniDec`
- `unidec`
- `unidec_modules`
- `unidec_tests`

Variables

- string `__author__` = 'Michael.Marty'

6.1.1 Variable Documentation

6.1.1.1 string `UniDec.__author__` = 'Michael.Marty'

6.2 UniDec.datacollector Namespace Reference

Classes

- class `DataCollector`
- class `ListCtrlPanel`
- class `NetworkFrame`
- class `XValueListCtrl`
- class `YValueListCtrl`

Variables

- string `__author__` = 'michael.marty'
- dictionary `datachoices` = {0: "Raw Data", 1: "Processed Data", 2: "Zero Charge Mass Spectrum"}
- dictionary `extractchoices` = {0: "Height", 1: "Local Max", 2: "Area", 3: "Center of Mass", 4: "Local Max Position"}
- dictionary `extractlabels` = {0: "Intensity", 1: "Intensity", 2: "Area", 3: "mass", 4: "mass"}

- dictionary `modelchoices`
- tuple `app = wx.App(False)`
- tuple `frame = DataCollector(None, "Collect Data")`

6.2.1 Variable Documentation

- 6.2.1.1 string `UniDec.datacollector.__author__ = 'michael.marty'`
- 6.2.1.2 tuple `UniDec.datacollector.app = wx.App(False)`
- 6.2.1.3 dictionary `UniDec.datacollector.datachoices = {0: "Raw Data", 1: "Processed Data", 2: "Zero Charge Mass Spectrum"}`
- 6.2.1.4 dictionary `UniDec.datacollector.extractchoices = {0: "Height", 1: "Local Max", 2: "Area", 3: "Center of Mass", 4: "Local Max Position"}`
- 6.2.1.5 dictionary `UniDec.datacollector.extractlabels = {0: "Intensity", 1: "Intensity", 2: "Area", 3: "mass", 4: "mass"}`
- 6.2.1.6 tuple `UniDec.datacollector.frame = DataCollector(None, "Collect Data")`
- 6.2.1.7 dictionary `UniDec.datacollector.modelchoices`

Initial value:

```
1 = {"Simple Single KD": "one", "Parallel KD's Chained": "parallel", "All KD's Free": "free",
2           "Test for Best Model": "test", "Series KD's Chained": "series"}
```

6.3 UniDec.GUniDec Namespace Reference

Classes

- class `Shell`
- class `UniDecApp`

Variables

- string `__author__ = 'Michael.Marty'`
- tuple `app = UniDecApp()`

6.3.1 Variable Documentation

- 6.3.1.1 string `UniDec.GUniDec.__author__ = 'Michael.Marty'`
- 6.3.1.2 tuple `UniDec.GUniDec.app = UniDecApp()`

6.4 UniDec.import_wizard Namespace Reference

Classes

- class `ImportWizard`

Variables

- tuple `app` = `wx.App(False)`
- tuple `frame` = `ImportWizard(None)`

6.4.1 Variable Documentation

6.4.1.1 tuple `UniDec.import_wizard.app` = `wx.App(False)`

6.4.1.2 tuple `UniDec.import_wizard.frame` = `ImportWizard(None)`

6.5 UniDec.test_UniDec Namespace Reference

Classes

- class `TestUniDec`

6.6 UniDec.unidec Namespace Reference

Classes

- class `DataContainer`
- class `UniDec`

Variables

- string `__author__` = 'Michael.Marty'
- tuple `eng` = `UniDec()`
- string `filename` = "0.txt"
- string `path` = "C:\\cprog\\UniDecDemo"
- list `files` = ["0.txt"]

6.6.1 Variable Documentation

6.6.1.1 string `UniDec.unidec.__author__` = 'Michael.Marty'

6.6.1.2 tuple `UniDec.unidec.eng` = `UniDec()`

6.6.1.3 string `UniDec.unidec.filename` = "0.txt"

6.6.1.4 list `UniDec.unidec.files` = ["0.txt"]

6.6.1.5 string `UniDec.unidec.path` = "C:\\cprog\\UniDecDemo"

6.7 UniDec.unidec_modules Namespace Reference

Namespaces

- `auto_peak`
- `AutocorrWindow`
- `ColorPlot`

- Extract2D
- fft_test
- fft_window
- GridDecon
- IM_functions
- IM_windows
- isolated_packages
- mainwindow
- ManualSelectionWindow
- MassDefects
- MassFitter
- MassSpecBuilder
- masstools
- miscwindows
- mzMLimporter
- nativez
- peaklists
- peakstructure
- peakwidthtools
- plot1d
- plot2d
- plot3d
- PlotAnimations
- PlottingWindow
- tims_import_wizard
- unidecstructure
- unidectools
- UniFit

Variables

- string __author__ = 'michael.marty'

6.7.1 Variable Documentation

6.7.1.1 string UniDec.unidec_modules.__author__ = 'michael.marty'

6.8 UniDec.unidec_modules.auto_peak Namespace Reference

Variables

- string __author__ = 'Michael.Marty'
- string file = "C:\\cprog\\UniDecDemo\\MTM_ADH_5_rawdata.txt"
- tuple data = np.loadtxt(file, skiprows=10)
- tuple thresh = auto_noise_level(data)
- tuple avgbs = average_bin_size(data)
- int window = fwhm/avgbs/4
- tuple cwtdata = np.transpose([data[:, 0], cwt])
- tuple peaks = peakdetect(cwtdata, None, window * 2., thresh)
- int zm = 1
- list ivals = peaks[:, 1]
- tuple maxpos = np.argmax(ivals)
- list mins = []

- tuple `x` = `np.abs(zm - zm[maxpos])`
- tuple `diffs` = `np.diff(x)`
- tuple `minpos` = `np.argmin(diffs)`
- tuple `minval` = `np.average(x[minpos:minpos + 2])`
- int `mass` = 1
- list `mz` = `peaks[maxpos, 0]`
- tuple `charge` = `np.round(mass / mz)`
- `tolerance` = `charge*fwhm`
- tuple `vec` = `np.array([mass, ival[maxpos], mz, charge, diffs[minpos], tolerance, zm[maxpos], False])`
- tuple `sindex` = `np.argsort(mins[:, 4])`
- list `peakassignments` = []
- list `row` = `mins[i]`
- list `swaps` = []
- list `topmass` = `row[0]`
- list `topcharge` = `row[3]`
- tuple `zms` = `np.abs(row[6] - mins[:, 6])`
- list `newmass` = `mins[j, 2]`
- int `newspot` = 0
- tuple `swaprows` = `deepcopy(mins[newspot:j])`
- list `boo1` = `mins[:, 7]`
- list `y` = `mins[boo1, 4]`
- tuple `m` = `np.array(m)`

6.8.1 Variable Documentation

- 6.8.1.1 string `UniDec.unidec_modules.auto_peak.__author__` = 'Michael.Marty'
- 6.8.1.2 tuple `UniDec.unidec_modules.auto_peak.avgbs` = `average_bin_size(data)`
- 6.8.1.3 list `UniDec.unidec_modules.auto_peak.boo1` = `mins[:, 7]`
- 6.8.1.4 tuple `UniDec.unidec_modules.auto_peak.charge` = `np.round(mass / mz)`
- 6.8.1.5 tuple `UniDec.unidec_modules.auto_peak.cwtdat` = `np.transpose([data[:, 0], cwt])`
- 6.8.1.6 tuple `UniDec.unidec_modules.auto_peak.data` = `np.loadtxt(file, skiprows=10)`
- 6.8.1.7 tuple `UniDec.unidec_modules.auto_peak.diffs` = `np.diff(x)`
- 6.8.1.8 string `UniDec.unidec_modules.auto_peak.file` = "C:\\cprog\\UniDecDemo\\MTM_ADH_5_rawdata.txt"
- 6.8.1.9 list `UniDec.unidec_modules.auto_peak.ivals` = `peaks[:, 1]`
- 6.8.1.10 tuple `UniDec.unidec_modules.auto_peak.m` = `np.array(m)`
- 6.8.1.11 int `UniDec.unidec_modules.auto_peak.mass` = 1
- 6.8.1.12 tuple `UniDec.unidec_modules.auto_peak.maxpos` = `np.argmax(ivals)`
- 6.8.1.13 tuple `UniDec.unidec_modules.auto_peak.minpos` = `np.argmin(diffs)`
- 6.8.1.14 list `UniDec.unidec_modules.auto_peak.mins` = []
- 6.8.1.15 tuple `UniDec.unidec_modules.auto_peak.minval` = `np.average(x[minpos:minpos + 2])`

- 6.8.1.16 list UniDec.unidec_modules.auto_peak.mz = peaks[maxpos, 0]
- 6.8.1.17 list UniDec.unidec_modules.auto_peak.newmass = mins[j, 2]
- 6.8.1.18 UniDec.unidec_modules.auto_peak.newspos = 0
- 6.8.1.19 list UniDec.unidec_modules.auto_peak.peakassignments = []
- 6.8.1.20 tuple UniDec.unidec_modules.auto_peak.peaks = peakdetect(cwtdata, None, window * 2., thresh)
- 6.8.1.21 list UniDec.unidec_modules.auto_peak.row = mins[i]
- 6.8.1.22 tuple UniDec.unidec_modules.auto_peak.sindex = np.argsort(mins[:, 4])
- 6.8.1.23 tuple UniDec.unidec_modules.auto_peak.swaprows = deepcopy(mins[newspos:j])
- 6.8.1.24 list UniDec.unidec_modules.auto_peak.swaps = []
- 6.8.1.25 tuple UniDec.unidec_modules.auto_peak.thresh = auto_noise_level(data)
- 6.8.1.26 list UniDec.unidec_modules.auto_peak.tolerance = charge*fwhm
- 6.8.1.27 list UniDec.unidec_modules.auto_peak.topcharge = row[3]
- 6.8.1.28 list UniDec.unidec_modules.auto_peak.topmass = row[0]
- 6.8.1.29 int UniDec.unidec_modules.auto_peak.vec = np.array([mass, ivals[maxpos], mz, charge, diffs[minpos], tolerance, zm[maxpos], False])
- 6.8.1.30 int UniDec.unidec_modules.auto_peak.window = fwhm/avgbs/4
- 6.8.1.31 list UniDec.unidec_modules.auto_peak.x = np.abs(zm - zm[maxpos])
- 6.8.1.32 list UniDec.unidec_modules.auto_peak.y = mins[boo1, 4]
- 6.8.1.33 int UniDec.unidec_modules.auto_peak.zm = 1
- 6.8.1.34 tuple UniDec.unidec_modules.auto_peak.zms = np.abs(row[6] - mins[:, 6])

6.9 UniDec.unidec_modules.AutocorrWindow Namespace Reference

Classes

- class [AutocorrWindow](#)
- class [CorrListCtrl](#)
- class [CorrListCtrlPanel](#)

Variables

- string [__author__](#) = 'Michael.Marty'

6.9.1 Variable Documentation

- 6.9.1.1 string UniDec.unidec_modules.AutocorrWindow.[__author__](#) = 'Michael.Marty'

6.10 UniDec.unidec_modules.ColorPlot Namespace Reference

Classes

- class [ColorPlot2D](#)

Variables

- string `__author__` = 'Michael.Marty'

6.10.1 Variable Documentation

6.10.1.1 string `UniDec.unidec_modules.ColorPlot.__author__` = 'Michael.Marty'

6.11 UniDec.unidec_modules.Extract2D Namespace Reference

Classes

- class [Extract2DPlot](#)

Variables

- string `__author__` = 'Michael.Marty'
- string `dir_name` = "C:\\MassLynx\\Mike.PRO\\Data\\150521\\mzML\\Aqpz_05_Ramp3\\MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_unidecfiles"
- string `file_name` = "MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_mass.txt"
- tuple `path` = `os.path.join(dir_name, file_name)`
- tuple `data` = `np.loadtxt(path)`
- tuple `data2` = `np.loadtxt(path)`
- tuple `data3` = `np.loadtxt(path)`
- list `datalist` = [data, data2, data3]
- tuple `app` = `wx.App(False)`
- tuple `frame` = `Extract2DPlot(None, datalist, yvals=np.array([100., 120., 180.]))`

6.11.1 Variable Documentation

6.11.1.1 string `UniDec.unidec_modules.Extract2D.__author__` = 'Michael.Marty'

6.11.1.2 tuple `UniDec.unidec_modules.Extract2D.app` = `wx.App(False)`

6.11.1.3 tuple `UniDec.unidec_modules.Extract2D.data` = `np.loadtxt(path)`

6.11.1.4 tuple `UniDec.unidec_modules.Extract2D.data2` = `np.loadtxt(path)`

6.11.1.5 tuple `UniDec.unidec_modules.Extract2D.data3` = `np.loadtxt(path)`

6.11.1.6 list `UniDec.unidec_modules.Extract2D.datalist` = [data, data2, data3]

6.11.1.7 string `UniDec.unidec_modules.Extract2D.dir_name` = "C:\\MassLynx\\Mike.PRO\\Data\\150521\\mzML\\Aqpz_05_Ramp3\\MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_unidecfiles"

```
6.11.1.8 string UniDec.unidec_modules.Extract2D.file_name = "MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_←
mass.txt"
```

```
6.11.1.9 tuple UniDec.unidec_modules.Extract2D.frame = Extract2DPlot(None, datalist, yvals=np.array([100., 120., 180.]))
```

```
6.11.1.10 tuple UniDec.unidec_modules.Extract2D.path = os.path.join(dir_name, file_name)
```

6.12 UniDec.unidec_modules.fft_test Namespace Reference

Functions

- def `MALDI_baseline` (`data`, `w`)
- def `calc_mediants` (`data`, `start`, `stop`, `w`)
- def `fit_mediants` (`data`, `start`, `stop`, `w`)
- def `old_cwt_2d`
- def `cwt_2d`
- def `fitfun` (`x`, `data`, `recon`)
- def `optimize_overlap` (`data`, `recon`)

Variables

- string `__author__` = 'michael.marty'
- string `datfile` = "C:\\NDDData\\PG25\\CG_07\\150820_CG_07_ramp90.txt"
- tuple `data` = np.loadtxt(`datfile`)
- float `mzbinsize` = 1.0
- int `baseline` = 30
- tuple `background` = np.sin((`data`[:, 0] - `data`[0, 0]) / (`data`[len(`data`) - 1, 0] - `data`[0, 0]) * np.pi)
- int `width` = 20
- int `num` = 10
- int `cutoff` = 5000
- string `wf` = "dog"
- int `param` = 2
- int `hpfilt` = 1
- tuple `lpfilt` = stats.norm.cdf(widths, `cutoff`, `cutoff` * 0.01)
- `filt` = `lpfilt`
- tuple `filtmat` = np.transpose([`filt` for `d` in `data`])
- tuple `recon` = mipy.wavelet.icwt(`cwt` * `filtmat`, `mzbinsize`, widths, `wf=wf`, `p=param`)
- tuple `reconscale` = `optimize_overlap`(`data`, `recon`)
- tuple `fdat` = np.average(`cwt`, axis=1)
- list `boo1` = `data`[:, 0]
- tuple `mindat` = min(`data`[:, 0])
- tuple `maxdat` = max(`data`[:, 0])
- tuple `mzdata` = linearize(`data`, 0.05, 3)
- tuple `xvals` = np.arange(`mindat`, `maxdat`, 500)
- tuple `results` = np.array([windowed_fft(`mzdata`, `x`, 2000) for `x` in `xvals`])
- list `intdat` = `results`[:, :, 1]
- tuple `yvals` = np.unique(`results`[:, :, 0])

6.12.1 Function Documentation

6.12.1.1 def UniDec.unidec_modules.fft_test.calc_medians (*data*, *start*, *stop*, *w*)

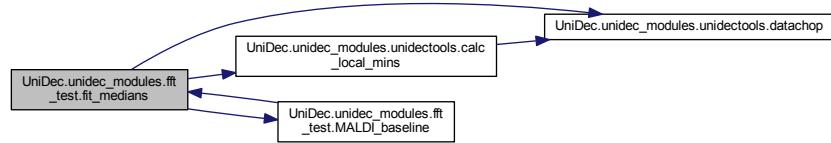
Here is the call graph for this function:



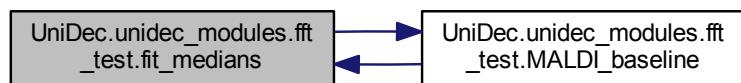
6.12.1.2 def UniDec.unidec_modules.fft_test.cwt_2d (*data*, *N*=20, *wf*="dog", *param*=2)

6.12.1.3 def UniDec.unidec_modules.fft_test.fit_medians (*data*, *start*, *stop*, *w*)

Here is the call graph for this function:



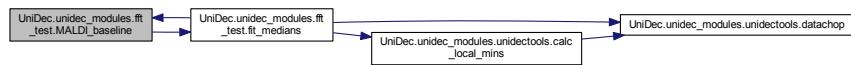
Here is the caller graph for this function:



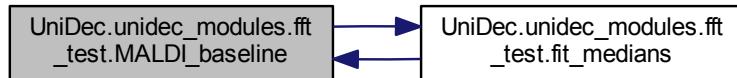
6.12.1.4 def UniDec.unidec_modules.fft_test.fitfun (*x*, *data*, *recon*)

6.12.1.5 def UniDec.unidec_modules.fft_test.MALDI_baseline (*data*, *w*)

Here is the call graph for this function:

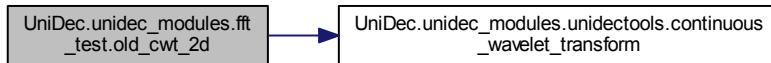


Here is the caller graph for this function:



6.12.1.6 def UniDec.unidec_modules.fft_test.old_cwt_2d (*data, N = 20*)

Here is the call graph for this function:



6.12.1.7 def UniDec.unidec_modules.fft_test.optimize_overlap (*data, recon*)

6.12.2 Variable Documentation

6.12.2.1 string UniDec.unidec_modules.fft_test.__author__ = 'michael.marty'

6.12.2.2 tuple UniDec.unidec_modules.fft_test.background = np.sin((data[:, 0] - data[0, 0]) / (data[len(data) - 1, 0] - data[0, 0]) * np.pi)

6.12.2.3 int UniDec.unidec_modules.fft_test.baseline = 30

6.12.2.4 list UniDec.unidec_modules.fft_test.boo1 = data[:, 0]

6.12.2.5 int UniDec.unidec_modules.fft_test.cutoff = 5000

6.12.2.6 list UniDec.unidec_modules.fft_test.data = np.loadtxt(datfile)

6.12.2.7 string UniDec.unidec_modules.fft_test.datfile = "C:\\NDDData\\PG25\\CG_07\\150820(CG_07_ramp90.txt"

6.12.2.8 tuple UniDec.unidec_modules.fft_test.fdat = np.average(cwt, axis=1)

6.12.2.9 UniDec.unidec_modules.fft_testfilt = lpfilt

6.12.2.10 tuple UniDec.unidec_modules.fft_testfiltmat = np.transpose([filt for d in data])

6.12.2.11 int UniDec.unidec_modules.fft_test.hpfilt = 1

6.12.2.12 list UniDec.unidec_modules.fft_test.intdat = results[:, :, 1]

- 6.12.2.13 tuple UniDec.unidec_modules.fft_test.lpfilt = stats.norm.cdf(widths, cutoff, cutoff * 0.01)
- 6.12.2.14 tuple UniDec.unidec_modules.fft_test.maxdat = max(data[:, 0])
- 6.12.2.15 tuple UniDec.unidec_modules.fft_test.mindat = min(data[:, 0])
- 6.12.2.16 float UniDec.unidec_modules.fft_test.mzbinsize = 1.0
- 6.12.2.17 tuple UniDec.unidec_modules.fft_test.mzdata = linearize(data, 0.05, 3)
- 6.12.2.18 int UniDec.unidec_modules.fft_test.num = 10
- 6.12.2.19 int UniDec.unidec_modules.fft_test.param = 2
- 6.12.2.20 tuple UniDec.unidec_modules.fft_test.recon = mipy.wavelet.icwt(cwt * filtmat, mzbinsize, widths, wf=wf, p=param)
- 6.12.2.21 tuple UniDec.unidec_modules.fft_test.reconscale = optimize_overlap(data, recon)
- 6.12.2.22 tuple UniDec.unidec_modules.fft_test.results = np.array([windowed_fft(mzdata, x, 2000) for x in xvals])
- 6.12.2.23 string UniDec.unidec_modules.fft_test.wf = "dog"
- 6.12.2.24 int UniDec.unidec_modules.fft_test.width = 20
- 6.12.2.25 tuple UniDec.unidec_modules.fft_test.xvals = np.arange(mindat, maxdat, 500)
- 6.12.2.26 tuple UniDec.unidec_modules.fft_test.yvals = np.unique(results[:, :, 0])

6.13 UniDec.unidec_modules.fft_window Namespace Reference

Classes

- class [FFTWindow](#)

Variables

- string `__author__` = 'Michael.Marty'
- string `datfile` = "C:\\NDData\\PG25\\CG_07\\150820(CG_07_ramp90.txt"
- tuple `data2` = np.loadtxt(`datfile`)
- tuple `app` = wx.App(False)
- tuple `frame` = [FFTWindow](#)(None, `data2`)

6.13.1 Variable Documentation

- 6.13.1.1 string UniDec.unidec_modules.fft_window.`__author__` = 'Michael.Marty'
- 6.13.1.2 tuple UniDec.unidec_modules.fft_window.`app` = wx.App(False)
- 6.13.1.3 tuple UniDec.unidec_modules.fft_window.`data2` = np.loadtxt(`datfile`)
- 6.13.1.4 string UniDec.unidec_modules.fft_window.`datfile` = "C:\\NDData\\PG25\\CG_07\\150820(CG_07_ramp90.txt"
- 6.13.1.5 tuple UniDec.unidec_modules.fft_window.`frame` = [FFTWindow](#)(None, `data2`)

6.14 UniDec.unidec_modules.GridDecon Namespace Reference

Classes

- class [GridDeconWindow](#)

Functions

- def [make_pmat](#) (mzgrid, fwhm)
- def [conv](#) (b, pmat)
- def [blur](#) (b, msig, zsig)
- def [grid_unidec](#)

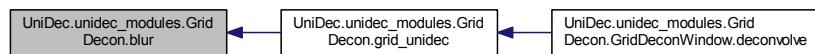
Variables

- string [__author__](#) = 'Michael.Marty'
- string [dir_name](#) = "C:\\MassLynx\\Mike.PRO\\Data\\150521\\mzML\\Aqpz_05_Ramp3\\"
- string [file_name](#) = "MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100.txt"
- tuple [path](#) = os.path.join([dir_name](#), [file_name](#))
- tuple [data](#) = np.loadtxt([path](#))
- tuple [app](#) = wx.App(False)
- tuple [frame](#) = [GridDeconWindow](#)(None, [data](#))

6.14.1 Function Documentation

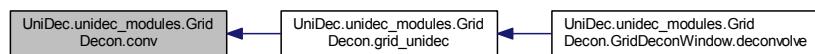
6.14.1.1 def UniDec.unidec_modules.GridDecon.blur (b, msig, zsig)

Here is the caller graph for this function:



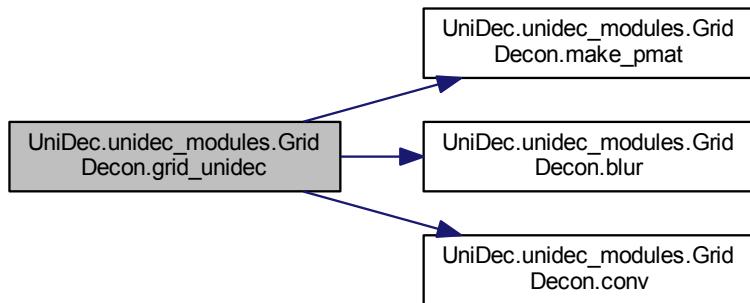
6.14.1.2 def UniDec.unidec_modules.GridDecon.conv (b, pmat)

Here is the caller graph for this function:

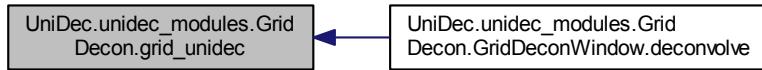


```
6.14.1.3 def UniDec.unidec_modules.GridDecon.grid_unidec( mzgrid, igrad, numit = 1000, fwhm = 5, mode = 0, msig = 0, zsig = 1 )
```

Here is the call graph for this function:

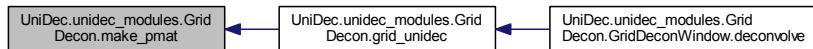


Here is the caller graph for this function:



```
6.14.1.4 def UniDec.unidec_modules.GridDecon.make_pmat( mzgrid, fwhm )
```

Here is the caller graph for this function:



6.14.2 Variable Documentation

```
6.14.2.1 string UniDec.unidec_modules.GridDecon.__author__ = 'Michael.Marty'
```

```
6.14.2.2 tuple UniDec.unidec_modules.GridDecon.app = wx.App(False)
```

```
6.14.2.3 tuple UniDec.unidec_modules.GridDecon.data = np.loadtxt(path)
```

```
6.14.2.4 string UniDec.unidec_modules.GridDecon.dir_name = "C:\\MassLynx\\Mike.PRO\\Data\\150521\\mzML\\Aqpz_05_Ramp3\\"
```

- 6.14.2.5 string UniDec.unidec_modules.GridDecon.file_name = "MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100.txt"
- 6.14.2.6 tuple UniDec.unidec_modules.GridDecon.frame = GridDeconWindow(None, data)
- 6.14.2.7 tuple UniDec.unidec_modules.GridDecon.path = os.path.join(dir_name, file_name)

6.15 UniDec.unidec_modules.IM_functions Namespace Reference

Functions

- def `smooth_2d` (igrid, smooth, smoothdt)
- def `min_array` (igrid, xwidth, ywidth)
- def `intensitythresh` (igrid, thresh)
- def `subtract_complex_2d` (igrid, config)
- def `compress_2d` (xgrid, ygrid, zgrid, num)
- def `linearize_2d` (xvals, yvals, igridd, binsize)
- def `detectoreff_2d` (igrid, xgrid, va)
- def `process_data_2d` (xgrid, ygrid, igridd, config)
- def `calc_twave_dt` (mass, z, ccs, config)
- def `calc_linear_dt` (mass, z, ccs, config)
- def `calc_native_ccs` (mass, gasmass)

Variables

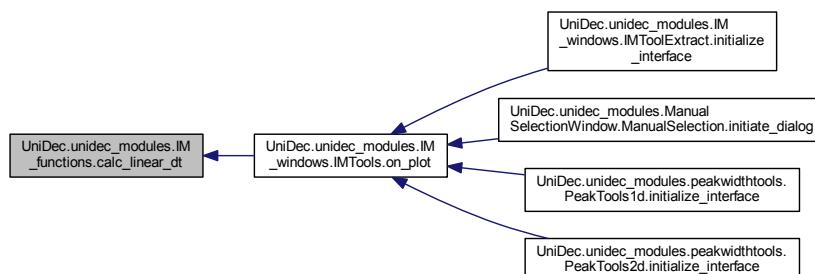
- string `__author__` = 'Michael.Marty'

6.15.1 Function Documentation

6.15.1.1 def UniDec.unidec_modules.IM_functions.calc_linear_dt(mass, z, ccs, config)

Calculate drift time in a linear cell
:param mass: Mass in Da
:param z: Charge
:param ccs: CCS in Angstrom^2
:param config: UniDecConfig object (carries the key parameters of temp, pressure, etc)
:return: Drift time (ms)

Here is the caller graph for this function:



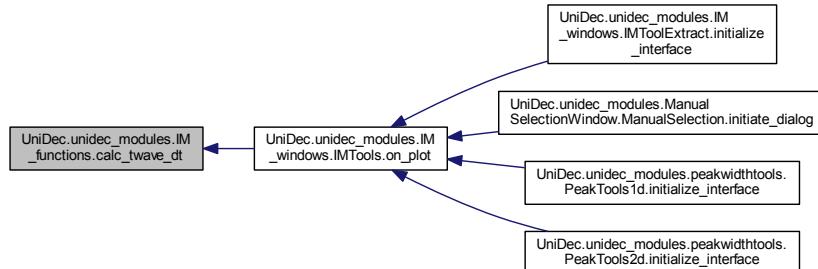
6.15.1.2 def UniDec.unidec_modules.IM_functions.calc_native_ccs(mass, gasmass)

```
Predict native CCS value for a particular mass in a given mass
:param mass: Mass of protein in Da
:param gasmass: Mass of IM background gas in Da
:return: Predicted CCS in Angstroms^2
```

6.15.1.3 def UniDec.unidec_modules.IM_functions.calc_twave_dt(mass, z, ccs, config)

```
Calculate drift time in a T-wave cell
:param mass: Mass in Da
:param z: Charge
:param ccs: CCS in Angstrom^2
:param config: UniDecConfig object (carries the key parameters of calibration)
:return: Drift time (ms)
```

Here is the caller graph for this function:



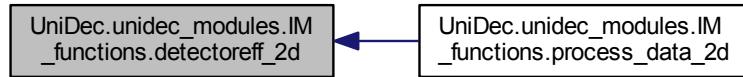
6.15.1.4 def UniDec.unidec_modules.IM_functions.compress_2d(xgrid, ygrid, zgrid, num)

```
Compresses a 2D grid in to smaller grids by merging n data points in the x dimension together as their average
:param xgrid: 2D numpy array
:param ygrid: 2D numpy array
:param zgrid: 2D numpy array
:param num: number of consecutive data points in the x-dimension to average together
:return: x, y, and z grids compressed along the x dimension to a new size
```

6.15.1.5 def UniDec.unidec_modules.IM_functions.detectoreff_2d(igridd, xgrid, va)

```
Corrects for Q-TOF detector efficiency
:param igridd: Intensity 2D numpy array
:param xgrid: 2D numpy array of m/z values
:param va: TOF acceleration voltage
:return: igridd corrected for detector efficiency
```

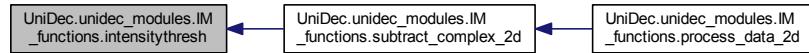
Here is the caller graph for this function:



6.15.1.6 def UniDec.unidec_modules.IM_functions.intensitythresh (*igrid, thresh*)

Intensity threshold for 2D grid
:param igrid: 2D numpy array
:param thresh: Threshold
:return: igrid with all elements below thresh set to 0

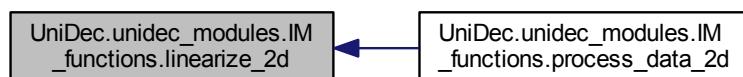
Here is the caller graph for this function:



6.15.1.7 def UniDec.unidec_modules.IM_functions.linearize_2d (*xvals, yvals, igridd, binsize*)

Linearize the x-axis of a 2D grid
:param xvals: 2D numpy array (x values)
:param yvals: 2D numpy array (y values)
:param igridd: 2D numpy array (intensity values)
:param binsize: difference between consecutive linear x points
:return: x, y, and z grid linearized along the x-axis

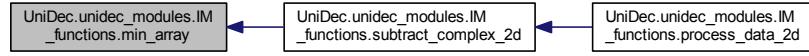
Here is the caller graph for this function:



6.15.1.8 def UniDec.unidec_modules.IM_functions.min_array (*igridd, xwidth, ywidth*)

Creates an array of local minimum values in a neighborhood of +/- width
:param igridd: 2D numpy array
:param xwidth: width in x direction
:param ywidth: width in y direction
:return: array of local minimum values in the same dimensions as igridd

Here is the caller graph for this function:



6.15.1.9 def UniDec.unidec_modules.IM_functions.process_data_2d (*xgrid*, *ygrid*, *igrid*, *config*)

Process IM-MS raw data.

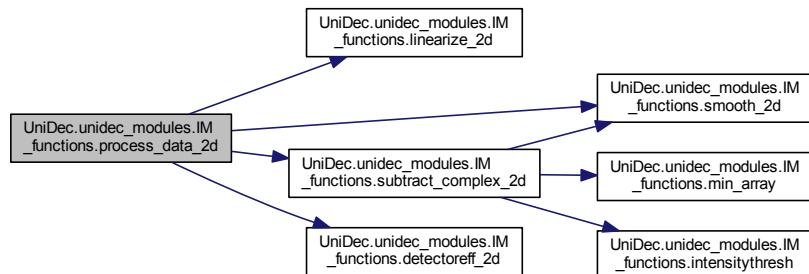
1. Chop data to defined limits
2. Linearize
3. Smooth
4. Subtract background
5. Detector efficiency correction
6. Normalize

```

:param xgrid: 2D numpy array (x values)
:param ygrid: 2D numpy array (y values)
:param igrid: 2D numpy array (intensity values values)
:param config: UniDecConfig object carrying parameters for processing
:return: x, y, and z grids of processed data

```

Here is the call graph for this function:



6.15.1.10 def UniDec.unidec_modules.IM_functions.smooth_2d (*igrid*, *smooth*, *smoothdt*)

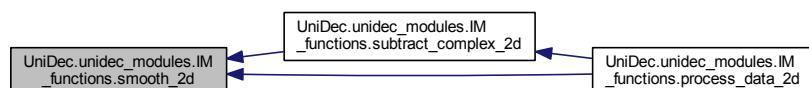
Gaussian smooth of 2D grid

```

:param igrid: 2D numpy array
:param smooth: width in x dimension (in data points)
:param smoothdt: width in y dimension (in data points)
:return: smoothed 2D numpy array

```

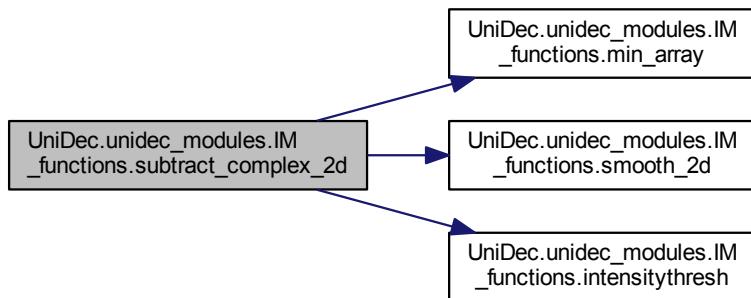
Here is the caller graph for this function:



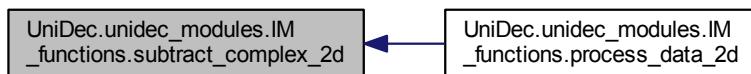
6.15.1.11 def UniDec.unidec_modules.IM_functions.subtract_complex_2d (*igrid, config*)

```
Subtract a complex curved baseline.
Creates a baseline using min_array, smooths it using smooth_2d, and subtracts it.
:param igrad: 2D numpy array
:param config: UniDecConfig object specifying width parameters in x and y dimensions
:return: igrad with background subtraction applied
```

Here is the call graph for this function:



Here is the caller graph for this function:



6.15.2 Variable Documentation

6.15.2.1 string UniDec.unidec_modules.IM_functions.__author__ = 'Michael.Marty'

6.16 UniDec.unidec_modules.IM_windows Namespace Reference

Classes

- class [IMListCtrl](#)
- class [IMListCtrlPanel](#)
- class [IMToolExtract](#)
- class [IMTools](#)

Variables

- string [__author__](#) = 'Michael.Marty'

6.16.1 Variable Documentation

6.16.1.1 string UniDec.unidec_modules.IM_windows.__author__ = 'Michael.Marty'

6.17 UniDec.unidec_modules.isolated_packages Namespace Reference

Namespaces

- [FileDialogs](#)
- [option_d](#)
- [texmaker](#)
- [twitter_interface](#)
- [ZoomBox](#)
- [ZoomSpan](#)

Variables

- string __author__ = 'Michael.Marty'

6.17.1 Variable Documentation

6.17.1.1 string UniDec.unidec_modules.isolated_packages.__author__ = 'Michael.Marty'

6.18 UniDec.unidec_modules.isolated_packages.FileDialogs Namespace Reference

Functions

- def [save_file_dialog](#)
- def [open_file_dialog](#)
- def [open_multiple_files_dialog](#)
- def [open_dir_dialog](#)
- def [open_multiple_dir_dialog](#) (message, default)
- def [open_single_dir_dialog](#) (message, default)

Variables

- tuple [default_dir](#) = os.path.abspath(os.path.join(os.getcwd(), os.path.pardir, 'data/'))

6.18.1 Function Documentation

6.18.1.1 def UniDec.unidec_modules.isolated_packages.FileDialogs.open_dir_dialog (*message* = "Select a Folder")

6.18.1.2 def UniDec.unidec_modules.isolated_packages.FileDialogs.open_file_dialog (*message* = "Open File", *file_types* = "*.*")

6.18.1.3 def UniDec.unidec_modules.isolated_packages.FileDialogs.open_multiple_dir_dialog (*message*, *default*)

6.18.1.4 def UniDec.unidec_modules.isolated_packages.FileDialogs.open_multiple_files_dialog (*message* = "Open Files", *file_type* = "*.*")

```
6.18.1.5 def UniDec.unidec_modules.isolated_packages.FileDialogs.open_single_dir_dialog( message, default )
6.18.1.6 def UniDec.unidec_modules.isolated_packages.FileDialogs.save_file_dialog( message = "Save File",
    file_types = "*.*", default_file = " " )
```

6.18.2 Variable Documentation

```
6.18.2.1 string UniDec.unidec_modules.isolated_packages.FileDialogs.default_dir = os.path.abspath(os.path.join(os.getcwd(),
    os.path.pardir, 'data/'))
```

6.19 UniDec.unidec_modules.isolated_packages.option_d Namespace Reference

Variables

- dictionary [parameters](#)
- list [cm_data](#)
- tuple [viridis](#) = LinearSegmentedColormap.from_list(__file__, cm_data)
- list [cm_data2](#)
- tuple [parula_map](#) = LinearSegmentedColormap.from_list('parula', cm_data2)
- list [cm_data3](#)
- tuple [fake_parula_map](#) = LinearSegmentedColormap.from_list(__file__, cm_data3)

6.19.1 Variable Documentation

```
6.19.1.1 list UniDec.unidec_modules.isolated_packages.option_d.cm_data
```

```
6.19.1.2 list UniDec.unidec_modules.isolated_packages.option_d.cm_data2
```

```
6.19.1.3 list UniDec.unidec_modules.isolated_packages.option_d.cm_data3
```

```
6.19.1.4 tuple UniDec.unidec_modules.isolated_packages.option_d.fake_parula_map = LinearSegmentedColormap.from_list(←
    __file__, cm_data3)
```

```
6.19.1.5 dictionary UniDec.unidec_modules.isolated_packages.option_d.parameters
```

Initial value:

```
1 = {
2     'xp': [22.674387857633945, 11.221508276482126, -14.356589454756971, -47.18817758739222, -34.59001004812
521,
3         -6.0516291196352654],
4     'yp': [-20.102530541012214, -33.08246073298429, -42.24476439790574, -5.595549738219887, 42.506544502617
8,
5         40.13395157135497],
6     'min_JK': 18.8671875,
7     'max_JK': 92.5}
```

```
6.19.1.6 tuple UniDec.unidec_modules.isolated_packages.option_d.parula_map = LinearSegmentedColormap.from_list('parula',
    cm_data2)
```

```
6.19.1.7 tuple UniDec.unidec_modules.isolated_packages.option_d.viridis = LinearSegmentedColormap.from_list(__file__,
    cm_data)
```

6.20 UniDec.unidec_modules.isolated_packages.texmaker Namespace Reference

Functions

- def [MakeTexReport](#) (fname, config, path, peaks, labels, names, color, figureflags)
- def [PDFTexReport](#) (fname)

6.20.1 Function Documentation

6.20.1.1 def UniDec.unidec_modules.isolated_packages.texmaker.MakeTexReport (*fname, config, path, peaks, labels, names, color, figureflags*)

6.20.1.2 def UniDec.unidec_modules.isolated_packages.texmaker.PDFTexReport (*fname*)

6.21 UniDec.unidec_modules.isolated_packages.twitter_interface Namespace Reference

Classes

- class [PinWindow](#)
- class [TwitterWindow](#)

Variables

- string [__author__](#) = 'Michael'

6.21.1 Variable Documentation

6.21.1.1 string UniDec.unidec_modules.isolated_packages.twitter_interface.[__author__](#) = 'Michael'

6.22 UniDec.unidec_modules.isolated_packages.ZoomBox Namespace Reference

Classes

- class [ZoomBox](#)

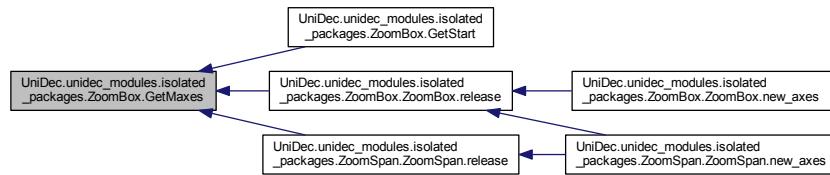
Functions

- def [GetMaxes](#)
- def [ResetVisible](#) (axes)
- def [GetStart](#) (axes)

6.22.1 Function Documentation

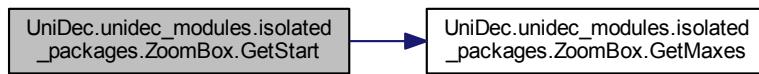
6.22.1.1 def UniDec.unidec_modules.isolated_packages.ZoomBox.GetMaxes (axes, xmin = None, xmax = None)

Here is the caller graph for this function:



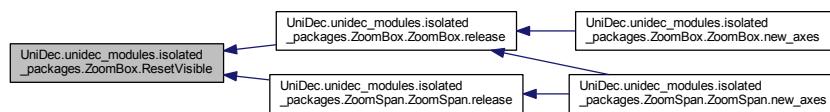
6.22.1.2 def UniDec.unidec_modules.isolated_packages.ZoomBox.GetStart (axes)

Here is the call graph for this function:



6.22.1.3 def UniDec.unidec_modules.isolated_packages.ZoomBox.ResetVisible (axes)

Here is the caller graph for this function:



6.23 UniDec.unidec_modules.isolated_packages.ZoomSpan Namespace Reference

Classes

- class [ZoomSpan](#)

6.24 UniDec.unidec_modules.mainwindow Namespace Reference

Classes

- class [Mainwindow](#)
- class [MyFileDropTarget](#)

Variables

- string `__author__` = 'Michael.Marty'

6.24.1 Variable Documentation

6.24.1.1 string `UniDec.unidec_modules/mainwindow.__author__` = 'Michael.Marty'

6.25 UniDec.unidec_modules.ManualSelectionWindow Namespace Reference

Classes

- class `ManualListCrtl`
- class `ManualListCtrlPanel`
- class `ManualSelection`

Functions

- def `closest` (`x, y, manlist`)
- def `correctassignments` (`manlist, xdat, ydat`)
- def `range_overlap` (`a_min, a_max, b_min, b_max`)
- def `checkoverlap` (`I1, I2`)
- def `detectoverlap` (`manlist`)

Variables

- string `__author__` = 'Michael.Marty'

6.25.1 Function Documentation

6.25.1.1 def `UniDec.unidec_modules.ManualSelectionWindow.checkoverlap(I1, I2)`

Check whether two lines of manual assignments are overlapping.

:param I1: Line 1 (1 x 5)
:param I2: Line 2 (1 x 5)
:return: True if overlapping, False if not.

Here is the call graph for this function:



Here is the caller graph for this function:



6.25.1.2 def UniDec.unidec_modules.ManualSelectionWindow.closest(x, y, manlist)

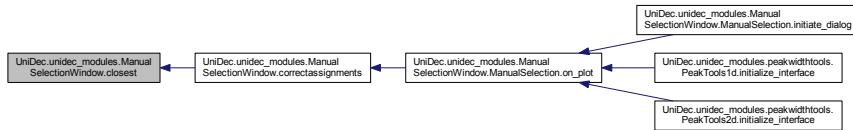
For manlist of manual assignments and an (x,y) point, finds the nearest manual assignment.
Used in correcting overlapping rectangles.

```

:param x: Float
:param y: Float
:param manlist: Array of manual assignment for IMMS (N x 5)
:return: out, pos
  
```

out is the line in manlist that is closest.
pos is the position of the line in manlist.

Here is the caller graph for this function:



6.25.1.3 def UniDec.unidec_modules.ManualSelectionWindow.correctassignments(manlist, xdat, ydat)

Correct the manual assignments so that they are not overlapping in IM-MS.

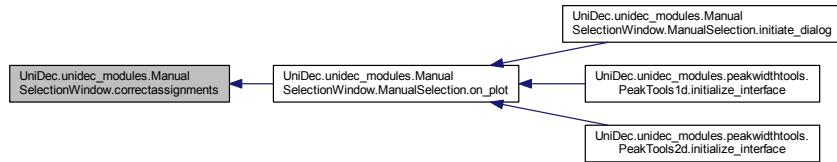
```

:param manlist: List of manual assignments in (N x 5) array.
:param xdat: x-axis (m/z)
:param ydat: y-axis (arrival time)
:return: manlist3, a new array of values corrected to eliminate overlap.
  
```

Here is the call graph for this function:



Here is the caller graph for this function:



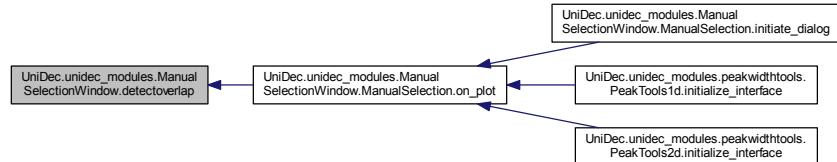
6.25.1.4 def UniDec.unidec_modules.ManualSelectionWindow.detectoverlap (*manlist*)

For a list of IM-MS manual assignments, check if any of the rectangles are overlapping.
:param manlist: Array of manual assignments (N x 5)
:return: True if overlapping, False if not.

Here is the call graph for this function:



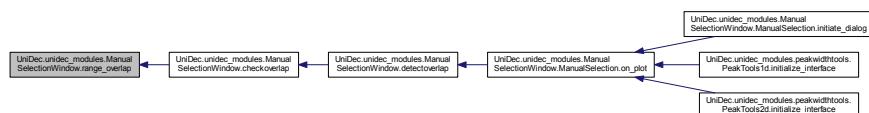
Here is the caller graph for this function:



6.25.1.5 def UniDec.unidec_modules.ManualSelectionWindow.range_overlap (*a_min*, *a_max*, *b_min*, *b_max*)

Checks whether two specific ranges of [*a_min*,*a_max*] and [*b_min*,*b_max*] overlap.
:param *a_min*:
:param *a_max*:
:param *b_min*:
:param *b_max*:
:return: True if overlapping, False if not.

Here is the caller graph for this function:



6.25.2 Variable Documentation

6.25.2.1 string UniDec.unidec_modules.ManualSelectionWindow.__author__ = 'Michael.Marty'

6.26 UniDec.unidec_modules.MassDefects Namespace Reference

Classes

- class [MassDefectWindow](#)

Variables

- string __author__ = 'Michael.Marty'
- string dir = "C:\\\\MassLynx\\\\Mike.PRO\\\\Data\\\\150521\\\\mzML\\\\Aqpz_05_Ramp3\\\\MTM_150521_AqpZ_05_P←
OPC_Ramp_1-5pbar_20mit100_unidecfiles"
- string file = "MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_mass.txt"
- tuple path = os.path.join(dir, file)
- tuple data = np.loadtxt(path)
- tuple data2 = np.loadtxt(path)
- list dataList = [data, data2]
- tuple app = wx.App(False)
- tuple frame = MassDefectWindow(None, dataList)

6.26.1 Variable Documentation

6.26.1.1 string UniDec.unidec_modules.MassDefects.__author__ = 'Michael.Marty'

6.26.1.2 tuple UniDec.unidec_modules.MassDefects.app = wx.App(False)

6.26.1.3 tuple UniDec.unidec_modules.MassDefects.data = np.loadtxt(path)

6.26.1.4 tuple UniDec.unidec_modules.MassDefects.data2 = np.loadtxt(path)

6.26.1.5 list UniDec.unidec_modules.MassDefects.dataList = [data, data2]

6.26.1.6 string UniDec.unidec_modules.MassDefects.dir = "C:\\\\MassLynx\\\\Mike.PRO\\\\Data\\\\150521\\\\mzML\\\\Aqpz_05_Ramp3\\\\M←
TM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_unidecfiles"

6.26.1.7 string UniDec.unidec_modules.MassDefects.file = "MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_mass.txt"

6.26.1.8 tuple UniDec.unidec_modules.MassDefects.frame = MassDefectWindow(None, dataList)

6.26.1.9 tuple UniDec.unidec_modules.MassDefects.path = os.path.join(dir, file)

6.27 UniDec.unidec_modules.MassFitter Namespace Reference

Classes

- class [MassFitter](#)

Functions

- def `make_mass_list` (`massdat`, `arrayin`, `psfun`, `startarray`, `args`)
- def `error_function` (`array`, `massdat`, `psfun`, `startarray`, `args`)
- def `least_squares_minimize` (`massdat`, `array`, `psfun`, `args`)

Variables

- string `__author__` = 'Michael.Marty'

6.27.1 Function Documentation

6.27.1.1 def UniDec.unidec_modules.MassFitter.error_function (`array`, `massdat`, `psfun`, `startarray`, `args`)

```
Error function for least_squares_minimize
:param array: Array of test parameters
:param massdat: Mass data to be fit
:param psfun: Peak shape function integer code
:param startarray: Starting array (not currently used but can be used to restrict some guesses)
:param args: Extra arguments for make_mass_list
:return: Squared errors array
```

Here is the call graph for this function:



6.27.1.2 def UniDec.unidec_modules.MassFitter.least_squares_minimize (`massdat`, `array`, `psfun`, `args`)

```
Perform least squares minimization of peaks defined in array to massdat.
:param massdat: Data to fit
:param array: Array of parameters for defining peaks that will be fit
:param psfun: Peak shape function integer code
:param args: Extra arguments for make_mass_list
:return: Best fit of values in array
```

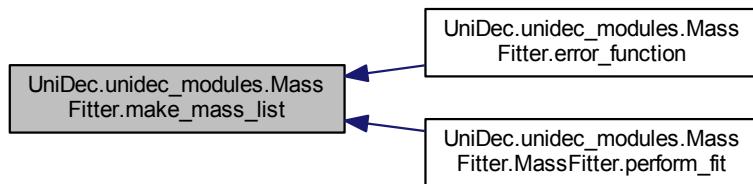
Here is the caller graph for this function:



6.27.1.3 def UniDec.unidec_modules.MassFitter.make_mass_list(massdat, arrayin, psfun, startarray, args)

For parameters in arrayin, make mass peaks to be fit to massdat.
 Arrayin must be P x 3 array of (mid, fwhm, area).
 :param massdat: Data to be fit
 :param arrayin: Parameters defining peaks
 :param psfun: Peak shape function integer code
 :param startarray: Starting array (not currently used but can be used to restrict some guesses)
 :param args: Extra arguments (such as nonorm to prevent normalization)
 :return:

Here is the caller graph for this function:



6.27.2 Variable Documentation

6.27.2.1 string UniDec.unidec_modules.MassFitter.__author__ = 'Michael.Marty'

6.28 UniDec.unidec_modules.MassSpecBuilder Namespace Reference

Functions

- def [make_mass_spectrum](#) (array, zrange=(10, 50, mzrange=(2000, 10000, mz_bin_size=1, adductmass=1.← 00727647, psfun=0, noise=0, baseline=0, kwargs))
- def [get_zrange](#) (params)
- def [get_mzrange](#) (params)
- def [simple_params](#) (masslist, intlist=None, resolution=1000, zwidth=2, rlist=None, kwargs)
- def [simple_spectrum](#) (masslist, kwargs)

Variables

- string [__author__](#) = 'Michael.Marty'

6.28.1 Function Documentation

6.28.1.1 def UniDec.unidec_modules.MassSpecBuilder.get_mzrange(params)

From parameters defining mass spectrum, pick a reasonable m/z range.
 :param params: P x 5 array of parameters [mass, mass fwhm, z avg, z std dev, intensity]
 :return: m/z range [min m/z , max m/z]

Here is the call graph for this function:



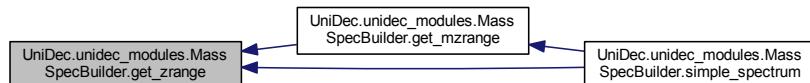
Here is the caller graph for this function:



6.28.1.2 def UniDec.unidec_modules.MassSpecBuilder.get_zrange (params)

From parameters defining mass spectrum, pick a reasonable charge state range.
:param params: P x 5 array of parameters [mass, mass fwhm, z avg, z std dev, intensity]
:return: charge state range [min z , max z]

Here is the caller graph for this function:



6.28.1.3 def UniDec.unidec_modules.MassSpecBuilder.make_mass_spectrum (array, zrange = (10, 50, mzrange = (2000, 10000, mz_bin_size = 1, adductmass = 1.00727647, psfun = 0, noise = 0, baseline = 0, kwargs))

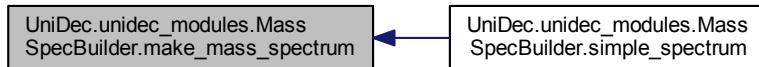
Create a new mass spectrum.

First, create the mzaxis from mzrange and the possible charge states from zrange.
Then, add in peaks at the appropriate mz values for the parameters defined in array.
Then, normalize and add optional background and noise.
Finally, renormalize.

:param array: P x 5 array of parameters [mass, mass fwhm, z avg, z std dev, intensity]
:param zrange: Tuple of list define range of allowed charge states
:param mzrange: Tuple or list defining range of m/z values
:param mz_bin_size: delta mz of mzaxis
:param adductmass: Mass of electrospray adduct species
:param psfun: Peak shape function integer code

```
:param noise: Std deviation of random Gaussian noise to be added to normalized spectrum
:param baseline: Peak intensity of sinusoidal baseline to be added to normalized spectrum
:param kwargs: Keyword catcher
:return: Spectrum, ztab (new spectrum in N x 2 (m/z, intensity) and charge states allowed)
```

Here is the caller graph for this function:



6.28.1.4 def UniDec.unidec_modules.MassSpecBuilder.simple_params (*masslist*, *intlist* = None, *resolution* = 1000, *zwidth* = 2, *rlist* = None, *kwargs*)

Set simple parameters [mass, mass fwhm, z avg, z std dev, intensity] for a mass list and optional arguments. Average charge is defined as the native charge state. Other parameters are defaults.

```
:param masslist: list of masses in Da
:param intlist: list of intensities (default is None which gives all as 1)
:param resolution: Mass resolution (delta m/m), Overridden if rlist is not None
:param zwidth: Standard deviation of charge state distribution
:param rlist: List of resolution values for each corresponding mass.
If None, will use a single resolution for all defined by resolution.
:param kwargs: Extra keywords
:return: P x 5 array of parameters [mass, mass fwhm, z avg, z std dev, intensity]
```

Here is the caller graph for this function:

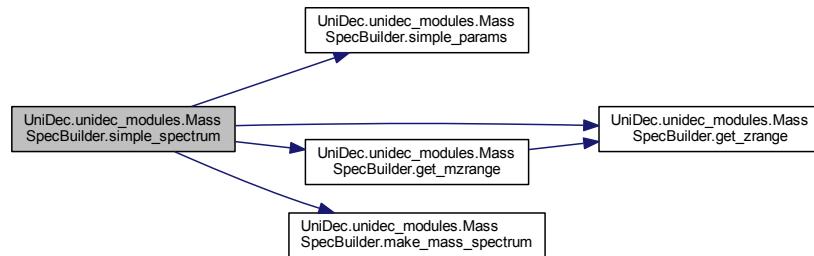


6.28.1.5 def UniDec.unidec_modules.MassSpecBuilder.simple_spectrum (*masslist*, *kwargs*)

For a mass list, create the parameters and ranges for a simple default spectrum.

```
:param masslist: Mass values
:param kwargs: Keywords of parameters to pass to simple_params and make_mass_spectrum
:return: N x 2 spectrum (m/z, intensity)
```

Here is the call graph for this function:



6.28.2 Variable Documentation

6.28.2.1 `string UniDec.unidec_modules.MassSpecBuilder.__author__ = 'Michael.Marty'`

6.29 UniDec.unidec_modules.masstools Namespace Reference

Classes

- class [MassListCrtl](#)
- class [MassListCrtlPanel](#)
- class [MassSelection](#)
- class [MatchListCrtl](#)
- class [MatchListCrtlPanel](#)
- class [OligomerListCrtlPanel](#)
- class [OligomerListCrtl](#)

6.30 UniDec.unidec_modules.misctools Namespace Reference

Classes

- class [AdditionalParameters](#)
- class [FileNameDialog](#)
- class [SaveFigureDialog](#)
- class [SingleInputDialog](#)

Functions

- def [setup_tab_box](#) (tab, plot)

Variables

- string [__author__](#) = 'Michael.Marty'

6.30.1 Function Documentation

6.30.1.1 def UniDec.unidec_modules.miscwindows.setup_tab_box (*tab, plot*)

Shortcut function for adding an object (plot) to a box sizer and fitting it to a notebook tab.
:param tab: wx.Notebook tab
:param plot: Object to add to box sizer
:return: None

6.30.2 Variable Documentation

6.30.2.1 string UniDec.unidec_modules.miscwindows.__author__ = 'Michael.Marty'

6.31 UniDec.unidec_modules.mzMLimporter Namespace Reference

Classes

- class [mzMLimporter](#)

Functions

- def [get_resolution](#) (*testdata*)
- def [merge_spectra](#) (*datalist*)

Variables

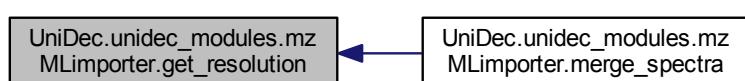
- string [__author__](#) = 'Michael.Marty'
- string [dir](#) = "C:\\cprog\\Joe"
- string [file](#) = "20150304_myo_70r_5u_full-ALL.mzML"
- tuple [tstart](#) = time.time()
- tuple [data](#) = [mzMLimporter](#)(os.path.join([dir](#), [file](#)))
- tuple [tend](#) = time.time()

6.31.1 Function Documentation

6.31.1.1 def UniDec.unidec_modules.mzMLimporter.get_resolution (*testdata*)

Get the median resolution of 1D MS data.
:param testdata: N x 2 data (mz, intensity)
:return: Median resolution (float)

Here is the caller graph for this function:



6.31.1.2 def UniDec.unidec_modules.mzMLimporter.merge_spectra (*datalist*)

Merge together a list of data.

Interpolates each data set in the list to a new nonlinear axis with the median resolution of the first element. Then, adds the interpolated data together to get the merged data.

:param datalist: M x N x 2 list of data sets
 :return: Merged N x 2 data set

Here is the call graph for this function:



6.31.2 Variable Documentation

6.31.2.1 string UniDec.unidec_modules.mzMLimporter.__author__ = 'Michael.Marty'

6.31.2.2 tuple UniDec.unidec_modules.mzMLimporter.data = mzMLimporter(os.path.join(dir, file))

6.31.2.3 string UniDec.unidec_modules.mzMLimporter.dir = "C:\\cprog\\Joe"

6.31.2.4 string UniDec.unidec_modules.mzMLimporter.file = "20150304_myo_70r_5u_full-ALL.mzML"

6.31.2.5 tuple UniDec.unidec_modules.mzMLimporter.tend = time.time()

6.31.2.6 tuple UniDec.unidec_modules.mzMLimporter.tstart = time.time()

6.32 UniDec.unidec_modules.nativez Namespace Reference

Classes

- class [ColorList](#)
- class [NativeZ](#)
- class [Zoffset](#)

Variables

- string __author__ = 'Michael.Marty'

6.32.1 Variable Documentation

6.32.1.1 string UniDec.unidec_modules.nativez.__author__ = 'Michael.Marty'

6.33 UniDec.unidec_modules.peaklistsorth Namespace Reference

Classes

- class [PeakListCtrlPanel](#)

6.34 UniDec.unidec_modules.peakstructure Namespace Reference

Classes

- class [Peak](#)
- class [Peaks](#)

Variables

- string [__author__](#) = 'Michael.Marty'

6.34.1 Variable Documentation

6.34.1.1 string UniDec.unidec_modules.peakstructure.[__author__](#) = 'Michael.Marty'

6.35 UniDec.unidec_modules.peakwidthtools Namespace Reference

Classes

- class [PeakTools1d](#)
- class [PeakTools2d](#)

Variables

- string [__author__](#) = 'Michael.Marty'

6.35.1 Variable Documentation

6.35.1.1 string UniDec.unidec_modules.peakwidthtools.[__author__](#) = 'Michael.Marty'

6.36 UniDec.unidec_modules.plot1d Namespace Reference

Classes

- class [Plot1d](#)

6.37 UniDec.unidec_modules.plot2d Namespace Reference

Classes

- class [Plot2d](#)

Variables

- string [__author__](#) = 'Michael.Marty'

6.37.1 Variable Documentation

6.37.1.1 string UniDec.unidec_modules.plot2d.__author__ = 'Michael.Marty'

6.38 UniDec.unidec_modules.plot3d Namespace Reference

Classes

- class [CubePlot](#)

Variables

- string __author__ = 'Michael.Marty'

6.38.1 Variable Documentation

6.38.1.1 string UniDec.unidec_modules.plot3d.__author__ = 'Michael.Marty'

6.39 UniDec.unidec_modules.PlotAnimations Namespace Reference

Classes

- class [AnimationWindow](#)

Variables

- string __author__ = 'Michael.Marty'
- tuple x = np.arange(0.0, 10.0)
- tuple dataList = np.array([np.transpose([x, x]), np.transpose([x, x * x]), np.transpose([x, x * x * x])])
- tuple app = wx.App(False)
- tuple frame = AnimationWindow(None, dataList)

6.39.1 Variable Documentation

6.39.1.1 string UniDec.unidec_modules.PlotAnimations.__author__ = 'Michael.Marty'

6.39.1.2 tuple UniDec.unidec_modules.PlotAnimations.app = wx.App(False)

6.39.1.3 tuple UniDec.unidec_modules.PlotAnimations.dataList = np.array([np.transpose([x, x]), np.transpose([x, x * x]), np.transpose([x, x * x * x])])

6.39.1.4 tuple UniDec.unidec_modules.PlotAnimations.frame = AnimationWindow(None, dataList)

6.39.1.5 tuple UniDec.unidec_modules.PlotAnimations.x = np.arange(0.0, 10.0)

6.40 UniDec.unidec_modules.PlottingWindow Namespace Reference

Classes

- class [PlottingWindow](#)

6.41 UniDec.unidec_modules.tims_import_wizard Namespace Reference

Namespaces

- `data_importer`
- `get_data_wrapper`
- `import_wizard_grid`
- `import_wizard_treectrl`
- `ImporterProgressGauge`
- `TagTypes`

Variables

- string `__author__` = 'michael.marty'

6.41.1 Variable Documentation

6.41.1.1 string `UniDec.unidec_modules.tims_import_wizard.__author__` = 'michael.marty'

6.42 UniDec.unidec_modules.tims_import_wizard.data_importer Namespace Reference

Functions

- def `auto_from_wizard` (`lines, exedir`)
- def `run_get_data` (`job_kwargs`)
- def `MakeUniDecConfig` (`job_kwargs`)
- def `process_from_wizard` (`kwargs`)
- def `mp_process_from_wizard` (`job_list`)
- def `data_import_worker` (`worker_queue, result_queue`)
- def `split_and_strip` (`line, delimiter=''`)
- def `parse_file`
- def `GetLines` (`InputFileName`)
- def `GetStartEndMass` (`RawFile`)
- def `get_stat_code`
- def `header_desc` (`file_path`)
- def `search_extern`

Variables

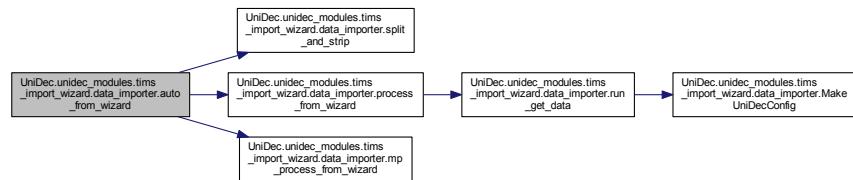
- `use_mp_import` = True
- dictionary `param_file_cache` = {}

6.42.1 Function Documentation

6.42.1.1 def `UniDec.unidec_modules.tims_import_wizard.data_importer.auto_from_wizard (lines, exedir)`

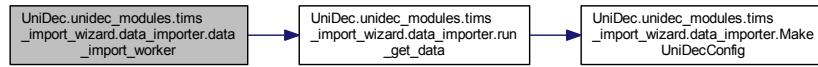
Auto load from the import wizard

Here is the call graph for this function:



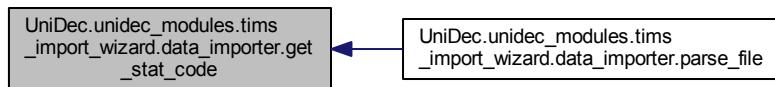
6.42.1.2 def UniDec.unidec_modules.tims_import_wizard.data_importer.data_import_worker (worker_queue, result_queue)

Here is the call graph for this function:



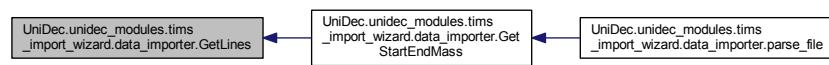
6.42.1.3 def UniDec.unidec_modules.tims_import_wizard.data_importer.get_stat_code (raw_file, stat_code, dir = None)

Here is the caller graph for this function:



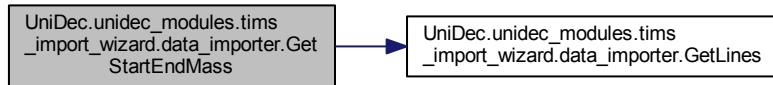
6.42.1.4 def UniDec.unidec_modules.tims_import_wizard.data_importer.GetLines (InputFileName)

Here is the caller graph for this function:

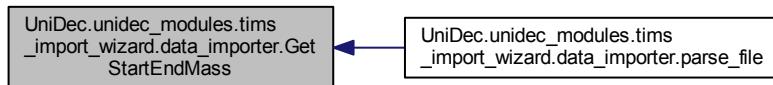


6.42.1.5 def UniDec.unidec_modules.tims_import_wizard.data_importer.GetStartEndMass (*RawFile*)

Here is the call graph for this function:

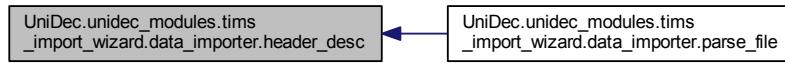


Here is the caller graph for this function:



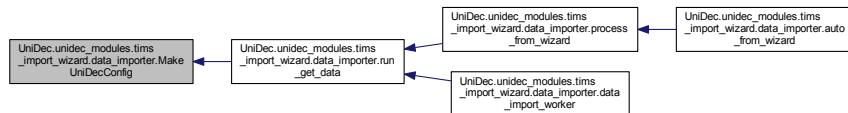
6.42.1.6 def UniDec.unidec_modules.tims_import_wizard.data_importer.header_desc (*file_path*)

Here is the caller graph for this function:



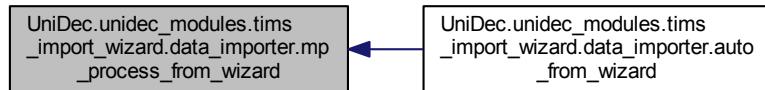
6.42.1.7 def UniDec.unidec_modules.tims_import_wizard.data_importer.MakeUniDecConfig (*job_kwargs*)

Here is the caller graph for this function:



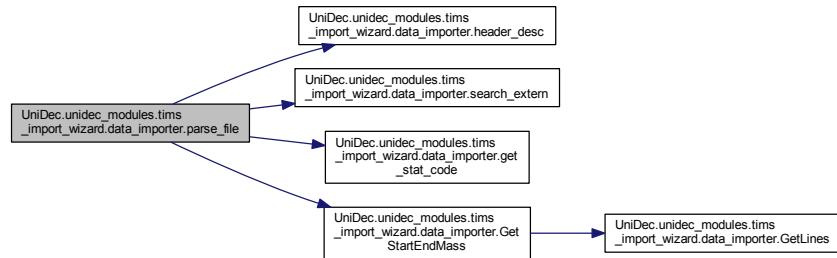
6.42.1.8 def UniDec.unidec_modules.tims_import_wizard.data_importer.mp_process_from_wizard (job_list)

Here is the caller graph for this function:



6.42.1.9 def UniDec.unidec_modules.tims_import_wizard.data_importer.parse_file (file_path, exp_type = 'linear', collision = None, debug = False, dir = None)

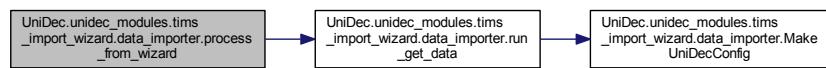
Here is the call graph for this function:



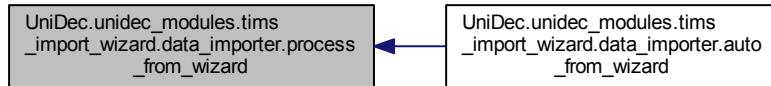
6.42.1.10 def UniDec.unidec_modules.tims_import_wizard.data_importer.process_from_wizard (kwargs)

Processes row in import wizard file
and adds to data model.

Here is the call graph for this function:

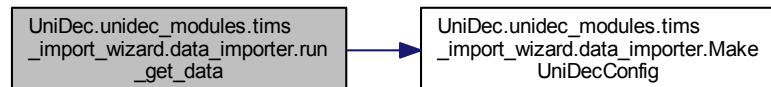


Here is the caller graph for this function:

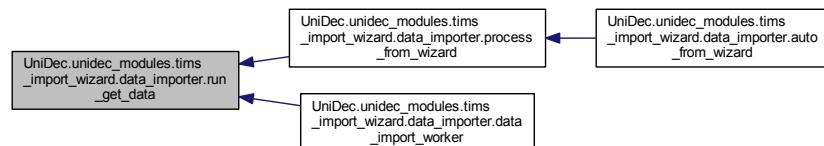


6.42.1.11 def UniDec.unidec_modules.tims_import_wizard.data_importer.run_get_data(job_kwargs)

Here is the call graph for this function:



Here is the caller graph for this function:



6.42.1.12 def UniDec.unidec_modules.tims_import_wizard.data_importer.search_extern(file_path, search_string, split_skip = False)

Pass in each string left of target value.

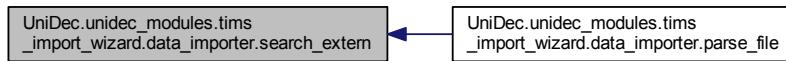
An example,

```

target
-----
Trap Wave Velocity (m/s)      300
search string='Trap Wave Velocity (m/s)'
returns :: 300

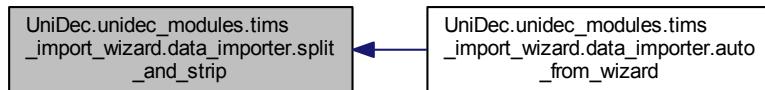
```

Here is the caller graph for this function:



6.42.1.13 def UniDec.unidec_modules.tims_import_wizard.data_importer.split_and_strip(*line*, *delimiter* = ')

Here is the caller graph for this function:



6.42.2 Variable Documentation

6.42.2.1 dictionary UniDec.unidec_modules.tims_import_wizard.data_importer.param_file_cache = {}

6.42.2.2 UniDec.unidec_modules.tims_import_wizard.data_importer.use_mp_import = True

6.43 UniDec.unidec_modules.tims_import_wizard.get_data_wrapper Namespace Reference

Functions

- def [new_get_data](#)
- def [new_get_data_MS](#)

6.43.1 Function Documentation

6.43.1.1 def UniDec.unidec_modules.tims_import_wizard.get_data_wrapper.new_get_data(*start*, *end*, *im_bin_size*, *raw_file*, *pusher*, *function_no*, *scan_start*, *scan_end*, *dir*=None)

6.43.1.2 def UniDec.unidec_modules.tims_import_wizard.get_data_wrapper.new_get_data_MS(*start*, *end*, *bin_size*, *raw_file*, *function_no*, *scan_start*, *scan_end*, *dir*=None)

6.44 UniDec.unidec_modules.tims_import_wizard.import_wizard_grid Namespace Reference

Classes

- class [WizardGrid](#)

6.45 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl Namespace Reference

Classes

- class [TreeCtrl](#)
- class [TreeCtrlPanel](#)

6.46 UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge Namespace Reference

Functions

- def [progress_dialog](#)
- def [on_callback\(\)](#)

Variables

- [dlg](#) = None
- int [counter](#) = 1
- int [maximum](#) = 1
- [pub_message](#) = None

6.46.1 Function Documentation

6.46.1.1 def UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.on_callback()

6.46.1.2 def UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.progress_dialog(*parent_window*, *title*, *message*, *num_files*, *pub_mess*=None)

6.46.2 Variable Documentation

6.46.2.1 int UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.counter = 1

6.46.2.2 UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.dlg = None

6.46.2.3 int UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.maximum = 1

6.46.2.4 UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.pub_message = None

6.47 UniDec.unidec_modules.tims_import_wizard.TagTypes Namespace Reference

Functions

- def [format_tag_name](#) (*tag_type*)

Variables

- string [SAMPLE](#) = 'sample'
- string [DESCRIPTION](#) = 'description'

- string **DRIFT_V** = 'dv'
- string **COLLISION_V** = 'cv'
- string **FILE_PATH** = 'file_path'
- string **FILE_NAME** = 'file_name'
- string **DRIFT_PRESSURE** = 'drift_pressure'
- string **TEMP** = 'temp'
- string **ATOM** = 'atom'
- string **WAVE_VELOCITY** = 'wave_velocity'
- string **WAVE_HEIGHT** = 'wave_height'
- string **EDC** = 'edc'
- string **CONE** = 'cone'
- string **EXTRACT** = 'extract'
- string **START** = 'start'
- string **END** = 'end'
- string **BIN** = 'bin'
- string **RANGE** = 'range'
- string **TYPE** = 'type'
- string **PUSHER** = 'pusher'
- string **FUNCTION** = 'function'
- string **SCAN_START** = 'scan_start'
- string **SCAN_END** = 'scan_end'
- string **TCAL1** = "tcal1"
- string **TCAL2** = "tcal2"
- dictionary **tag_type_formatting**

6.47.1 Function Documentation

6.47.1.1 def UniDec.unidec_modules.tims_import_wizard.TagTypes.format_tag_name (*tag_type*)

6.47.2 Variable Documentation

6.47.2.1 string UniDec.unidec_modules.tims_import_wizard.TagTypes.ATOM = 'atom'

6.47.2.2 string UniDec.unidec_modules.tims_import_wizard.TagTypes.BIN = 'bin'

6.47.2.3 string UniDec.unidec_modules.tims_import_wizard.TagTypes.COLLISION_V = 'cv'

6.47.2.4 string UniDec.unidec_modules.tims_import_wizard.TagTypes.CONE = 'cone'

6.47.2.5 string UniDec.unidec_modules.tims_import_wizard.TagTypes.DESCRIPTION = 'description'

6.47.2.6 string UniDec.unidec_modules.tims_import_wizard.TagTypes.DRIFT_PRESSURE = 'drift_pressure'

6.47.2.7 string UniDec.unidec_modules.tims_import_wizard.TagTypes.DRIFT_V = 'dv'

6.47.2.8 string UniDec.unidec_modules.tims_import_wizard.TagTypes.EDC = 'edc'

6.47.2.9 string UniDec.unidec_modules.tims_import_wizard.TagTypes.END = 'end'

6.47.2.10 string UniDec.unidec_modules.tims_import_wizard.TagTypes.EXTRACT = 'extract'

6.47.2.11 string UniDec.unidec_modules.tims_import_wizard.TagTypes.FILE_NAME = 'file_name'

6.47.2.12 string UniDec.unidec_modules.tims_import_wizard.TagTypes.FILE_PATH = 'file_path'

- 6.47.2.13 string UniDec.unidec_modules.tims_import_wizard.TagTypes.FUNCTION = 'function'
- 6.47.2.14 string UniDec.unidec_modules.tims_import_wizard.TagTypes.PUSHER = 'pusher'
- 6.47.2.15 string UniDec.unidec_modules.tims_import_wizard.TagTypes.RANGE = 'range'
- 6.47.2.16 string UniDec.unidec_modules.tims_import_wizard.TagTypes.SAMPLE = 'sample'
- 6.47.2.17 string UniDec.unidec_modules.tims_import_wizard.TagTypes.SCAN_END = 'scan_end'
- 6.47.2.18 string UniDec.unidec_modules.tims_import_wizard.TagTypes.SCAN_START = 'scan_start'
- 6.47.2.19 string UniDec.unidec_modules.tims_import_wizard.TagTypes.START = 'start'
- 6.47.2.20 dictionary UniDec.unidec_modules.tims_import_wizard.TagTypes.tag_type_formatting

Initial value:

```

1 = {SAMPLE: 'Sample',
2                 DESCRIPTION: 'Description',
3                 DRIFT_V: 'Drift Voltage',
4                 COLLISION_V: 'Collision Voltage',
5                 FILE_PATH: 'File Path',
6                 FILE_NAME: 'File Name',
7                 DRIFT_PRESSURE: 'Drift Pressure',
8                 TEMP: 'Temperature',
9                 ATOM: 'Atom',
10                WAVE_VELOCITY: 'Wave Velocity',
11                WAVE_HEIGHT: 'Wave Height',
12                EDC: 'EDC',
13                CONE: 'Cone Voltage',
14                EXTRACT: 'Extract',
15                START: 'Start',
16                END: 'End',
17                BIN: 'm/z Bin Size',
18                RANGE: 'm/z Range',
19                TYPE: 'Experiment Type',
20                PUSHER: 'Pusher',
21                FUNCTION: 'Function',
22                SCAN_START: 'Scan Start',
23                SCAN_END: 'Scan End',
24                TCAL1:"Calibration 1",
25                TCAL2:"Calibration 2"
26}

```

- 6.47.2.21 string UniDec.unidec_modules.tims_import_wizard.TagTypes.TCAL1 = "tcal1"
- 6.47.2.22 string UniDec.unidec_modules.tims_import_wizard.TagTypes.TCAL2 = "tcal2"
- 6.47.2.23 string UniDec.unidec_modules.tims_import_wizard.TagTypes.TEMP = 'temp'
- 6.47.2.24 string UniDec.unidec_modules.tims_import_wizard.TagTypes.TYPE = 'type'
- 6.47.2.25 string UniDec.unidec_modules.tims_import_wizard.TagTypes.WAVE_HEIGHT = 'wave_height'
- 6.47.2.26 string UniDec.unidec_modules.tims_import_wizard.TagTypes.WAVE_VELOCITY = 'wave_velocity'

6.48 UniDec.unidec_modules.unidecstructure Namespace Reference

Classes

- class [UniDecConfig](#)

Variables

- string `__author__` = 'Michael.Marty'

6.48.1 Variable Documentation

6.48.1.1 string UniDec.unidec_modules.unidecstructure.`__author__` = 'Michael.Marty'

6.49 UniDec.unidec_modules.unidectools Namespace Reference

Functions

- def `isempty` (thing)
- def `string_to_value` (s)
- def `simp_string_to_value` (s)
- def `string_to_int`
- def `safedivide` (a, b)
- def `weighted_std` (values, weights)
- def `interp_pos` (array, target)
- def `interp_val` (data, target)
- def `nearestunsorted` (array, target)
- def `nearest` (array, target)
- def `get_z_offset` (mass, charge)
- def `predict_charge` (mass)
- def `simchargefit` (x2)
- def `get_tvalue`
- def `get_zvalue`
- def `integrate` (data, start, end)
- def `center_of_mass`
- def `stepmax` (array, index)
- def `localmax` (array, start, end)
- def `localmaxpos` (data, start, end)
- def `localmax2` (array, index, window)
- def `simple_extract`
- def `data_extract` (data, x, extract_method, window=None, kwargs)
- def `data_extract_grid`
- def `kendrick_analysis`
- def `solve_for_mass`
- def `header_test` (path)
- def `load_mz_file` (path, config)
- def `zipdir` (path, zip_handle)
- def `zip_folder` (save_path)
- def `dataexport` (datatop, fname)
- def `mergedata` (data1, data2)
- def `mergedata2d` (x1, y1, x2, y2, z2)
- def `auto_peak_width` (datatop)
- def `auto_noise_level`
- def `average_bin_size` (datatop)
- def `cal_data`
- def `datachop` (datatop, newmin, newmax)
- def `datasimsub` (datatop, buff)
- def `datacompsub` (datatop, buff)
- def `calc_local_mins` (data, w)
- def `polynomial_background_subtract`

- def `savgol`
- def `savgol_background_subtract`
- def `intensitythresh` (datatop, thresh)
- def `gsmooth` (datatop, sig)
- def `nonlinear_axis` (start, end, res)
- def `linear_interpolation` (x1, x2, x)
- def `lintegrate` (datatop, intx)
- def `linterpolate` (datatop, intx)
- def `linearize` (datatop, binsize, linflag)
- def `nonlinearize` (datatop, num_compressed)
- def `removeduplicates` (datatop)
- def `normalize` (datatop)
- def `detectoreff` (datatop, va)
- def `dataprep` (datatop, config)
- def `unidec_call` (exepath, configfile, silent=False, kwargs)
- def `peakdetect`
- def `mergepeaks` (peaks1, peaks2, window)
- def `make_peaks_mztab` (mzgrid, pks, adductmass)
- def `makespecfun` (i, k, peaks_masses, adductmass, charges, xvals, ftab, xmax, xmin)
- def `make_peaks_mztab_spectrum` (mzgrid, pks, data2, mztab)
- def `makeconvspecies` (processed_data, pks, config)
- def `nonlinstickconv` (xvals, mztab, fwhm, psfun)
- def `stickconv` (mztab, kernel)
- def `make_alpha_cmap` (rgb_tuple, alpha)
- def `color_map_array` (array, cmap, alpha)
- def `lengths` (array)
- def `combine` (array2)
- def `combine_all` (array2)
- def `make_isolated_match` (oligos)
- def `make_all_matches` (oligos)
- def `match`
- def `ndis_std`
- def `ndis` (x, mid, fwhm, kwargs)
- def `ndis_fit` (x, s, m, a, b)
- def `ldis`
- def `ldis_fit` (x, s, m, a, b)
- def `spltdis`
- def `spltdis_fit` (x, s, m, a, b)
- def `voigt`
- def `cconv` (a, b)
- def `single_cwt`
- def `continuous_wavelet_transform`
- def `autocorr`
- def `cconvolve` (xvals, mztab, fwhm, psfun)
- def `conv_peak_shape_kernel` (xaxis, psfun, fwhm)
- def `make_peak_shape`
- def `gaussfit`
- def `psfit` (x, s, m, a, b, psfun)
- def `voigt_fit`
- def `fit_peak` (xvals, yvals, psfun, midguess, fwhmguess, aguess, bguess)
- def `isolated_peak_fit` (xvals, yvals, psfun, kwargs)
- def `fft` (data)
- def `fft_diff` (data, diffrange=[500.])
- def `pad_data`
- def `pad_two_power` (data)

- def `double_fft_diff`
- def `windowed_fft`
- def `win_fft_grid` (rawdata, binsize, wbin, window_fwhm, diffrange)
- def `win_fft_diff`
- def `correlation_integration` (dat1, dat2, alpha=0.01, plot_corr=False, kwargs)
- def `wide_sse` (dat1, dat2, sig)
- def `broaden` (aligned)

Variables

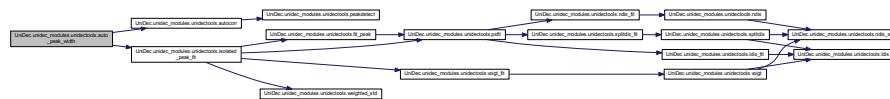
- int `is_64bits` = sys.maxsize>2
- string `dllname` = "libmypfunc"
- `testpath` = `dllname`
- `dllpath` = `testpath`
- tuple `pathoffile` = os.path.dirname(os.path.abspath(__file__))
- tuple `libs` = cdll.LoadLibrary(`dllpath`)

6.49.1 Function Documentation

6.49.1.1 def UniDec.unidec_modules.unidectools.auto_noise_level (`datatop, buffer=10`)

6.49.1.2 def UniDec.unidec_modules.unidectools.auto_peak_width (`datatop`)

Here is the call graph for this function:

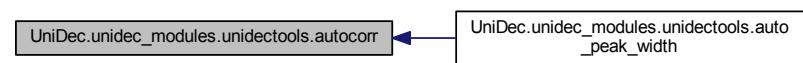


6.49.1.3 def UniDec.unidec_modules.unidectools.autocorr (`datatop, config=None`)

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.4 def UniDec.unidec_modules.unidectools.average_bin_size (*datatop*)

6.49.1.5 def UniDec.unidec_modules.unidectools.broaden (*aligned*)

Take a list of aligned peaks and broaden each so that they achieve maximum overlap with the broadest one.
:param aligned: Array (N x M x 2). N is the number of peaks, M is the number of data points, 2 is (x,y)
:return: combined, aligned: The combined total of all the aligned and broaded individual peaks.

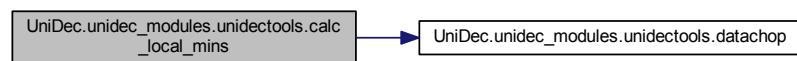
Here is the call graph for this function:



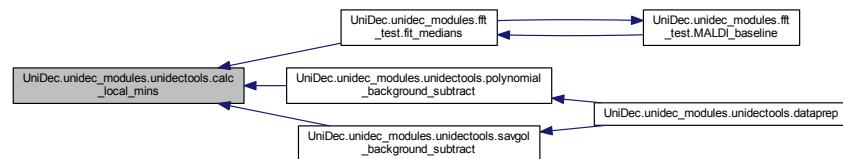
6.49.1.6 def UniDec.unidec_modules.unidectools.cal_data (*datatop*, *poly_coeff=None*)

6.49.1.7 def UniDec.unidec_modules.unidectools.calc_local_mins (*data*, *w*)

Here is the call graph for this function:



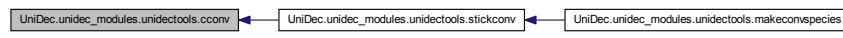
Here is the caller graph for this function:



6.49.1.8 def UniDec.unidec_modules.unidectools.cconv (*a*, *b*)

Circular convolution of two lists
:param a: N-length array
:param b: N-length array
:return: Convolution

Here is the caller graph for this function:



6.49.1.9 def UniDec.unidec_modules.unidectools.cconvolve (*xvals*, *mztab*, *fwhm*, *psfun*)

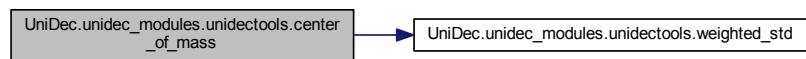
```
Fast nonlinear convolution algorithm using C dll.
:param xvals: x-axis
:param mztab: mztab from make_peaks_mztab()
:param fwhm: Full width half max of peak
:param psfun: Peak shape function code (0=Gauss, 1=Lorentzian, 2=Split G/L)
:return: Convolved output
```

Here is the caller graph for this function:

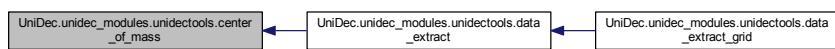


6.49.1.10 def UniDec.unidec_modules.unidectools.center_of_mass (*data*, *start*=None, *end*=None)

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.11 def UniDec.unidec_modules.unidectools.color_map_array (*array*, *cmap*, *alpha*)

```
For a specified array of values, map the intensity to a specified RGB color defined by cmap (output as topcm).
For each color, create a color map where the color is constant but the transparency changes (output as cmarr).
:param array: Values
:param cmap: Color map
:param alpha: Max Alpha value (transparency) [0,1]
:return: cmarr, topcm (list of transparent color maps, list of RGB colors for array values)
```

Here is the call graph for this function:



6.49.1.12 def UniDec.unidec_modules.unidectools.combine (array2)

Here is the call graph for this function:

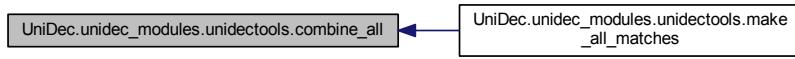


6.49.1.13 def UniDec.unidec_modules.unidectools.combine_all (array2)

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.14 def UniDec.unidec_modules.unidectools.continuous_wavelet_transform (a, widths, wavelet_type = "Ricker")

Perform a continuous wavelet transform at multiple widths.

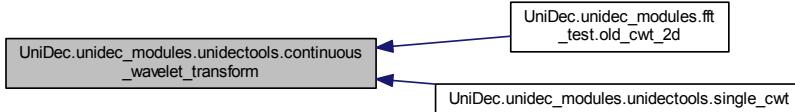
:param a: 1D numpy array of data (length N)

:param widths: List of widths (length W) of transform defined with respect to the data points in a

:param wavelet_type: Type of wavelet. Either "Ricker" (Mexican Hat) or "Morlet" (Gabor)

:return: cwt_matrix (The continuous wavelet transform at the defined widths in a (W x N) array)

Here is the caller graph for this function:



6.49.1.15 def UniDec.unidec_modules.unidectools.conv_peak_shape_kernel(*xaxis*, *psfun*, *fwhm*)

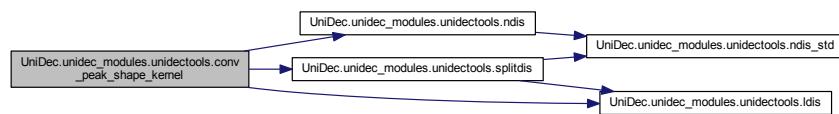
Creation of an efficient peak shape kernel for circular convolutions.

Note: peak width must be in units of index not value of x-axis. To get this take fwhm/binsize.
 :param xaxis: Array of x axis values
 :param psfun: Integer

0=Gaussian
 1=Lorentzian
 2=Split Gaussian/Lorentzian

:param fwhm: Full width half max of peak (in units matching data indexes not values)
 :return: Peak shape kernel centered at 0.

Here is the call graph for this function:



Here is the caller graph for this function:



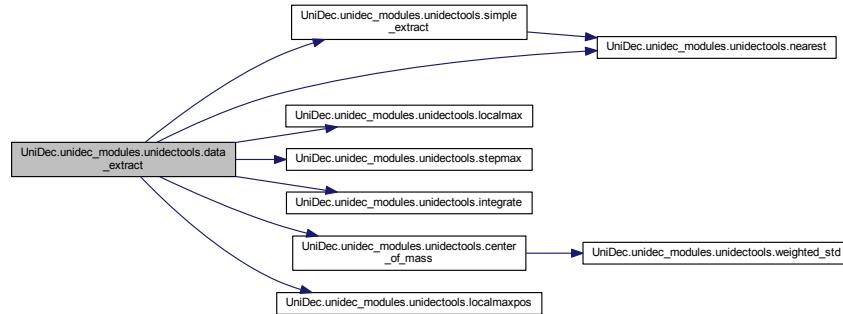
6.49.1.16 def UniDec.unidec_modules.unidectools.correlation_integration(*dat1*, *dat2*, *alpha* = 0.01, *plot_corr* = False, *kwargs*)

Perform MacCoss method (<http://pubs.acs.org/doi/pdf/10.1021/ac034790h>) of getting peak intensities
 :param dat1: Denominator peak
 :param dat2: Numerator peak
 :param alpha: 1-confidence level
 :param plot_corr: Boolean flag, if True, will plot the results
 :param kwargs: keywords (unused dump)
 :return: slope, cierr, rsquared, slope_std_error * np.sqrt(n), pvalue
 slope of line (ratio of peak areas)
 cierr (confidence interval for error)
 rsquared (R squared value for linear fit)
 slope_std_error * np.sqrt(n) (standard deviation of slope fit)
 pvalue (probability that slope is nonzero)

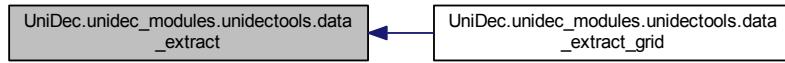
6.49.1.17 def UniDec.unidec_modules.unidectools.data_extract(*data*, *x*, *extract_method*, *window* = None, *kwargs*)

Assumes a sorted array in data[:,0]
 :param data:
 :param x:
 :param extract_method:
 :param window:
 :return:

Here is the call graph for this function:

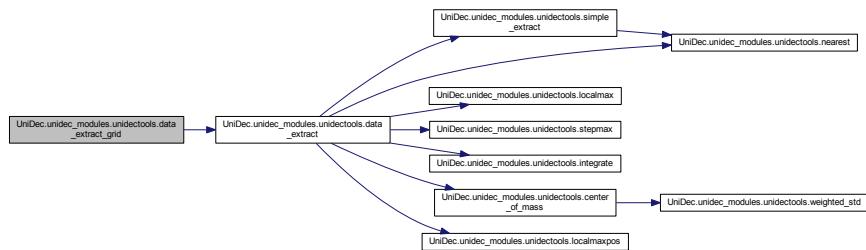


Here is the caller graph for this function:



6.49.1.18 def UniDec.unidec_modules.unidectools.data_extract_grid (`data`, `xarray`, `extract_method = 1`, `window = 0`)

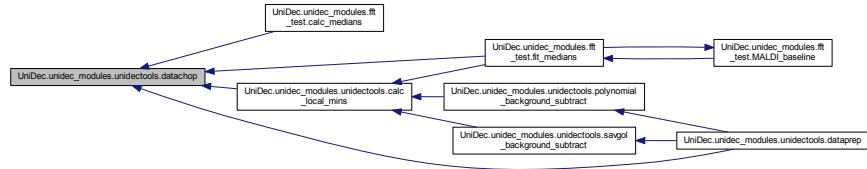
Here is the call graph for this function:



6.49.1.19 def UniDec.unidec_modules.unidectools.datachop (`datatop`, `newmin`, `newmax`)

Chops the range of the data. The `[:,0]` column of the data is the column that will be indexed.
:param datatop: Data array
:param newmin: Minimum value of chopped data
:param newmax: Maximum value of chopped data
:return: New data limited between the two bounds

Here is the caller graph for this function:



6.49.1.20 def UniDec.unidec_modules.unidectools.datacompsub (*datatop, buff*)

Complex background subtraction.

Taken from MassSpec Paper

First creates an array that matches the data but has the minimum value within a window of +/- *buff*. Then, smooths the minimum array with a Gaussian filter of width *buff* * 2 to form the background array. Finally, subtracts the background array from the data intensities.

```
:param datatop: Data array
:param buff: Width parameter
:returns: Subtracted data
```

Here is the caller graph for this function:



6.49.1.21 def UniDec.unidec_modules.unidectools.dataexport (*datatop, fname*)

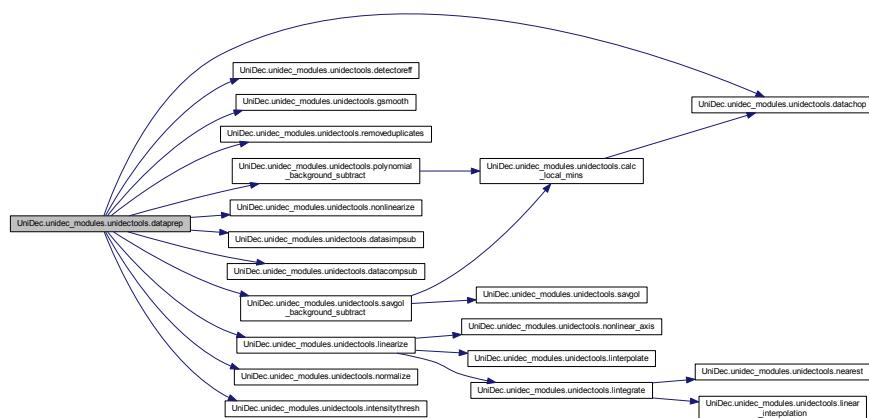
6.49.1.22 def UniDec.unidec_modules.unidectools.dataprep (*datatop, config*)

Main function to process 1D MS data. The order is:

```
Crop Data (datacrop)
Correct for detector efficiency (detectoreff)
Smooth (gsmooth)
Remove duplicates (removeduplicates)
Linearize (linearize or nonlinearize)
Baseline subtraction (datasimpsub or datacompsub or simply data[:,1]-np.amin(data[:,1]))
Normalization (normalize)
Intensity Threshold with a threshold of 0 (intthresh)

:param datatop: Raw data array (N x 2)
:param config: UniDecConfig object
:returns: Processed data
```

Here is the call graph for this function:



6.49.1.23 def UniDec.unidec_modules.unidectools.datasimpsub (*datatop*, *buff*)

Simple subtraction of a linear background.

The first n and last n data points are averaged. A line is drawn between the two averages. This line is then subtracted from the `[:,1]` column of the data.

`:param datatop: Data array (N x 2) (m/z, intensity)`
`:param buff: Integer, n.`
`:return: Subtracted data`

Here is the caller graph for this function:



6.49.1.24 def UniDec.unidec_modules.unidectools.detectoreff (*datatop*, *va*)

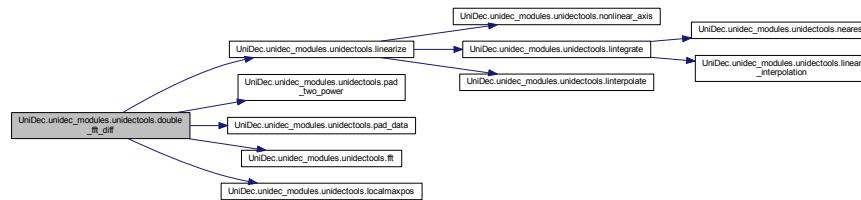
Incorporate a model of TOF detector efficiency used by CHAMP to correct the intensity values.
`:param datatop: Data array (N x 2)`
`:param va: TOF acceleration voltage in kV (I think...)`
`:return: Detector corrected data (N x 2)`

Here is the caller graph for this function:



```
6.49.1.25 def UniDec.unidec_modules.unidectools.double_fft_diff( mzdata, diffrange = None, binsize = 0.1, pad = None, preprocessed = False )
```

Here is the call graph for this function:

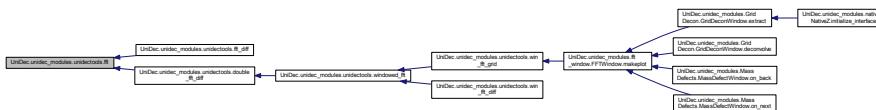


Here is the caller graph for this function:



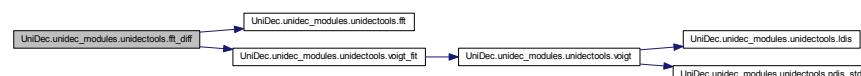
```
6.49.1.26 def UniDec.unidec_modules.unidectools.fft( data )
```

Here is the caller graph for this function:



```
6.49.1.27 def UniDec.unidec_modules.unidectools.fft_diff( data, diffrange = [ 500. ] )
```

Here is the call graph for this function:

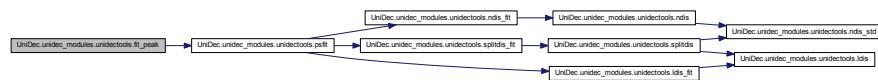


```
6.49.1.28 def UniDec.unidec_modules.unidectools.fit_peak( xvals, yvals, psfun, midguess, fwhmguess, aguess, bguess )
```

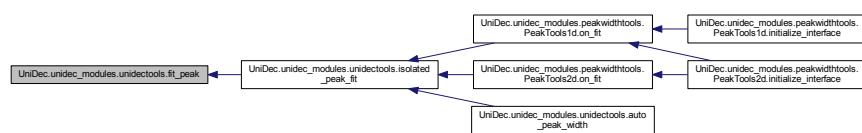
Fit peak from xvals and yvals data to defined peak shape function.
:param xvals: x values of data
:param yvals: y values of data
:param psfun: peak shape function integer code

```
:param midguess: midpoint guess
:param fwhmguess: fwhm guess
:param aguess: amplitude guess
:param bguess: background guess
:return: popt, perr, fitdat (optimized parameters [fwhm, mid, a, b], std error of parameters, fit to data)
```

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.29 def UniDec.unidec_modules.unidectools.gaussfit(xvals, yvals, mguess =None, sguess = 0.1, aguess = None, cleanup = True)

Simple gaussian fitting function.

```
:param xvals: X values
:param yvals: Y values
:param mguess: Guess for midpoint
:param sguess: Guess for standard deviation
:param aguess: Guess for amplitude
:param cleanup: Boolean Flag, if True, will clean up data to remove background and normalize
:return: Gaussian fit parameters [mid, sig, amp]
```

6.49.1.30 def UniDec.unidec_modules.unidectools.get_tvalue(dof, ci = 0.99)

Get t-value for a given degrees of freedom and confidence interval

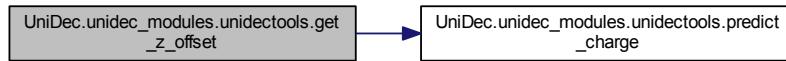
```
:param dof: Degrees of freedom
:param ci: Confidence interval level (default is 0.99, 99% confidence)
:return: T value
```

6.49.1.31 def UniDec.unidec_modules.unidectools.get_z_offset(mass, charge)

For a given mass and charge combination, calculate the charge offset parameter.

```
:param mass: Mass in Da
:param charge: Charge State
:return: Difference between charge and predicted native charge of the mass
```

Here is the call graph for this function:



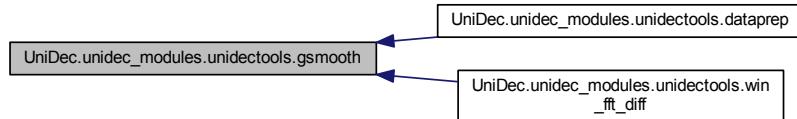
6.49.1.32 def UniDec.unidec_modules.unidectools.get_zvalue(ci=0.99)

Get z-value for area under a Gaussian for a given confidence level
:param ci: Confidence interval level (default is 0.99, 99% confidence)
:return: Z-value

6.49.1.33 def UniDec.unidec_modules.unidectools.gsmooth(datatop, sig)

Smooths the data with a Gaussian filter of width sig.
:param datatop: Data array
:param sig: Width of Gaussian Array
:return: Smoothed Data

Here is the caller graph for this function:



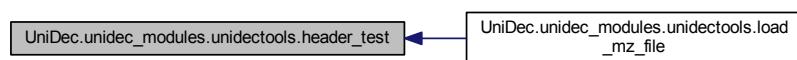
6.49.1.34 def UniDec.unidec_modules.unidectools.header_test(path)

A quick test of a file to remove any problems from the header.

If scans through each line of an input file specified by path and count the number of lines that cannot be completely converted to floats. It breaks the loop on the first hit that is entirely floats, so any header lines below that will not be counted.

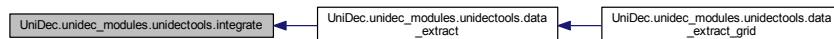
:param path: Path of file to be scanned
:return: Integer length of the number of header lines

Here is the caller graph for this function:



6.49.1.35 def UniDec.unidec_modules.unidectools.integrate (*data, start, end*)

Here is the caller graph for this function:



6.49.1.36 def UniDec.unidec_modules.unidectools.intensitythresh (*datatop, thresh*)

Sets an intensity threshold. Everything below the threshold is set to 0.

```
:param datatop: Data array
:param thresh: Threshold value
:returns: Thresholded array.
```

Here is the caller graph for this function:



6.49.1.37 def UniDec.unidec_modules.unidectools.interp_pos (*array, target*)

On a given array, interpolate the position of the target

```
:param array: Array
:param target: Value
:returns: Interpolated index of value in array.
```

6.49.1.38 def UniDec.unidec_modules.unidectools.interp_val (*data, target*)

On a given array, interpolate the value of the target

```
:param array: data
:param target: Value
:returns: Interpolated index of value in array.
```

6.49.1.39 def UniDec.unidec_modules.unidectools.isempty (*thing*)

Checks whether the thing, a list or array, is empty

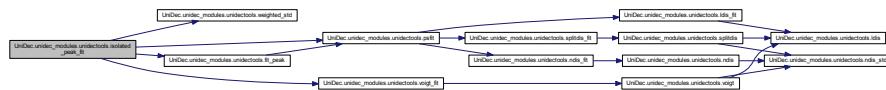
```
:param thing: Object to check
:returns: Boolean, True if not empty
```

6.49.1.40 def UniDec.unidec_modules.unidectools.isolated_peak_fit (*xvals, yvals, psfun, kwargs*)

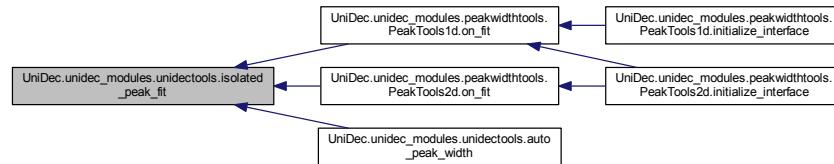
Fit an isolated peak to the peak shape model.

```
:param xvals: x values of data
:param yvals: y values of data
:param psfun: peak shape function integer code
:param kwargs: keywords (unused)
:returns: fit_array, fit_data (4 x 2 array of (fit, error) for [fwhm,mid,amp,background], fit to data)
```

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.41 def UniDec.unidec_modules.unidectools.kendrick_analysis (massdat, kendrickmass, centermode = 1, nbins = 50, transformmode = 1, xaxistype = 1)

Here is the call graph for this function:

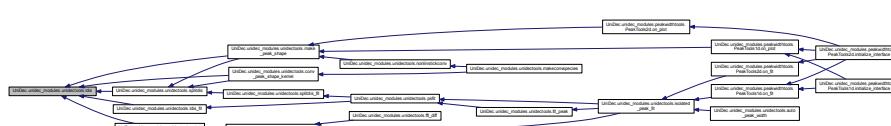


6.49.1.42 def UniDec.unidec_modules.unidectools.idis (x, mid, fwhm, a = 1, norm_area = False)

Lorentzian function normalized to a max of 1.

Note: x and mid are interchangable. At least one should be a single float. The other may be an array.
:param x: x values
:param mid: Mean
:param fwhm: Full Width at Half Max
:param a: Amplitude (default is 1)
:param norm_area: Boolean, Whether to normalize so that the area under the distribution is 1.
:return: Lorentzian distribution at x values

Here is the caller graph for this function:



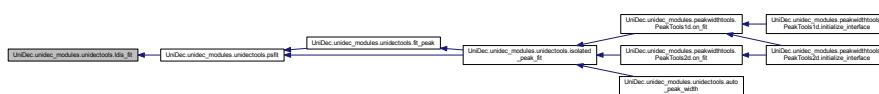
6.49.1.43 def UniDec.unidec_modules.unidectools.ldis_fit(x, s, m, a, b)

Function for fitting Lorentzian distribution to peak.
 Adds a background to ldis.
 Prevents negative background, amplitude, and standard deviation.
 :param x: x value
 :param s: full width half max
 :param m: mean
 :param a: amplitude
 :param b: linear background
 :return: peak shape

Here is the call graph for this function:

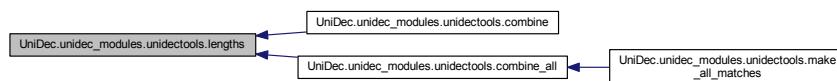


Here is the caller graph for this function:



6.49.1.44 def UniDec.unidec_modules.unidectools.lengths(array)

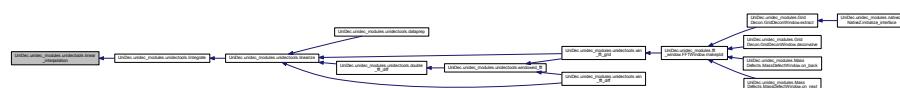
Here is the caller graph for this function:



6.49.1.45 def UniDec.unidec_modules.unidectools.linear_interpolation(x1, x2, x)

:param x1:
 :param x2:
 :param x:
 :return: float(x - x1) / float(x2 - x1)

Here is the caller graph for this function:

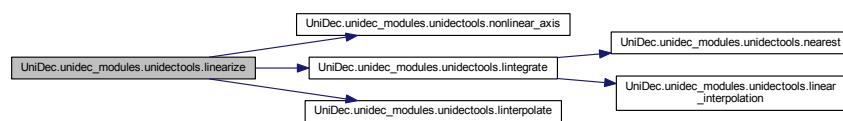


6.49.1.46 def UniDec.unidec_modules.unidectools.linearize (*datatop*, *binsize*, *linflag*)

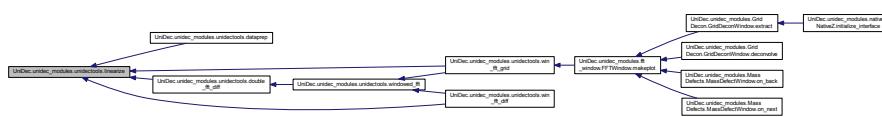
Linearize data by defined x-axis bin size by either interpolation or integration
 :param datatop: Data array (N x 2)
 :param binsize: Spacing between first two m/z points
 :param linflag: Integer flag indicating the type of linearization.

0=Integration with Linear Axis (constant m/z)
 1=Integration with Nonlinear Axis (constant resolution: mz / delta mz)
 3=Interpolation with Linear Axis
 4=Interpolation with Nonlinear Axis
 :return: Linearized data

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.47 def UniDec.unidec_modules.unidectools.integrate (*datatop*, *intx*)

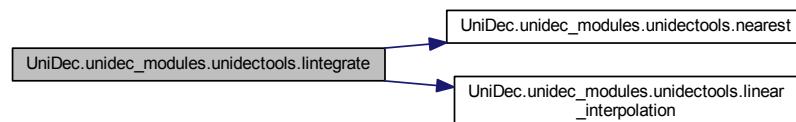
Linearize x-axis by integration.

Each intensity value in the old data gets proportionally added into the new x-axis.

The total sum of the intensity values should be constant.

:param datatop: Data array
 :param intx: New x-axis for data
 :return: Integration of intensity from original data onto the new x-axis.
 Same shape as the old data but new length.

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.48 def UniDec.unidec_modules.unidectools.interpolate(datatop, intx)

Linearize x-axis by interpolation.

The new x-axis is interpolated on the old data and the corresponding intensities are picked out.

```
:param datatop: Data array
:param intx: New x-axis
:return: Interpolation of intensity from original data onto the new x-axis.
        Same shape as the old data but new length.
```

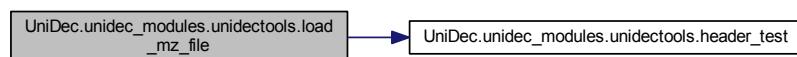
Here is the caller graph for this function:



6.49.1.49 def UniDec.unidec_modules.unidectools.load_mz_file(path, config)

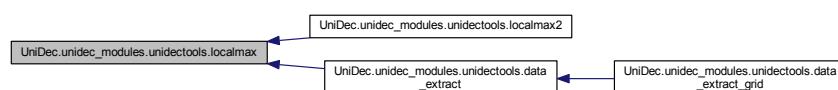
Loads a text or mzml file
:param path: File path to load
:param config: UniDecConfig object
:return: Data array

Here is the call graph for this function:



6.49.1.50 def UniDec.unidec_modules.unidectools.localmax(array, start, end)

Here is the caller graph for this function:



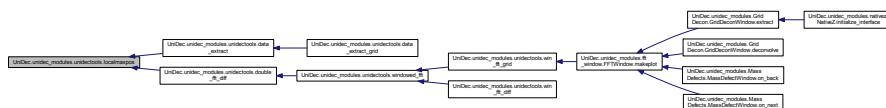
6.49.1.51 def UniDec.unidec_modules.unidectools.localmax2 (array, index, window)

Here is the call graph for this function:



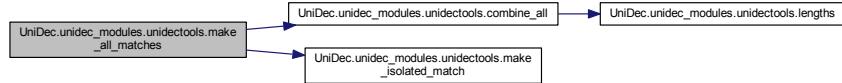
6.49.1.52 def UniDec.unidec_modules.unidectools.localmaxpos (data, start, end)

Here is the caller graph for this function:



6.49.1.53 def UniDec.unidec_modules.unidectools.make_all_matches (oligos)

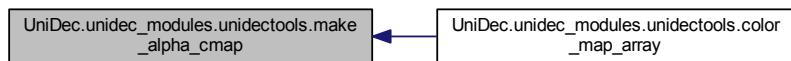
Here is the call graph for this function:



6.49.1.54 def UniDec.unidec_modules.unidectools.make_alpha_cmap (rgb_tuple, alpha)

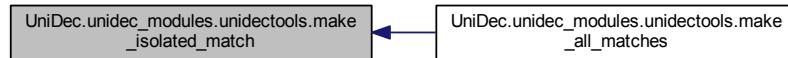
Make color map where RGB specified in tup
:param rgb_tuple: Tuple of RGB vaalues [0,1]
:param alpha: Maximum Alpha (Transparency) [0,1]
:return: Color map dictionary with a constant color but varying transparency

Here is the caller graph for this function:



6.49.1.55 def UniDec.unidec_modules.unidectools.make_isolated_match(oligos)

Here is the caller graph for this function:



6.49.1.56 def UniDec.unidec_modules.unidectools.make_peak_shape(xaxis, psfun, fwhm, mid, norm_area=False)

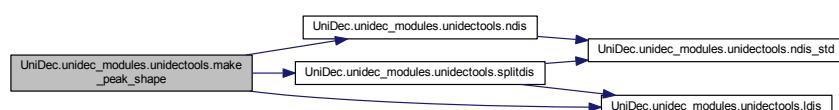
Make a peak of width fwhm centered at mid for given x axis.

Note: peak width must be in units of index not value of x-axis. To get this take fwhm/binsize.
:param xaxis: Array of x axis values
:param psfun: Integer

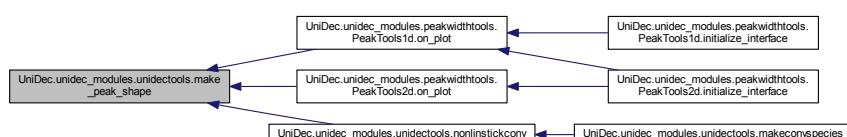
0=Gaussian
1=Lorentzian
2=Split Gaussian/Lorentzian

:param fwhm: Full width half max of peak (in units matching data indexes not values)
:param mid: Midpoint of peak
:return: Peak shape centered at midpoint .

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.57 def UniDec.unidec_modules.unidectools.make_peaks_mztab(mzgrid, pks, adductmass)

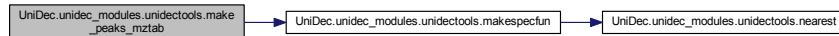
For each peak in pks, get the charge state distribution.

The intensity at each charge state is determined from mzgrid and stored in a list as peak.mztab. An array of the results is also output for help speeding up make_peaks_mztab_spectrum

:param mzgrid: 2D grid of m/z vs charge (N x Z)
:param pks: Peaks object (length P)

```
:param adductmass: Mass of electrospray adduct.
:return: P x Z array
```

Here is the call graph for this function:



6.49.1.58 def UniDec.unidec_modules.unidectools.make_peaks_mztab_spectrum (mzgrid, pks, data2, mztab)

Used for plotting the dots in plot 4.

Perform the same things as make_peaks_mztab, but instead of using the deconvolved intensities, it takes the intensity directly from the spectrum.

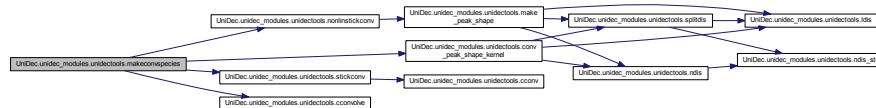
```
:param mzgrid: m/z grid (N x Z)
:param pks: Peaks object
:param data2: Processed data 1D
:param mztab: Prior mztab from make_peaks_mztab
:return: mztab but with intensities replaced by value at the spectrum.
```

6.49.1.59 def UniDec.unidec_modules.unidectools.makeconvspecies (processed_data, pks, config)

For data and peaks, create a simulated spectrum of each peak.
Assumes p.mztab has been set for each p in pks.peaks by make_peaks_mztab
Also makes pks.composite, which is a sum of all the simulated spectra.

```
:param processed_data: Processed 2D MS data (data2, N x 2)
:param pks: Peaks object (P Peak objects in pks.peaks)
:param config: UniDecConfig object
:return: Array of simulated spectra (P x N)
```

Here is the call graph for this function:



6.49.1.60 def UniDec.unidec_modules.unidectools.makespecfun (i, k, peaks_masses, adductmass, charges, xvals, ftab, xmax, xmin)

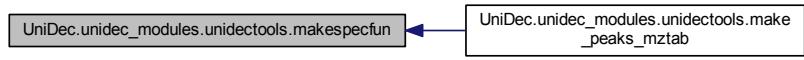
Small helper function to speed things up. May be more better way to do this, but I found this to be fastest.

```
:param i: peak mass index
:param k: charge index
:param peaks_masses: peak masses list
:param adductmass: Adduct mass
:param charges: charge list
:param xvals: x-values from data
:param ftab: List of interpolation functions
:param xmax: Maximum x value
:param xmin: Minimum x value
:return:
```

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.61 def UniDec.unidec_modules.unidectools.match (*pks*, *oligomasslist*, *oligonames*, *tolerance*=None)

Here is the call graph for this function:



6.49.1.62 def UniDec.unidec_modules.unidectools.mergedata (*data1*, *data2*)

Uses a 1D interpolation to merge the intensity of data2 into the axis of data1
:param data1: Reference data (N x 2 array)
:param data2: Data to merge (M x 2 array)
:return: data2 interpolated into the same axis as data1 (N x 2)

6.49.1.63 def UniDec.unidec_modules.unidectools.mergedata2d (*x1*, *y1*, *x2*, *y2*, *z2*)

Uses a 2D interpolation to merge a 2D grid of data from one set of axes to another.

Requires rectangular grids of all inputs such as might be created by numpy.meshgrid.
:param x1: Reference x-value grid (N x M)
:param y1: Reference y-value grid (N x M)
:param x2: Data x-value grid (N2 x M2)
:param y2: Data y-value grid (N2 x M2)
:param z2: Data intensity grid (N2 x M2)
:return: z2 interpolated onto x1 y1 2D grid (N x M)

6.49.1.64 def UniDec.unidec_modules.unidectools.mergepeaks (*peaks1*, *peaks2*, *window*)

Merge a test list of peaks to a reference list.

Each peak in peaks2 is matched to the closest peak in peak1.

If it within some defined threshold, the new peak replaces that closes peak in the matched list.
If no new peaks are matched to a reference peak, that peaks mass is unchanged but intensity is set to 0.

```
:param peaks1: Reference peaks (P x 2)
:param peaks2: Test peaks (R x 2)
:param window: Tolerance window of the x values
:return: Intensity of peaks2 matched to values of peaks1 (P x 2)
```

6.49.1.65 def UniDec.unidec_modules.unidectools.ndis(x, mid, fwhm, kwargs)

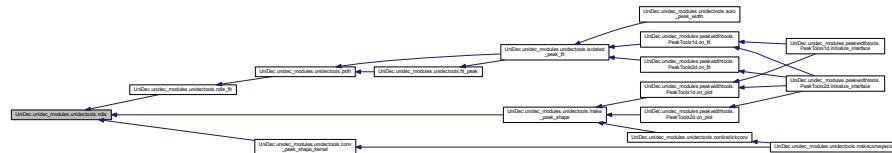
Gaussian function normalized to a max of 1.

Note: x and mid are interchangable. At least one should be a single float. The other may be an array.
 :param x: x values
 :param mid: Mean
 :param fwhm: Full Width at Half Max ($2.35482 * \text{standard deviation}$)
 :param kwargs: Allows norm_area flag to be passed
 :return: Gaussian distribution at x values

Here is the call graph for this function:



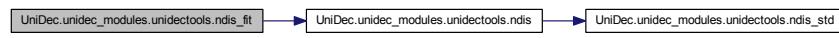
Here is the caller graph for this function:



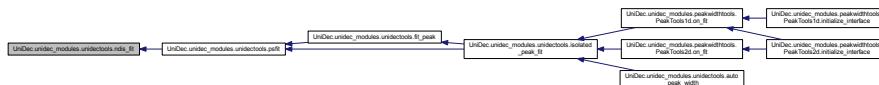
6.49.1.66 def UniDec.unidec_modules.unidectools.ndis_fit(x, s, m, a, b)

Function for fitting normal distribution to peak.
 Adds a background to ndis.
 Prevents negative background, amplitude, and standard deviation.
 :param x: x value
 :param s: full width half max
 :param m: mean
 :param a: amplitude
 :param b: linear background
 :return: peak shape

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.67 def UniDec.unidec_modules.unidectools.ndis_std(x, mid, sig, a=1, norm_area=False)

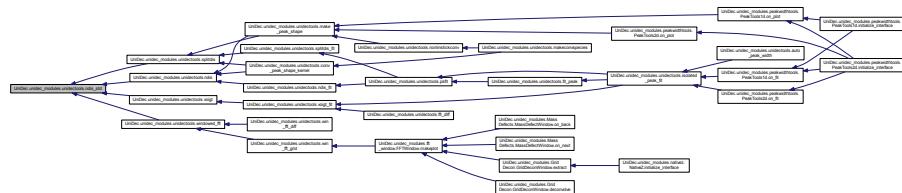
Normal Gaussian function normalized to the max of 1.

```

:param x: x values
:param mid: Mean of Gaussian
:param sig: Standard Deviation
:param a: Maximum amplitude (default is 1)
:param norm_area: Boolean, Whether to normalize so that the area under the distribution is 1.
:returns: Gaussian distribution at x values

```

Here is the caller graph for this function:



6.49.1.68 def UniDec.unidec_modules.unidectools.nearest(array, target)

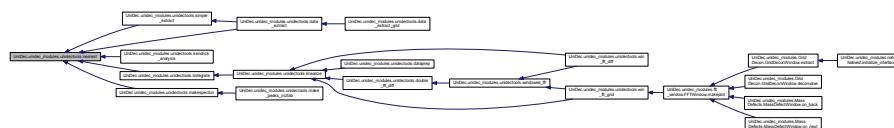
In an sorted array, quickly find the position of the element closest to the target.

```

:param array: Array
:param target: Value
:returns: np.argmin(np.abs(array - target))

```

Here is the caller graph for this function:



6.49.1.69 def UniDec.unidec_modules.unidectools.nearestunsorted(array, target)

In an unsorted array, find the position of the element closest to the target.

For a sorted array, the method nearest will be faster.

```

:param array: Array
:param target: Value
:returns: np.argmin(np.abs(array - target))

```

Here is the caller graph for this function:



6.49.1.70 def UniDec.unidec_modules.unidectools.nonlinear_axis(start, end, res)

Creates a nonlinear axis with the m/z values spaced with a defined and constant resolution.
:param start: Minimum m/z value
:param end: Maximum m/z value
:param res: Resolution of the axis (m / delta m)
:return: One dimensional array of the nonlinear axis.

Here is the caller graph for this function:



6.49.1.71 def UniDec.unidec_modules.unidectools.nonlinearize(datatop, num_compressed)

Compress the data in a simple and nonlinear way.
:param datatop: Data array (N x 2)
:param num_compressed:
:return:

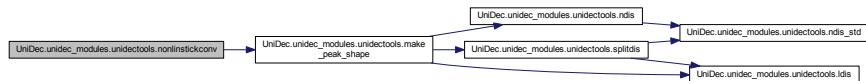
Here is the caller graph for this function:



6.49.1.72 def UniDec.unidec_modules.unidectools.nonlinstickconv(xvals, mztab, fwhm, psfun)

Python-based Nonlinear convolution. First makes a stick spectrum. Then, convolved with peak shape kernel.
:param xvals: x-axis
:param mztab: mztab from make_peaks_mztab
:param fwhm: Full width half max
:param psfun: Peak shape function integer
:return: Convolved output

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.73 def UniDec.unidec_modules.unidectools.normalize(datatop)

Normalize the data so that the maximum intensity is 1.

```

maxval = npamax(datatop[:, 1])
datatop[:, 1] = datatop[:, 1] / maxval

:param datatop: Data array (N x 2)
:returns: Normalized data array (N x 2)
  
```

Here is the caller graph for this function:



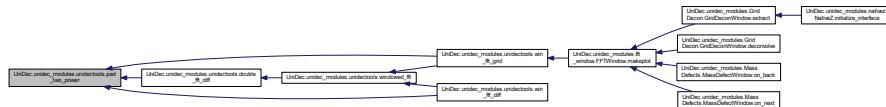
6.49.1.74 def UniDec.unidec_modules.unidectools.pad_data(linear_mzdata, pad_until = 50000)

Here is the caller graph for this function:



6.49.1.75 def UniDec.unidec_modules.unidectools.pad_two_power(*data*)

Here is the caller graph for this function:



6.49.1.76 def UniDec.unidec_modules.unidectools.peakdetect(*data*, *config*=None, *window*=10, *threshold*=0)

Simple peak detection algorithm.

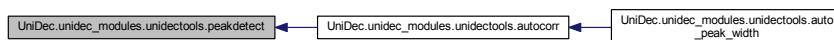
Detects a peak if a given data point is a local maximum within plus or minus config.peakwindow. Peaks must also be above a threshold of config.peakthresh * max_data_intensity.

The mass and intensity of peaks meeting these criteria are output as a P x 2 array.

```

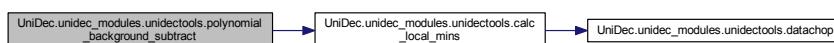
:param data: Mass data array (N x 2) (mass intensity)
:param config: UniDecConfig object
:return: Array of peaks positions and intensities (P x 2) (mass intensity)
    
```

Here is the caller graph for this function:

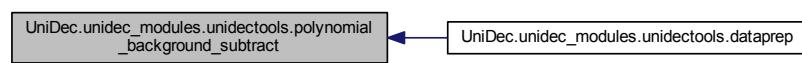


6.49.1.77 def UniDec.unidec_modules.unidectools.polynomial_background_subtract(*datatop*, *polynomial_order*=4, *width*=20, *cutoff_percent*=0.25)

Here is the call graph for this function:



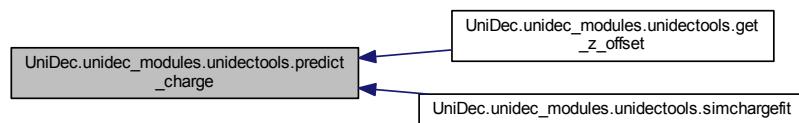
Here is the caller graph for this function:



6.49.1.78 def UniDec.unidec_modules.unidectools.predict_charge(mass)

```
Give predicted native charge state of species of defined mass
:param mass: Mass in Da
:return: Float, predicted average native charge state
```

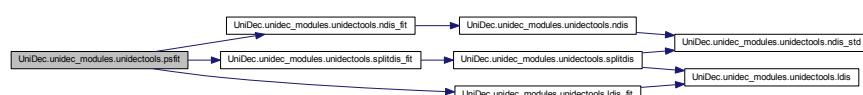
Here is the caller graph for this function:



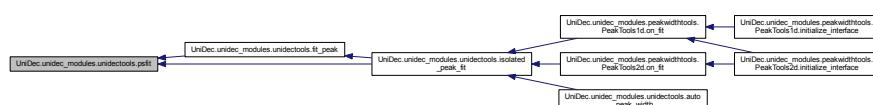
6.49.1.79 def UniDec.unidec_modules.unidectools.psfit(x, s, m, a, b, psfun)

```
Make peak shape from fit
:param x: x values
:param s: fwhm
:param m: max position
:param a: amplitude
:param b: background
:param psfun: peak shape function integer code
:return: peak shape fit data
```

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.80 def UniDec.unidec_modules.unidectools.removeduplicates(datatop)

```
Cleans up data that may have the same x value multiple times.
Each nonunique x gets merged into a single unique x with the sum of all of the nonunique intensities.
:param datatop: Data array (N x 2)
:return: Data with unique x values
```

Here is the caller graph for this function:

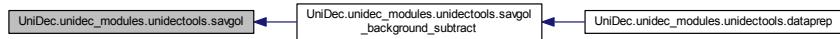


6.49.1.81 def UniDec.unidec_modules.unidectools.safedivide(a, b)

```
Divide numpy arrays b from a. Define a/0=0 to avoid zero division error.
:param a: Numerator
:param b: Denominator
:return: a/b
```

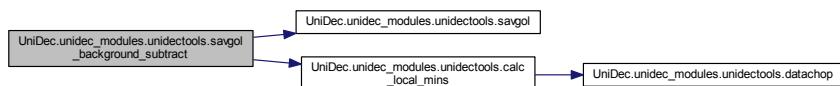
6.49.1.82 def UniDec.unidec_modules.unidectools.savgol(ydata, window=None, order=2)

Here is the caller graph for this function:

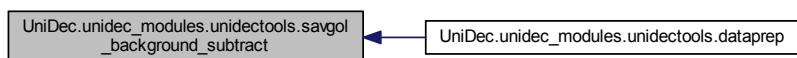


6.49.1.83 def UniDec.unidec_modules.unidectools.savgol_background_subtract(datatop, width, cutoff_percent=0.25)

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.84 def UniDec.unidec_modules.unidectools.simchargefit(x2)

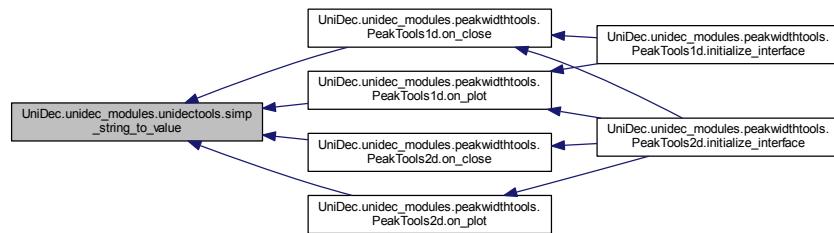
Here is the call graph for this function:



6.49.1.85 def UniDec.unidec_modules.unidectools.simp_string_to_value(s)

Try to convert string to float. Raise False if not possible.
:param s: String
:return: Float if possible. Otherwise, False

Here is the caller graph for this function:

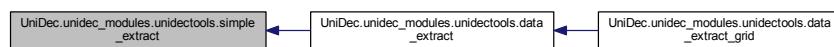


6.49.1.86 def UniDec.unidec_modules.unidectools.simple_extract(data, x, zero_edge = True)

Here is the call graph for this function:



Here is the caller graph for this function:

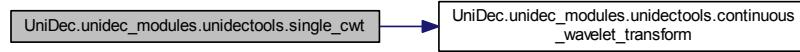


6.49.1.87 def UniDec.unidec_modules.unidectools.single_cwt(*a*, *width*, *wavelet_type* = "Ricker")

Perform a continuous wavelet transform at a single defined width.

```
:param a: 1D numpy array of data (length N)
:param width: Width of transform defined with respect to the data points in a
:param wavelet_type: Type of wavelet. Either "Ricker" (Mexican Hat) or "Morlet" (Gabor)
:return: cwt, wavelet
Continuous wavelet transform and wavelet of choice, both as numpy arrays of length N.
```

Here is the call graph for this function:



6.49.1.88 def UniDec.unidec_modules.unidectools.solve_for_mass(*mz1*, *mz2*, *adductmass* = 1.007276467)

Simple function to solve for mass from two adjacent charge state peaks in m/z.

```
:param mz1: Smaller m/z value (charge = z1)
:param mz2: Larger m/z value (charge = z2 = z1 + 1)
:param adductmass: Mass of electrospray adduct (default = Hydrogen)
:return: mass, z1, z2
```

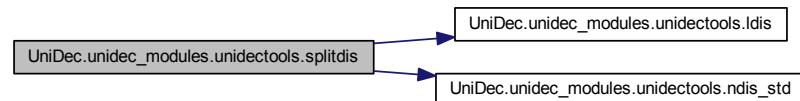
6.49.1.89 def UniDec.unidec_modules.unidectools.splitdis(*x*, *mid*, *fwhm*, *a*=1, *norm_area*=False)

Split Gaussain/Lorentzian function normalized to a max of 1.

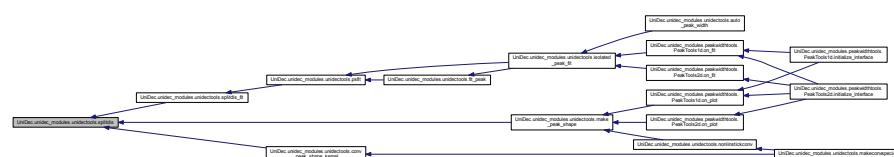
Gaussian < mid. Lorentzian > mid.

```
:param mid: Mid point (point of peak intensity)
:param x: x value or values
:param fwhm: Full Width at Half Max
:return: Split Gaussian/Lorentzian distribution at x value
```

Here is the call graph for this function:



Here is the caller graph for this function:



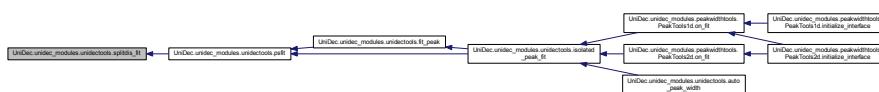
6.49.1.90 def UniDec.unidec_modules.unidectools.splitdis_fit(x, s, m, a, b)

Function for fitting Split G/L distribution to peak.
 Adds a background to splitdis.
 Prevents negative background, amplitude, and standard deviation.
 :param x: x value
 :param s: full width half max
 :param m: mean
 :param a: amplitude
 :param b: linear background
 :return: peak shape

Here is the call graph for this function:

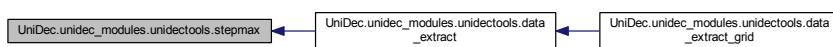


Here is the caller graph for this function:



6.49.1.91 def UniDec.unidec_modules.unidectools.stepmax(array, index)

Here is the caller graph for this function:



6.49.1.92 def UniDec.unidec_modules.unidectools.stickconv(mztab, kernel)

Make stick spectrum and then convolves with kernel.
 :param mztab: mztab from make_peaks_mztab
 :param kernel: peak shape kernel
 :return: Convolved output

Here is the call graph for this function:



Here is the caller graph for this function:



6.49.1.93 def UniDec.unidec_modules.unidectools.string_to_int(s, default=False)

Try to convert string to integer.
:param s: String
:return: Integer if possible. Otherwise, False

6.49.1.94 def UniDec.unidec_modules.unidectools.string_to_value(s)

Try to convert string to float.
:param s: String
:return: Float if possible. Otherwise, empty string.

6.49.1.95 def UniDec.unidec_modules.unidectools.unidec_call(exepath, configfile, silent=False, kwargs)

Run the UniDec binary specified by exepath with the configuration file specified by configfile. If silent is False (default), the output from exepath will be printed to the standard out. If silent is True, the output is suppressed.

The binary is run as a commandline subprocess with a call of (for example):

```
UniDec.exe conf.dat

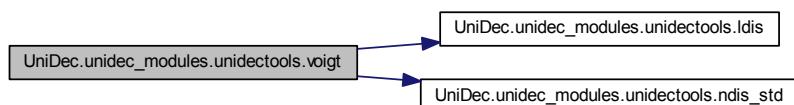
:param exepath: Path to UniDec or UniDecIM binary
:param configfile: Path to configuration file
:param silent: Whether to print the output of exepath to the standard out
:param kwargs:
:return: Standard error of exepath execution
```

6.49.1.96 def UniDec.unidec_modules.unidectools.voigt(x, mu=0, sigma=1, gamma=1, amp=1, background=0)

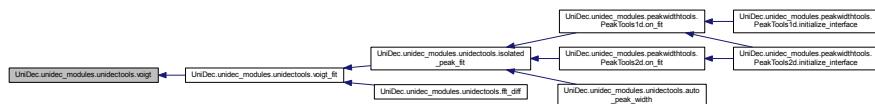
```
\voigt profile

V(x,sig,gam) = Re(w(z))/(sig*sqrt(2*pi))
z = (x+i*gam)/(sig*sqrt(2))
```

Here is the call graph for this function:

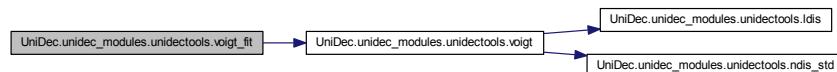


Here is the caller graph for this function:

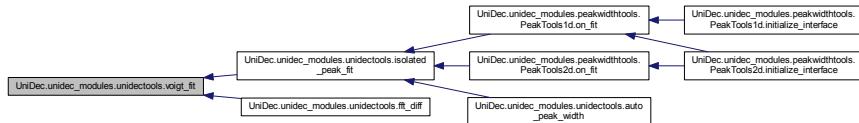


6.49.1.97 def UniDec.unidec_modules.unidectools.voigt_fit (*xvals*, *yvals*, *mguess* = 0, *sguess* = 0 . 1, *gguess* = 0, *aguess* = 0, *bguess* = 0)

Here is the call graph for this function:



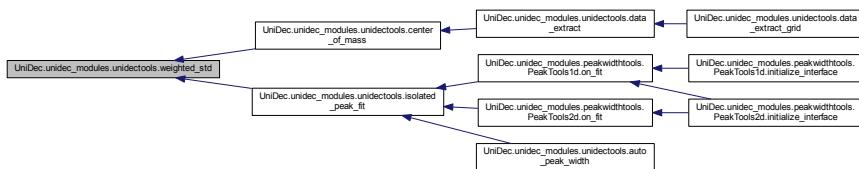
Here is the caller graph for this function:



6.49.1.98 def UniDec.unidec_modules.unidectools.weighted_std (*values*, *weights*)

Calculate weighted standard deviation.
:param values: Values
:param weights: Weights
:return: Weighted standard deviation.

Here is the caller graph for this function:



6.49.1.99 def UniDec.unidec_modules.unidectools.wide_sse (dat1, dat2, sig)

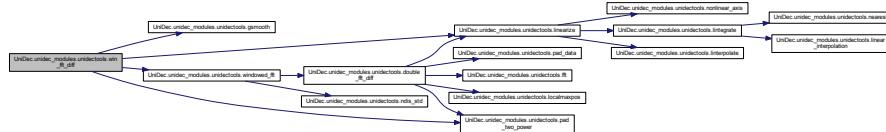
```
Tests the sum of squared errors between two sets of data where the second has been convolved with a Gaussian
:param dat1: Reference list of intensities.
:param dat2: Test spectrum list of intensities to broaden.
:param sig: Sigma for Gaussian filter
:return: SSE between dat1 and broadened dat1 (float)
```

Here is the caller graph for this function:



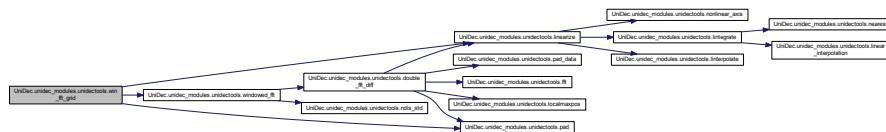
6.49.1.100 def UniDec.unidec_modules.unidectools.win_fft_diff (rawdata, binsize = 0.05, sigma = 1000, diffrange = None)

Here is the call graph for this function:

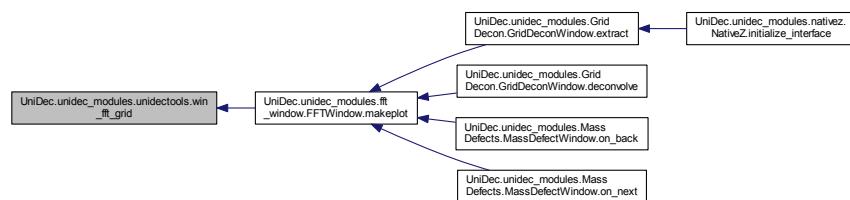


6.49.1.101 def UniDec.unidec_modules.unidectools.win_fft_grid (rawdata, binsize, wbin, window_fwhm, diffrange)

Here is the call graph for this function:

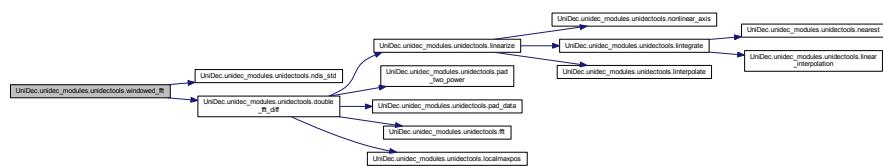


Here is the caller graph for this function:

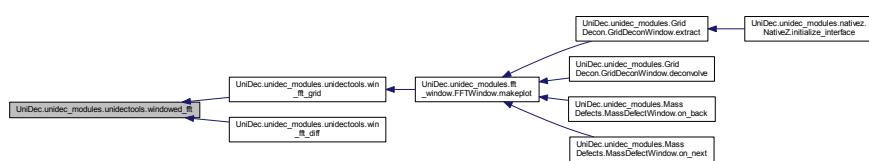


6.49.1.102 def UniDec.unidec_modules.unidectools.windowed_fft(*data*, *mean*, *sigma*, *diffrange*=None)

Here is the call graph for this function:



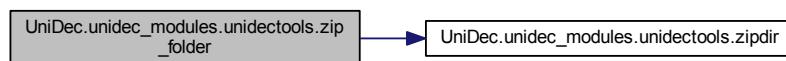
Here is the caller graph for this function:



6.49.1.103 def UniDec.unidec_modules.unidectools.zip_folder(*save_path*)

Zips a directory specified by *save_path* into a zip file for saving.
:param *save_path*: Path to save to zip
:return: None

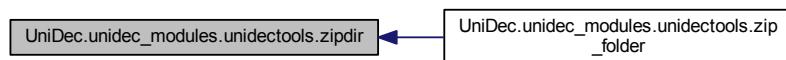
Here is the call graph for this function:



6.49.1.104 def UniDec.unidec_modules.unidectools.zipdir(*path*, *zip_handle*)

Zips all the files in the path into the *zip_handle*
:param *path*: Directory path
:param *zip_handle*: Handle of the zip file that is being created
:return: None

Here is the caller graph for this function:



6.49.2 Variable Documentation

- 6.49.2.1 string UniDec.unidec_modules.unidectools.dllname = "libmypfunc"
- 6.49.2.2 UniDec.unidec_modules.unidectools.dllpath = testpath
- 6.49.2.3 int UniDec.unidec_modules.unidectools.is_64bits = sys.maxsize>2
- 6.49.2.4 tuple UniDec.unidec_modules.unidectools.libs = cdll.LoadLibrary(dllpath)
- 6.49.2.5 tuple UniDec.unidec_modules.unidectools.pathtofile = os.path.dirname(os.path.abspath(__file__))
- 6.49.2.6 tuple UniDec.unidec_modules.unidectools.testpath = dllname

6.50 UniDec.unidec_modules.UniFit Namespace Reference

Classes

- class KDmodel
- class kdstruct

Functions

- def safedivide (a, b)
- def fixlists (list1, list2)
- def sortarray (a)
- def CompareModels (e1, e2, p1, p2, n, thresh)
- def Ftest (e1, e2, p1, p2, n)
- def findend (reactions, end)
- def findpaths (reactions)
- def GetError (data, pfree, lfree, ureact, prottab, ligtab, paths, kds, weights, nodelist, nfactors)
- def MinFree (ptot, ltot, ureact, prottab, ligtab, paths, kds, pguess, lguess, nfactors)
- def GetFree (pO, ptot, ltot, ureact, prottab, ligtab, paths, kds, nfactors)
- def MakeGrid (pfree, lfree, ureact, prottab, ligtab, paths, kds, nfactors)
- def draw_graph_structure
- def draw_graph
- def MinFreeError (kds, data, weights, kdargs)
- def GetDegenKD (kds, kdargs)
- def Minimize (data, kdargs, kwargs)
- def BootMin (data, kdargs, weights)
- def BootMinWorker (queue, results_queue)

Variables

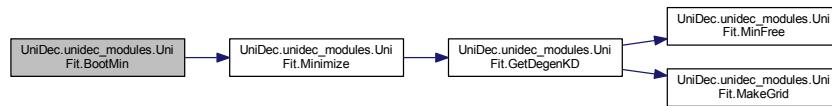
- string __author__ = 'Michael.Marty'
- int switch = 3
- string path = "C:\\cprog\\Tim\\raw"
- string file_name = "man7.inp"
- tuple data = np.loadtxt(file_name)
- list pconc = data[0]
- list lconc = data[1]
- tuple header = string.split(file_name, ".")
- int nprot = 1

- int `nlig` = 4
- int `maxsites` = 4
- list `nodelist` = [[1, j] for j in xrange(0, `nlig` + 1)]
- `dims` = data.shape
- tuple `fit`

6.50.1 Function Documentation

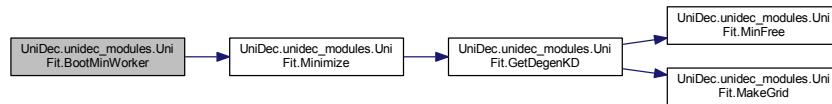
6.50.1.1 def UniDec.unidec_modules.UniFit.BootMin (`data`, `kdargs`, `weights`)

Here is the call graph for this function:



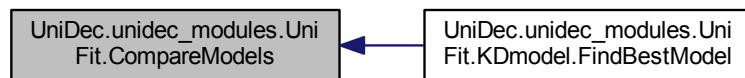
6.50.1.2 def UniDec.unidec_modules.UniFit.BootMinWorker (`queue`, `results_queue`)

Here is the call graph for this function:



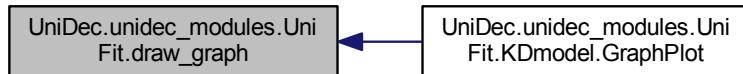
6.50.1.3 def UniDec.unidec_modules.UniFit.CompareModels (`e1`, `e2`, `p1`, `p2`, `n`, `thresh`)

Here is the caller graph for this function:



```
6.50.1.4 def UniDec.unidec_modules.UniFit.draw_graph( graph1, graph2, kds, errors, kdmap, header, ax=None )
```

Here is the caller graph for this function:



```
6.50.1.5 def UniDec.unidec_modules.UniFit.draw_graph_structure( graph1, graph2, kdmap, ax=None )
```

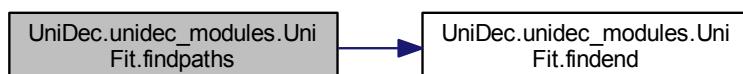
```
6.50.1.6 def UniDec.unidec_modules.UniFit.findend( reactions, end )
```

Here is the caller graph for this function:



```
6.50.1.7 def UniDec.unidec_modules.UniFit.findpaths( reactions )
```

Here is the call graph for this function:

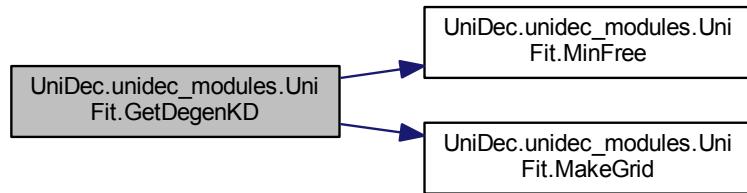


```
6.50.1.8 def UniDec.unidec_modules.UniFit.fixlists( list1, list2 )
```

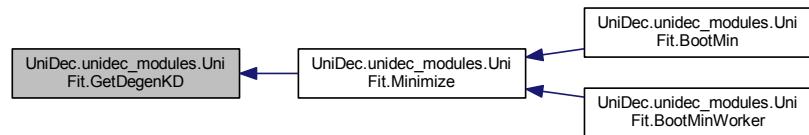
```
6.50.1.9 def UniDec.unidec_modules.UniFit.Ftest( e1, e2, p1, p2, n )
```

6.50.1.10 def UniDec.unidec_modules.UniFit.GetDegenKD (*kds*, *kdargs*)

Here is the call graph for this function:



Here is the caller graph for this function:

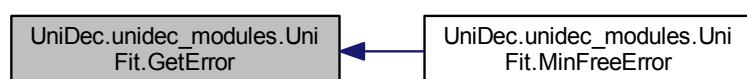


6.50.1.11 def UniDec.unidec_modules.UniFit.GetError (*data*, *pfree*, *lfree*, *ureact*, *prottab*, *ligtab*, *paths*, *kds*, *weights*, *nodelist*, *nfactors*)

Here is the call graph for this function:



Here is the caller graph for this function:



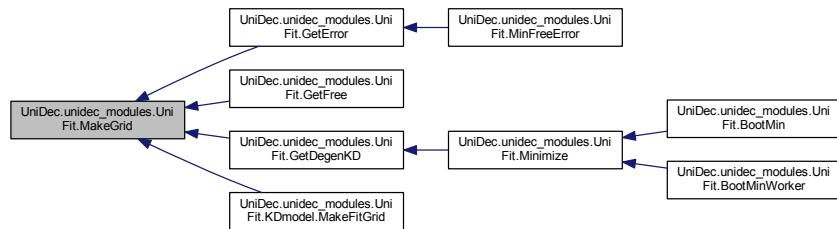
6.50.1.12 def UniDec.unidec_modules.UniFit.GetFree(*pO*, *ptot*, *ltot*, *ureact*, *prottab*, *littab*, *paths*, *kds*, *nfactors*)

Here is the call graph for this function:



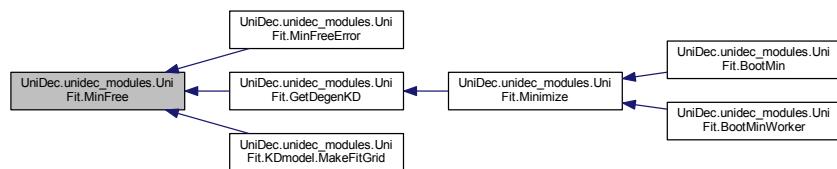
6.50.1.13 def UniDec.unidec_modules.UniFit.MakeGrid(*pfree*, *lfree*, *ureact*, *prottab*, *littab*, *paths*, *kds*, *nfactors*)

Here is the caller graph for this function:



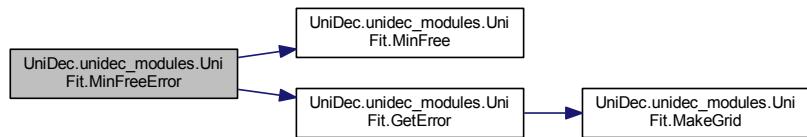
6.50.1.14 def UniDec.unidec_modules.UniFit.MinFree(*ptot*, *ltot*, *ureact*, *prottab*, *littab*, *paths*, *kds*, *pguess*, *lguess*, *nfactors*)

Here is the caller graph for this function:



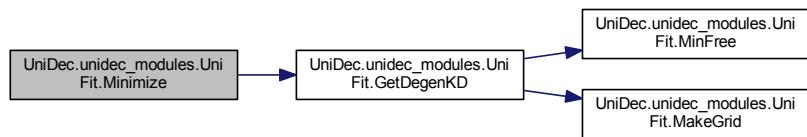
6.50.1.15 def UniDec.unidec_modules.UniFit.MinFreeError (*kds*, *data*, *weights*, *kdargs*)

Here is the call graph for this function:

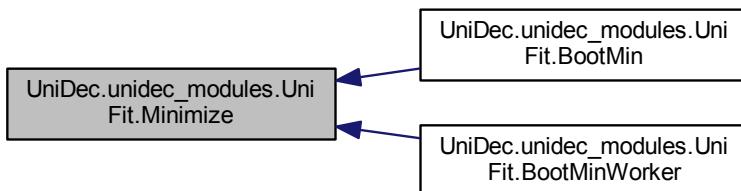


6.50.1.16 def UniDec.unidec_modules.UniFit.Minimize (*data*, *kdargs*, *kwargs*)

Here is the call graph for this function:



Here is the caller graph for this function:



6.50.1.17 def UniDec.unidec_modules.UniFit.safedivide (*a*, *b*)

6.50.1.18 def UniDec.unidec_modules.UniFit.sortarray (*a*)

6.50.2 Variable Documentation

6.50.2.1 string UniDec.unidec_modules.UniFit.__author__ = 'Michael.Marty'

6.50.2.2 tuple UniDec.unidec_modules.UniFit.data = np.loadtxt(file_name)

6.50.2.3 UniDec.unidec_modules.UniFit.dims = data.shape

6.50.2.4 string UniDec.unidec_modules.UniFit.file_name = "man7.inp"

6.50.2.5 tuple UniDec.unidec_modules.UniFit.fit

Initial value:

```
1 = KDmodel(nprot, nlig, data, pconc, lconc, nodelist, header, prot="free", lig="parallel", bootnum=0,
2                         maxsites=maxsites)
```

6.50.2.6 tuple UniDec.unidec_modules.UniFit.header = string.split(file_name, ".")

6.50.2.7 list UniDec.unidec_modules.UniFit.lconc = data[1]

6.50.2.8 int UniDec.unidec_modules.UniFit.maxsites = 4

6.50.2.9 int UniDec.unidec_modules.UniFit.nlig = 4

6.50.2.10 list UniDec.unidec_modules.UniFit.nodelist = [[1, j] for j in xrange(0, nlig + 1)]

6.50.2.11 int UniDec.unidec_modules.UniFit.nprot = 1

6.50.2.12 string UniDec.unidec_modules.UniFit.path = "C:\\cprog\\Tim\\raw"

6.50.2.13 list UniDec.unidec_modules.UniFit.pconc = data[0]

6.50.2.14 int UniDec.unidec_modules.UniFit.switch = 3

6.51 UniDec.unidec_tests Namespace Reference

Classes

- class [UniDecTest](#)

Variables

- string [__author__](#) = 'Michael.Marty'
- tuple [eng](#) = [UniDecTest\(\)](#)

6.51.1 Variable Documentation

6.51.1.1 string UniDec.unidec_tests.__author__ = 'Michael.Marty'

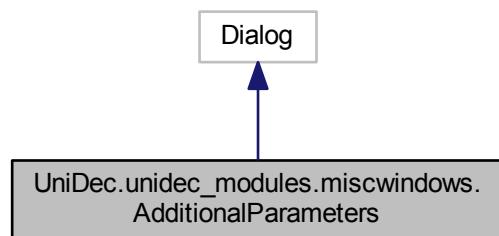
6.51.1.2 tuple UniDec.unidec_tests.eng = [UniDecTest\(\)](#)

Chapter 7

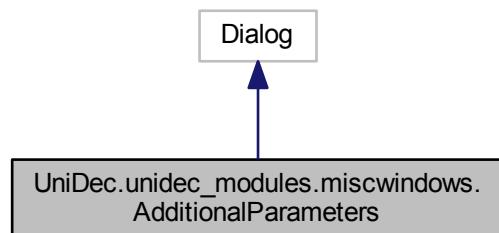
Class Documentation

7.1 UniDec.unidec_modules.miscwindows.AdditionalParameters Class Reference

Inheritance diagram for UniDec.unidec_modules.miscwindows.AdditionalParameters:



Collaboration diagram for UniDec.unidec_modules.miscwindows.AdditionalParameters:



Public Member Functions

- def `__init__` (self, args, kwargs)

- def `initialize_interface` (`self, config`)
- def `on_close` (`self, e`)
- def `on_close_cancel` (`self, e`)

Public Attributes

- `config`
- `inputbox5`
- `inputbox6`
- `inputbox6b`

7.1.1 Constructor & Destructor Documentation

7.1.1.1 def UniDec.unidec_modules.miscwindows.AdditionalParameters.`__init__` (`self, args, kwargs`)

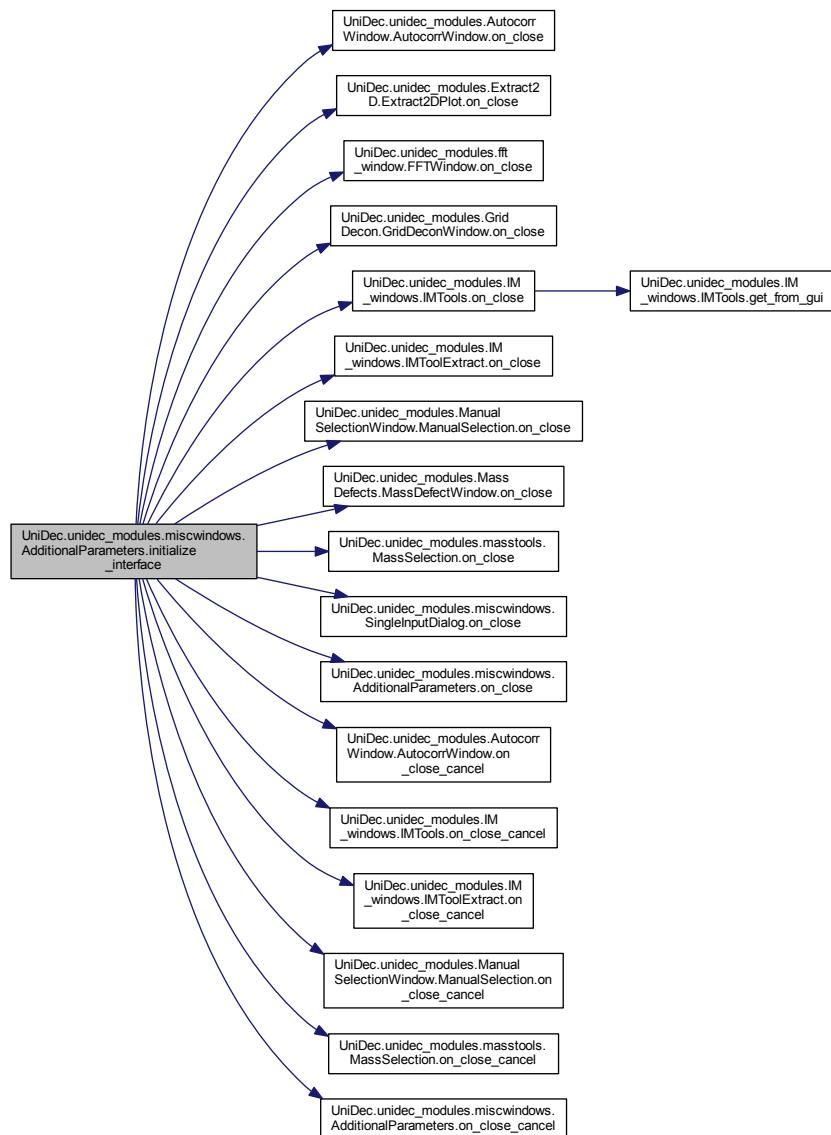
Create a dialog for setting some obscure additional parameters.
:param args: Passed to `wx.Dialog`
:param kwargs: Passed to `wx.Dialog`
:return: None

7.1.2 Member Function Documentation

7.1.2.1 def UniDec.unidec_modules.miscwindows.AdditionalParameters.`initialize_interface` (`self, config`)

Initialize the GUI.
:param config: `UniDecConfig` object
:return: None

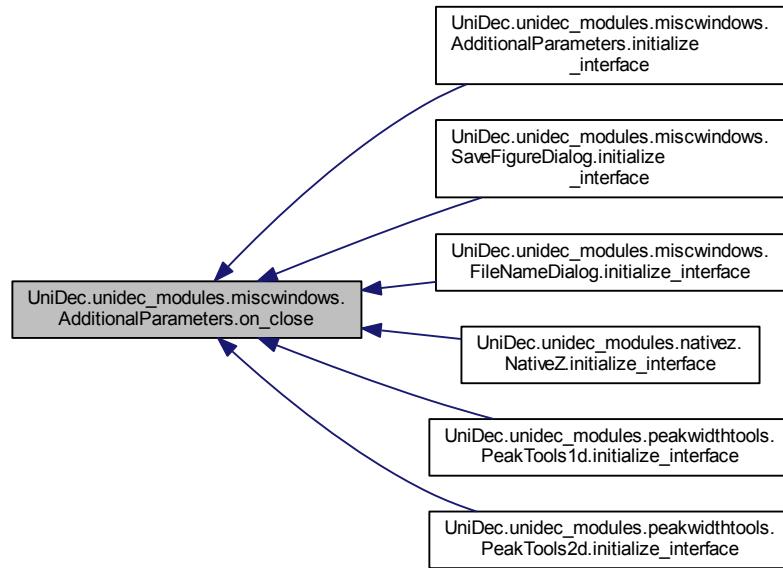
Here is the call graph for this function:



7.1.2.2 def UniDec.unidec_modules.misctools.AdditionalParameters.on_close (self, e)

Update parameters in self.config from the GUI. Close the window.
:param e: Unused Event
:return: None

Here is the caller graph for this function:

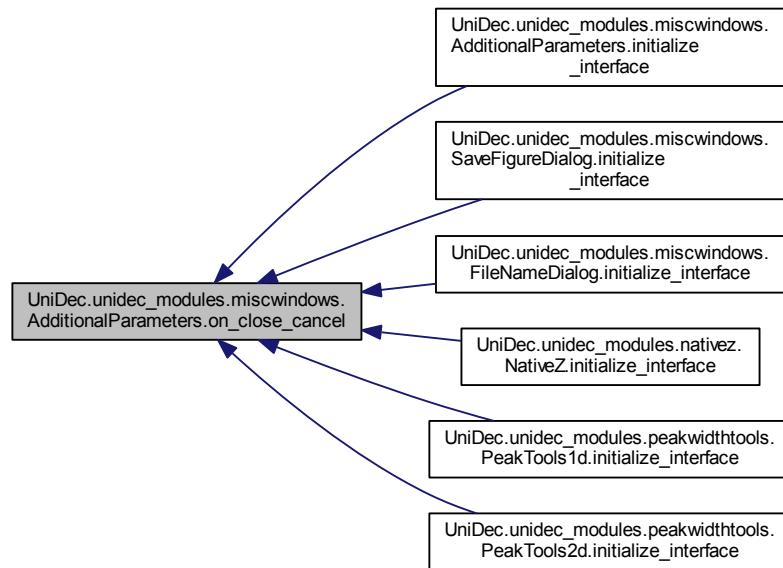


7.1.2.3 def UniDec.unidec_modules.miscwindows.AdditionalParameters.on_close_cancel (*self*, *e*)

```

Close the window but don't update the parameters in self.config.
:param e: Unused event
:return: None
  
```

Here is the caller graph for this function:



7.1.3 Member Data Documentation

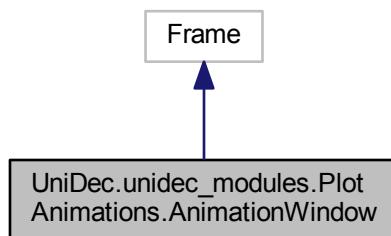
- 7.1.3.1 [UniDec.unidec_modules.miscwindows.AdditionalParameters.config](#)
- 7.1.3.2 [UniDec.unidec_modules.miscwindows.AdditionalParameters.inputbox5](#)
- 7.1.3.3 [UniDec.unidec_modules.miscwindows.AdditionalParameters.inputbox6](#)
- 7.1.3.4 [UniDec.unidec_modules.miscwindows.AdditionalParameters.inputbox6b](#)

The documentation for this class was generated from the following file:

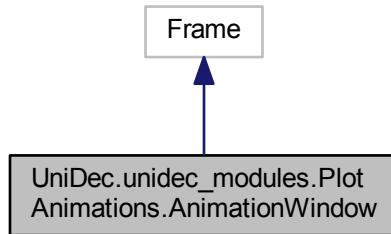
- C:/Python/UniDec/unidec_modules/[miscwindows.py](#)

7.2 UniDec.unidec_modules.PlotAnimations.AnimationWindow Class Reference

Inheritance diagram for UniDec.unidec_modules.PlotAnimations.AnimationWindow:



Collaboration diagram for UniDec.unidec_modules.PlotAnimations.AnimationWindow:



Public Member Functions

- def [`__init__`](#) (self, parent, data_list, config=None, yvals=None, mode="1D", args, kwargs)

- def `on_close` (self, e)
- def `update` (self, frame_number)
- def `update_plot` (self)
- def `init` (self)
- def `on_play` (self, e)
- def `refresh_plot` (self)
- def `on_next` (self, e)
- def `on_back` (self, e)
- def `update_framerate` (self, e)

Public Attributes

- `mode`
- `config`
- `datalist`
- `yvals`
- `dim`
- `pos`
- `play`
- `animation`
- `plot`
- `frslider`
- `playbutton`
- `nextbutton`
- `backbutton`
- `ctlautoscale`

7.2.1 Constructor & Destructor Documentation

7.2.1.1 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.`__init__` (`self`, `parent`, `data_list`, `config` = `None`, `yvals` = `None`, `mode` = "1D", `args`, `kwargs`)

A simple window for animating multiple 1D or 2D plots in a sequence.

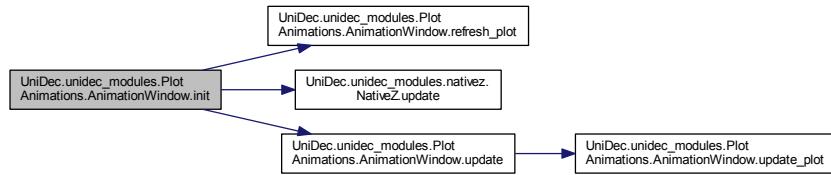
:param parent: Parent window. Passed to `wx.Frame`.
 :param data_list: List of data to be plotted
 :param config: `UniDecConfig` object
 :param yvals: Titles for the plots.
 :param mode: 1 = 1D plots, 2 = 2D plots
 :param args:
 :param kwargs:
 :return: None

7.2.2 Member Function Documentation

7.2.2.1 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.`init` (`self`)

Create a fresh plot and start the animation.
 :return: None

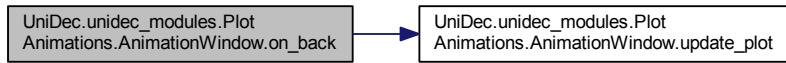
Here is the call graph for this function:



7.2.2.2 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.on_back (self, e)

Plot the previous data set in data_list.
:param e: Unused event
:return: None

Here is the call graph for this function:



7.2.2.3 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.on_close (self, e)

Stop the animation and close the window.
:param e: Unused event
:return: None

7.2.2.4 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.on_next (self, e)

Plot the next data set in data_list.
:param e: Unused event
:return: None

Here is the call graph for this function:



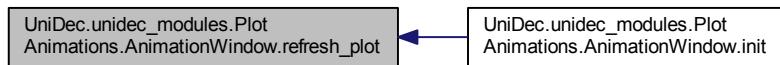
7.2.2.5 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.on_play(self, e)

```
Toggles self.play on or off. Will break the while loop in self.update if self.play = False.
:param e: Unused event
:return: None
```

7.2.2.6 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.refresh_plot(self)

```
Create a fresh plot from the top.
:return: None
```

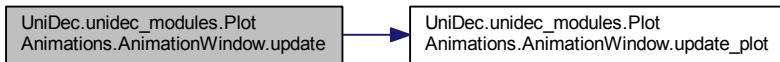
Here is the caller graph for this function:



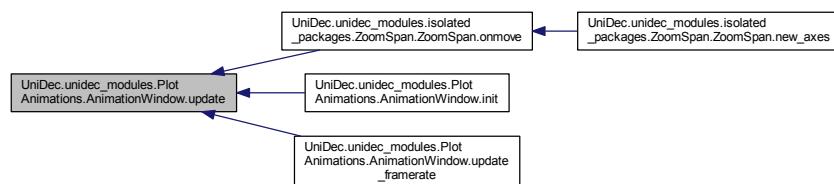
7.2.2.7 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.update(self, frame_number)

```
Continues to increment the plot to the next value in the data_list. Will stop if self.play is False.
:param frame_number: Required but unused. Filled by FuncAnimation.
:return: 0
```

Here is the call graph for this function:



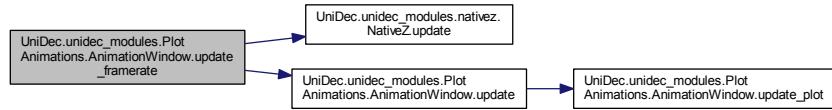
Here is the caller graph for this function:



7.2.2.8 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.update_framerate(self, e)

```
Change the frame rate. Restart the animation with fresh frame rate.
:param e: Unused event
:return: None
```

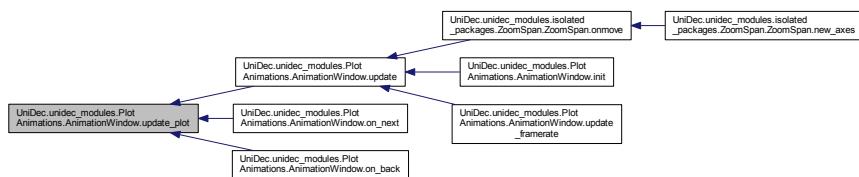
Here is the call graph for this function:



7.2.2.9 def UniDec.unidec_modules.PlotAnimations.AnimationWindow.update_plot (self)

Increment to the next data set and update teh plot with the new data.
 Tries to keep some of the old plotting parameters like the zoom the same.
 Stops the animation if an error occurs.
 :return: None

Here is the caller graph for this function:



7.2.3 Member Data Documentation

7.2.3.1 UniDec.unidec_modules.PlotAnimations.AnimationWindow.animation

7.2.3.2 UniDec.unidec_modules.PlotAnimations.AnimationWindow.backbutton

7.2.3.3 UniDec.unidec_modules.PlotAnimations.AnimationWindow.config

7.2.3.4 UniDec.unidec_modules.PlotAnimations.AnimationWindow.ctlautoscale

7.2.3.5 UniDec.unidec_modules.PlotAnimations.AnimationWindow.datalist

7.2.3.6 UniDec.unidec_modules.PlotAnimations.AnimationWindow.dim

7.2.3.7 UniDec.unidec_modules.PlotAnimations.AnimationWindow.frslider

7.2.3.8 UniDec.unidec_modules.PlotAnimations.AnimationWindow.mode

7.2.3.9 UniDec.unidec_modules.PlotAnimations.AnimationWindow.nextbutton

7.2.3.10 UniDec.unidec_modules.PlotAnimations.AnimationWindow.play

7.2.3.11 UniDec.unidec_modules.PlotAnimations.AnimationWindow.playbutton

7.2.3.12 UniDec.unidec_modules.PlotAnimations.AnimationWindow.plot

7.2.3.13 UniDec.unidec_modules.PlotAnimations.AnimationWindow.pos

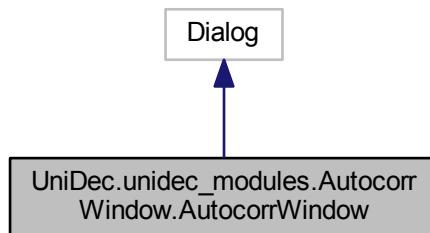
7.2.3.14 UniDec.unidec_modules.PlotAnimations.AnimationWindow.yvals

The documentation for this class was generated from the following file:

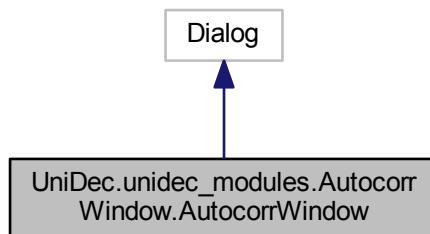
- C:/Python/UniDec/unidec_modules/[PlotAnimations.py](#)

7.3 UniDec.unidec_modules.AutocorrWindow.AutocorrWindow Class Reference

Inheritance diagram for UniDec.unidec_modules.AutocorrWindow.AutocorrWindow:



Collaboration diagram for UniDec.unidec_modules.AutocorrWindow.AutocorrWindow:



Public Member Functions

- def [`__init__`](#) (self, args, kwargs)
- def [`initialize_dialog`](#) (self, config, massdat)
- def [`run_autocorr`](#) (self, e)
- def [`on_close`](#) (self, e)
- def [`on_close_cancel`](#) (self, e)

Public Attributes

- [config](#)
- [massdat](#)
- [plot1](#)
- [listpanel](#)

7.3.1 Detailed Description

Dialog window for autocorrelation.

7.3.2 Constructor & Destructor Documentation

7.3.2.1 def UniDec.unidec_modules.AutocorrWindow.AutocorrWindow.[__init__](#)(*self, args, kwargs*)

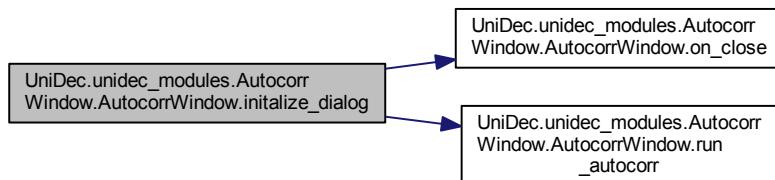
```
Creates a dialog.
:param args: Passed to wx.Dialog
:param kwargs: Passed to wx.Dialog
:return: None
```

7.3.3 Member Function Documentation

7.3.3.1 def UniDec.unidec_modules.AutocorrWindow.AutocorrWindow.[initialize_dialog](#)(*self, config, massdat*)

```
Initializes dialog and the layout. Calls run_autocorr.
:param config: UniDecConfig object
:param massdat: Array of mass distribution (N x 2)
:return: None
```

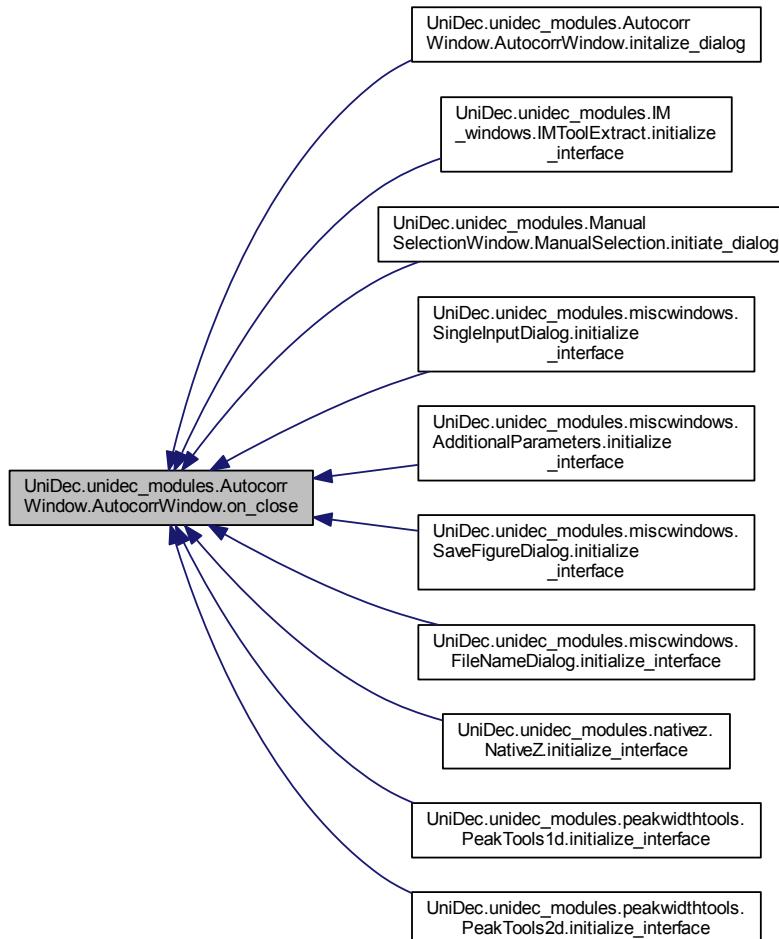
Here is the call graph for this function:



7.3.3.2 def UniDec.unidec_modules.AutocorrWindow.AutocorrWindow.[on_close](#)(*self, e*)

```
Close dialog.
:param e: Unused event
:return: None
```

Here is the caller graph for this function:



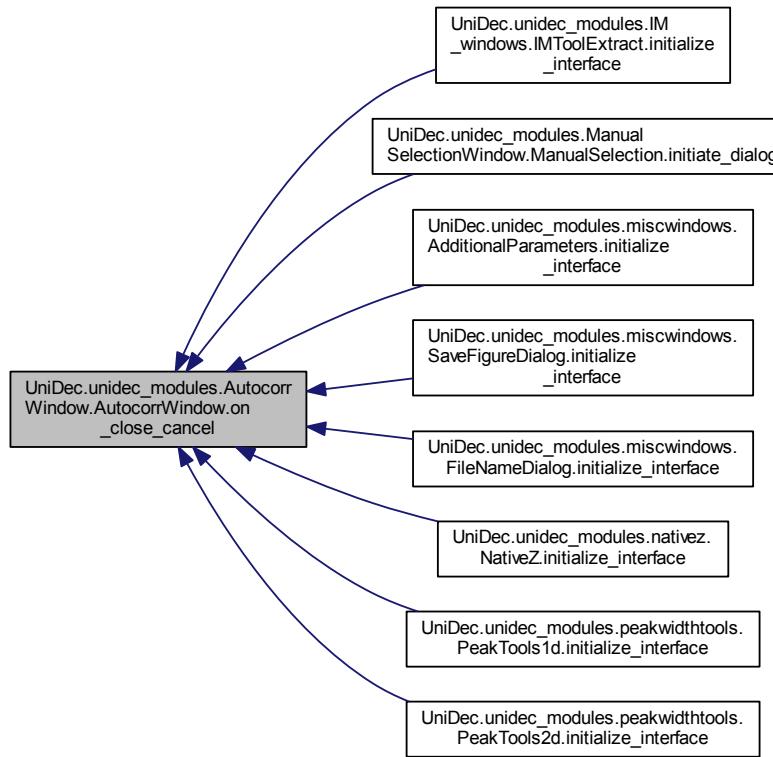
7.3.3.3 def UniDec.unidec_modules.AutocorrWindow.AutocorrWindow.on_close_cancel (self, e)

```

Cancel the dialog.
:param e: Unused event
:return: None

```

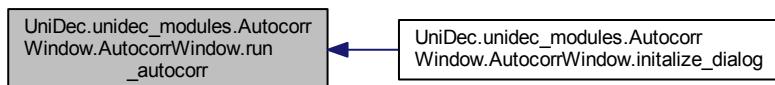
Here is the caller graph for this function:



7.3.3.4 def UniDec.unidec_modules.AutocorrWindow.AutocorrWindow.run_autocorr (self, e)

Performs autocorrelation using ud.autocorr from unidectools.
 Plots the results and adds peaks to listctrl.
 :param e: Unused event
 :return: None

Here is the caller graph for this function:



7.3.4 Member Data Documentation

7.3.4.1 UniDec.unidec_modules.AutocorrWindow.AutocorrWindow.config

7.3.4.2 UniDec.unidec_modules.AutocorrWindow.AutocorrWindow.listpanel

7.3.4.3 UniDec.unidec_modules.AutocorrWindow.AutocorrWindow.massdat

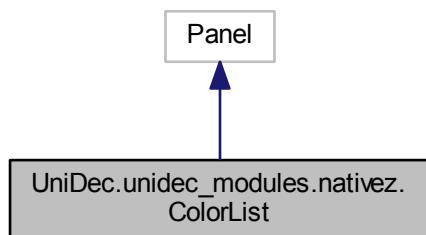
7.3.4.4 UniDec.unidec_modules.AutocorrWindow.AutocorrWindow.plot1

The documentation for this class was generated from the following file:

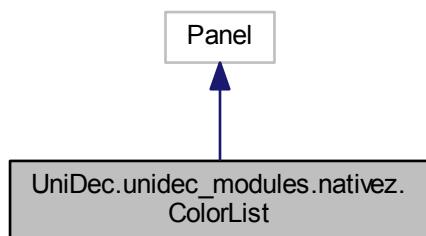
- C:/Python/UniDec/unidec_modules/AutocorrWindow.py

7.4 UniDec.unidec_modules.nativez.ColorList Class Reference

Inheritance diagram for UniDec.unidec_modules.nativez.ColorList:



Collaboration diagram for UniDec.unidec_modules.nativez.ColorList:



Public Member Functions

- def [__init__](#) (self, parent)
- def [add_empty_line](#) (self)
- def [add_line](#) (self, zoff)
- def [return_data](#) (self)
- def [super_delete](#) (self)

Public Attributes

- `ultimateList`
- `butontot`

7.4.1 Constructor & Destructor Documentation

7.4.1.1 def UniDec.unidec_modules.nativez.ColorList.__init__(self, parent)

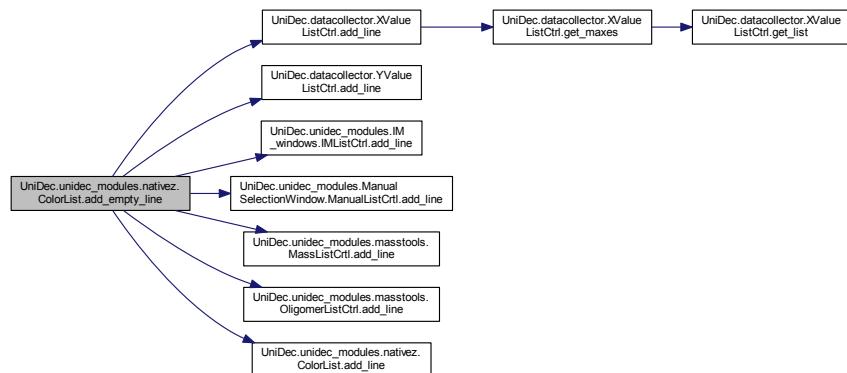
Create an ultimape list control panel.
:param parent: Parent passed to wx.Panel
:return: None

7.4.2 Member Function Documentation

7.4.2.1 def UniDec.unidec_modules.nativez.ColorList.add_empty_line(self)

Add an empty line by adding a default Zoffset object.
:return: None

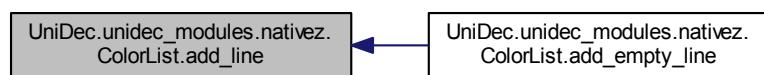
Here is the call graph for this function:



7.4.2.2 def UniDec.unidec_modules.nativez.ColorList.add_line(self, zoff)

Adds a new line from a Zoffset object.
:param zoff: Zoffset object.
:return:

Here is the caller graph for this function:



7.4.2.3 def UniDec.unidec_modules.nativez.ColorList.return_data (self)

Make each line from the listctrl into a Zoffset object and return the list.
:return: List of Zoffset objects

7.4.2.4 def UniDec.unidec_modules.nativez.ColorList.super_delete (self)

Delete all items in the ultimate list control.
:return: None

7.4.3 Member Data Documentation

7.4.3.1 UniDec.unidec_modules.nativez.ColorList.buttontot

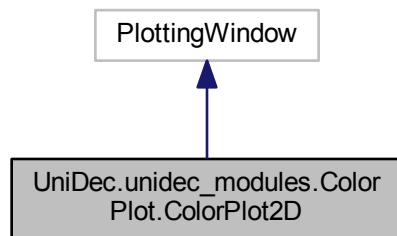
7.4.3.2 UniDec.unidec_modules.nativez.ColorList.ultimateList

The documentation for this class was generated from the following file:

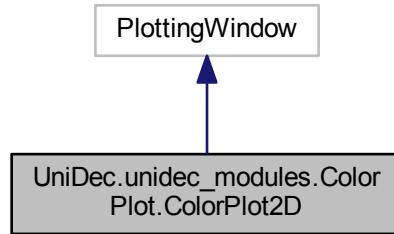
- C:/Python/UniDec/unidec_modules/nativez.py

7.5 UniDec.unidec_modules.ColorPlot.ColorPlot2D Class Reference

Inheritance diagram for UniDec.unidec_modules.ColorPlot.ColorPlot2D:



Collaboration diagram for UniDec.unidec_modules.ColorPlot.ColorPlot2D:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `make_color_plot` (self, mzgrid, mzax, dtax, ztab)

Public Attributes

- `datalims`
- `subplot1`
- `cbar`
- `flag`

7.5.1 Detailed Description

Method to perform a 3D plot by plotting the Z axis as 2D slices of a different color. Each 2D slice uses the alpha (trasparency) parameter to indicate intensity in square root scale.

7.5.2 Constructor & Destructor Documentation

7.5.2.1 def UniDec.unidec_modules.ColorPlot.ColorPlot2D.__init__(self, args, kwargs)

Initialize by inheriting from Plotting Window and setting the axes dimensions.
:param args:
:param kwargs:
:return: ColorPlot2D object

7.5.3 Member Function Documentation

7.5.3.1 def UniDec.unidec_modules.ColorPlot.ColorPlot2D.make_color_plot(self, mzgrid, mzax, dtax, ztab)

Creates the color plot
:param mzgrid: mz x dt x z numpy array of intensity values
:param mzax: m/z axis
:param dtax: drift time axis
:param ztab: charge axis
:return: None

7.5.4 Member Data Documentation

7.5.4.1 UniDec.unidec_modules.ColorPlot.ColorPlot2D.cbar

7.5.4.2 UniDec.unidec_modules.ColorPlot.ColorPlot2D.datalims

7.5.4.3 UniDec.unidec_modules.ColorPlot.ColorPlot2D.flag

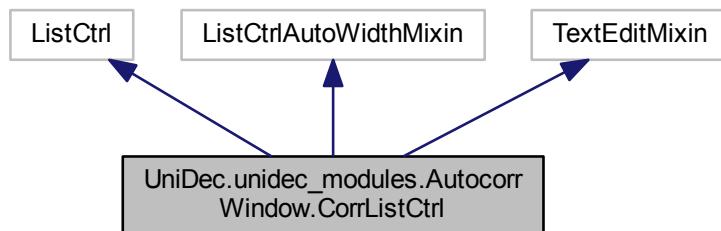
7.5.4.4 UniDec.unidec_modules.ColorPlot.ColorPlot2D.subplot1

The documentation for this class was generated from the following file:

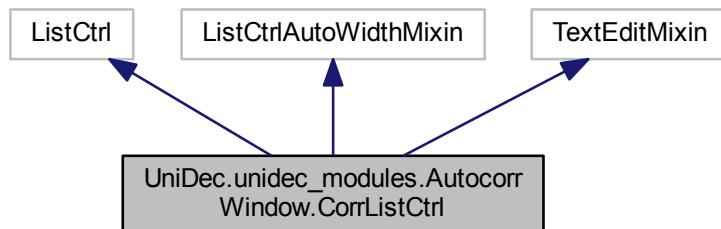
- C:/Python/UniDec/unidec_modules/[ColorPlot.py](#)

7.6 UniDec.unidec_modules.AutocorrWindow.CorrListCtrl Class Reference

Inheritance diagram for UniDec.unidec_modules.AutocorrWindow.CorrListCtrl:



Collaboration diagram for UniDec.unidec_modules.AutocorrWindow.CorrListCtrl:



Public Member Functions

- def [__init__](#)
- def [populate](#) (self, pks)

- def [clear_list](#) (*self*)

7.6.1 Detailed Description

Class for the list control of peak values

7.6.2 Constructor & Destructor Documentation

7.6.2.1 def UniDec.unidec_modules.AutocorrWindow.CorrListCtrl.__init__ (*self*, *parent*, *id_value*, *pos* = wx.DefaultPosition, *size* = wx.DefaultSize, *style* = 0)

```
Create a two column list control
:param parent: Parent window or panel
:param id_value: ID passed to wx.ListCtrl
:param pos: pos passed to wx.ListCtrl
:param size: size passed to wx.ListCtrl
:param style: styl passed to wx.ListCtrl
:return: None
```

7.6.3 Member Function Documentation

7.6.3.1 def UniDec.unidec_modules.AutocorrWindow.CorrListCtrl.clear_list (*self*)

```
Clears the list.
:return: None
```

7.6.3.2 def UniDec.unidec_modules.AutocorrWindow.CorrListCtrl.populate (*self*, *pks*)

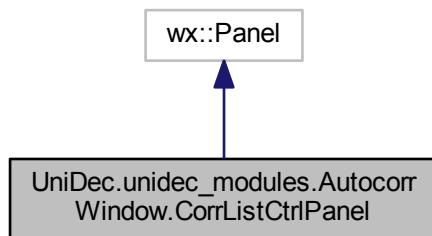
```
Add Peaks class object to the panel. Adds p.textmarker to the first column and p.mass to the second.
The background color is set to p.color.
:param pks: Peaks object
:return: None
```

The documentation for this class was generated from the following file:

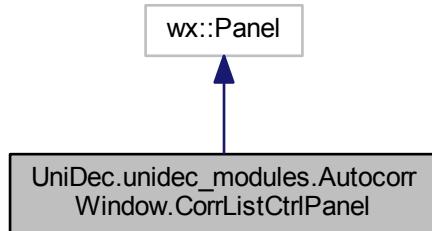
- C:/Python/UniDec/unidec_modules/[AutocorrWindow.py](#)

7.7 UniDec.unidec_modules.AutocorrWindow.CorrListCtrlPanel Class Reference

Inheritance diagram for UniDec.unidec_modules.AutocorrWindow.CorrListCtrlPanel:



Collaboration diagram for UniDec.unidec_modules.AutocorrWindow.CorrListCtrlPanel:



Public Member Functions

- def [__init__](#) (self, parent)

Public Attributes

- [list](#)

7.7.1 Detailed Description

Panel for the ListCtrl

7.7.2 Constructor & Destructor Documentation

7.7.2.1 def UniDec.unidec_modules.AutocorrWindow.CorrListCtrlPanel.[__init__](#) (self, parent)

Creates the panel.
:param parent: Parent panel or window
:return: None

7.7.3 Member Data Documentation

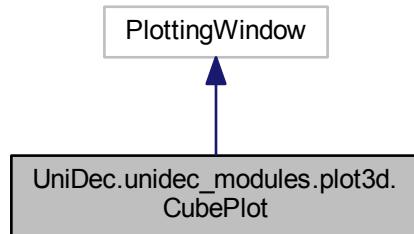
7.7.3.1 UniDec.unidec_modules.AutocorrWindow.CorrListCtrlPanel.list

The documentation for this class was generated from the following file:

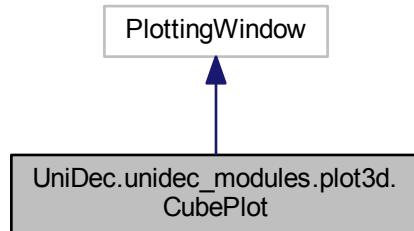
- C:/Python/UniDec/unidec_modules/[AutocorrWindow.py](#)

7.8 UniDec.unidec_modules.plot3d.CubePlot Class Reference

Inheritance diagram for UniDec.unidec_modules.plot3d.CubePlot:



Collaboration diagram for UniDec.unidec_modules.plot3d.CubePlot:



Public Member Functions

- def [__init__](#) (self, args, kwargs)
- def [cubeplot](#)
- def [make_isomatrices](#) (self)
- def [isometric_projection](#) (self, x, y, z)
- def [isogrids](#) (self)
- def [isoticks](#) (self, ax, col)
- def [isolabels](#) (self, [xticlab](#), [yticlab](#), [zticlab](#), ax, col)
- def [isolines](#) (self)

Public Attributes

- [normalticks](#)
- [subplot1](#)
- [alpha](#)
- [beta](#)

- [cmap](#)
- [xlen](#)
- [ylen](#)
- [zlen](#)
- [xticlab](#)
- [yticlab](#)
- [zticlab](#)
- [xticloc](#)
- [yticloc](#)
- [zticloc](#)
- [cbar](#)
- [datalims](#)
- [flag](#)
- [pc](#)

7.8.1 Detailed Description

Plotting class for cube plots. Performs isometric projections of three 2D plots onto three faces of a cube.

7.8.2 Constructor & Destructor Documentation

7.8.2.1 def UniDec.unidec_modules.plot3d.CubePlot.__init__(self, args, kwargs)

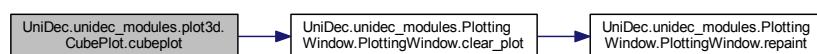
Initialize the plotting window. Specify axes. Specify that the plot does not have normal tick marks to repaint
:param args:
:param kwargs:
:return: CubePlot Object

7.8.3 Member Function Documentation

7.8.3.1 def UniDec.unidec_modules.plot3d.CubePlot.cubeplot(self, xaxis, yaxis, zaxis, C, C2, C3, xlab = "", ylab = "", zlab = "", cmap = "jet")

Make 2D isometric projection plot of three cube faces
:param xaxis: X-axis values
:param yaxis: Y-axis values
:param zaxis: Z-axis values
:param C: Intensity grid for X v. Y face
:param C2: Intensity grid for X v. Z face
:param C3: Intensity grid for Y v. Z face
:param xlab: X-axis label
:param ylab: Y-axis label
:param zlab: Z-axis label
:param cmap: Colormap for 2D plot
:return: None

Here is the call graph for this function:



7.8.3.2 def UniDec.unidec_modules.plot3d.CubePlot.isogrids (self)

```
Sets jsometric projections of X, Y, and Z axis grids
:return: None
```

Here is the call graph for this function:

**7.8.3.3 def UniDec.unidec_modules.plot3d.CubePlot.isolabels (self, xticlab, yticlab, zticlab, ax, col)**

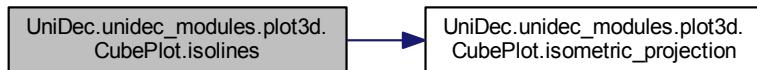
```
Draw isometric projection of axis labels
:param xticlab: X-axis label (string)
:param yticlab: Y-axis label (string)
:param zticlab: Z-axis label (string)
:param ax: Axis object
:param col: Color (not presently used)
:return: None
```

Here is the call graph for this function:

**7.8.3.4 def UniDec.unidec_modules.plot3d.CubePlot.isolines (self)**

```
Draw isometric projection of lines at the edge of the cube.
:return: None
```

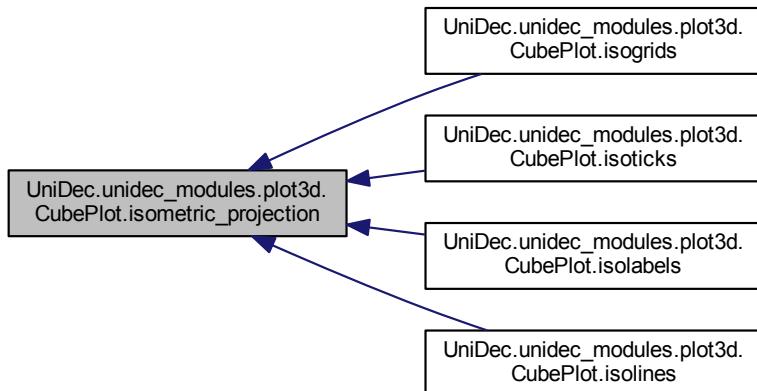
Here is the call graph for this function:



7.8.3.5 def UniDec.unidec_modules.plot3d.CubePlot.isometric_projection(self, x, y, z)

Give the isometric projection of a given (x,y,z) onto a plane set by self.alpha and self.beta
:param x: x value (float)
:param y: y value (float)
:param z: z value (float)
:return: o, isometric projection vector

Here is the caller graph for this function:



7.8.3.6 def UniDec.unidec_modules.plot3d.CubePlot.isoticks(self, ax, col)

Draws isometric projection of tick marks.
:param ax: Axis object
:param col: Color of ticks
:return: None

Here is the call graph for this function:



7.8.3.7 def UniDec.unidec_modules.plot3d.CubePlot.make_isomatrices(self)

Make projection matrix, self.pc, for calculating isometric projection
:return: None

7.8.4 Member Data Documentation

7.8.4.1 UniDec.unidec_modules.plot3d.CubePlot.alpha

7.8.4.2 UniDec.unidec_modules.plot3d.CubePlot.beta

7.8.4.3 UniDec.unidec_modules.plot3d.CubePlot.cbar

7.8.4.4 UniDec.unidec_modules.plot3d.CubePlot.cmap

7.8.4.5 UniDec.unidec_modules.plot3d.CubePlot.datalims

7.8.4.6 UniDec.unidec_modules.plot3d.CubePlot.flag

7.8.4.7 UniDec.unidec_modules.plot3d.CubePlot.normalticks

7.8.4.8 UniDec.unidec_modules.plot3d.CubePlot.pc

7.8.4.9 UniDec.unidec_modules.plot3d.CubePlot.subplot1

7.8.4.10 UniDec.unidec_modules.plot3d.CubePlot.xlen

7.8.4.11 UniDec.unidec_modules.plot3d.CubePlot.xticlab

7.8.4.12 UniDec.unidec_modules.plot3d.CubePlot.xticloc

7.8.4.13 UniDec.unidec_modules.plot3d.CubePlot.ylen

7.8.4.14 UniDec.unidec_modules.plot3d.CubePlot.yticlab

7.8.4.15 UniDec.unidec_modules.plot3d.CubePlot.yticloc

7.8.4.16 UniDec.unidec_modules.plot3d.CubePlot.zlen

7.8.4.17 UniDec.unidec_modules.plot3d.CubePlot.zticlab

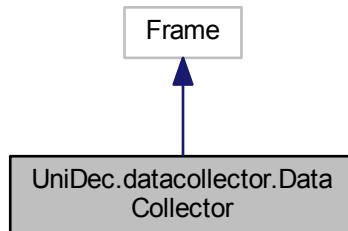
7.8.4.18 UniDec.unidec_modules.plot3d.CubePlot.zticloc

The documentation for this class was generated from the following file:

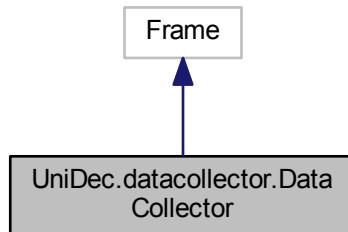
- C:/Python/UniDec/unidec_modules/[plot3d.py](#)

7.9 UniDec.datacollector.DataCollector Class Reference

Inheritance diagram for UniDec.datacollector.DataCollector:



Collaboration diagram for UniDec.datacollector.DataCollector:



Public Member Functions

- def `__init__` (self, parent, title, config=None, pks=None, args, kwargs)
- def `load_x_from_peaks` (self, e)
- def `on_save` (self, e)
- def `on_load` (self, e)
- def `load` (self, savename)
- def `on_add_x` (self, e)
- def `on_add_y` (self, e)
- def `on_choose_dir` (self, e)
- def `on_motion` (self, xpos, ypos)
- def `update_get` (self, e)
- def `update_set` (self, e)
- def `on_run`
- def `make_grid_plots` (self, e)
- def `makeplot2` (self)
- def `on_save_fig` (self, e)
- def `on_save_figPDF` (self, e)

- def `on_kd_fit` (self, e)
- def `on_animate` (self, e)
- def `on_animate2` (self, e)
- def `on_2dgrid` (self, e)
- def `on_defect` (self, e)
- def `on_autocorr` (self, e)
- def `on_local_path` (self, e)
- def `on_absolute_path` (self, e)
- def `on_export` (self, e)
- def `on_msms_norm` (self, e)
- def `on_ylabel` (self, e)

Public Attributes

- `directory`
- `config`
- `pks`
- `gridparams`
- `filemenu`
- `menuSave`
- `menuLoad`
- `menuSaveFigPNG`
- `menuSaveFigPDF`
- `toolsmenu`
- `experimentalmenu`
- `menuAnimation`
- `menuAnimation2`
- `menu2dGrid`
- `menudefect`
- `menulocalpath`
- `menuabsolutepath`
- `menumssnorm`
- `menuautocorr`
- `menuylabel`
- `menuBar`
- `panel`
- `sizer`
- `inputsizer`
- `ypanelsizer`
- `ypanel`
- `ypanelsizer2`
- `addybutton`
- `dirinput`
- `dirbutton`
- `xpanel`
- `xpanelsizer`
- `addxbutton`
- `plotwindow`
- `tab1`
- `tab2`
- `tab3`
- `plot1`
- `plot2d`
- `plot4`

- [plot2](#)
- [plotwindow2](#)
- [tab12](#)
- [tab22](#)
- [plot3](#)
- [plot3h](#)
- [runsizer](#)
- [ctldata](#)
- [ctlmin](#)
- [ctlmax](#)
- [ctlnorm](#)
- [runbutton](#)
- [ctlnorm2](#)
- [ctlextract](#)
- [ctlwindow](#)
- [runsizer2](#)
- [ctlprot](#)
- [ctllig](#)
- [ctlbootstrap](#)
- [kdbutton](#)
- [ctlprotmodel](#)
- [ctlligmodel](#)
- [ctlmaxsites](#)
- [ctloutliers](#)
- [plotsizer](#)
- [xvals](#)
- [yvals](#)
- [range](#)
- [extract](#)
- [normflag](#)
- [normflag2](#)
- [protflag](#)
- [ligflag](#)
- [datachoice](#)
- [numprot](#)
- [numlig](#)
- [bootstrap](#)
- [window](#)
- [maxsites](#)
- [extractchoice](#)
- [savename](#)
- [localpath](#)
- [molig](#)
- [xcolors](#)
- [data](#)
- [grid](#)
- [var1](#)
- [xlabel](#)
- [ylabel](#)

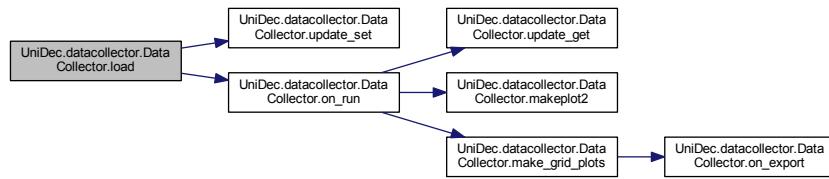
7.9.1 Constructor & Destructor Documentation

7.9.1.1 def UniDec.datacollector.DataCollector.__init__(*self*, *parent*, *title*, *config*=None, *pks*=None, *args*, *kwargs*)

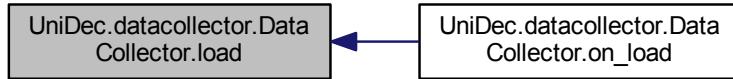
7.9.2 Member Function Documentation

7.9.2.1 def UniDec.datacollector.DataCollector.load(*self*, *savename*)

Here is the call graph for this function:



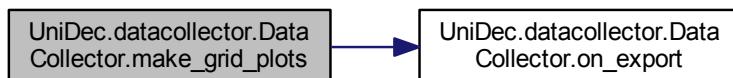
Here is the caller graph for this function:



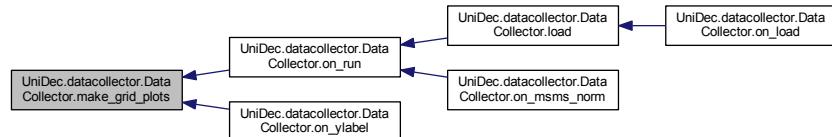
7.9.2.2 def UniDec.datacollector.DataCollector.load_x_from_peaks(*self*, *e*)

7.9.2.3 def UniDec.datacollector.DataCollector.make_grid_plots(*self*, *e*)

Here is the call graph for this function:

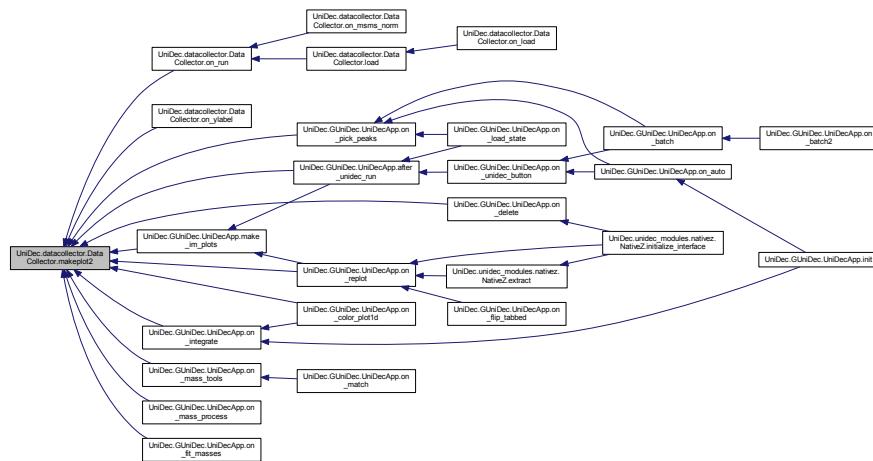


Here is the caller graph for this function:



7.9.2.4 def UniDec.datacollector.DataCollector.makeplot2 (self)

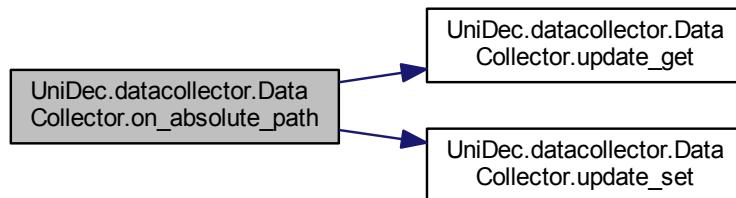
Here is the caller graph for this function:



7.9.2.5 def UniDec.datacollector.DataCollector.on_2dgrid (self, e)

7.9.2.6 def UniDec.datacollector.DataCollector.on_absolute_path (self, e)

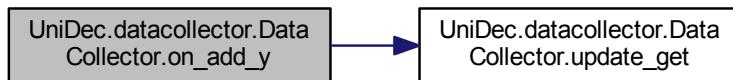
Here is the call graph for this function:



7.9.2.7 def UniDec.datacollector.DataCollector.on_add_x (self, e)

7.9.2.8 def UniDec.datacollector.DataCollector.on_add_y (self, e)

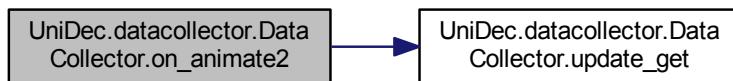
Here is the call graph for this function:



7.9.2.9 def UniDec.datacollector.DataCollector.on_animate (self, e)

7.9.2.10 def UniDec.datacollector.DataCollector.on_animate2 (self, e)

Here is the call graph for this function:



7.9.2.11 def UniDec.datacollector.DataCollector.on_autocorr (self, e)

7.9.2.12 def UniDec.datacollector.DataCollector.on_choose_dir (self, e)

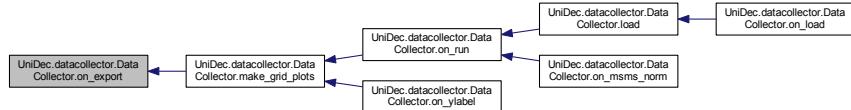
Here is the caller graph for this function:



7.9.2.13 def UniDec.datacollector.DataCollector.on_defect (self, e)

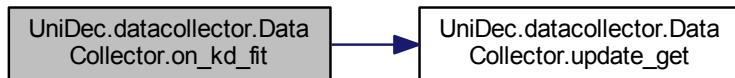
7.9.2.14 def UniDec.datacollector.DataCollector.on_export(self, e)

Here is the caller graph for this function:



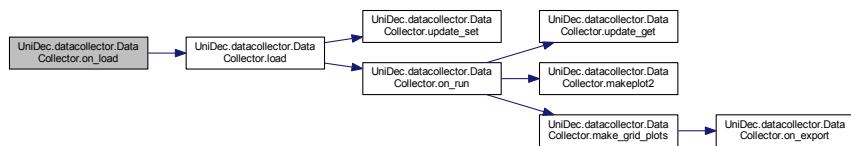
7.9.2.15 def UniDec.datacollector.DataCollector.on_kd_fit(self, e)

Here is the call graph for this function:



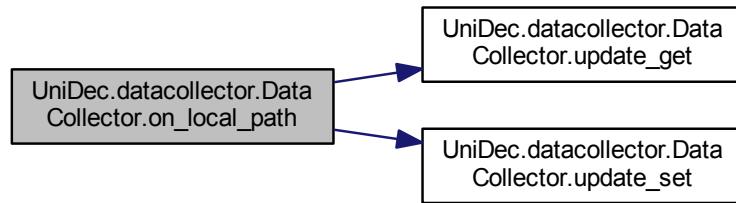
7.9.2.16 def UniDec.datacollector.DataCollector.on_load(self, e)

Here is the call graph for this function:



7.9.2.17 def UniDec.datacollector.DataCollector.on_local_path (*self*, *e*)

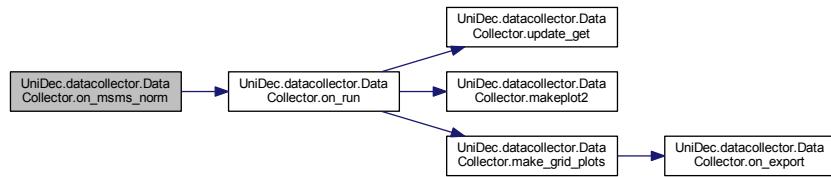
Here is the call graph for this function:



7.9.2.18 def UniDec.datacollector.DataCollector.on_motion (*self*, *xpos*, *ypos*)

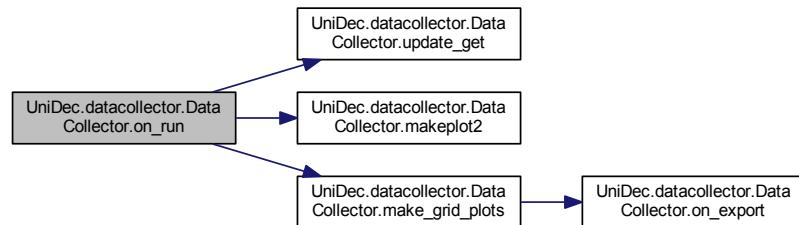
7.9.2.19 def UniDec.datacollector.DataCollector.on_msms_norm (*self*, *e*)

Here is the call graph for this function:

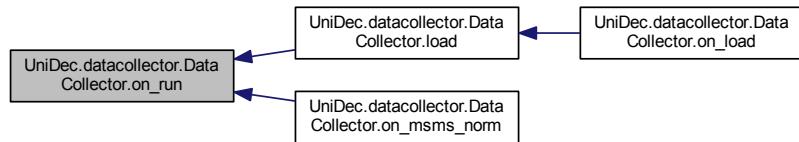


7.9.2.20 def UniDec.datacollector.DataCollector.on_run (*self*, *e*, *vals*=None)

Here is the call graph for this function:

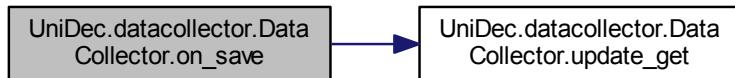


Here is the caller graph for this function:



7.9.2.21 def UniDec.datacollector.DataCollector.on_save (self, e)

Here is the call graph for this function:

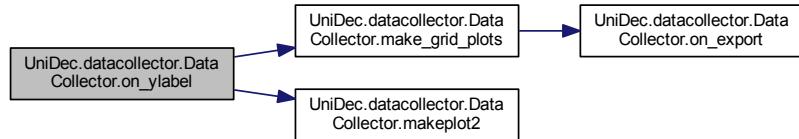


7.9.2.22 def UniDec.datacollector.DataCollector.on_save_fig (self, e)

7.9.2.23 def UniDec.datacollector.DataCollector.on_save_figPDF (self, e)

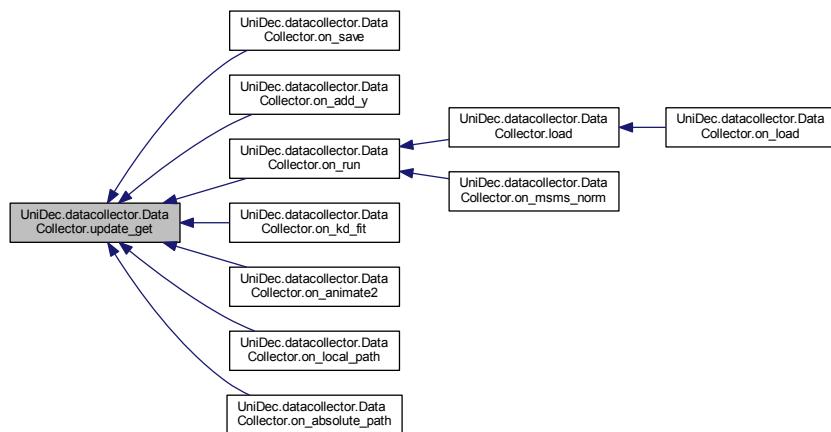
7.9.2.24 def UniDec.datacollector.DataCollector.on_ylabel (self, e)

Here is the call graph for this function:



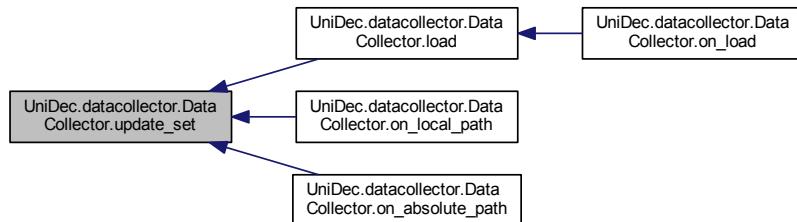
7.9.2.25 def UniDec.datacollector.DataCollector.update_get(self, e)

Here is the caller graph for this function:



7.9.2.26 def UniDec.datacollector.DataCollector.update_set(self, e)

Here is the caller graph for this function:



7.9.3 Member Data Documentation

7.9.3.1 UniDec.datacollector.DataCollector.addxbutton

7.9.3.2 UniDec.datacollector.DataCollector.addybutton

7.9.3.3 UniDec.datacollector.DataCollector.bootstrap

7.9.3.4 UniDec.datacollector.DataCollector.config

7.9.3.5 UniDec.datacollector.DataCollector.ctlbootstrap

7.9.3.6 UniDec.datacollector.DataCollector.ctldata

7.9.3.7 UniDec.datacollector.DataCollector.ctlextract

- 7.9.3.8 UniDec.datacollector.DataCollector.ctllig
- 7.9.3.9 UniDec.datacollector.DataCollector.ctlligmodel
- 7.9.3.10 UniDec.datacollector.DataCollector.ctlmax
- 7.9.3.11 UniDec.datacollector.DataCollector.ctlmaxsites
- 7.9.3.12 UniDec.datacollector.DataCollector.ctlmin
- 7.9.3.13 UniDec.datacollector.DataCollector.ctlnorm
- 7.9.3.14 UniDec.datacollector.DataCollector.ctlnorm2
- 7.9.3.15 UniDec.datacollector.DataCollector.ctloutliers
- 7.9.3.16 UniDec.datacollector.DataCollector.ctlprot
- 7.9.3.17 UniDec.datacollector.DataCollector.ctlprotmodel
- 7.9.3.18 UniDec.datacollector.DataCollector.ctlwindow
- 7.9.3.19 UniDec.datacollector.DataCollector.data
- 7.9.3.20 UniDec.datacollector.DataCollector.datachoice
- 7.9.3.21 UniDec.datacollector.DataCollector.dirbutton
- 7.9.3.22 UniDec.datacollector.DataCollector.directory
- 7.9.3.23 UniDec.datacollector.DataCollector.dirinput
- 7.9.3.24 UniDec.datacollector.DataCollector.experimentalmenu
- 7.9.3.25 UniDec.datacollector.DataCollector.extract
- 7.9.3.26 UniDec.datacollector.DataCollector.extractchoice
- 7.9.3.27 UniDec.datacollector.DataCollector.filemenu
- 7.9.3.28 UniDec.datacollector.DataCollector.grid
- 7.9.3.29 UniDec.datacollector.DataCollector.gridparams
- 7.9.3.30 UniDec.datacollector.DataCollector.inputsizer
- 7.9.3.31 UniDec.datacollector.DataCollector.kdbutton
- 7.9.3.32 UniDec.datacollector.DataCollector.ligflag
- 7.9.3.33 UniDec.datacollector.DataCollector.localpath
- 7.9.3.34 UniDec.datacollector.DataCollector.maxsites
- 7.9.3.35 UniDec.datacollector.DataCollector.menu2dGrid

- 7.9.3.36 UniDec.datacollector.DataCollector.menuabsolutepath
- 7.9.3.37 UniDec.datacollector.DataCollector.menuAnimation
- 7.9.3.38 UniDec.datacollector.DataCollector.menuAnimation2
- 7.9.3.39 UniDec.datacollector.DataCollector.menuautocorr
- 7.9.3.40 UniDec.datacollector.DataCollector.menuBar
- 7.9.3.41 UniDec.datacollector.DataCollector.menudefect
- 7.9.3.42 UniDec.datacollector.DataCollector.menuLoad
- 7.9.3.43 UniDec.datacollector.DataCollector menulocalpath
- 7.9.3.44 UniDec.datacollector.DataCollector.menumssmsnorm
- 7.9.3.45 UniDec.datacollector.DataCollector.menuSave
- 7.9.3.46 UniDec.datacollector.DataCollector.menuSaveFigPDF
- 7.9.3.47 UniDec.datacollector.DataCollector.menuSaveFigPNG
- 7.9.3.48 UniDec.datacollector.DataCollector.menuylabel
- 7.9.3.49 UniDec.datacollector.DataCollector.molig
- 7.9.3.50 UniDec.datacollector.DataCollector.normflag
- 7.9.3.51 UniDec.datacollector.DataCollector.normflag2
- 7.9.3.52 UniDec.datacollector.DataCollector.numlig
- 7.9.3.53 UniDec.datacollector.DataCollector.numprot
- 7.9.3.54 UniDec.datacollector.DataCollector.panel
- 7.9.3.55 UniDec.datacollector.DataCollector.pks
- 7.9.3.56 UniDec.datacollector.DataCollector.plot1
- 7.9.3.57 UniDec.datacollector.DataCollector.plot2
- 7.9.3.58 UniDec.datacollector.DataCollector.plot2d
- 7.9.3.59 UniDec.datacollector.DataCollector.plot3
- 7.9.3.60 UniDec.datacollector.DataCollector.plot3h
- 7.9.3.61 UniDec.datacollector.DataCollector.plot4
- 7.9.3.62 UniDec.datacollector.DataCollector.plotsizer
- 7.9.3.63 UniDec.datacollector.DataCollector.plotwindow

- 7.9.3.64 UniDec.datacollector.DataCollector.plotwindow2
- 7.9.3.65 UniDec.datacollector.DataCollector.protflag
- 7.9.3.66 UniDec.datacollector.DataCollector.range
- 7.9.3.67 UniDec.datacollector.DataCollector.runbutton
- 7.9.3.68 UniDec.datacollector.DataCollector.runsizer
- 7.9.3.69 UniDec.datacollector.DataCollector.runsizer2
- 7.9.3.70 UniDec.datacollector.DataCollector.savename
- 7.9.3.71 UniDec.datacollector.DataCollector.sizer
- 7.9.3.72 UniDec.datacollector.DataCollector.tab1
- 7.9.3.73 UniDec.datacollector.DataCollector.tab12
- 7.9.3.74 UniDec.datacollector.DataCollector.tab2
- 7.9.3.75 UniDec.datacollector.DataCollector.tab22
- 7.9.3.76 UniDec.datacollector.DataCollector.tab3
- 7.9.3.77 UniDec.datacollector.DataCollector.toolsmenu
- 7.9.3.78 UniDec.datacollector.DataCollector.var1
- 7.9.3.79 UniDec.datacollector.DataCollector.window
- 7.9.3.80 UniDec.datacollector.DataCollector.xcolors
- 7.9.3.81 UniDec.datacollector.DataCollector.xlabel
- 7.9.3.82 UniDec.datacollector.DataCollector.xpanel
- 7.9.3.83 UniDec.datacollector.DataCollector.xpanelsizer
- 7.9.3.84 UniDec.datacollector.DataCollector.xvals
- 7.9.3.85 UniDec.datacollector.DataCollector.ylabel
- 7.9.3.86 UniDec.datacollector.DataCollector.ypanel
- 7.9.3.87 UniDec.datacollector.DataCollector.ypanelsizer
- 7.9.3.88 UniDec.datacollector.DataCollector.ypanelsizer2
- 7.9.3.89 UniDec.datacollector.DataCollector.yvals

The documentation for this class was generated from the following file:

- C:/Python/UniDec/[datacollector.py](#)

7.10 UniDec.unidec.DataContainer Class Reference

Public Member Functions

- def [__init__](#) (*self*)

Public Attributes

- [fitdat](#)
- [fitdat2d](#)
- [rawdata](#)
- [rawdata3](#)
- [data2](#)
- [data3](#)
- [massdat](#)
- [mzgrid](#)
- [massgrid](#)
- [ztab](#)
- [massccs](#)
- [ccsz](#)
- [ccsdata](#)

7.10.1 Constructor & Destructor Documentation

7.10.1.1 def UniDec.unidec.DataContainer.[__init__](#) (*self*)

Initialize DataContainer with empty arrays.
:return: None

7.10.2 Member Data Documentation

7.10.2.1 UniDec.unidec.DataContainer.[ccsdata](#)

7.10.2.2 UniDec.unidec.DataContainer.[ccsz](#)

7.10.2.3 UniDec.unidec.DataContainer.[data2](#)

7.10.2.4 UniDec.unidec.DataContainer.[data3](#)

7.10.2.5 UniDec.unidec.DataContainer.[fitdat](#)

7.10.2.6 UniDec.unidec.DataContainer.[fitdat2d](#)

7.10.2.7 UniDec.unidec.DataContainer.[massccs](#)

7.10.2.8 UniDec.unidec.DataContainer.[massdat](#)

7.10.2.9 UniDec.unidec.DataContainer.[massgrid](#)

7.10.2.10 UniDec.unidec.DataContainer.[mzgrid](#)

7.10.2.11 UniDec.unidec.DataContainer.[rawdata](#)

7.10.2.12 UniDec.unidec.DataContainer.[rawdata3](#)

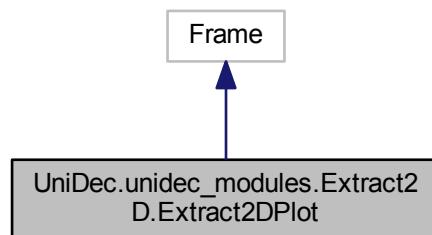
7.10.2.13 UniDec.unidec.DataContainer.ztab

The documentation for this class was generated from the following file:

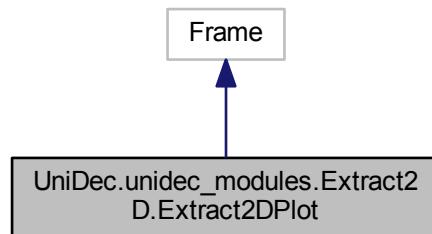
- C:/Python/UniDec/unidec.py

7.11 UniDec.unidec_modules.Extract2D.Extract2DPlot Class Reference

Inheritance diagram for UniDec.unidec_modules.Extract2D.Extract2DPlot:



Collaboration diagram for UniDec.unidec_modules.Extract2D.Extract2DPlot:



Public Member Functions

- def `__init__`
- def `getfromgui` (self)
- def `makegrid` (self)
- def `extractall` (self)
- def `makeplot` (self)
- def `makeplottotal` (self)
- def `makeplotwap` (self)
- def `on_close`
- def `on_back`

- def `on_next`
- def `on_total`
- def `on_wap` (self, e)
- def `on_save_fig` (self, e)
- def `on_save_figPDF` (self, e)

Public Attributes

- `filemenu`
- `menuSaveFigPNG`
- `menuSaveFigPDF`
- `menuBar`
- `config`
- `directory`
- `header`
- `params`
- `datalist`
- `dlen`
- `pos`
- `yvals`
- `storediscrete`
- `plot1`
- `plot2`
- `ctlm0`
- `ctlm1`
- `ctlm2`
- `ctlm1min`
- `ctlm1max`
- `ctlm2min`
- `ctlm2max`
- `ctlwindow`
- `ctlnorm`
- `normflag`
- `m1range`
- `m2range`
- `m2grid`
- `massgrid`
- `igrid`

7.11.1 Constructor & Destructor Documentation

7.11.1.1 def UniDec.unidec_modules.Extract2D.Extract2DPlot.__init__ (self, parent, data_list, config = None, yvals = None, directory = None, header = None, params = None)

Create wx.Frame and initialize components
:param parent: Parent window or panel passed to wx.Frame
:param data_list: Input data for extraction in a list of arrays (N x 2)
:param config: UniDecConfig object. If None, will use defaults.
:param yvals: Position values for corresponding data_list elements.
For plots, these become the titles. For the Weighted-Average-of-Position (WAP) these are the position values.
:param directory: Directory for saving files. Default is current working directory.
:param header: Header for files that are written. Default is "Extract"
:param params: List of 8 values that define the parameters for extraction.

```
0=mass 0
1=mass 1
2=mass 2
```

```

3=minimum oligomeric state of mass 1
4=maximum oligomeric state of mass 1
5=minimum oligomeric state of mass 2
6=maximum oligomeric state of mass 2
7>Error window for finding intensity value

masses = m0 + m1 * range(min m1, max m1 +1) + m2 * range(min m2, max m2 +1)

:returns: None

```

7.11.2 Member Function Documentation

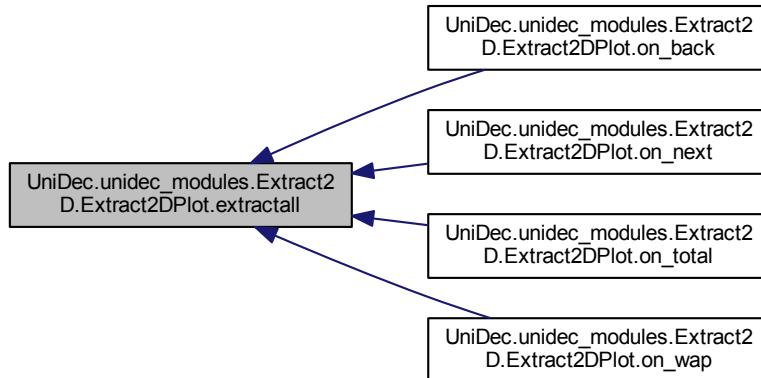
7.11.2.1 def UniDec.unidec_modules.Extract2D.Extract2DPlot.extractall (self)

```

Extract intensity values from self.datalist for mass values in self.massgrid.
:returns: None

```

Here is the caller graph for this function:



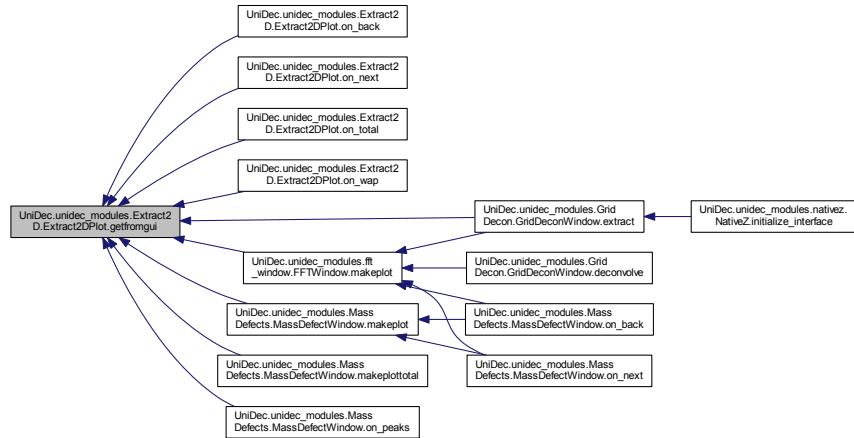
7.11.2.2 def UniDec.unidec_modules.Extract2D.Extract2DPlot.getfromgui (self)

```

Extract parameters from GUI to self.params
:returns:

```

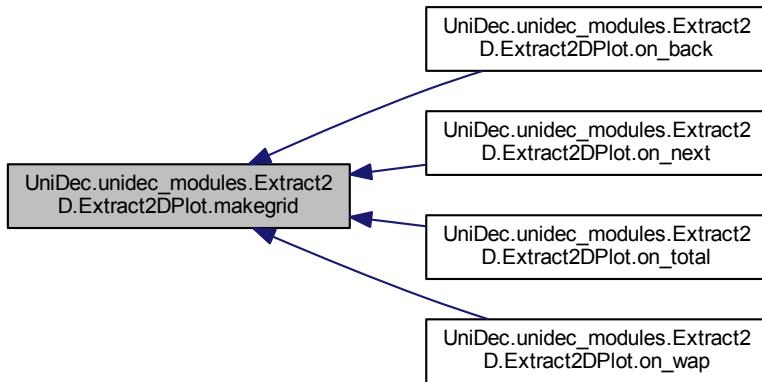
Here is the caller graph for this function:



7.11.2.3 def UniDec.unidec_modules.Extract2D.Extract2DPlot.makegrid (self)

```
Make grid of mass values for potential combinations of m1 and m2 + m0.
:returns: None
```

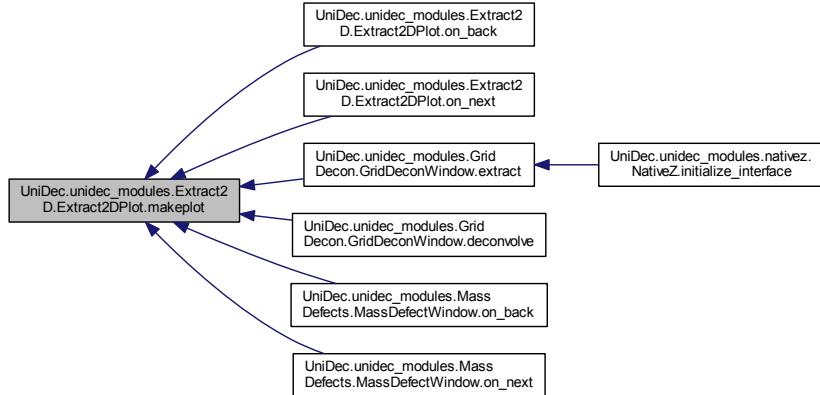
Here is the caller graph for this function:



7.11.2.4 def UniDec.unidec_modules.Extract2D.Extract2DPlot.makeplot (self)

```
Make the 2D and 1D plots for element self.pos in data_list.
:returns: None
```

Here is the caller graph for this function:



7.11.2.5 def UniDec.unidec_modules.Extract2D.Extract2DPlot.makeplottotal (self)

Make the 2D and 1D plots for the sum of all arrays in `data_list`. Write outputs to `_grid_2D_extract.txt` and `_total_2D_extract.txt`.
`:return:`

Here is the caller graph for this function:



7.11.2.6 def UniDec.unidec_modules.Extract2D.Extract2DPlot.makeplotwap (self)

Calculates the weighted average of position (WAP) for each element in the intensity grid.
 Writes 1D output to `_WAP_2D_Extract.txt`.
`:return:` None

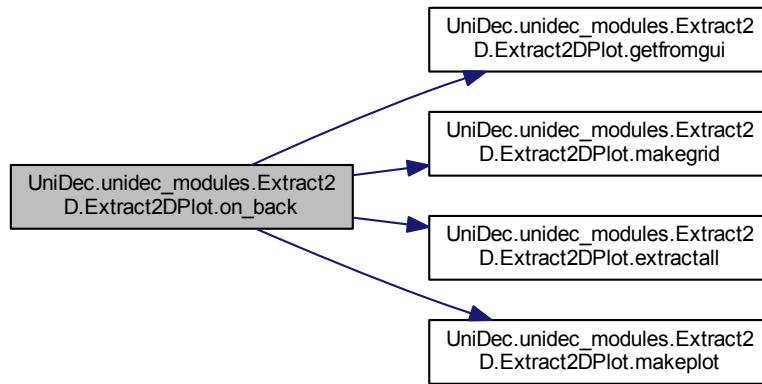
Here is the caller graph for this function:



7.11.2.7 def UniDec.unidec_modules.Extract2D.Extract2DPlot.on_back(self, e=None)

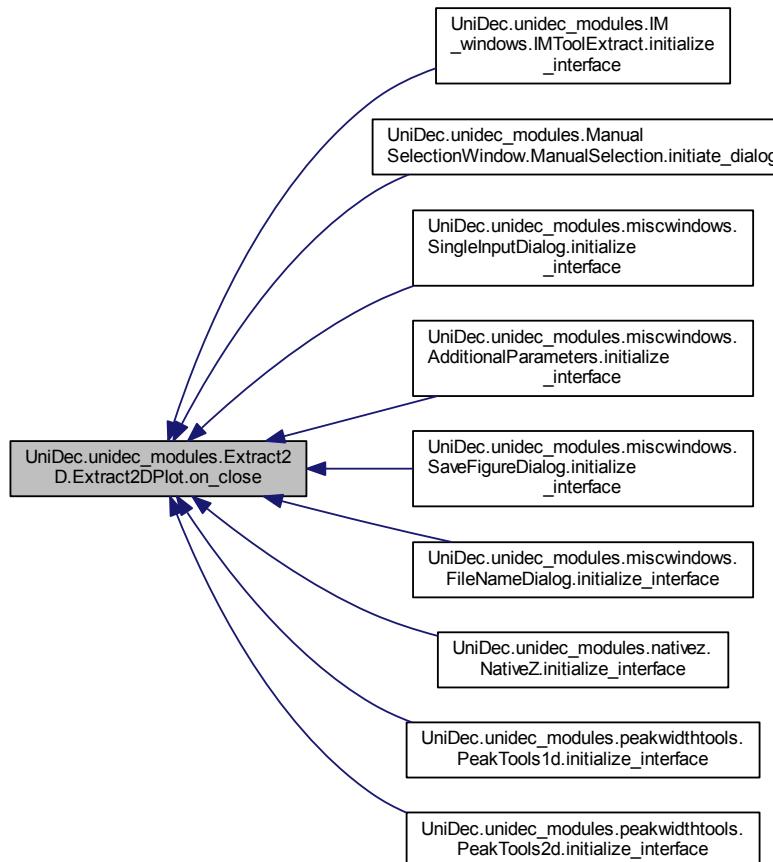
```
Plot the extraction from the previous array in data_list.  
:param e: Unused event  
:return:
```

Here is the call graph for this function:

**7.11.2.8 def UniDec.unidec_modules.Extract2D.Extract2DPlot.on_close(self, e=None)**

```
Close the window. Return self.config.discreteplot to its original value.  
:param e:  
:return:
```

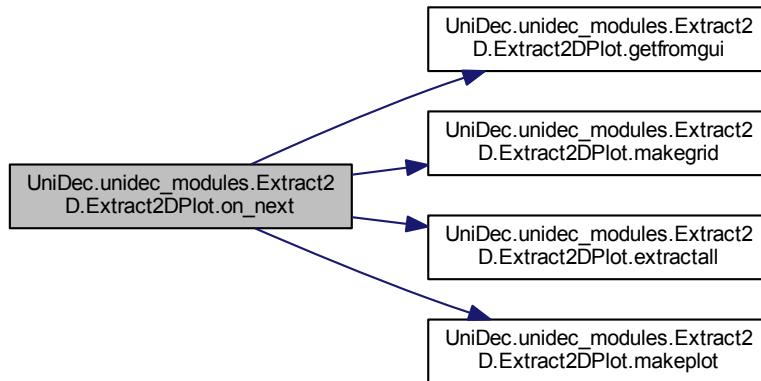
Here is the caller graph for this function:



7.11.2.9 def UniDec.unidec_modules.Extract2D.Extract2DPlot.on_next(self, e=None)

Plot the extraction from the next array in data_list.
:param e: Unused event
:return: None

Here is the call graph for this function:



7.11.2.10 def UniDec.unidec_modules.Extract2D.Extract2DPlot.on_save_fig(self, e)

Save figures as a PNG in self.directory.
:param e: Unused event
:return: None

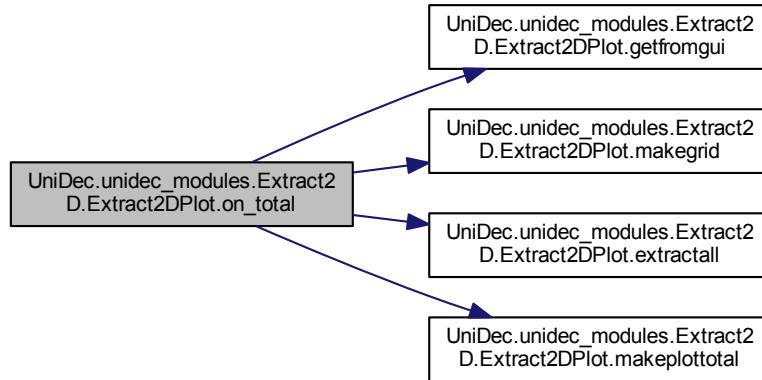
7.11.2.11 def UniDec.unidec_modules.Extract2D.Extract2DPlot.on_save_figPDF(self, e)

Save figures as a PDF in self.directory.
:param e: Unused event
:return: None

7.11.2.12 def UniDec.unidec_modules.Extract2D.Extract2DPlot.on_total(self, e =None)

Extract all and plot total.
:param e: Unused event
:return: None

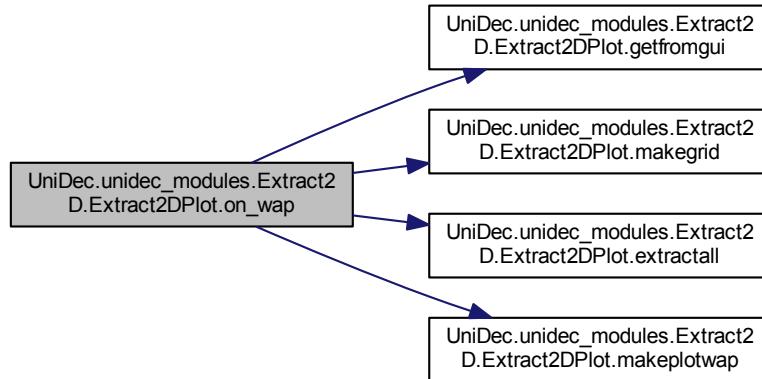
Here is the call graph for this function:



7.11.2.13 def UniDec.unidec_modules.Extract2D.Extract2DPlot.on_wap (self, e)

Extract all and plot weighted average of position.
:param e: Unused event
:return: None

Here is the call graph for this function:



7.11.3 Member Data Documentation

7.11.3.1 UniDec.unidec_modules.Extract2D.Extract2DPlot.config

7.11.3.2 UniDec.unidec_modules.Extract2D.Extract2DPlot.ctlm0

7.11.3.3 UniDec.unidec_modules.Extract2D.Extract2DPlot.ctlm1

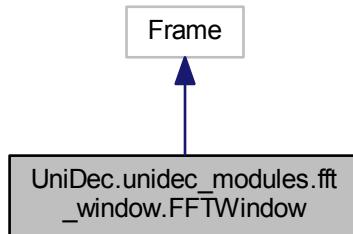
- 7.11.3.4 `UniDec.unidec_modules.Extract2D.Extract2DPlot.ctlm1max`
- 7.11.3.5 `UniDec.unidec_modules.Extract2D.Extract2DPlot.ctlm1min`
- 7.11.3.6 `UniDec.unidec_modules.Extract2D.Extract2DPlot.ctlm2`
- 7.11.3.7 `UniDec.unidec_modules.Extract2D.Extract2DPlot.ctlm2max`
- 7.11.3.8 `UniDec.unidec_modules.Extract2D.Extract2DPlot.ctlm2min`
- 7.11.3.9 `UniDec.unidec_modules.Extract2D.Extract2DPlot.ctlnorm`
- 7.11.3.10 `UniDec.unidec_modules.Extract2D.Extract2DPlot.ctlwindow`
- 7.11.3.11 `UniDec.unidec_modules.Extract2D.Extract2DPlot.datalist`
- 7.11.3.12 `UniDec.unidec_modules.Extract2D.Extract2DPlot.directory`
- 7.11.3.13 `UniDec.unidec_modules.Extract2D.Extract2DPlot.dlen`
- 7.11.3.14 `UniDec.unidec_modules.Extract2D.Extract2DPlot.filemenu`
- 7.11.3.15 `UniDec.unidec_modules.Extract2D.Extract2DPlot.header`
- 7.11.3.16 `UniDec.unidec_modules.Extract2D.Extract2DPlot.igrid`
- 7.11.3.17 `UniDec.unidec_modules.Extract2D.Extract2DPlot.m1range`
- 7.11.3.18 `UniDec.unidec_modules.Extract2D.Extract2DPlot.m2grid`
- 7.11.3.19 `UniDec.unidec_modules.Extract2D.Extract2DPlot.m2range`
- 7.11.3.20 `UniDec.unidec_modules.Extract2D.Extract2DPlot.massgrid`
- 7.11.3.21 `UniDec.unidec_modules.Extract2D.Extract2DPlot.menuBar`
- 7.11.3.22 `UniDec.unidec_modules.Extract2D.Extract2DPlot.menuSaveFigPDF`
- 7.11.3.23 `UniDec.unidec_modules.Extract2D.Extract2DPlot.menuSaveFigPNG`
- 7.11.3.24 `UniDec.unidec_modules.Extract2D.Extract2DPlot.normflag`
- 7.11.3.25 `UniDec.unidec_modules.Extract2D.Extract2DPlot.params`
- 7.11.3.26 `UniDec.unidec_modules.Extract2D.Extract2DPlot.plot1`
- 7.11.3.27 `UniDec.unidec_modules.Extract2D.Extract2DPlot.plot2`
- 7.11.3.28 `UniDec.unidec_modules.Extract2D.Extract2DPlot.pos`
- 7.11.3.29 `UniDec.unidec_modules.Extract2D.Extract2DPlot.storeddiscrete`
- 7.11.3.30 `UniDec.unidec_modules.Extract2D.Extract2DPlot.yvals`

The documentation for this class was generated from the following file:

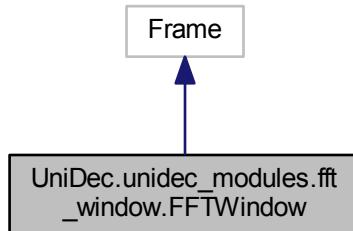
- C:/Python/UniDec/unidec_modules/[Extract2D.py](#)

7.12 UniDec.unidec_modules.fft_window.FFTWindow Class Reference

Inheritance diagram for UniDec.unidec_modules.fft_window.FFTWindow:



Collaboration diagram for UniDec.unidec_modules.fft_window.FFTWindow:



Public Member Functions

- def `__init__`
- def `on_close` (self, e)
- def `getfromgui` (self)
- def `makeplot`
- def `on_save_fig` (self, e)
- def `on_save_fig_pdf` (self, e)
- def `on_add_line` (self, e)

Public Attributes

- `directory`
- `config`
- `window_fwhm`
- `binsize`
- `wbin`

- `diffrange`
- `rawdata`
- `xlims`
- `plotmenu`
- `menuaddline`
- `plot1`
- `plot2`
- `ctlfwhm`
- `ctlwbin`
- `ctlbinsize`
- `ctlmin`
- `ctlmax`

7.12.1 Constructor & Destructor Documentation

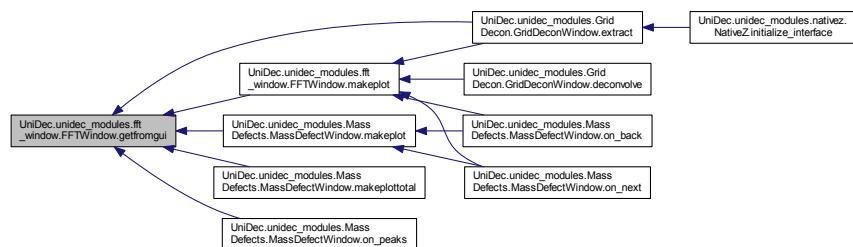
7.12.1.1 `def UniDec.unidec_modules.fft_window.FFTWindow.__init__ (self, parent, data, config=None, directory = None)`

7.12.2 Member Function Documentation

7.12.2.1 `def UniDec.unidec_modules.fft_window.FFTWindow.getfromgui (self)`

Update parameters from GUI.
`:return:` None

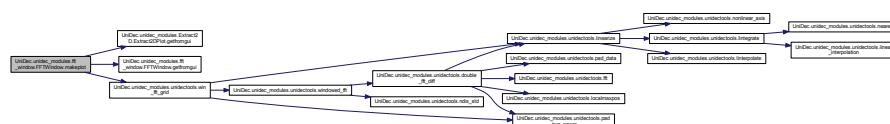
Here is the caller graph for this function:



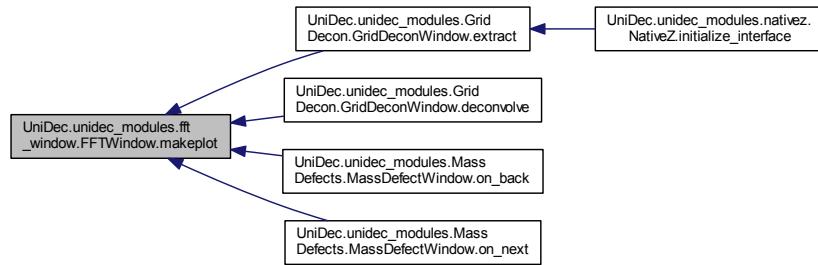
7.12.2.2 `def UniDec.unidec_modules.fft_window.FFTWindow.makeplot (self, e = None)`

Runs the kendrick analysis on a single of the mass distributions in `self.datalist` set by `self.pos`.
Plots the results in 1D and 2D.
`:return:` None

Here is the call graph for this function:



Here is the caller graph for this function:



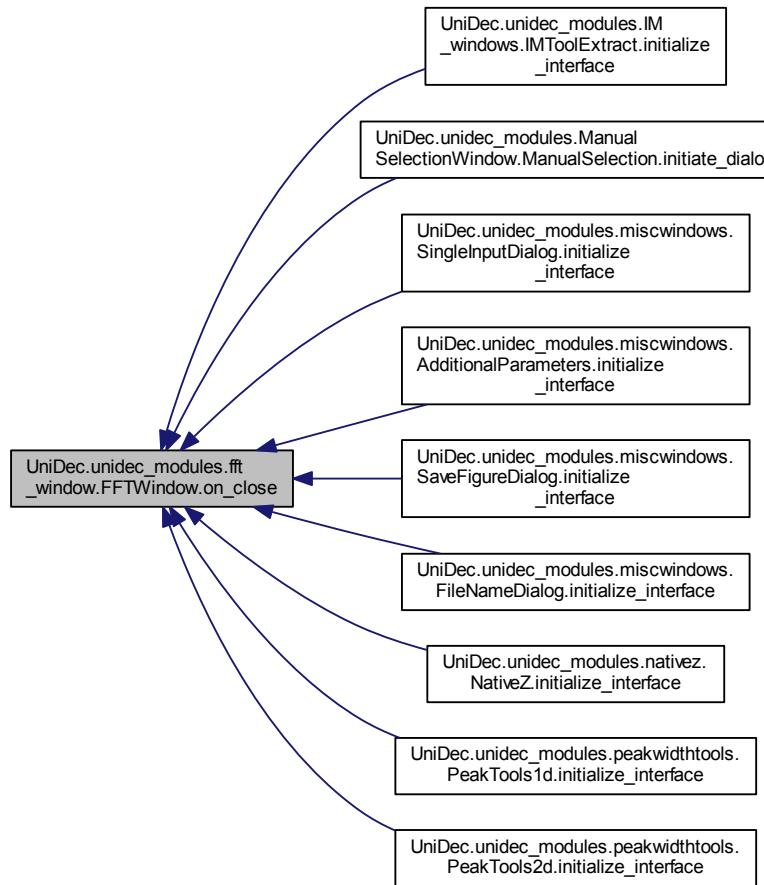
7.12.2.3 def UniDec.unidec_modules.fft_window.FFTWindow.on_add_line(self, e)

Add a horizontal line to the plot to visualize a predicted mass defect.
 Opens a dialog to input the value. Can be called more than once to add multiple lines.
 :param e: Unused event
 :return: None

7.12.2.4 def UniDec.unidec_modules.fft_window.FFTWindow.on_close(self, e)

Close the window. Will try to set self.config.molig as self.m0.
 :param e: Unused event
 :return: None

Here is the caller graph for this function:



7.12.2.5 def UniDec.unidec_modules.fft_window.FFTWindow.on_save_fig(self, e)

Saves the figures in self.directory as PNGs.
:param e: Unused event
:return: None

7.12.2.6 def UniDec.unidec_modules.fft_window.FFTWindow.on_save_fig_pdf(self, e)

Saves the figures in self.directory as PDFs.
:param e: Unused event
:return: None

7.12.3 Member Data Documentation

7.12.3.1 UniDec.unidec_modules.fft_window.FFTWindow.binsize

7.12.3.2 UniDec.unidec_modules.fft_window.FFTWindow.config

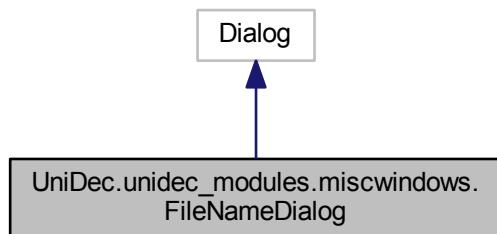
- 7.12.3.3 UniDec.unidec_modules.fft_window.FFTWindow.ctlbinsize
- 7.12.3.4 UniDec.unidec_modules.fft_window.FFTWindow.ctlfwhm
- 7.12.3.5 UniDec.unidec_modules.fft_window.FFTWindow.ctlmax
- 7.12.3.6 UniDec.unidec_modules.fft_window.FFTWindow.ctlmin
- 7.12.3.7 UniDec.unidec_modules.fft_window.FFTWindow.ctlwbin
- 7.12.3.8 UniDec.unidec_modules.fft_window.FFTWindow.diffrange
- 7.12.3.9 UniDec.unidec_modules.fft_window.FFTWindow.directory
- 7.12.3.10 UniDec.unidec_modules.fft_window.FFTWindow.menuaddline
- 7.12.3.11 UniDec.unidec_modules.fft_window.FFTWindow.plot1
- 7.12.3.12 UniDec.unidec_modules.fft_window.FFTWindow.plot2
- 7.12.3.13 UniDec.unidec_modules.fft_window.FFTWindow.plotmenu
- 7.12.3.14 UniDec.unidec_modules.fft_window.FFTWindow.rawdata
- 7.12.3.15 UniDec.unidec_modules.fft_window.FFTWindow.wbin
- 7.12.3.16 UniDec.unidec_modules.fft_window.FFTWindow.window_fwhm
- 7.12.3.17 UniDec.unidec_modules.fft_window.FFTWindow.xlims

The documentation for this class was generated from the following file:

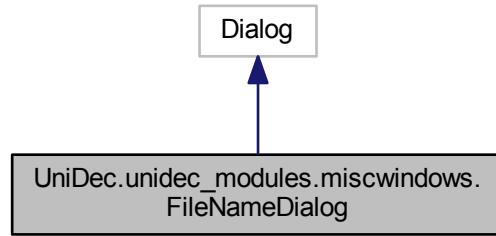
- C:/Python/UniDec/unidec_modules/[fft_window.py](#)

7.13 UniDec.unidec_modules.misctools.FileNameDialog Class Reference

Inheritance diagram for UniDec.unidec_modules.misctools.FileNameDialog:



Collaboration diagram for UniDec.unidec_modules.miscwindows.FileNameDialog:



Public Member Functions

- def `__init__` (`self, args, kwargs`)
- def `initialize_interface` (`self, config`)
- def `on_close` (`self, e`)
- def `on_close_cancel` (`self, e`)

Public Attributes

- `config`
- `inputbox`
- `dirbox`
- `confbox`
- `outputbox`
- `massbox`
- `manualbox`
- `obox`
- `matchbox`
- `peakbox`

7.13.1 Constructor & Destructor Documentation

7.13.1.1 def UniDec.unidec_modules.miscwindows.FileNameDialog.__init__ (`self, args, kwargs`)

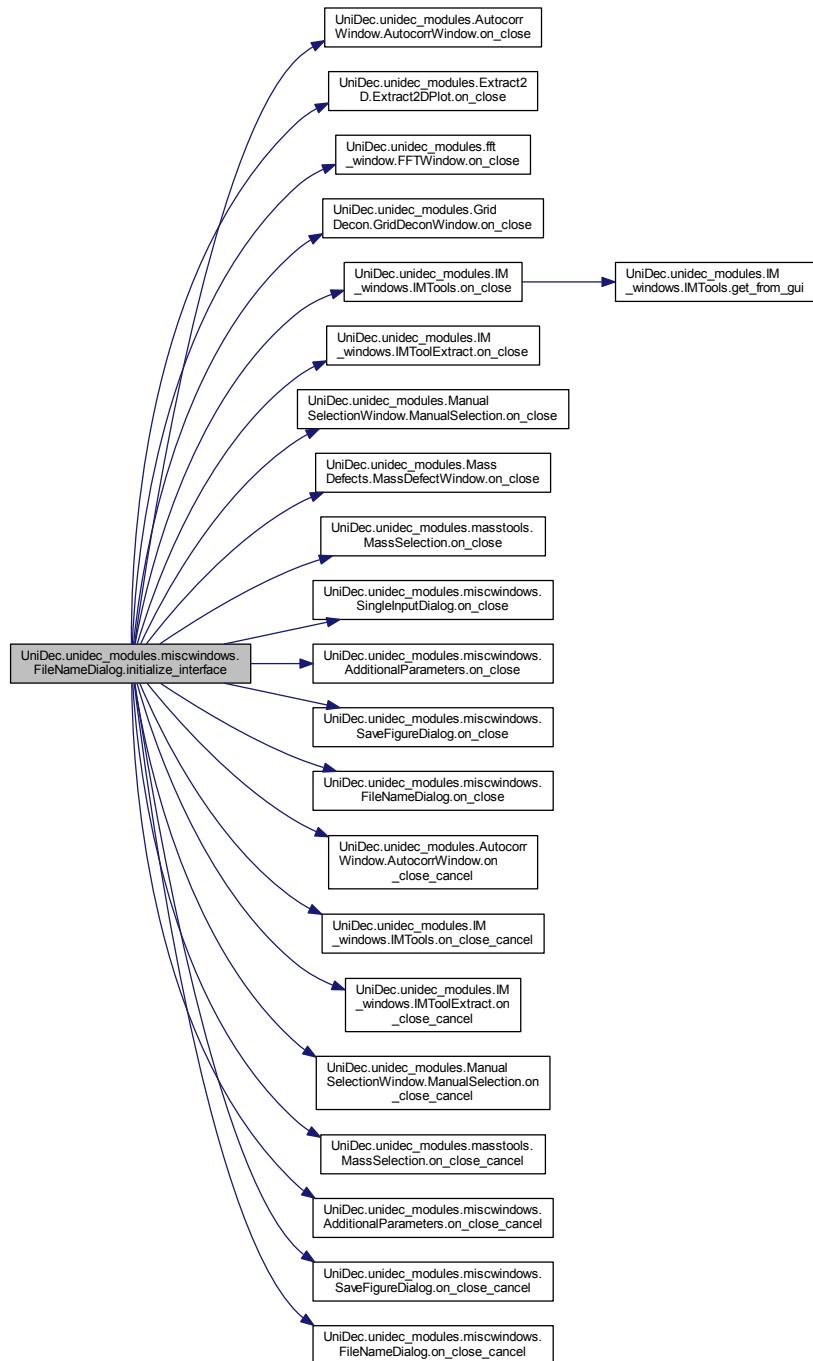
Window for renaming default file names.
:param args: Passed to `wx.Dialog`
:param kwargs: Passed to `wx.Dialog`
:return: None

7.13.2 Member Function Documentation

7.13.2.1 def UniDec.unidec_modules.miscwindows.FileNameDialog.initialize_interface (`self, config`)

Initialize the interface.
:param config: `UniDecConfig` object
:return: None

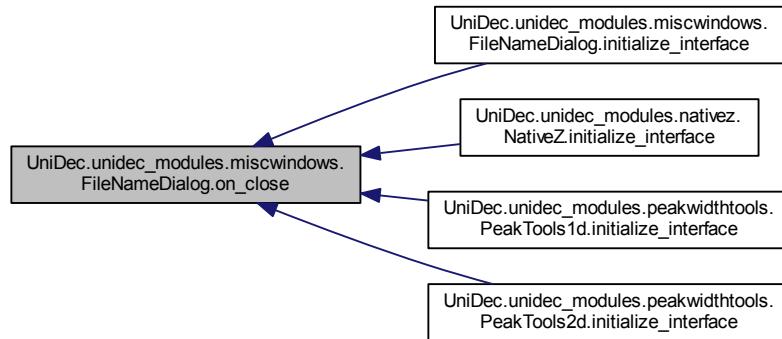
Here is the call graph for this function:



7.13.2.2 def UniDec.unidec_modules.misctools.FileNameDialog.on_close(self, e)

Get the new filenames from the window.
 If each is not blank, update self.config.
 Close the window.
 :param e: Unused event
 :return: None

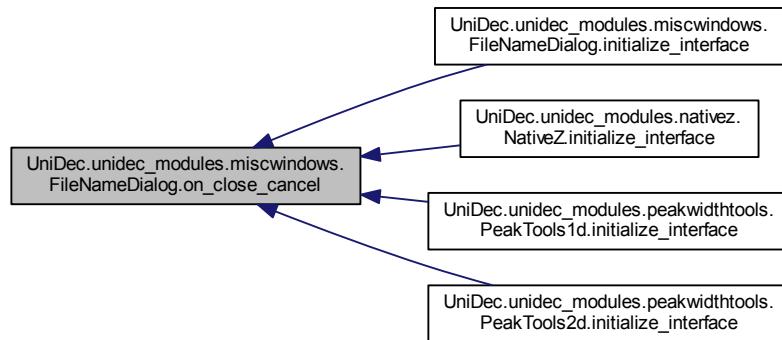
Here is the caller graph for this function:



7.13.2.3 def UniDec.unidec_modules.mscwindows.FileNameDialog.on_close_cancel (self, e)

Close the window but don't update any of the parameters.
`:param e: Unused event`
`:return: None`

Here is the caller graph for this function:



7.13.3 Member Data Documentation

7.13.3.1 UniDec.unidec_modules.mscwindows.FileNameDialog.confbox

7.13.3.2 UniDec.unidec_modules.mscwindows.FileNameDialog.config

7.13.3.3 UniDec.unidec_modules.mscwindows.FileNameDialog.dirbox

7.13.3.4 UniDec.unidec_modules.mscwindows.FileNameDialog.inputbox

7.13.3.5 UniDec.unidec_modules.mscwindows.FileNameDialog.manualbox

7.13.3.6 UniDec.unidec_modules.miscwindows.FileNameDialog.massbox

7.13.3.7 UniDec.unidec_modules.miscwindows.FileNameDialog.matchbox

7.13.3.8 UniDec.unidec_modules.miscwindows.FileNameDialogobox

7.13.3.9 UniDec.unidec_modules.miscwindows.FileNameDialog.outputbox

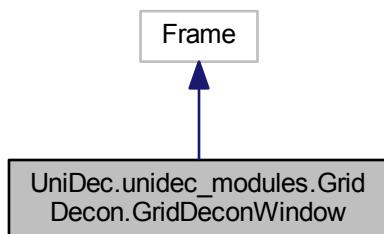
7.13.3.10 UniDec.unidec_modules.miscwindows.FileNameDialog.peakbox

The documentation for this class was generated from the following file:

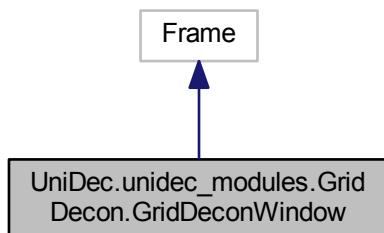
- C:/Python/UniDec/unidec_modules/[miscwindows.py](#)

7.14 UniDec.unidec_modules.GridDecon.GridDeconWindow Class Reference

Inheritance diagram for UniDec.unidec_modules.GridDecon.GridDeconWindow:



Collaboration diagram for UniDec.unidec_modules.GridDecon.GridDeconWindow:



Public Member Functions

- def [__init__](#)

- def `getfromgui` (self)
- def `extract` (self, e)
- def `makegrids` (self)
- def `deconvolve` (self, e)
- def `makeplot`
- def `on_close`
- def `on_save_fig` (self, e)
- def `on_save_figPDF` (self, e)

Public Attributes

- `filemenu`
- `menuSaveFigPNG`
- `menuSaveFigPDF`
- `menuBar`
- `data`
- `config`
- `directory`
- `params`
- `storediscrete`
- `plot1`
- `plot2`
- `ctlm0`
- `ctlm1`
- `ctlm1min`
- `ctlm1max`
- `ctlm2min`
- `ctlm2max`
- `ctlwindow`
- `ctlfwhm`
- `ctlmsig`
- `ctlzzsig`
- `mrange`
- `zrange`
- `zgrid`
- `mzgrid`
- `igrid`

7.14.1 Constructor & Destructor Documentation

7.14.1.1 def `UniDec.unidec_modules.GridDecon.GridDeconWindow.__init__` (`self, parent, data, config=None, directory=None`)

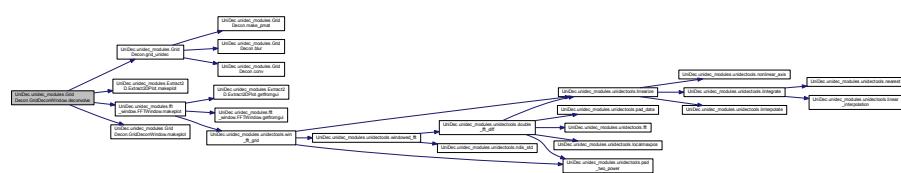
```
masses = m0 + m1 * range(min m1, max m1 +1)

:return: None
```

7.14.2 Member Function Documentation

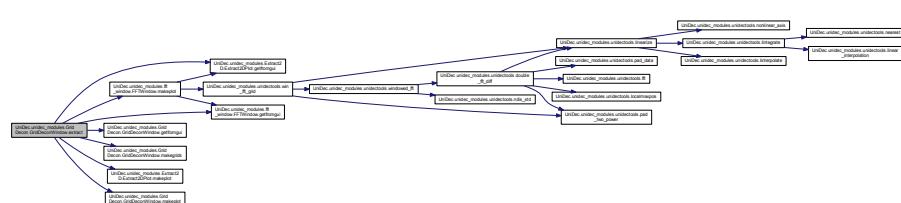
7.14.2.1 def UniDec.unidec_modules.GridDecon.GridDeconWindow.deconvolve (self, e)

Here is the call graph for this function:

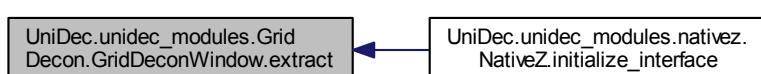


7.14.2.2 def UniDec.unidec_modules.GridDecon.GridDeconWindow.extract (self, e)

Here is the call graph for this function:



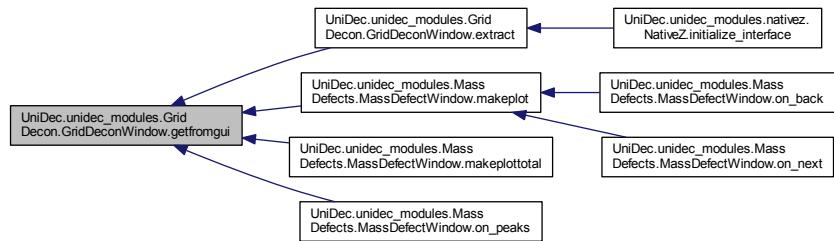
Here is the caller graph for this function:



7.14.2.3 def UniDec.unidec_modules.GridDecon.GridDeconWindow.getfromgui (self)

```
Extract parameters from GUI to self.params
:returns:
```

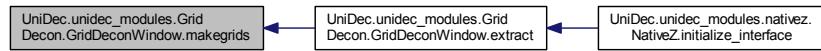
Here is the caller graph for this function:



7.14.2.4 def UniDec.unidec_modules.GridDecon.GridDeconWindow.makegrids (self)

Make grid of mass values for potential combinations of m1 and m2 + m0.
:return: None

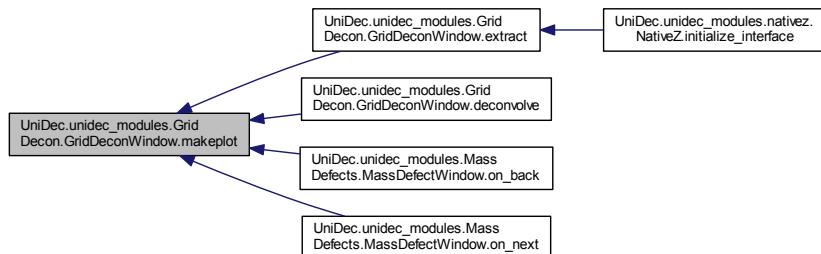
Here is the caller graph for this function:



7.14.2.5 def UniDec.unidec_modules.GridDecon.GridDeconWindow.makeplot (self, title = "Extracted Data")

Make the 2D and 1D plots for element self.pos in data_list.
:return: None

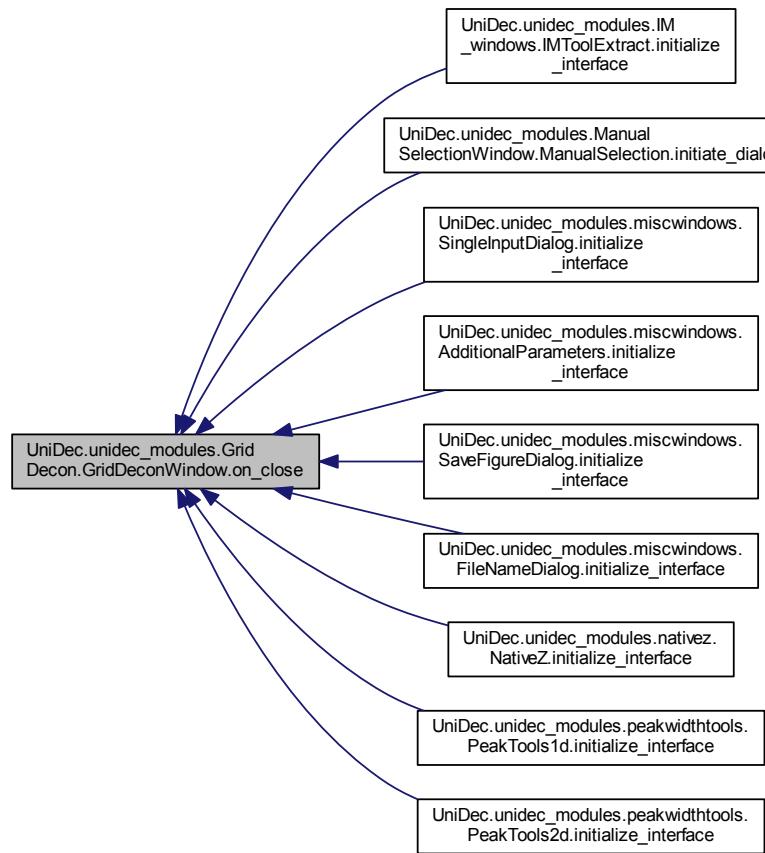
Here is the caller graph for this function:



7.14.2.6 def UniDec.unidec_modules.GridDecon.GridDeconWindow.on_close (self, e = None)

Close the window. Return self.config.discreteplot to its original value.
:param e:
:return:

Here is the caller graph for this function:



7.14.2.7 def UniDec.unidec_modules.GridDecon.GridDeconWindow.on_save_fig (self, e)

Save figures as a PNG in self.directory.
:param e: Unused event
:return: None

7.14.2.8 def UniDec.unidec_modules.GridDecon.GridDeconWindow.on_save_figPDF (self, e)

Save figures as a PDF in self.directory.
:param e: Unused event
:return: None

7.14.3 Member Data Documentation

7.14.3.1 UniDec.unidec_modules.GridDecon.GridDeconWindow.config

7.14.3.2 UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlfwhm

7.14.3.3 UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlm0

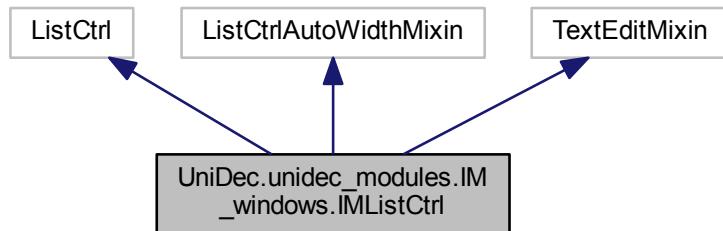
- 7.14.3.4 `UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlm1`
- 7.14.3.5 `UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlm1max`
- 7.14.3.6 `UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlm1min`
- 7.14.3.7 `UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlm2max`
- 7.14.3.8 `UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlm2min`
- 7.14.3.9 `UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlmsig`
- 7.14.3.10 `UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlwindow`
- 7.14.3.11 `UniDec.unidec_modules.GridDecon.GridDeconWindow.ctlzzsig`
- 7.14.3.12 `UniDec.unidec_modules.GridDecon.GridDeconWindow.data`
- 7.14.3.13 `UniDec.unidec_modules.GridDecon.GridDeconWindow.directory`
- 7.14.3.14 `UniDec.unidec_modules.GridDecon.GridDeconWindow.filemenu`
- 7.14.3.15 `UniDec.unidec_modules.GridDecon.GridDeconWindow.igrid`
- 7.14.3.16 `UniDec.unidec_modules.GridDecon.GridDeconWindow.menuBar`
- 7.14.3.17 `UniDec.unidec_modules.GridDecon.GridDeconWindow.menuSaveFigPDF`
- 7.14.3.18 `UniDec.unidec_modules.GridDecon.GridDeconWindow.menuSaveFigPNG`
- 7.14.3.19 `UniDec.unidec_modules.GridDecon.GridDeconWindow.mrange`
- 7.14.3.20 `UniDec.unidec_modules.GridDecon.GridDeconWindow.mzgrid`
- 7.14.3.21 `UniDec.unidec_modules.GridDecon.GridDeconWindow.params`
- 7.14.3.22 `UniDec.unidec_modules.GridDecon.GridDeconWindow.plot1`
- 7.14.3.23 `UniDec.unidec_modules.GridDecon.GridDeconWindow.plot2`
- 7.14.3.24 `UniDec.unidec_modules.GridDecon.GridDeconWindow.storediscrete`
- 7.14.3.25 `UniDec.unidec_modules.GridDecon.GridDeconWindow.zgrid`
- 7.14.3.26 `UniDec.unidec_modules.GridDecon.GridDeconWindow.zrange`

The documentation for this class was generated from the following file:

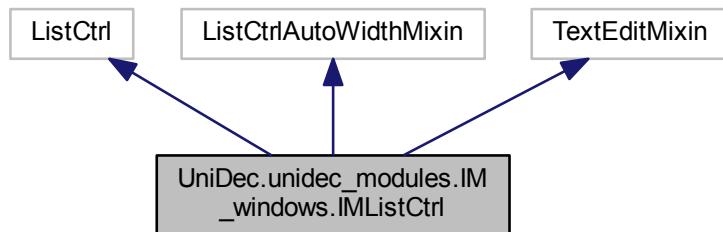
- C:/Python/UniDec/unidec_modules/[GridDecon.py](#)

7.15 UniDec.unidec_modules.IM_windows.ILListCtrl Class Reference

Inheritance diagram for UniDec.unidec_modules.IM_windows.ILListCtrl:



Collaboration diagram for UniDec.unidec_modules.IM_windows.ILListCtrl:



Public Member Functions

- def `__init__`
- def `clear_list` (self)
- def `add_line`
- def `populate`
- def `get_list` (self)
- def `on_right_click` (self, event)
- def `on_delete` (self, event)

Public Attributes

- `popupID1`

7.15.1 Constructor & Destructor Documentation

```
7.15.1.1 def UniDec.unidec_modules.IM_windows.ILMListCtrl.__init__( self, parent, id_val, pos =
    wx.DefaultPosition, size = wx.DefaultSize, style = 0 )
```

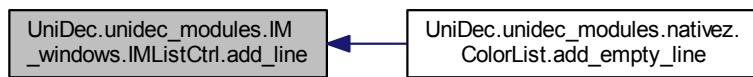
Create listctrl with 2 columns.
:param parent: Passed to wx.ListCtrl
:param id_val: Passed to wx.ListCtrl
:param pos: Passed to wx.ListCtrl
:param size: Passed to wx.ListCtrl
:param style: Passed to wx.ListCtrl
:return: None

7.15.2 Member Function Documentation

```
7.15.2.1 def UniDec.unidec_modules.IM_windows.ILMListCtrl.add_line( self, val = 0 )
```

Add a new line to the list.
:param val: Value for the first column. Default is 0. Default for second column is 0.
:return: None

Here is the caller graph for this function:



```
7.15.2.2 def UniDec.unidec_modules.IM_windows.ILMListCtrl.clear_list( self )
```

Clear list.
:return: None

```
7.15.2.3 def UniDec.unidec_modules.IM_windows.ILMListCtrl.get_list( self )
```

Return the list of values in the listctrl.
:return: Nested list of listctrl output

```
7.15.2.4 def UniDec.unidec_modules.IM_windows.ILMListCtrl.on_delete( self, event )
```

Delete the selected item.
:param event: Unused event.
:return: None

Here is the caller graph for this function:



7.15.2.5 def UniDec.unidec_modules.IM_windows.ILListCtrl.on_right_click (self, event)

```
Create a right click menu.  
:param event: Unused event  
:return: None
```

7.15.2.6 def UniDec.unidec_modules.IM_windows.ILListCtrl.populate (self, data, colors=None)

```
Add data from array or nested list to the listctrl.  
:param data: List or array of data values.  
:param colors: Background colors list  
:return: None
```

7.15.3 Member Data Documentation

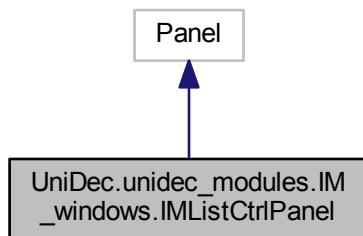
7.15.3.1 UniDec.unidec_modules.IM_windows.ILListCtrl.popupID1

The documentation for this class was generated from the following file:

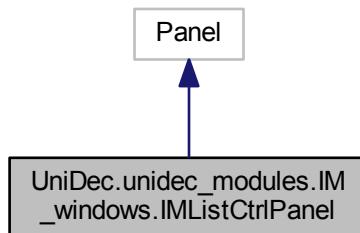
- C:/Python/UniDec/unidec_modules/[IM_windows.py](#)

7.16 UniDec.unidec_modules.IM_windows.ILListCtrlPanel Class Reference

Inheritance diagram for UniDec.unidec_modules.IM_windows.ILListCtrlPanel:



Collaboration diagram for UniDec.unidec_modules.IM_windows.ILMListCtrlPanel:



Public Member Functions

- def [__init__](#) (self, parent, size=(200, 200))

Public Attributes

- [list](#)

7.16.1 Constructor & Destructor Documentation

7.16.1.1 def UniDec.unidec_modules.IM_windows.ILMListCtrlPanel.__init__(self, parent, size = (200, 200))

```
Creates the panel for the ILMListCtrl
:param parent: Parent window or panel
:param size: Size in pixels for list control
:return: None
```

7.16.2 Member Data Documentation

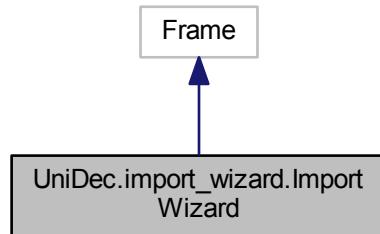
7.16.2.1 UniDec.unidec_modules.IM_windows.ILMListCtrlPanel.list

The documentation for this class was generated from the following file:

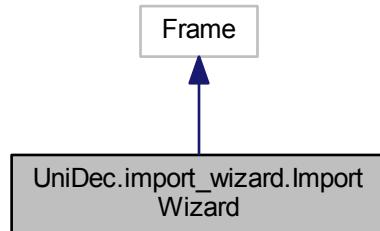
- C:/Python/UniDec/unidec_modules/[IM_windows.py](#)

7.17 UniDec.import_wizard.ImportWizard Class Reference

Inheritance diagram for UniDec.import_wizard.ImportWizard:



Collaboration diagram for UniDec.import_wizard.ImportWizard:



Public Member Functions

- def `__init__`
- def `setup_frame` (self)
- def `get_folder_path` (self, evt)
- def `on_folder_path_change` (self, evt)
- def `add_file` (self, evt)
- def `export_then_load` (self, evt)
- def `auto`
- def `export_file` (self, evt)
- def `close` (self, evt)

Public Attributes

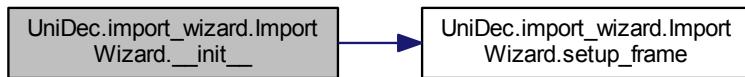
- `exedir`
- `Title`
- `file_set`

- [rb](#)
- [folder_path](#)
- [my_grid](#)
- [my_tree](#)
- [tree](#)
- [desc](#)

7.17.1 Constructor & Destructor Documentation

7.17.1.1 `def UniDec.import_wizard.ImportWizard.__init__(self, parent, dir=None)`

Here is the call graph for this function:

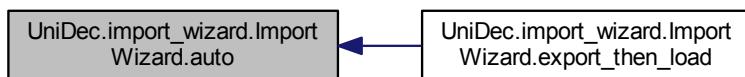


7.17.2 Member Function Documentation

7.17.2.1 `def UniDec.import_wizard.ImportWizard.add_file(self, evt)`

7.17.2.2 `def UniDec.import_wizard.ImportWizard.auto(self, evt, file_path=None, filtered_lines=None)`

Here is the caller graph for this function:



7.17.2.3 `def UniDec.import_wizard.ImportWizard.close(self, evt)`

7.17.2.4 `def UniDec.import_wizard.ImportWizard.export_file(self, evt)`

Export import file for later import

7.17.2.5 `def UniDec.import_wizard.ImportWizard.export_then_load(self, evt)`

save file then load it

Here is the call graph for this function:



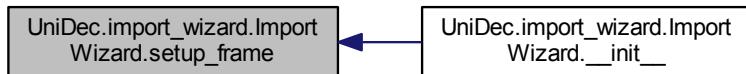
7.17.2.6 def UniDec.import_wizard.ImportWizard.get_folder_path (self, evt)

Get path to folder and place in txtctrl

7.17.2.7 def UniDec.import_wizard.ImportWizard.on_folder_path_change (self, evt)

7.17.2.8 def UniDec.import_wizard.ImportWizard.setup_frame (self)

Here is the caller graph for this function:



7.17.3 Member Data Documentation

7.17.3.1 UniDec.import_wizard.ImportWizard.desc

7.17.3.2 UniDec.import_wizard.ImportWizard.exedir

7.17.3.3 UniDec.import_wizard.ImportWizard.file_set

7.17.3.4 UniDec.import_wizard.ImportWizard.folder_path

7.17.3.5 UniDec.import_wizard.ImportWizard.my_grid

7.17.3.6 UniDec.import_wizard.ImportWizard.my_tree

7.17.3.7 UniDec.import_wizard.ImportWizard.rb

7.17.3.8 UniDec.import_wizard.ImportWizard.Title

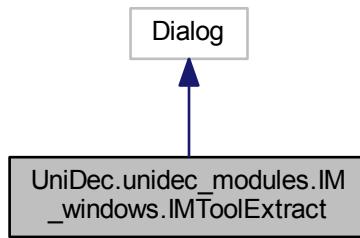
7.17.3.9 UniDec.import_wizard.ImportWizard.tree

The documentation for this class was generated from the following file:

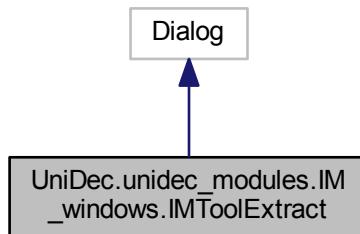
- C:/Python/UniDec/import_wizard.py

7.18 UniDec.unidec_modules.IM_windows.IMToolExtract Class Reference

Inheritance diagram for UniDec.unidec_modules.IM_windows.IMToolExtract:



Collaboration diagram for UniDec.unidec_modules.IM_windows.IMToolExtract:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `initialize_interface` (self, massdat, ccsdat, mccsgrid, config, pks)
- def `on_close` (self, e)
- def `on_close_cancel` (self, e)
- def `loadpeaks` (self, e)
- def `get_from_gui` (self, e)
- def `on_add` (self, e)
- def `on_plot` (self, e)

Public Attributes

- `plot1`

- [plot2](#)
- [masspanel](#)
- [ctlzout](#)
- [config](#)
- [massdat](#)
- [ccsdat](#)
- [totalgrid](#)
- [pk5](#)
- [ztab](#)
- [zout](#)

7.18.1 Constructor & Destructor Documentation

7.18.1.1 def UniDec.unidec_modules.IM_windows.IMToolExtract.__init__(self, args, kwargs)

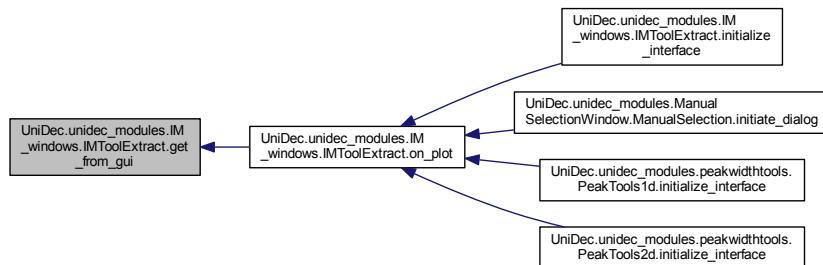
Creates dialog window for performing extraction of IM data slices.
:param args: Passed to wx.Dialog
:param kwargs: Passed to wx.Dialog
:return: None

7.18.2 Member Function Documentation

7.18.2.1 def UniDec.unidec_modules.IM_windows.IMToolExtract.get_from_gui(self, e)

Load from GUI to self.zout. If nothing is set, self.zout = 0.
:param e: Unused event
:return: None

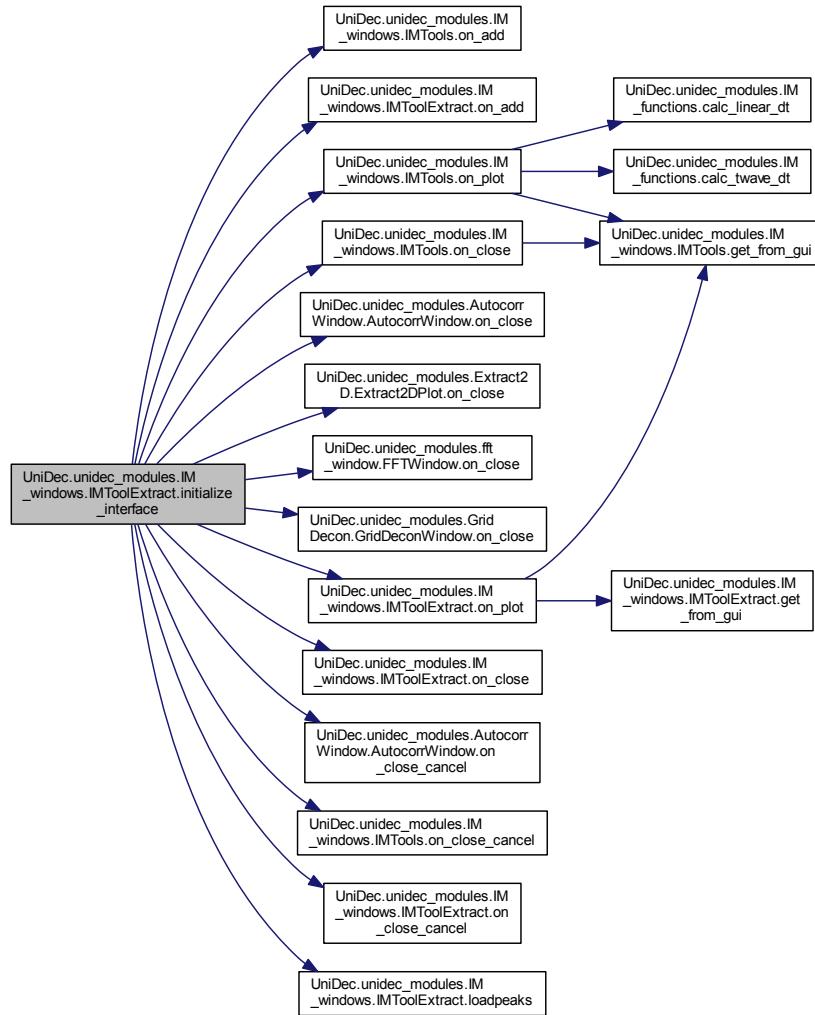
Here is the caller graph for this function:



7.18.2.2 def UniDec.unidec_modules.IM_windows.IMToolExtract.initialize_interface(self, massdat, ccsdat, mccsgrid, config, pk5)

Initializes the interface and plots the initial results.
:param massdat: Mass distribution array (N x 2)
:param ccsdat: CCS distribution array (M x 2)
:param mccsgrid: Array of intensity values for corresponding mass and CCS values (N x M) array
:param config: UniDecConfig object
:param pk5: Peaks object
:return: None

Here is the call graph for this function:

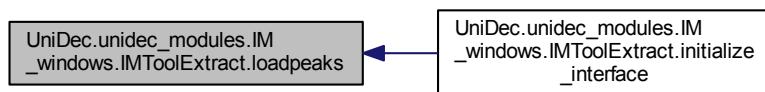


7.18.2.3 def UniDec.unidec_modules.IM_windows.IMToolExtract.loadpeaks (self, e)

```

Load masses from self.pks.peaks into the masspanel.
:param e: Unused event
:return: None
  
```

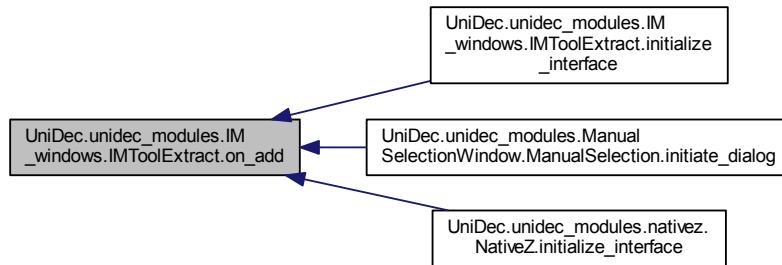
Here is the caller graph for this function:



7.18.2.4 def UniDec.unidec_modules.IM_windows.IMToolExtract.on_add (self, e)

Add a blank line to the masspanel.
:param e: Unused event
:return: None

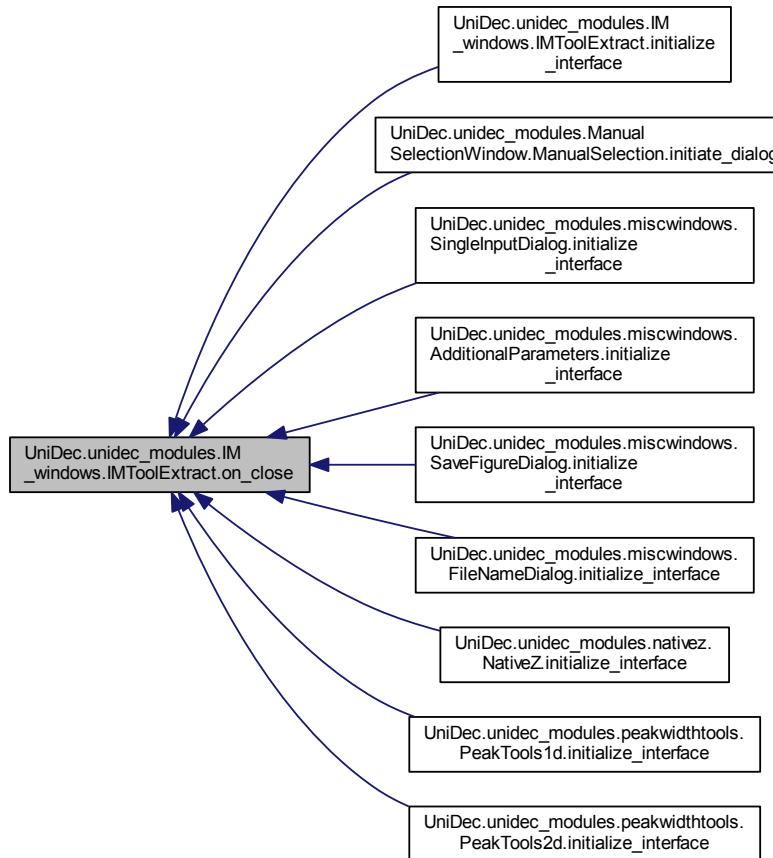
Here is the caller graph for this function:



7.18.2.5 def UniDec.unidec_modules.IM_windows.IMToolExtract.on_close (self, e)

Close the dialog and set `self.config.zout` to `self.zout`.
:param e: Unused event
:return: None

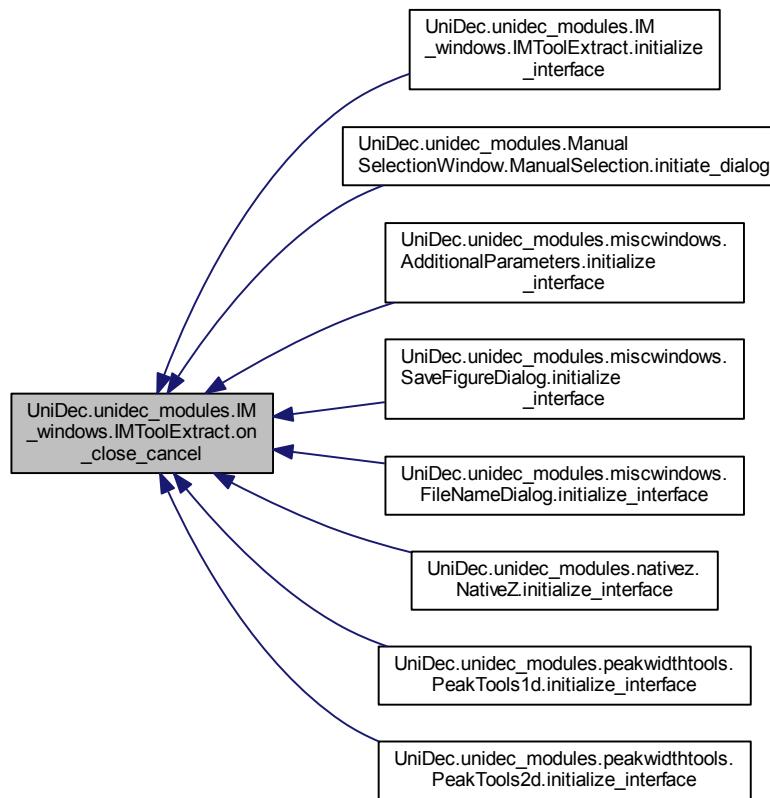
Here is the caller graph for this function:



7.18.2.6 def UniDec.unidec_modules.IM_windows.IMToolExtract.on_close_cancel (self, e)

```
Close the dialog but do not update self.config.zout.  
:param e: Unused event  
:return: None
```

Here is the caller graph for this function:

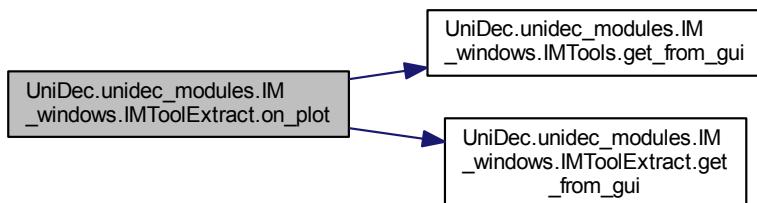


7.18.2.7 def UniDec.unidec_modules.IM_windows.IMToolExtract.on_plot(self, e)

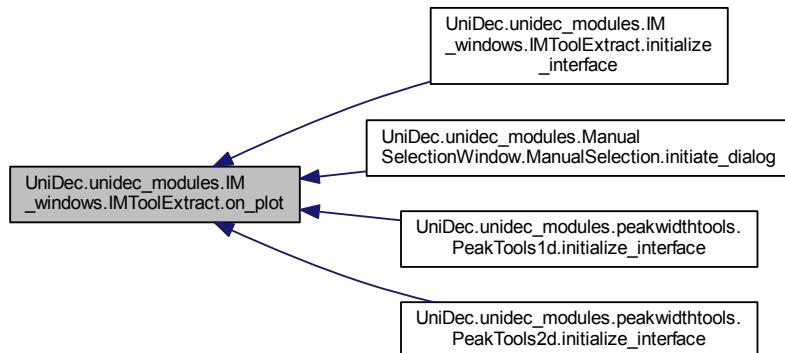
```

First, it updates from the GUI.
Second, if _zout_str(self.zout).bin file exists, it will be imported.
This allows slices of specific charge states to be extracted. Otherwise, the default is all charge states.
Third, the values are extracted and plotted.
:param e: Unused event
:return: None
  
```

Here is the call graph for this function:



Here is the caller graph for this function:



7.18.3 Member Data Documentation

7.18.3.1 `UniDec.unidec_modules.IM_windows.IMToolExtract.ccsdat`

7.18.3.2 `UniDec.unidec_modules.IM_windows.IMToolExtract.config`

7.18.3.3 `UniDec.unidec_modules.IM_windows.IMToolExtract.ctlzout`

7.18.3.4 `UniDec.unidec_modules.IM_windows.IMToolExtract.massdat`

7.18.3.5 `UniDec.unidec_modules.IM_windows.IMToolExtract.masspanel`

7.18.3.6 `UniDec.unidec_modules.IM_windows.IMToolExtract.pks`

7.18.3.7 `UniDec.unidec_modules.IM_windows.IMToolExtract.plot1`

7.18.3.8 `UniDec.unidec_modules.IM_windows.IMToolExtract.plot2`

7.18.3.9 `UniDec.unidec_modules.IM_windows.IMToolExtract.totalgrid`

7.18.3.10 `UniDec.unidec_modules.IM_windows.IMToolExtract.zout`

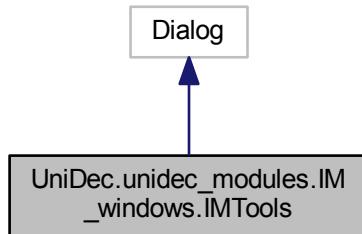
7.18.3.11 `UniDec.unidec_modules.IM_windows.IMToolExtract.ztab`

The documentation for this class was generated from the following file:

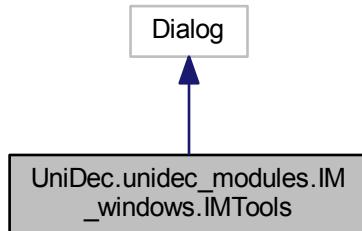
- C:/Python/UniDec/unidec_modules/[IM_windows.py](#)

7.19 UniDec.unidec_modules.IM_windows.IMTools Class Reference

Inheritance diagram for UniDec.unidec_modules.IM_windows.IMTools:



Collaboration diagram for UniDec.unidec_modules.IM_windows.IMTools:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `initialize_interface` (self, `data3`, `config`)
- def `setup_panel` (self)
- def `on_close` (self, e)
- def `on_close_cancel` (self, e)
- def `load_to_gui` (self, e)
- def `get_from_gui` (self, e)
- def `on_add` (self, e)
- def `on_plot` (self, e)
- def `on_flip_twave` (self, e)

Public Attributes

- `pnl`
- `pnl2`

- [plot](#)
- [ctlwave](#)
- [masspanel](#)
- [twave](#)
- [flag](#)
- [data3](#)
- [config](#)
- [defaultconfig](#)
- [ctlvolt](#)
- [ctlpressure](#)
- [ctltemp](#)
- [ctlgasmass](#)
- [ctlto](#)
- [ctldriftlength](#)
- [ctlcal1](#)
- [ctlcal2](#)
- [ctledc](#)

7.19.1 Constructor & Destructor Documentation

7.19.1.1 def UniDec.unidec_modules.IM_windows.IMTools.__init__(self, args, kwargs)

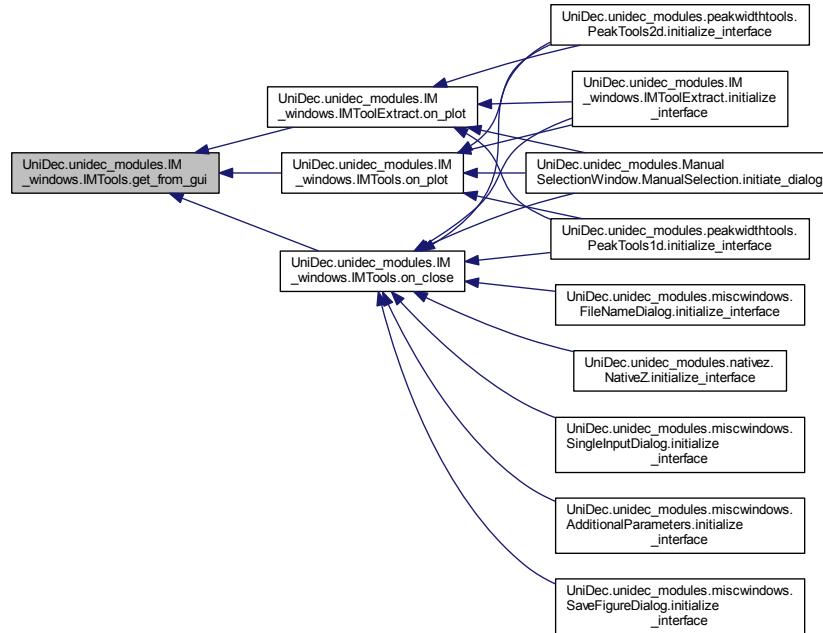
Initialize the dialog window.
:param args: Passed to wx.Dialog
:param kwargs: Passed to wx.Dialog
:return: None

7.19.2 Member Function Documentation

7.19.2.1 def UniDec.unidec_modules.IM_windows.IMTools.get_from_gui(self, e)

Load from GUI to self.config
:param e: Unused event
:return: None

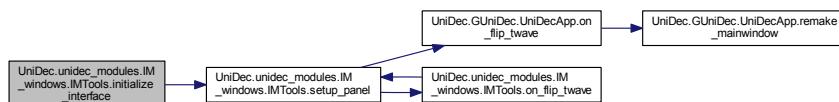
Here is the caller graph for this function:



7.19.2.2 def UniDec.unidec_modules.IM_windows.IMTools.initialize_interface (self, data3, config)

Initialize the parameters, setup the panels, and display the interface.
:param data3: IM-MS raw or processed data
:param config: UniDecConfig object
:return: None

Here is the call graph for this function:



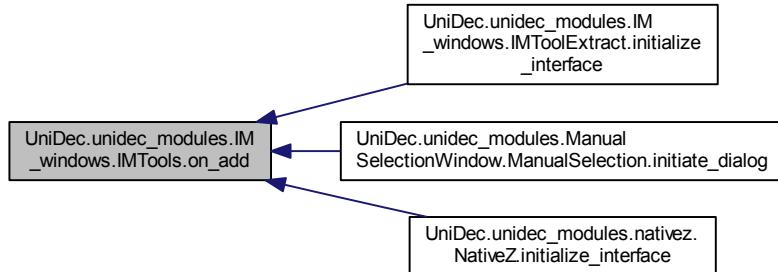
7.19.2.3 def UniDec.unidec_modules.IM_windows.IMTools.load_to_gui (self, e)

Load from self.config into the GUI control boxes.
:param e: Unused event
:return: None

7.19.2.4 def UniDec.unidec_modules.IM_windows.IMTools.on_add (self, e)

Add lines to the masspanel.
:param e: Unused event
:return: None

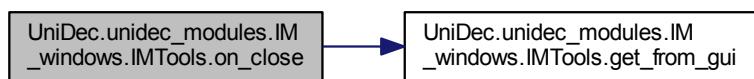
Here is the caller graph for this function:



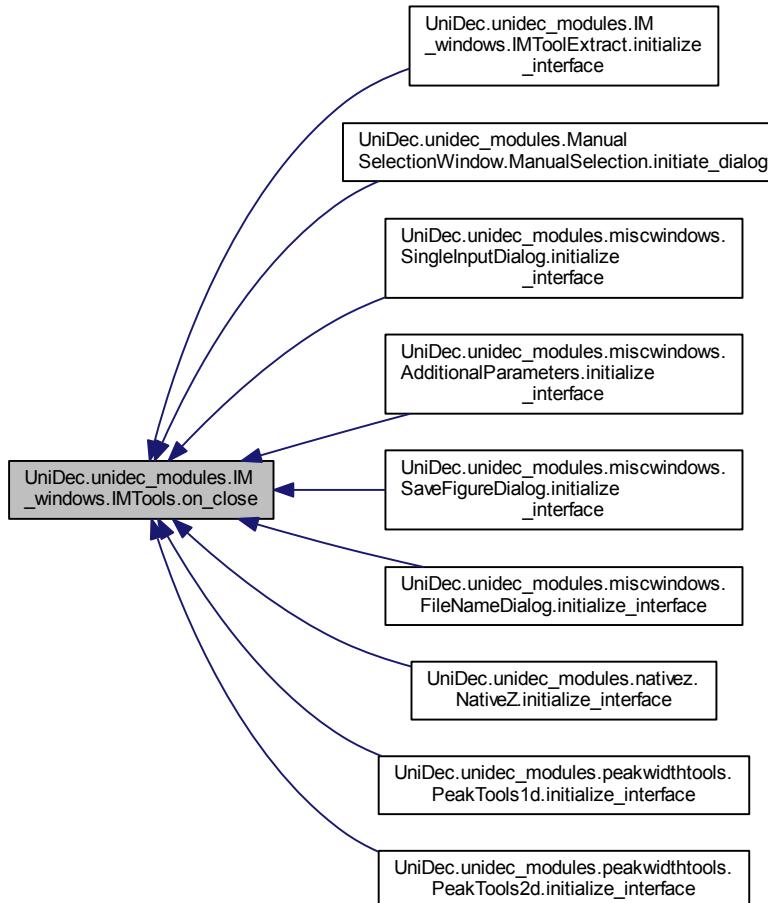
7.19.2.5 def UniDec.unidec_modules.IM_windows.IMTools.on_close (self, e)

```
Close the window and set self.defaultconfig to the new self.config.  
:param e: Unused event  
:return: None
```

Here is the call graph for this function:



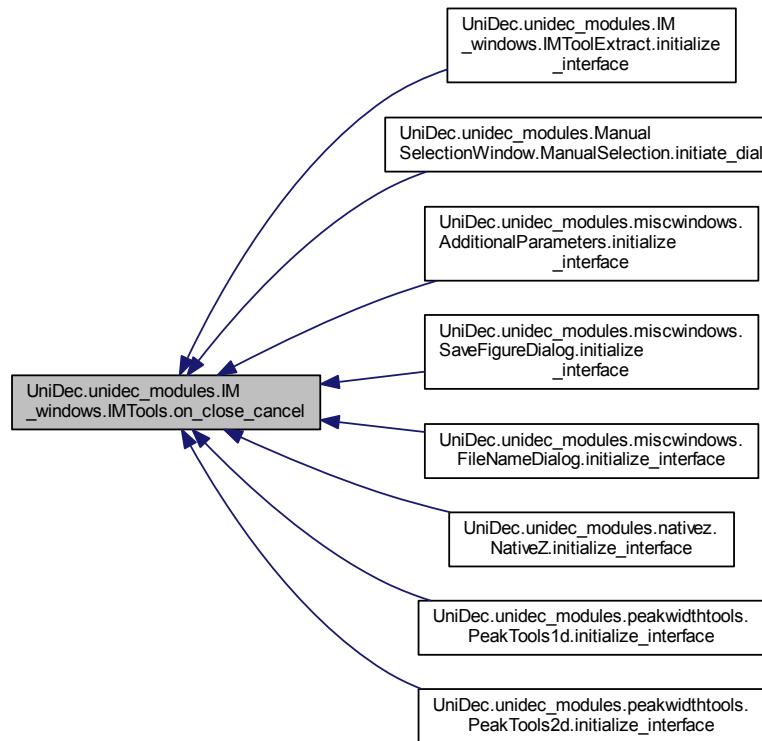
Here is the caller graph for this function:



7.19.2.6 def UniDec.unidec_modules.IM_windows.IMTools.on_close_cancel(self, e)

Close the window but do not update self.defaultconfig.
:param e: Unused event
:return: None

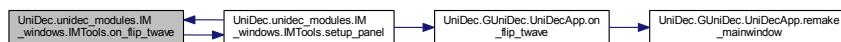
Here is the caller graph for this function:



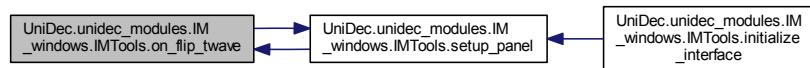
7.19.2.7 def UniDec.unidec_modules.IM_windows.IMTools.on_flip_twave (self, e)

Flip configuration from linear to t-wave. Changes the gas from Ni to He or visa versa. Remakes the GUI.
 :param e: Unused event
 :return: None

Here is the call graph for this function:



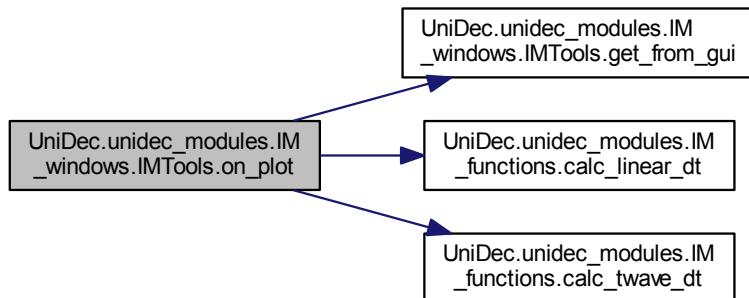
Here is the caller graph for this function:



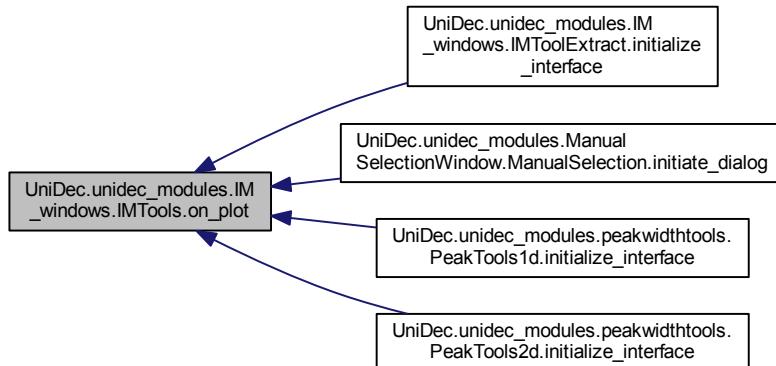
7.19.2.8 def UniDec.unidec_modules.IM_windows.IMTools.on_plot(self, e)

Gathers all of the parameters and simulates the m/z and dt values. Plots the results.
:param e: wx.Event
:return: None

Here is the call graph for this function:



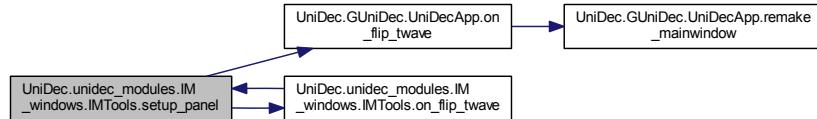
Here is the caller graph for this function:



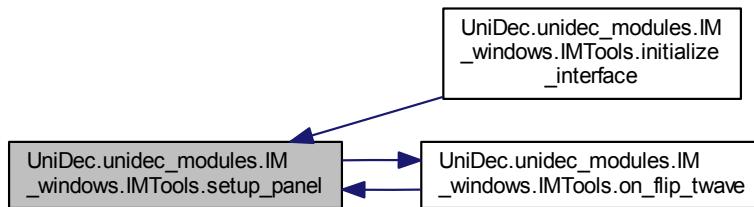
7.19.2.9 def UniDec.unidec_modules.IM_windows.IMTools.setup_panel(self)

Make/remake the main panel.
:return: None

Here is the call graph for this function:



Here is the caller graph for this function:



7.19.3 Member Data Documentation

7.19.3.1 UniDec.unidec_modules.IM_windows.IMTools.config

7.19.3.2 UniDec.unidec_modules.IM_windows.IMTools.ctldriftlength

7.19.3.3 UniDec.unidec_modules.IM_windows.IMTools.ctledc

7.19.3.4 UniDec.unidec_modules.IM_windows.IMTools.ctlgasmass

7.19.3.5 UniDec.unidec_modules.IM_windows.IMTools.ctlpressure

7.19.3.6 UniDec.unidec_modules.IM_windows.IMTools.ctltcal1

7.19.3.7 UniDec.unidec_modules.IM_windows.IMTools.ctltcal2

7.19.3.8 UniDec.unidec_modules.IM_windows.IMTools.ctlttemp

7.19.3.9 UniDec.unidec_modules.IM_windows.IMTools.ctlto

7.19.3.10 UniDec.unidec_modules.IM_windows.IMTools.ctltwave

7.19.3.11 UniDec.unidec_modules.IM_windows.IMTools.ctlvolt

7.19.3.12 UniDec.unidec_modules.IM_windows.IMTools.data3

7.19.3.13 UniDec.unidec_modules.IM_windows.IMTools.defaultconfig

- 7.19.3.14 [UniDec.unidec_modules.IM_windows.IMTools.flag](#)
- 7.19.3.15 [UniDec.unidec_modules.IM_windows.IMTools.masspanel](#)
- 7.19.3.16 [UniDec.unidec_modules.IM_windows.IMTools.plot](#)
- 7.19.3.17 [UniDec.unidec_modules.IM_windows.IMTools.pnl](#)
- 7.19.3.18 [UniDec.unidec_modules.IM_windows.IMTools.pnl2](#)
- 7.19.3.19 [UniDec.unidec_modules.IM_windows.IMTools.twave](#)

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/[IM_windows.py](#)

7.20 UniDec.unidec_modules.UniFit.KDmodel Class Reference

Public Member Functions

- def [__init__](#) (self, numtotprot, numtotlig, data, pconc, lconc, nodelist, header, removeoutliers=False, plot1=None, plot2=None, plot3=None, bootnum=1, maxsites=0, kwargs)
- def [FindBestModel](#) (self, fixedprotmodel, fixedligmodel)
- def [RunKDFit](#) (self, kwargs)
- def [Return](#) (self)
- def [SetupModel](#) (self, kwargs)
- def [ModPaths](#) (self)
- def [MakeFitGrid](#) (self)
- def [OutlierTest](#) (self)
- def [Bootstrap](#) (self, std, numpnts)
- def [RunBootstrap](#) (self)
- def [GraphPlot](#)
- def [PlotTrace](#)
- def [PlotHist](#)

Public Attributes

- [outlierflag](#)
- [plot1](#)
- [plot2](#)
- [plot3](#)
- [protflag](#)
- [ligflag](#)
- [mode](#)
- [header](#)
- [maxsites](#)
- [kdargs](#)
- [randfit](#)
- [bootnum](#)
- [numtotprot](#)
- [numtotlig](#)
- [nprot](#)
- [nlig](#)

- [data](#)
- [fixedligmodel](#)
- [fixedprotmodel](#)
- [findmodelflag](#)
- [plotflag](#)
- [ligmodel](#)
- [fit](#)
- [degenkds](#)
- [residuals](#)
- [stdres](#)
- [error](#)
- [reactions](#)
- [nodes](#)
- [kdmap](#)
- [numkd](#)
- [graph](#)
- [ugraph](#)
- [nodenames](#)
- [fitgrid](#)
- [stddevs](#)
- [meanfit](#)

7.20.1 Constructor & Destructor Documentation

```
7.20.1.1 def UniDec.unidec_modules.UniFit.KDmodel.__init__( self, numtotprot, numtotlig, data, pconc, lconc, nodelist, header, removeoutliers = False, plot1 = None, plot2 = None, plot3 = None, bootnum = 1, maxsites = 0, kwargs )
```

7.20.2 Member Function Documentation

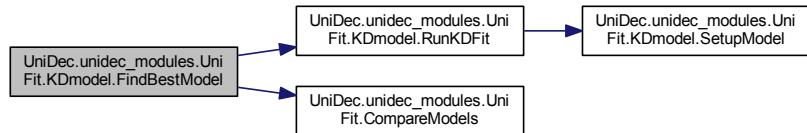
```
7.20.2.1 def UniDec.unidec_modules.UniFit.KDmodel.Bootstrap( self, std, numpts )
```

Here is the call graph for this function:



7.20.2.2 def UniDec.unidec_modules.UniFit.KDmodel.FindBestModel (*self*, *fixedprotmodel*, *fixedligmodel*)

Here is the call graph for this function:



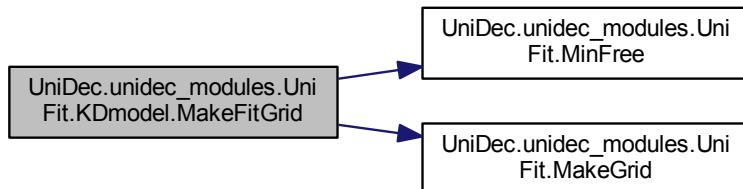
7.20.2.3 def UniDec.unidec_modules.UniFit.KDmodel.GraphPlot (*self*, *ax=None*)

Here is the call graph for this function:



7.20.2.4 def UniDec.unidec_modules.UniFit.KDmodel.MakeFitGrid (*self*)

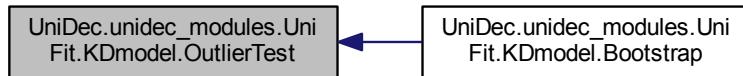
Here is the call graph for this function:



7.20.2.5 def UniDec.unidec_modules.UniFit.KDmodel.ModPaths (*self*)

7.20.2.6 def UniDec.unidec_modules.UniFit.KDmodel.OutlierTest (*self*)

Here is the caller graph for this function:



7.20.2.7 def UniDec.unidec_modules.UniFit.KDmodel.PlotHist (*self*, *topax* = None)

7.20.2.8 def UniDec.unidec_modules.UniFit.KDmodel.PlotTrace (*self*, *topax* = None)

7.20.2.9 def UniDec.unidec_modules.UniFit.KDmodel.Return (*self*)

7.20.2.10 def UniDec.unidec_modules.UniFit.KDmodel.RunBootstrap (*self*)

7.20.2.11 def UniDec.unidec_modules.UniFit.KDmodel.RunKDFit (*self*, *kwargs*)

Here is the call graph for this function:

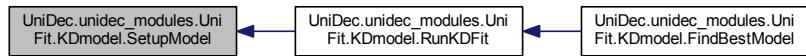


Here is the caller graph for this function:



7.20.2.12 def UniDec.unidec_modules.UniFit.KDmodel.SetupModel (*self*, *kwargs*)

Here is the caller graph for this function:



7.20.3 Member Data Documentation

7.20.3.1 UniDec.unidec_modules.UniFit.KDmodel.bootnum

7.20.3.2 UniDec.unidec_modules.UniFit.KDmodel.data

7.20.3.3 UniDec.unidec_modules.UniFit.KDmodel.degenkds

7.20.3.4 UniDec.unidec_modules.UniFit.KDmodel.error

7.20.3.5 UniDec.unidec_modules.UniFit.KDmodel.findmodelflag

7.20.3.6 UniDec.unidec_modules.UniFit.KDmodel.fit

7.20.3.7 UniDec.unidec_modules.UniFit.KDmodel.fitgrid

7.20.3.8 UniDec.unidec_modules.UniFit.KDmodel.fixedligmodel

7.20.3.9 UniDec.unidec_modules.UniFit.KDmodel.fixedprotmodel

7.20.3.10 UniDec.unidec_modules.UniFit.KDmodel.graph

7.20.3.11 UniDec.unidec_modules.UniFit.KDmodel.header

7.20.3.12 UniDec.unidec_modules.UniFit.KDmodel.kdargs

7.20.3.13 UniDec.unidec_modules.UniFit.KDmodel.kdmap

7.20.3.14 UniDec.unidec_modules.UniFit.KDmodel.ligflag

7.20.3.15 UniDec.unidec_modules.UniFit.KDmodel.ligmodel

7.20.3.16 UniDec.unidec_modules.UniFit.KDmodel.maxsites

7.20.3.17 UniDec.unidec_modules.UniFit.KDmodel.meanfit

7.20.3.18 UniDec.unidec_modules.UniFit.KDmodel.mode

7.20.3.19 UniDec.unidec_modules.UniFit.KDmodel.nlig

7.20.3.20 UniDec.unidec_modules.UniFit.KDmodel.nodenames

7.20.3.21 UniDec.unidec_modules.UniFit.KDmodel.nodes

- 7.20.3.22 `UniDec.unidec_modules.UniFit.KDmodel.nprot`
- 7.20.3.23 `UniDec.unidec_modules.UniFit.KDmodel.numkd`
- 7.20.3.24 `UniDec.unidec_modules.UniFit.KDmodel.numtotlig`
- 7.20.3.25 `UniDec.unidec_modules.UniFit.KDmodel.numtotprot`
- 7.20.3.26 `UniDec.unidec_modules.UniFit.KDmodel.outlierflag`
- 7.20.3.27 `UniDec.unidec_modules.UniFit.KDmodel.plot1`
- 7.20.3.28 `UniDec.unidec_modules.UniFit.KDmodel.plot2`
- 7.20.3.29 `UniDec.unidec_modules.UniFit.KDmodel.plot3`
- 7.20.3.30 `UniDec.unidec_modules.UniFit.KDmodel.plotflag`
- 7.20.3.31 `UniDec.unidec_modules.UniFit.KDmodel.protflag`
- 7.20.3.32 `UniDec.unidec_modules.UniFit.KDmodel.randfit`
- 7.20.3.33 `UniDec.unidec_modules.UniFit.KDmodel.reactions`
- 7.20.3.34 `UniDec.unidec_modules.UniFit.KDmodel.residuals`
- 7.20.3.35 `UniDec.unidec_modules.UniFit.KDmodel.stddevs`
- 7.20.3.36 `UniDec.unidec_modules.UniFit.KDmodel.stdres`
- 7.20.3.37 `UniDec.unidec_modules.UniFit.KDmodel.ugraph`

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/[UniFit.py](#)

7.21 UniDec.unidec_modules.UniFit.kdstruct Class Reference

Public Member Functions

- def [__init__](#) (`self`)

Public Attributes

- [`pconc`](#)
- [`lconc`](#)
- [`ureact`](#)
- [`nprottab`](#)
- [`nligtab`](#)
- [`paths`](#)
- [`pfree`](#)
- [`lfree`](#)
- [`weights`](#)
- [`nodelist`](#)

- [kds](#)
- [degen](#)
- [maxsites](#)
- [nfactors](#)

7.21.1 Constructor & Destructor Documentation

7.21.1.1 [def UniDec.unidec_modules.UniFit.kdstruct.__init__ \(self \)](#)

7.21.2 Member Data Documentation

7.21.2.1 [UniDec.unidec_modules.UniFit.kdstruct.degen](#)

7.21.2.2 [UniDec.unidec_modules.UniFit.kdstruct.kds](#)

7.21.2.3 [UniDec.unidec_modules.UniFit.kdstruct.lconc](#)

7.21.2.4 [UniDec.unidec_modules.UniFit.kdstruct.lfrees](#)

7.21.2.5 [UniDec.unidec_modules.UniFit.kdstruct.maxsites](#)

7.21.2.6 [UniDec.unidec_modules.UniFit.kdstruct.nfactors](#)

7.21.2.7 [UniDec.unidec_modules.UniFit.kdstruct.nligtab](#)

7.21.2.8 [UniDec.unidec_modules.UniFit.kdstruct.nodelist](#)

7.21.2.9 [UniDec.unidec_modules.UniFit.kdstruct.nprottab](#)

7.21.2.10 [UniDec.unidec_modules.UniFit.kdstruct.paths](#)

7.21.2.11 [UniDec.unidec_modules.UniFit.kdstruct.pconc](#)

7.21.2.12 [UniDec.unidec_modules.UniFit.kdstruct.pfrees](#)

7.21.2.13 [UniDec.unidec_modules.UniFit.kdstruct.ureact](#)

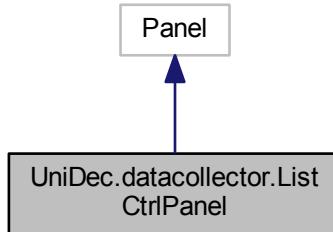
7.21.2.14 [UniDec.unidec_modules.UniFit.kdstruct.weights](#)

The documentation for this class was generated from the following file:

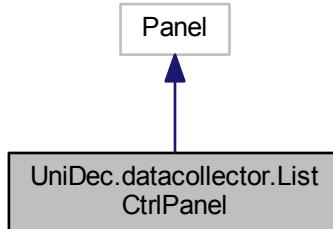
- C:/Python/UniDec/unidec_modules/[UniFit.py](#)

7.22 UniDec.datacollector.ListCtrlPanel Class Reference

Inheritance diagram for UniDec.datacollector.ListCtrlPanel:



Collaboration diagram for UniDec.datacollector.ListCtrlPanel:



Public Member Functions

- def [__init__](#) (self, parent, list_type="X", size=(200, 400))
- def [on_right_click](#) (self, event)
- def [on_popup_one](#) (self, event)
- def [on_popup_two](#) (self, event)
- def [on_popup_three](#) (self, event)
- def [on_popup_four](#) (self, event)

Public Attributes

- [selection](#)
- [list](#)
- [popupID1](#)
- [popupID2](#)
- [popupID3](#)
- [popupID4](#)

7.22.1 Constructor & Destructor Documentation

7.22.1.1 def UniDec.datacollector.ListCtrlPanel.__init__ (*self*, *parent*, *list_type* = "X", *size* = (200, 400))

7.22.2 Member Function Documentation

7.22.2.1 def UniDec.datacollector.ListCtrlPanel.on_popup_four (*self*, *event*)

7.22.2.2 def UniDec.datacollector.ListCtrlPanel.on_popup_one (*self*, *event*)

7.22.2.3 def UniDec.datacollector.ListCtrlPanel.on_popup_three (*self*, *event*)

7.22.2.4 def UniDec.datacollector.ListCtrlPanel.on_popup_two (*self*, *event*)

7.22.2.5 def UniDec.datacollector.ListCtrlPanel.on_right_click (*self*, *event*)

7.22.3 Member Data Documentation

7.22.3.1 UniDec.datacollector.ListCtrlPanel.list

7.22.3.2 UniDec.datacollector.ListCtrlPanel.popupID1

7.22.3.3 UniDec.datacollector.ListCtrlPanel.popupID2

7.22.3.4 UniDec.datacollector.ListCtrlPanel.popupID3

7.22.3.5 UniDec.datacollector.ListCtrlPanel.popupID4

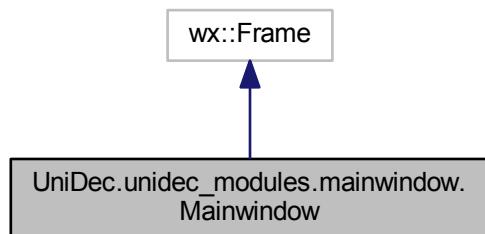
7.22.3.6 UniDec.datacollector.ListCtrlPanel.selection

The documentation for this class was generated from the following file:

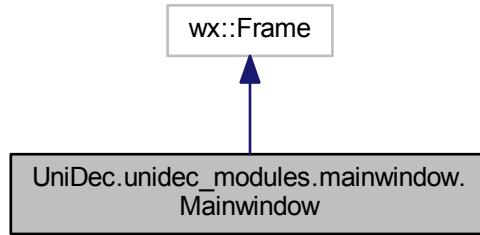
- C:/Python/UniDec/[datacollector.py](#)

7.23 UniDec.unidec_modules.mainwindow.Mainwindow Class Reference

Inheritance diagram for UniDec.unidec_modules.mainwindow.Mainwindow:



Collaboration diagram for UniDec.unidec_modules/mainwindow.Mainwindow:



Public Member Functions

- def `__init__`
- def `setup_shortcuts` (self)
- def `setup_menu` (self)
- def `on_defaults` (self, e)
- def `setup_main_panel` (self)
- def `setup_tool_tips` (self)
- def `import_config_to_gui` (self)
- def `export_gui_to_config` (self)
- def `menu_401_403` (self, event)
- def `clear_all_plots`
- def `on_motion` (self, xpos, ypos)
- def `on_about` (self, e)
- def `on_exit` (self, e)
- def `save_all_figures` (self, extension, extension2="", e=0, header=None, kwargs)
- def `on_save_figure_eps` (self, e)
- def `on_save_figure_png` (self, e, kwargs)
- def `on_save_figure_pdf` (self, e)
- def `on_save_figure_dialog` (self, e)
- def `shrink_figure` (self, plot)
- def `shrink_all_figures` (self)
- def `on_save_figure_small` (self, e)
- def `on_check_manual` (self, e)
- def `on_mass_list` (self, e)

Public Attributes

- `pres`
- `config`
- `title`
- `version`
- `icon_path`
- `open_bmp`
- `next_bmp`
- `report_bmp`
- `A_bmp`

- [ud_bmp](#)
- [system](#)
- [displaysize](#)
- [tabbed](#)
- [imflag](#)
- [twave](#)
- [backgroundchoices](#)
- [filemenu](#)
- [toolsmenu](#)
- [analysismenu](#)
- [advancedmenu](#)
- [experimentalmenu](#)
- [menuOpen](#)
- [menuOpenRaw](#)
- [menuLoadState](#)
- [menuSaveState](#)
- [menupastespectrum](#)
- [menuLoad](#)
- [menuLoadDefault](#)
- [menuSaveDefault](#)
- [defaultmenu](#)
- [menuDefault1](#)
- [menuDefault2](#)
- [menuDefault3](#)
- [menufigdialog](#)
- [figmenu](#)
- [menuSaveFigure0](#)
- [menuSaveFigure1s](#)
- [menuSaveFigure1](#)
- [menuSaveFigure2](#)
- [menuSaveFigure4](#)
- [menuAbout](#)
- [menuExit](#)
- [menuBatch](#)
- [menuBatch2](#)
- [menuBatchRaw](#)
- [menulimportWizard](#)
- [menuAutoWidth](#)
- [menuWidth](#)
- [menuManualFile](#)
- [menuMassFile](#)
- [menuPlotZ](#)
- [menucollect](#)
- [menuExport](#)
- [menuFitNorm](#)
- [menukendrick](#)
- [menu2Dgrid](#)
- [menuautocorr](#)
- [menuintegrate](#)
- [menumatch](#)
- [menucom](#)
- [menuchargeplot](#)
- [menuoffset](#)
- [menuimtools](#)
- [menuimtools2](#)

- menunativeccs
- menuReset
- menuUnidecPath
- menuFileName
- menuflipmode
- menufliptabbed
- Tweet
- menuAdditionalParameters
- menuDeisotope
- menuCrossValidate
- menucolor1d
- menusuperbatch
- menumassprocess
- menuerrors
- menucal
- menufft
- menugriddecon
- menuBar
- plot1
- plot2
- plot3
- plot4
- plot5
- plot6
- plot1im
- plot1fit
- plot2ccs
- plot5mccs
- plot5ccsz
- plot3color
- plot9
- plot10
- peakpanel
- openbutton
- procbutton
- udbutton
- ppbutton
- autobutton
- ctlminmz
- ctlmaxmz
- ctlimindt
- ctlmaxdt
- ctlsmoothdt
- ctlsubbuffdt
- subtypectl
- dataprepbutton
- ctlbuff
- ctlsmooth
- ctlbinsize
- ctlpusher
- ctlinthresh
- ctladductmass
- ctlaccelvolt
- ctlbintype
- ctlconvertflag

- [ctlwave](#)
- [ctlvolt](#)
- [ctlpressure](#)
- [ctltemp](#)
- [ctlgasmass](#)
- [ctlto](#)
- [ctldriftlength](#)
- [ctlcal1](#)
- [ctlcal2](#)
- [ctledc](#)
- [ctlstartz](#)
- [ctlendz](#)
- [ctlmasslb](#)
- [ctlmassub](#)
- [ctlccslb](#)
- [ctlccsub](#)
- [ctlccsbins](#)
- [ctldtsig](#)
- [ctlmassbins](#)
- [ctlmzsig](#)
- [ctlpsfun](#)
- [rununidec](#)
- [ctlzzsig](#)
- [ctlmolig](#)
- [ctlmsig](#)
- [ctlcsig](#)
- [ctlnumit](#)
- [ctlpoolflag](#)
- [ctlisotopemode](#)
- [ctlmanualassign](#)
- [ctlmasslistflag](#)
- [ctlmtabsig](#)
- [ctlminnativez](#)
- [ctlmaxnativez](#)
- [ctlnativeeccslb](#)
- [ctlnativeeccsub](#)
- [ctlwindow](#)
- [ctlthresh](#)
- [ctlnorm](#)
- [plotbutton](#)
- [plotbutton2](#)
- [ctl2dcm](#)
- [ctlpeakcm](#)
- [ctldiscrete](#)
- [ctlpublicationmode](#)
- [ctlrawflag](#)
- [ctlthresh2](#)
- [ctlsep](#)
- [ctlintlb](#)
- [ctlintub](#)
- [replotbutton](#)
- [compositebutton](#)
- [cubeplotbutton](#)
- [pngs](#)
- [figsize](#)
- [rect](#)

7.23.1 Detailed Description

Main UniDec GUI Window.

7.23.2 Constructor & Destructor Documentation

7.23.2.1 `def UniDec.unidec_modules/mainwindow.Mainwindow.__init__ (self, parent, title, config, iconfile = "logo.ico", tabbed = None)`

initialize window and feed in links to presenter and config.

:param parent: GUUniDec Presenter -> self.pres
:param title: Window title (string)
:param config: UniDecConfig object ->self.config
:return: None

7.23.3 Member Function Documentation

7.23.3.1 `def UniDec.unidec_modules/mainwindow.Mainwindow.clear_all_plots (self, flag = 0)`

Clear All Plots
:return: None

7.23.3.2 `def UniDec.unidec_modules/mainwindow.Mainwindow.export_gui_to_config (self)`

Exports parameters from the GUI to the config object.
:return: None

7.23.3.3 `def UniDec.unidec_modules/mainwindow.Mainwindow.import_config_to_gui (self)`

Imports parameters from the config object to the GUI.
:return: None

7.23.3.4 `def UniDec.unidec_modules/mainwindow.Mainwindow.menu_401_403 (self, event)`

Menu function to adjust the UniDec core function (agreesiveflag).
:param event: wx Event
:return: None

7.23.3.5 `def UniDec.unidec_modules/mainwindow.Mainwindow.on_about (self, e)`

Displays message about program
:param e:
:return:

7.23.3.6 `def UniDec.unidec_modules/mainwindow.Mainwindow.on_check_manual (self, e)`

Checks the configuration to see if values for manual mode are set. If they are not, it opens the window to set the manual assignments.
:param e: Dummy wx event passed on.
:return: None

7.23.3.7 def UniDec.unidec_modules/mainwindow.Mainwindow.on_defaults(self, e)

Resets the configuration to a default predefined in the unidecstructure file.
:param e: Menu event
:return: None

7.23.3.8 def UniDec.unidec_modules/mainwindow.Mainwindow.on_exit(self, e)

Exit the Program
:param e: Dummy wx event
:return: None

Here is the caller graph for this function:



7.23.3.9 def UniDec.unidec_modules/mainwindow.Mainwindow.on_mass_list(self, e)

Checks the configuration to see if values for the mass list are set. If they are not, it opens the window to set the mass list.
:param e: Dummy wx event passed on.
:return: None

7.23.3.10 def UniDec.unidec_modules/mainwindow.Mainwindow.on_motion(self, xpos, ypos)

Triggered by pubsub from plot windows. Reports text in Status Bar.
:param xpos: x position fed from event
:param ypos: y position fed from event
:return: None

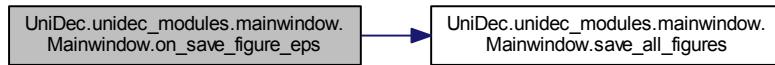
7.23.3.11 def UniDec.unidec_modules/mainwindow.Mainwindow.on_save_figure_dialog(self, e)

Open dialog box to set the parameters for figure type, size, and path to save.
:param e: Dummy wx event
:return: None

7.23.3.12 def UniDec.unidec_modules/mainwindow.Mainwindow.on_save_figure_eps(self, e)

Save all figures as EPS
:param e: Dummy wx event
:return: None

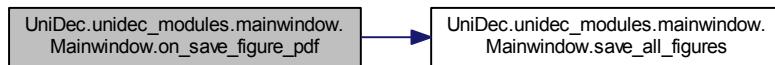
Here is the call graph for this function:



7.23.3.13 def UniDec.unidec_modules/mainwindow.Mainwindow.on_save_figure_pdf (self, e)

```
Saves all figures as PDF
:param e: Dummy wx event
:return: None
```

Here is the call graph for this function:



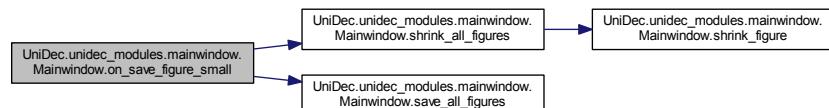
7.23.3.14 def UniDec.unidec_modules/mainwindow.Mainwindow.on_save_figure_png (self, e, kwargs)

```
Save all figures as PNG
:param e: Dummy wx event
:param kwargs: keywords to pass to matplotlib savefig
:return: None
```

7.23.3.15 def UniDec.unidec_modules/mainwindow.Mainwindow.on_save_figure_small (self, e)

```
Preset to shrink figures to 4.5 in by 3 in and save as PDF.
:param e: Dummy wx event
:return: None
```

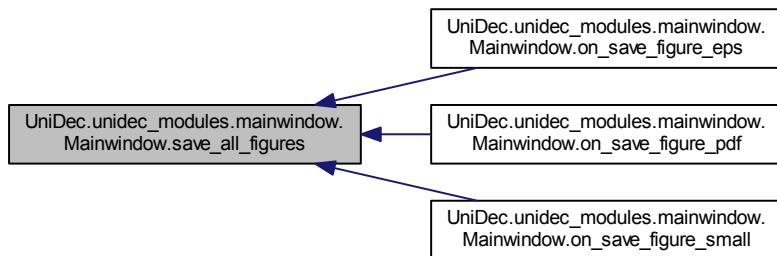
Here is the call graph for this function:



7.23.3.16 def UniDec.unidec_modules/mainwindow.Mainwindow.save_all_figures (self, extension, extension2 = ' ', e = 0, header = None, kwargs)

Save All of the Figures. Will name as header+extension2+_FigureX.+exetension
:param extension: Figure type (pdf, eps, png). Anything accepted by matplotlib
:param extension2: Additional text to include in the figure header.
:param e: Dummy wx Event
:param header: Option to add different header. Default of none yields self.outfname as the path header
:param kwargs: Any keywords to pass to the matplotlib savefig command such as Transparent or DPI
:return: figureflags, files (the figures that were successfully saved and the files that they were saved to)

Here is the caller graph for this function:



7.23.3.17 def UniDec.unidec_modules/mainwindow.Mainwindow.setup_main_panel (self)

Lays Out Main Panel. Binds some functions to presenter.
:return: None

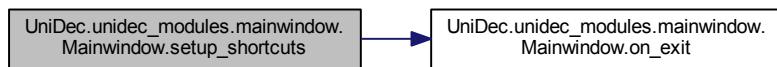
7.23.3.18 def UniDec.unidec_modules/mainwindow.Mainwindow.setup_menu (self)

Sets menu and binds menu objects to functions in presenter and window
:return: None

7.23.3.19 def UniDec.unidec_modules/mainwindow.Mainwindow.setup_shortcuts (self)

Setup shortcuts in GUI. Binds key combinations to functions in presenter (self.pres)
:return: None

Here is the call graph for this function:



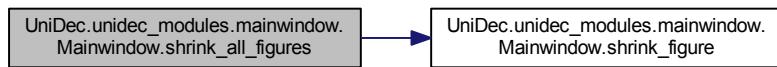
7.23.3.20 def UniDec.unidec_modules/mainwindow.Mainwindow.setup_tool_tips (self)

Sets Tool Tips for items on the Main Panel
:return: None

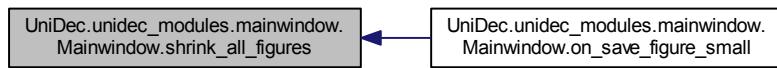
7.23.3.21 def UniDec.unidec_modules/mainwindow.Mainwindow.shrink_all_figures (self)

Shrinks all figures to the size specified in self.figsize
:return: A list of plot objects that we shrunk

Here is the call graph for this function:



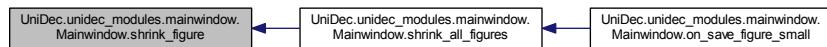
Here is the caller graph for this function:



7.23.3.22 def UniDec.unidec_modules/mainwindow.Mainwindow.shrink_figure (self, plot)

Automatically shrinks the plot to a figure size in inches set in self.figsize.
:param plot: Plot object to shrink
:return: None

Here is the caller graph for this function:



7.23.4 Member Data Documentation

7.23.4.1 UniDec.unidec_modules/mainwindow.Mainwindow.A_bmp

7.23.4.2 UniDec.unidec_modules/mainwindow.Mainwindow.advancedmenu

7.23.4.3 UniDec.unidec_modules/mainwindow.Mainwindow.analysismenu

- 7.23.4.4 UniDec.unidec_modules/mainwindow.Mainwindow.autobutton
- 7.23.4.5 UniDec.unidec_modules/mainwindow.Mainwindow.backgroundchoices
- 7.23.4.6 UniDec.unidec_modules/mainwindow.Mainwindow.compositebutton
- 7.23.4.7 UniDec.unidec_modules/mainwindow.Mainwindow.config
- 7.23.4.8 UniDec.unidec_modules/mainwindow.Mainwindow.ctl2dcm
- 7.23.4.9 UniDec.unidec_modules/mainwindow.Mainwindow.ctlaccelvolt
- 7.23.4.10 UniDec.unidec_modules/mainwindow.Mainwindow.ctladductmass
- 7.23.4.11 UniDec.unidec_modules/mainwindow.Mainwindow.ctlbinsize
- 7.23.4.12 UniDec.unidec_modules/mainwindow.Mainwindow.ctlbintype
- 7.23.4.13 UniDec.unidec_modules/mainwindow.Mainwindow.ctlbuff
- 7.23.4.14 UniDec.unidec_modules/mainwindow.Mainwindow.ctlccsbins
- 7.23.4.15 UniDec.unidec_modules/mainwindow.Mainwindow.ctlccslb
- 7.23.4.16 UniDec.unidec_modules/mainwindow.Mainwindow.ctlccsub
- 7.23.4.17 UniDec.unidec_modules/mainwindow.Mainwindow.ctlconvertflag
- 7.23.4.18 UniDec.unidec_modules/mainwindow.Mainwindow.ctlcsg
- 7.23.4.19 UniDec.unidec_modules/mainwindow.Mainwindow.ctldiscrete
- 7.23.4.20 UniDec.unidec_modules/mainwindow.Mainwindow.ctldriftlength
- 7.23.4.21 UniDec.unidec_modules/mainwindow.Mainwindow.ctldtsig
- 7.23.4.22 UniDec.unidec_modules/mainwindow.Mainwindow.ctledc
- 7.23.4.23 UniDec.unidec_modules/mainwindow.Mainwindow.ctlendz
- 7.23.4.24 UniDec.unidec_modules/mainwindow.Mainwindow.ctlgasmass
- 7.23.4.25 UniDec.unidec_modules/mainwindow.Mainwindow.ctlintlb
- 7.23.4.26 UniDec.unidec_modules/mainwindow.Mainwindow.ctlintthresh
- 7.23.4.27 UniDec.unidec_modules/mainwindow.Mainwindow.ctlintub
- 7.23.4.28 UniDec.unidec_modules/mainwindow.Mainwindow.ctlisotopemode
- 7.23.4.29 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmanualassign
- 7.23.4.30 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmassbins
- 7.23.4.31 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmasslb

- 7.23.4.32 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmasslistflag
- 7.23.4.33 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmassub
- 7.23.4.34 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmaxdt
- 7.23.4.35 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmaxmz
- 7.23.4.36 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmaxnativez
- 7.23.4.37 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmindt
- 7.23.4.38 UniDec.unidec_modules/mainwindow.Mainwindow.ctlminmz
- 7.23.4.39 UniDec.unidec_modules/mainwindow.Mainwindow.ctlminnativez
- 7.23.4.40 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmolig
- 7.23.4.41 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmsig
- 7.23.4.42 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmtabsig
- 7.23.4.43 UniDec.unidec_modules/mainwindow.Mainwindow.ctlmzsig
- 7.23.4.44 UniDec.unidec_modules/mainwindow.Mainwindow.ctlnativeccslb
- 7.23.4.45 UniDec.unidec_modules/mainwindow.Mainwindow.ctlnativeccsub
- 7.23.4.46 UniDec.unidec_modules/mainwindow.Mainwindow.ctlnorm
- 7.23.4.47 UniDec.unidec_modules/mainwindow.Mainwindow.ctlnumit
- 7.23.4.48 UniDec.unidec_modules/mainwindow.Mainwindow.ctlpeakcm
- 7.23.4.49 UniDec.unidec_modules/mainwindow.Mainwindow.ctlpoolflag
- 7.23.4.50 UniDec.unidec_modules/mainwindow.Mainwindow.ctlpressure
- 7.23.4.51 UniDec.unidec_modules/mainwindow.Mainwindow.ctlpsfun
- 7.23.4.52 UniDec.unidec_modules/mainwindow.Mainwindow.ctlpublicationmode
- 7.23.4.53 UniDec.unidec_modules/mainwindow.Mainwindow.ctlpusher
- 7.23.4.54 UniDec.unidec_modules/mainwindow.Mainwindow.ctlrawflag
- 7.23.4.55 UniDec.unidec_modules/mainwindow.Mainwindow.ctlsept
- 7.23.4.56 UniDec.unidec_modules/mainwindow.Mainwindow.ctlsmooth
- 7.23.4.57 UniDec.unidec_modules/mainwindow.Mainwindow.ctlsmoothdt
- 7.23.4.58 UniDec.unidec_modules/mainwindow.Mainwindow.ctlstartz
- 7.23.4.59 UniDec.unidec_modules/mainwindow.Mainwindow.ctlsubbuffdt

- 7.23.4.60 UniDec.unidec_modules/mainwindow.Mainwindow.ctltcal1
- 7.23.4.61 UniDec.unidec_modules/mainwindow.Mainwindow.ctltcal2
- 7.23.4.62 UniDec.unidec_modules/mainwindow.Mainwindow.ctltemp
- 7.23.4.63 UniDec.unidec_modules/mainwindow.Mainwindow.ctlthresh
- 7.23.4.64 UniDec.unidec_modules/mainwindow.Mainwindow.ctlthresh2
- 7.23.4.65 UniDec.unidec_modules/mainwindow.Mainwindow.ctlto
- 7.23.4.66 UniDec.unidec_modules/mainwindow.Mainwindow.ctltwave
- 7.23.4.67 UniDec.unidec_modules/mainwindow.Mainwindow.ctlvolt
- 7.23.4.68 UniDec.unidec_modules/mainwindow.Mainwindow.ctlwindow
- 7.23.4.69 UniDec.unidec_modules/mainwindow.Mainwindow.ctlzzsig
- 7.23.4.70 UniDec.unidec_modules/mainwindow.Mainwindow.cubeplotbutton
- 7.23.4.71 UniDec.unidec_modules/mainwindow.Mainwindow.dataprepbutton
- 7.23.4.72 UniDec.unidec_modules/mainwindow.Mainwindow.defaultmenu
- 7.23.4.73 UniDec.unidec_modules/mainwindow.Mainwindow.displaysize
- 7.23.4.74 UniDec.unidec_modules/mainwindow.Mainwindow.experimentalmenu
- 7.23.4.75 UniDec.unidec_modules/mainwindow.Mainwindow.figmenu
- 7.23.4.76 UniDec.unidec_modules/mainwindow.Mainwindow.figsize
- 7.23.4.77 UniDec.unidec_modules/mainwindow.Mainwindow.filemode
- 7.23.4.78 UniDec.unidec_modules/mainwindow.Mainwindow.icon_path
- 7.23.4.79 UniDec.unidec_modules/mainwindow.Mainwindow.imflag
- 7.23.4.80 UniDec.unidec_modules/mainwindow.Mainwindow.menu2Dgrid
- 7.23.4.81 UniDec.unidec_modules/mainwindow.Mainwindow.menuAbout
- 7.23.4.82 UniDec.unidec_modules/mainwindow.Mainwindow.menuAdditionalParameters
- 7.23.4.83 UniDec.unidec_modules/mainwindow.Mainwindow.menuautocorr
- 7.23.4.84 UniDec.unidec_modules/mainwindow.Mainwindow.menuAutoWidth
- 7.23.4.85 UniDec.unidec_modules/mainwindow.Mainwindow.menuBar
- 7.23.4.86 UniDec.unidec_modules/mainwindow.Mainwindow.menuBatch
- 7.23.4.87 UniDec.unidec_modules/mainwindow.Mainwindow.menuBatch2

- 7.23.4.88 [UniDec.unidec_modules/mainwindow.Mainwindow.menuBatchRaw](#)
- 7.23.4.89 [UniDec.unidec_modules/mainwindow.Mainwindow.menuCal](#)
- 7.23.4.90 [UniDec.unidec_modules/mainwindow.Mainwindow.menuChargePlot](#)
- 7.23.4.91 [UniDec.unidec_modules/mainwindow.Mainwindow.menuCollect](#)
- 7.23.4.92 [UniDec.unidec_modules/mainwindow.Mainwindow.menuColor1d](#)
- 7.23.4.93 [UniDec.unidec_modules/mainwindow.Mainwindow.menuCom](#)
- 7.23.4.94 [UniDec.unidec_modules/mainwindow.Mainwindow.menuCrossValidate](#)
- 7.23.4.95 [UniDec.unidec_modules/mainwindow.Mainwindow.menuDefault1](#)
- 7.23.4.96 [UniDec.unidec_modules/mainwindow.Mainwindow.menuDefault2](#)
- 7.23.4.97 [UniDec.unidec_modules/mainwindow.Mainwindow.menuDefault3](#)
- 7.23.4.98 [UniDec.unidec_modules/mainwindow.Mainwindow.menuDeisotope](#)
- 7.23.4.99 [UniDec.unidec_modules/mainwindow.Mainwindow.menuErrors](#)
- 7.23.4.100 [UniDec.unidec_modules/mainwindow.Mainwindow.menuExit](#)
- 7.23.4.101 [UniDec.unidec_modules/mainwindow.Mainwindow.menuExport](#)
- 7.23.4.102 [UniDec.unidec_modules/mainwindow.Mainwindow.menuFFT](#)
- 7.23.4.103 [UniDec.unidec_modules/mainwindow.Mainwindow.menuFileDialog](#)
- 7.23.4.104 [UniDec.unidec_modules/mainwindow.Mainwindow.menuFileName](#)
- 7.23.4.105 [UniDec.unidec_modules/mainwindow.Mainwindow.menuFitNorm](#)
- 7.23.4.106 [UniDec.unidec_modules/mainwindow.Mainwindow.menuFlipMode](#)
- 7.23.4.107 [UniDec.unidec_modules/mainwindow.Mainwindow.menuFlippedTabbed](#)
- 7.23.4.108 [UniDec.unidec_modules/mainwindow.Mainwindow.menuGridDecon](#)
- 7.23.4.109 [UniDec.unidec_modules/mainwindow.Mainwindow.menuImportWizard](#)
- 7.23.4.110 [UniDec.unidec_modules/mainwindow.Mainwindow.menuIMTools](#)
- 7.23.4.111 [UniDec.unidec_modules/mainwindow.Mainwindow.menuIMTools2](#)
- 7.23.4.112 [UniDec.unidec_modules/mainwindow.Mainwindow.menuIntegrate](#)
- 7.23.4.113 [UniDec.unidec_modules/mainwindow.Mainwindow.menuKendrick](#)
- 7.23.4.114 [UniDec.unidec_modules/mainwindow.Mainwindow.menuLoad](#)
- 7.23.4.115 [UniDec.unidec_modules/mainwindow.Mainwindow.menuLoadDefault](#)

- 7.23.4.116 UniDec.unidec_modules/mainwindow.Mainwindow.menuLoadState
- 7.23.4.117 UniDec.unidec_modules/mainwindow.Mainwindow.menuManualFile
- 7.23.4.118 UniDec.unidec_modules/mainwindow.Mainwindow.menuMassFile
- 7.23.4.119 UniDec.unidec_modules/mainwindow.Mainwindow.menumassprocess
- 7.23.4.120 UniDec.unidec_modules/mainwindow.Mainwindow.menumatch
- 7.23.4.121 UniDec.unidec_modules/mainwindow.Mainwindow.menunativeccs
- 7.23.4.122 UniDec.unidec_modules/mainwindow.Mainwindow.menuoffset
- 7.23.4.123 UniDec.unidec_modules/mainwindow.Mainwindow.menuOpen
- 7.23.4.124 UniDec.unidec_modules/mainwindow.Mainwindow.menuOpenRaw
- 7.23.4.125 UniDec.unidec_modules/mainwindow.Mainwindow.menuPastespectrum
- 7.23.4.126 UniDec.unidec_modules/mainwindow.Mainwindow.menuPlotZ
- 7.23.4.127 UniDec.unidec_modules/mainwindow.Mainwindow.menuReset
- 7.23.4.128 UniDec.unidec_modules/mainwindow.Mainwindow.menuSaveDefault
- 7.23.4.129 UniDec.unidec_modules/mainwindow.Mainwindow.menuSaveFigure0
- 7.23.4.130 UniDec.unidec_modules/mainwindow.Mainwindow.menuSaveFigure1
- 7.23.4.131 UniDec.unidec_modules/mainwindow.Mainwindow.menuSaveFigure1s
- 7.23.4.132 UniDec.unidec_modules/mainwindow.Mainwindow.menuSaveFigure2
- 7.23.4.133 UniDec.unidec_modules/mainwindow.Mainwindow.menuSaveFigure4
- 7.23.4.134 UniDec.unidec_modules/mainwindow.Mainwindow.menuSaveState
- 7.23.4.135 UniDec.unidec_modules/mainwindow.Mainwindow.menusuperbatch
- 7.23.4.136 UniDec.unidec_modules/mainwindow.Mainwindow.menuUnidecPath
- 7.23.4.137 UniDec.unidec_modules/mainwindow.Mainwindow.menuWidth
- 7.23.4.138 UniDec.unidec_modules/mainwindow.Mainwindow.next_bmp
- 7.23.4.139 UniDec.unidec_modules/mainwindow.Mainwindow.open_bmp
- 7.23.4.140 UniDec.unidec_modules/mainwindow.Mainwindow.openbutton
- 7.23.4.141 UniDec.unidec_modules/mainwindow.Mainwindow.peakpanel
- 7.23.4.142 UniDec.unidec_modules/mainwindow.Mainwindow.plot1
- 7.23.4.143 UniDec.unidec_modules/mainwindow.Mainwindow.plot10

- 7.23.4.144 UniDec.unidec_modules/mainwindow.Mainwindow.plot1fit
- 7.23.4.145 UniDec.unidec_modules/mainwindow.Mainwindow.plot1im
- 7.23.4.146 UniDec.unidec_modules/mainwindow.Mainwindow.plot2
- 7.23.4.147 UniDec.unidec_modules/mainwindow.Mainwindow.plot2ccs
- 7.23.4.148 UniDec.unidec_modules/mainwindow.Mainwindow.plot3
- 7.23.4.149 UniDec.unidec_modules/mainwindow.Mainwindow.plot3color
- 7.23.4.150 UniDec.unidec_modules/mainwindow.Mainwindow.plot4
- 7.23.4.151 UniDec.unidec_modules/mainwindow.Mainwindow.plot5
- 7.23.4.152 UniDec.unidec_modules/mainwindow.Mainwindow.plot5ccsz
- 7.23.4.153 UniDec.unidec_modules/mainwindow.Mainwindow.plot5mccs
- 7.23.4.154 UniDec.unidec_modules/mainwindow.Mainwindow.plot6
- 7.23.4.155 UniDec.unidec_modules/mainwindow.Mainwindow.plot9
- 7.23.4.156 UniDec.unidec_modules/mainwindow.Mainwindow.plotbutton
- 7.23.4.157 UniDec.unidec_modules/mainwindow.Mainwindow.plotbutton2
- 7.23.4.158 UniDec.unidec_modules/mainwindow.Mainwindow.pngs
- 7.23.4.159 UniDec.unidec_modules/mainwindow.Mainwindow.pppbutton
- 7.23.4.160 UniDec.unidec_modules/mainwindow.Mainwindow.pres
- 7.23.4.161 UniDec.unidec_modules/mainwindow.Mainwindow.procbutton
- 7.23.4.162 UniDec.unidec_modules/mainwindow.Mainwindow.rect
- 7.23.4.163 UniDec.unidec_modules/mainwindow.Mainwindow.replotbutton
- 7.23.4.164 UniDec.unidec_modules/mainwindow.Mainwindow.report_bmp
- 7.23.4.165 UniDec.unidec_modules/mainwindow.Mainwindow.rununidec
- 7.23.4.166 UniDec.unidec_modules/mainwindow.Mainwindow.subtypecl
- 7.23.4.167 UniDec.unidec_modules/mainwindow.Mainwindow.system
- 7.23.4.168 UniDec.unidec_modules/mainwindow.Mainwindow.tabbed
- 7.23.4.169 UniDec.unidec_modules/mainwindow.Mainwindow.title
- 7.23.4.170 UniDec.unidec_modules/mainwindow.Mainwindow.toolsmenu
- 7.23.4.171 UniDec.unidec_modules/mainwindow.Mainwindow.twave

7.23.4.172 UniDec.unidec_modules/mainwindow.Mainwindow.Tweet

7.23.4.173 UniDec.unidec_modules/mainwindow.Mainwindow.ud_bmp

7.23.4.174 UniDec.unidec_modules/mainwindow.Mainwindow.udbutton

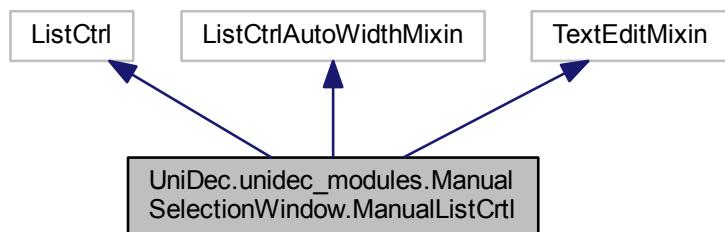
7.23.4.175 UniDec.unidec_modules/mainwindow.Mainwindow.version

The documentation for this class was generated from the following file:

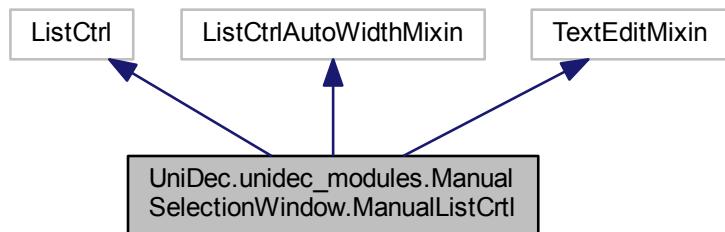
- C:/Python/UniDec/unidec_modules/[mainwindow.py](#)

7.24 UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl Class Reference

Inheritance diagram for UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl:



Collaboration diagram for UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl:



Public Member Functions

- def [__init__](#)
- def [clear](#) (self)
- def [add_line](#)

- def [populate](#)
- def [get_list](#) (self)

Public Attributes

- [imflag](#)

7.24.1 Constructor & Destructor Documentation

7.24.1.1 def UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl.__init__ (self, parent, id_value, pos = wx.DefaultPosition, size = wx.DefaultSize, style = 0, imflag = 0)

```
Create a listctrl with either three or five columns depending on whether it is IM or MS mode.
:param parent: Passed to wx.ListCtrl
:param id_value: Passed to wx.ListCtrl
:param pos: Passed to wx.ListCtrl
:param size: Passed to wx.ListCtrl
:param style: Passed to wx.ListCtrl
:param imflag: Whether the listctrl should have 3 columns for MS (0) or 5 columns for IMMS (1)
:return: None
```

7.24.2 Member Function Documentation

7.24.2.1 def UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl.add_line (self, line = None)

```
Insert a new line into the listctrl.
:param line: Optional list of values for the new line. Default is [0,0,0,0]
:return: None
```

Here is the caller graph for this function:



7.24.2.2 def UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl.clear (self)

```
Clear the list.
:return: None
```

7.24.2.3 def UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl.get_list (self)

```
Return a nested list of the values in the listctrl.
:return: Nested list of the outputs.
```

7.24.2.4 def UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl.populate (self, data, colors = None)

```
Add data from an array to the listctrl.
:param data: Data array to be added
:param colors: Optional list of background colors.
:return: None
```

7.24.3 Member Data Documentation

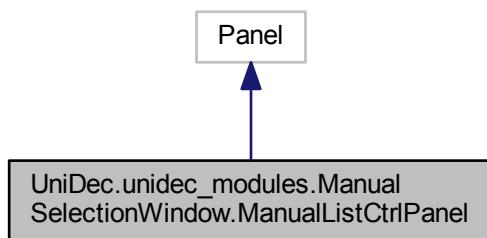
7.24.3.1 UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl.imflag

The documentation for this class was generated from the following file:

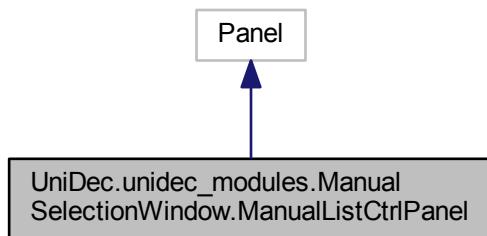
- C:/Python/UniDec/unidec_modules/[ManualSelectionWindow.py](#)

7.25 UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel Class Reference

Inheritance diagram for UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel:



Collaboration diagram for UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel:



Public Member Functions

- def [__init__](#)
- def [on_right_click](#)
- def [on_popup_one](#)

Public Attributes

- [list](#)
- [selection](#)
- [popupID1](#)

7.25.1 Constructor & Destructor Documentation

7.25.1.1 def UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel.__init__ (self, parent, imflag = 0)

```
Create the panel for the ManualListCtrl. Binds right click options.  
:param parent: Parent window or panel.  
:param imflag: Whether it should be IM-MS mode (1) or just MS (0).  
:return: None
```

7.25.2 Member Function Documentation

7.25.2.1 def UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel.on_popup_one (self, e =None)

```
Delete the selected items.  
:param e: Unused event  
:return: None
```

7.25.2.2 def UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel.on_right_click (self, e =None)

```
Open right click menu.  
:param e: Unused event  
:return: None
```

7.25.3 Member Data Documentation

7.25.3.1 UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel.list

7.25.3.2 UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel.popupID1

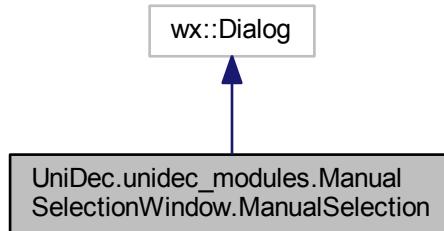
7.25.3.3 UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel.selection

The documentation for this class was generated from the following file:

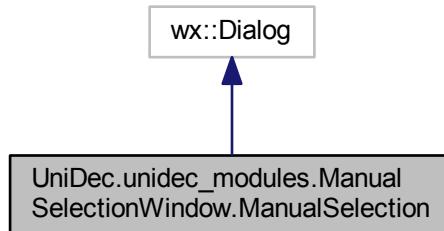
- C:/Python/UniDec/unidec_modules/[ManualSelectionWindow.py](#)

7.26 UniDec.unidec_modules.ManualSelectionWindow.ManualSelection Class Reference

Inheritance diagram for UniDec.unidec_modules.ManualSelectionWindow.ManualSelection:



Collaboration diagram for UniDec.unidec_modules.ManualSelectionWindow.ManualSelection:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `initiate_dialog` (self, config, data)
- def `on_close` (self, e)
- def `on_close_cancel` (self, e)
- def `on_clear` (self, e)
- def `on_add` (self, e)
- def `on_add_from_plot` (self, e)
- def `on_plot` (self, e)
- def `on_import` (self, e)

Public Attributes

- `config`
- `data`
- `plot1`
- `masslistbox`

7.26.1 Constructor & Destructor Documentation

7.26.1.1 def UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.__init__(self, args, kwargs)

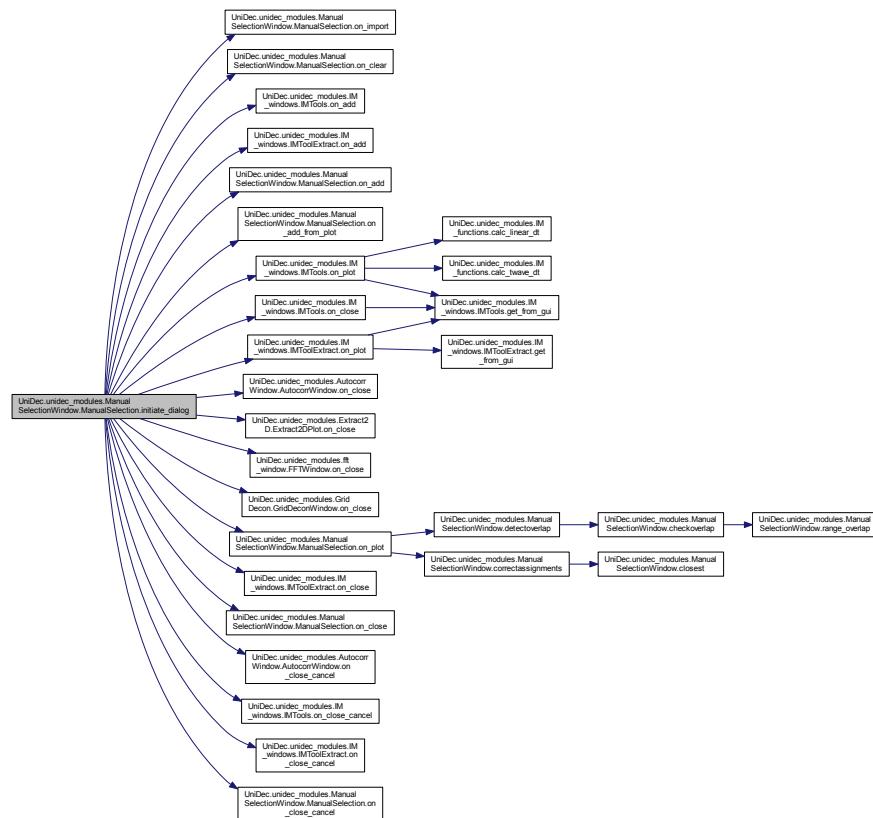
```
Create the initial dialog.
:param args: Passed to wx.Dialog
:param kwargs: Passed to wx.Dialog
:return: None
```

7.26.2 Member Function Documentation

7.26.2.1 def UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.initiate_dialog(self, config, data)

```
Initiate the dialog window, lay everything out, and plot the intial results
:param config: UniDecConfig object
:param data: Data to plot (either MS or IM-MS)
:return: None
```

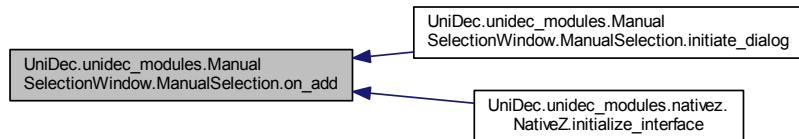
Here is the call graph for this function:



7.26.2.2 def UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.on_add(self, e)

```
Add a new blank line to the listctrl.
:param e: Unused event
:return: None
```

Here is the caller graph for this function:



7.26.2.3 def UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.on_add_from_plot (self, e)

Grab the limits of the plot and make that the limits of the manual assignment.
 :param e: Unused event
 :return: None

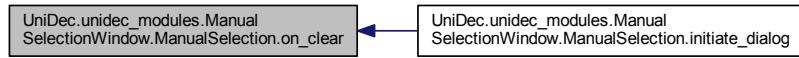
Here is the caller graph for this function:



7.26.2.4 def UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.on_clear (self, e)

Clear the listctrl.
 :param e: Unused event
 :return: None

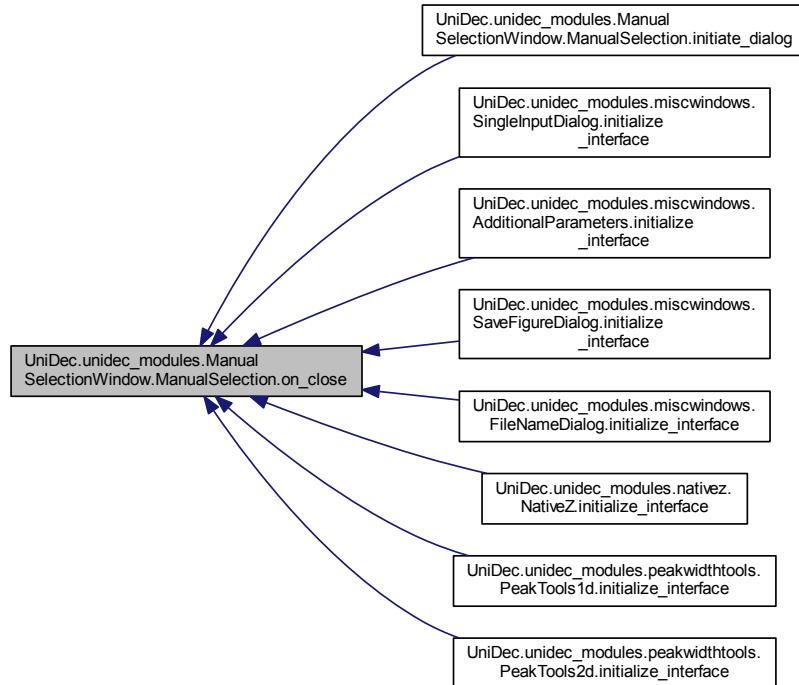
Here is the caller graph for this function:



7.26.2.5 def UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.on_close (self, e)

Get manuallist from listctrl, clean up, write it to self.config.manuallist, and then destroy the window.
 :param e: Unused event
 :return: None

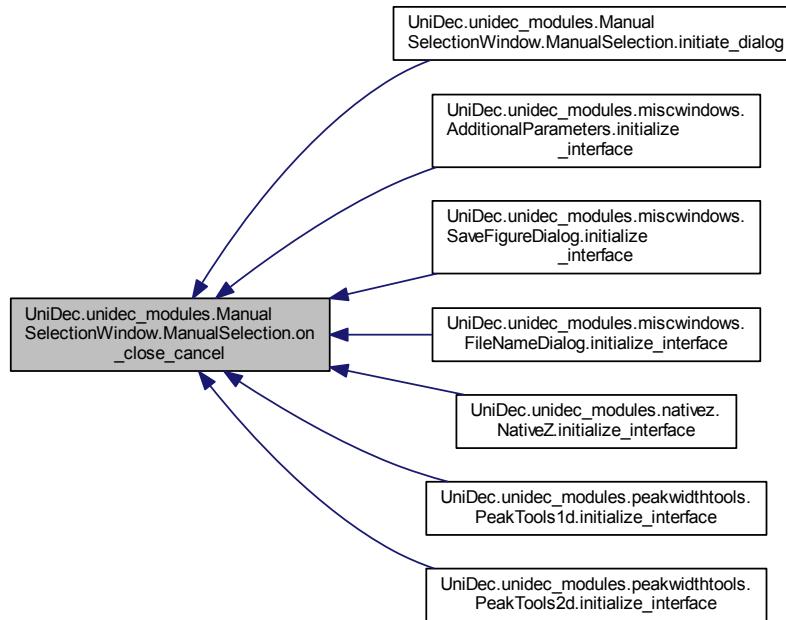
Here is the caller graph for this function:



7.26.2.6 def UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.on_close_cancel (self, e)

Destroy the dialog without updating the manual assignment list in `UniDecConfig`.
:param e: Unused event
:return: None

Here is the caller graph for this function:



7.26.2.7 def UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.on_import(self, e)

Open a file dialog and import a N x 3 (MS) or N x 5 (IMMS) array of manual assignment.
 Add the array to the listctrl.
 :param e: Unused event
 :return: None

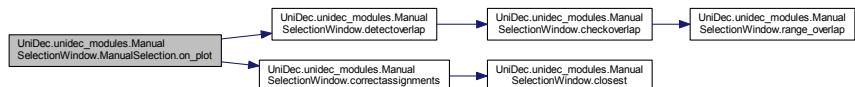
Here is the caller graph for this function:



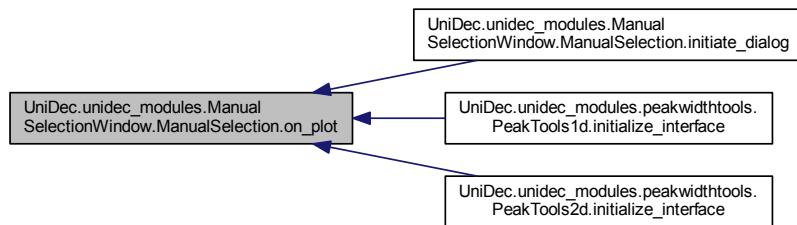
7.26.2.8 def UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.on_plot(self, e)

Attempts to correct and plot the manual assignments.
 :param e: Unused event
 :return: None

Here is the call graph for this function:



Here is the caller graph for this function:



7.26.3 Member Data Documentation

7.26.3.1 UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.config

7.26.3.2 UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.data

7.26.3.3 UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.masslistbox

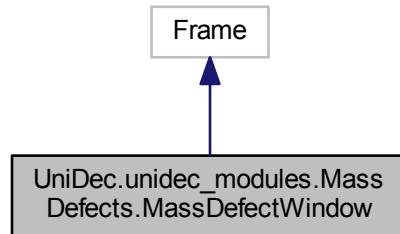
7.26.3.4 UniDec.unidec_modules.ManualSelectionWindow.ManualSelection.plot1

The documentation for this class was generated from the following file:

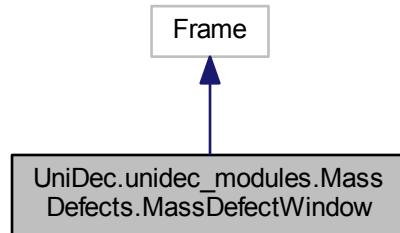
- C:/Python/UniDec/unidec_modules/[ManualSelectionWindow.py](#)

7.27 UniDec.unidec_modules.MassDefects.MassDefectWindow Class Reference

Inheritance diagram for UniDec.unidec_modules.MassDefects.MassDefectWindow:



Collaboration diagram for UniDec.unidec_modules.MassDefects.MassDefectWindow:



Public Member Functions

- def `__init__`
- def `on_close` (self, e)
- def `getfromgui` (self)
- def `makeplot` (self)
- def `makeplottotal`
- def `on_back` (self, e)
- def `on_next` (self, e)
- def `on_peaks` (self, e)
- def `on_save_fig` (self, e)
- def `on_save_fig_pdf` (self, e)
- def `on_add_line` (self, e)

Public Attributes

- `directory`

- parent
- m0
- config
- pos
- yvals
- ylab
- nbins
- transformmode
- centermode
- xtype
- factor
- xlabel
- datalist
- plotmenu
- menuaddline
- plot1
- plot2
- ctlm0
- ctlwindow
- pks
- radiobox
- radiobox2
- radiobox3

7.27.1 Constructor & Destructor Documentation

7.27.1.1 def UniDec.unidec_modules.MassDefects.MassDefectWindow.`__init__`(*self*, *parent*, *data_list*, *config* = None, *yvals* = None, *pks* = None, *value* = None, *directory* = None)

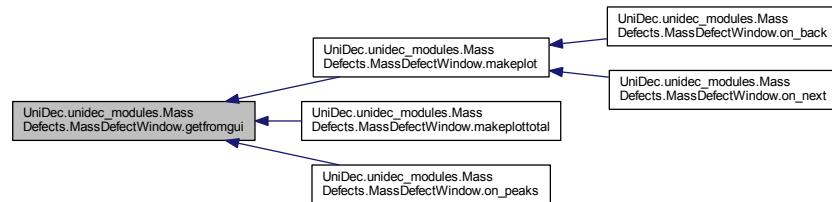
Creates a window for visualizing high-mass mass defects.
:param parent: Passed to wx.Frame
:param data_list: List of mass distribution data.
:param config: UniDecConfig object
:param yvals: List of titles for each mass distribution in data_list
:param pks: Peaks object
:param value: Kendrick reference mass (default is 760.076, the mass of POPC)
:param directory: Directory to save files to (default is os.getcwd())
:return: None

7.27.2 Member Function Documentation

7.27.2.1 def UniDec.unidec_modules.MassDefects.MassDefectWindow.getfromgui(*self*)

Update parameters from GUI.
:return: None

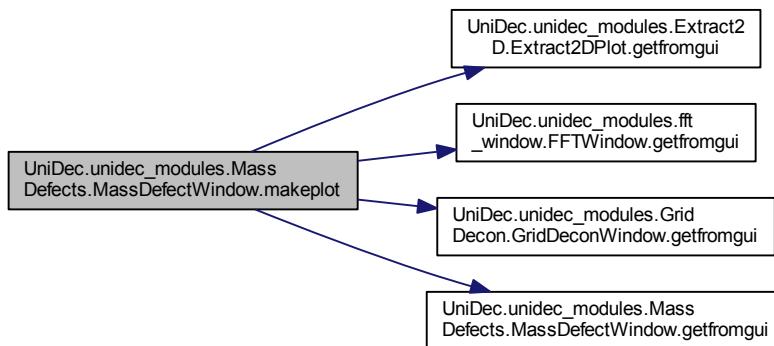
Here is the caller graph for this function:



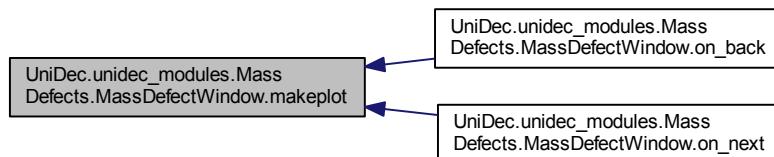
7.27.2.2 def UniDec.unidec_modules.MassDefectWindow.makeplot(self)

Runs the kendrick analysis on a single of the mass distributions in self.datalist set by self.pos.
 Plots the results in 1D and 2D.
 :return: None

Here is the call graph for this function:



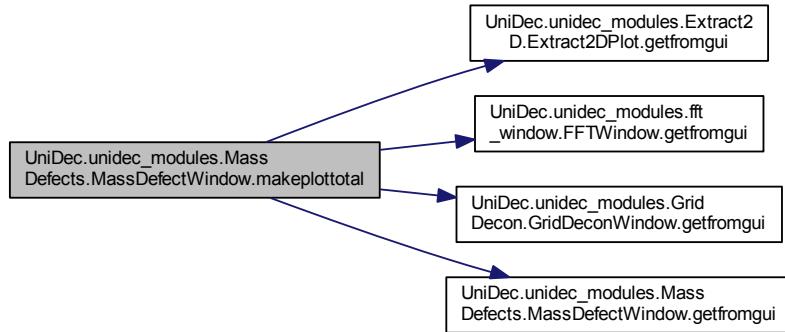
Here is the caller graph for this function:



7.27.2.3 def UniDec.unidec_modules.MassDefectWindow.makeplottotal(self, e=None)

Runs the kendrick analysis on all of the mass distributions in self.datalist.
 Assumes they are all the same dimensions, which is why we run mergedata when it is loaded.
 Sums the results and plots the sums in 1D and 2D.
 :param e: Unused event
 :return: None

Here is the call graph for this function:



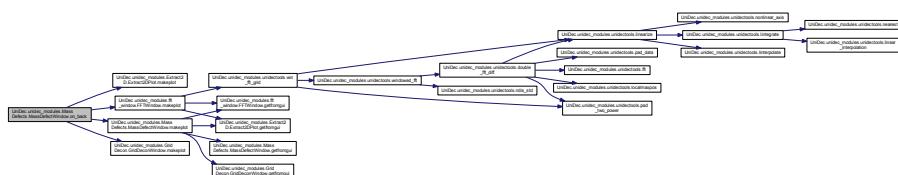
7.27.2.4 def UniDec.unidec_modules.MassDefectWindow.on_add_line(self, e)

Add a horizontal line to the plot to visualize a predicted mass defect.
 Opens a dialog to input the value. Can be called more than once to add multiple lines.
 :param e: Unused event
 :return: None

7.27.2.5 def UniDec.unidec_modules.MassDefectWindow.on_back(self, e)

Plot the mass defect of the previous thing in the mass defect list.
 :param e: Unused event
 :return: None

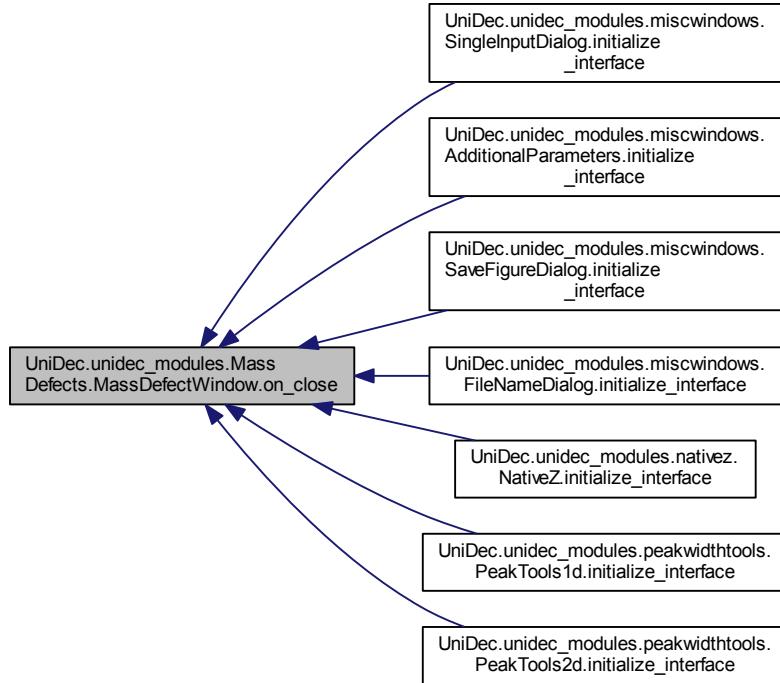
Here is the call graph for this function:



7.27.2.6 def UniDec.unidec_modules.MassDefectWindow.on_close(self, e)

Close the window. Will try to set self.config.molig as self.m0.
 :param e: Unused event
 :return: None

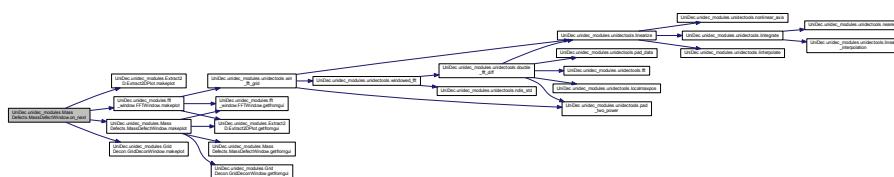
Here is the caller graph for this function:



7.27.2.7 def UniDec.unidec_modules.MassDefects.MassDefectWindow.on_next(self, e)

Plot the mass defect of the next thing in the mass defect list.
 :param e: Unused event
 :return: None

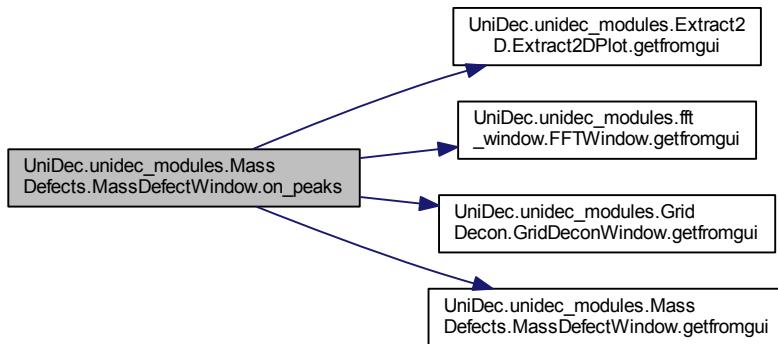
Here is the call graph for this function:



7.27.2.8 def UniDec.unidec_modules.MassDefects.MassDefectWindow.on_peaks(self, e)

For each peak in self.pks, get the mass defects and plot them.
 :param e: Unused event
 :return: None

Here is the call graph for this function:



7.27.2.9 def UniDec.unidec_modules.MassDefects.MassDefectWindow.on_save_fig (self, e)

Saves the figures in self.directory as PNGs.
:param e: Unused event
:return: None

7.27.2.10 def UniDec.unidec_modules.MassDefects.MassDefectWindow.on_save_fig_pdf (self, e)

Saves the figures in self.directory as PDFs.
:param e: Unused event
:return: None

7.27.3 Member Data Documentation

7.27.3.1 UniDec.unidec_modules.MassDefects.MassDefectWindow.centermode

7.27.3.2 UniDec.unidec_modules.MassDefects.MassDefectWindow.config

7.27.3.3 UniDec.unidec_modules.MassDefects.MassDefectWindow.ctlm0

7.27.3.4 UniDec.unidec_modules.MassDefects.MassDefectWindow.ctlwindow

7.27.3.5 UniDec.unidec_modules.MassDefects.MassDefectWindow.datalist

7.27.3.6 UniDec.unidec_modules.MassDefects.MassDefectWindow.directory

7.27.3.7 UniDec.unidec_modules.MassDefects.MassDefectWindow.factor

7.27.3.8 UniDec.unidec_modules.MassDefects.MassDefectWindow.m0

7.27.3.9 UniDec.unidec_modules.MassDefects.MassDefectWindow.menuaddline

7.27.3.10 UniDec.unidec_modules.MassDefects.MassDefectWindow.nbins

7.27.3.11 UniDec.unidec_modules.MassDefects.MassDefectWindow.parent

- 7.27.3.12 `UniDec.unidec_modules.MassDefects.MassDefectWindow.pks`
- 7.27.3.13 `UniDec.unidec_modules.MassDefects.MassDefectWindow.plot1`
- 7.27.3.14 `UniDec.unidec_modules.MassDefects.MassDefectWindow.plot2`
- 7.27.3.15 `UniDec.unidec_modules.MassDefects.MassDefectWindow.plotmenu`
- 7.27.3.16 `UniDec.unidec_modules.MassDefects.MassDefectWindow.pos`
- 7.27.3.17 `UniDec.unidec_modules.MassDefects.MassDefectWindow.radiobox`
- 7.27.3.18 `UniDec.unidec_modules.MassDefects.MassDefectWindow.radiobox2`
- 7.27.3.19 `UniDec.unidec_modules.MassDefects.MassDefectWindow.radiobox3`
- 7.27.3.20 `UniDec.unidec_modules.MassDefects.MassDefectWindow.transformmode`
- 7.27.3.21 `UniDec.unidec_modules.MassDefects.MassDefectWindow.xlab`
- 7.27.3.22 `UniDec.unidec_modules.MassDefects.MassDefectWindow xtype`
- 7.27.3.23 `UniDec.unidec_modules.MassDefects.MassDefectWindow.ylab`
- 7.27.3.24 `UniDec.unidec_modules.MassDefects.MassDefectWindow.yvals`

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/[MassDefects.py](#)

7.28 UniDec.unidec_modules.MassFitter.MassFitter Class Reference

Public Member Functions

- def [`__init__`](#) (`self`, `massdat`, `guessarray`, `psfun`, `args`)
- def [`perform_fit`](#) (`self`, `args`)

Public Attributes

- `massdat`
- `finarray`
- `psfun`
- `fit`
- `fitdat`
- `initguess`

7.28.1 Detailed Description

Class for fitting zero-charge mass spectrum to overlapping peaks.

7.28.2 Constructor & Destructor Documentation

7.28.2.1 def UniDec.unidec_modules.MassFitter.MassFitter.__init__(self, massdat, guessarray, psfun, args)

Initialize values and set initial guesses.

Guess array can be fed in several things. If there are five columns, it expects a P x 5 grid.

[mass, mass fwhm, charge (not used), charge std (not used), intensity]

If there are only two columns, it expects a P x 2 grid

[mass, intensity]

```
:param massdat: Mass data to be fit
:param guessarray: Array of initial peak parameters
:param psfun: Peak shape function integer code
:param args: Arguments passed to fits and guesses.
:return: fitdat
```

7.28.3 Member Function Documentation

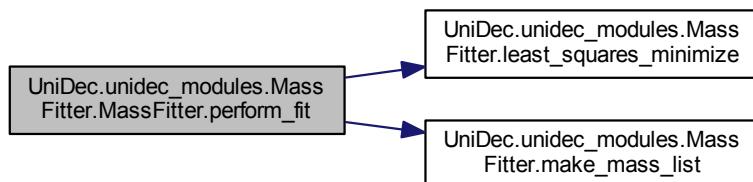
7.28.3.1 def UniDec.unidec_modules.MassFitter.MassFitter.perform_fit(self, args)

Run least squares fitting

:param args: Arguments passed to fitting

:return: fitdat, fit (fit to data and fit parameters in a P x 3 array of (mid, fwhm, area))

Here is the call graph for this function:



7.28.4 Member Data Documentation

7.28.4.1 UniDec.unidec_modules.MassFitter.MassFitter.finarray

7.28.4.2 UniDec.unidec_modules.MassFitter.MassFitter.fit

7.28.4.3 UniDec.unidec_modules.MassFitter.MassFitter.fitdat

7.28.4.4 UniDec.unidec_modules.MassFitter.MassFitter.initguess

7.28.4.5 UniDec.unidec_modules.MassFitter.MassFitter.massdat

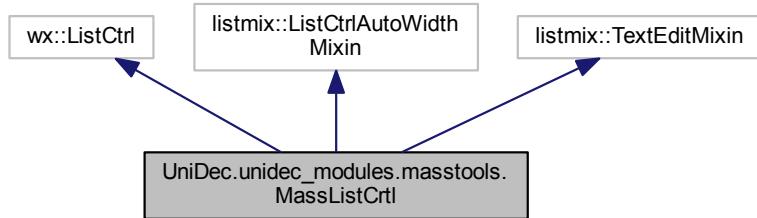
7.28.4.6 UniDec.unidec_modules.MassFitter.MassFitter.psfun

The documentation for this class was generated from the following file:

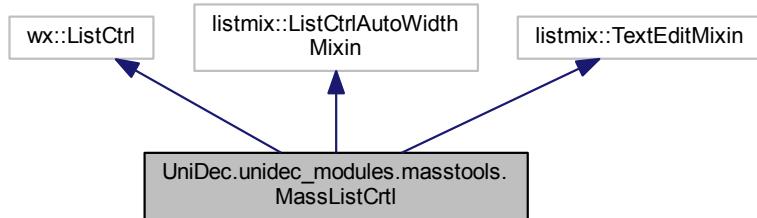
- C:/Python/UniDec/unidec_modules/[MassFitter.py](#)

7.29 UniDec.unidec_modules.masstools.MassListCtrl Class Reference

Inheritance diagram for UniDec.unidec_modules.masstools.MassListCtrl:



Collaboration diagram for UniDec.unidec_modules.masstools.MassListCtrl:



Public Member Functions

- def [`__init__`](#)
- def [`populate`](#) (`self`, `listctrldata`)
- def [`clear`](#) (`self`)
- def [`add_line`](#) (`self`)
- def [`get_list`](#) (`self`)
- def [`on_right_click_masslist`](#) (`self`, `event`)
- def [`on_masslist_delete`](#) (`self`, `event`)

Public Attributes

- [`popupID1`](#)

7.29.1 Constructor & Destructor Documentation

7.29.1.1 def `UniDec.unidec_modules.masstools.MassListCtrl.__init__ (self, parent, id_value, pos = wx.DefaultPosition, size = wx.DefaultSize, style = 0)`

Create the mass list ctrl with one column.

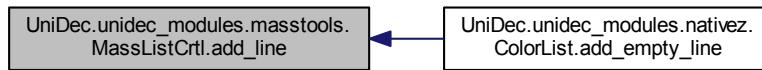
```
:param parent: Passed to wx.ListCtrl
:param id_value: Passed to wx.ListCtrl
:param pos: Passed to wx.ListCtrl
:param size: Passed to wx.ListCtrl
:param style: Passed to wx.ListCtrl
:return: None
```

7.29.2 Member Function Documentation

7.29.2.1 def UniDec.unidec_modules.masstools.MassListCtrl.add_line(*self*)

Add a new line, default of 0.
:return: None

Here is the caller graph for this function:



7.29.2.2 def UniDec.unidec_modules.masstools.MassListCtrl.clear(*self*)

Clear the list.
:return: None

7.29.2.3 def UniDec.unidec_modules.masstools.MassListCtrl.get_list(*self*)

Return the list as a list of mass values
:return: List of mass values

7.29.2.4 def UniDec.unidec_modules.masstools.MassListCtrl.on_masslist_delete(*self, event*)

Delete the selected item.
:param event: Unused event.
:return: None

7.29.2.5 def UniDec.unidec_modules.masstools.MassListCtrl.on_right_click_masslist(*self, event*)

Create a right click menu.
:param event: Unused event
:return: None

7.29.2.6 def UniDec.unidec_modules.masstools.MassListCtrl.populate(*self, listctrldata*)

Populate the the listctrl from a list of mass values
:param listctrldata: mass value list
:return: None

7.29.3 Member Data Documentation

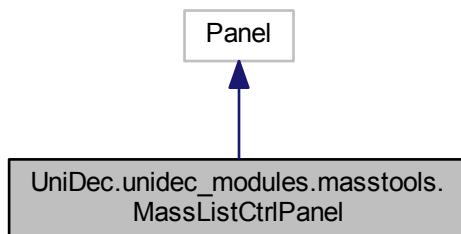
7.29.3.1 UniDec.unidec_modules.masstools.MassListCtrl.populID1

The documentation for this class was generated from the following file:

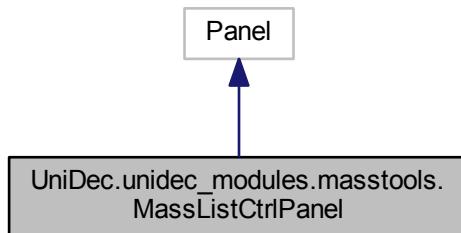
- C:/Python/UniDec/unidec_modules/[masstools.py](#)

7.30 UniDec.unidec_modules.masstools.MassListCtrlPanel Class Reference

Inheritance diagram for UniDec.unidec_modules.masstools.MassListCtrlPanel:



Collaboration diagram for UniDec.unidec_modules.masstools.MassListCtrlPanel:



Public Member Functions

- def [__init__](#) (self, parent)

Public Attributes

- [list](#)

7.30.1 Constructor & Destructor Documentation

7.30.1.1 def UniDec.unidec_modules.masstools.MassListCtrlPanel.__init__(self, parent)

```
ListCtrlPanel for the Mass list
:param parent: Parent panel or window
:return: None
```

7.30.2 Member Data Documentation

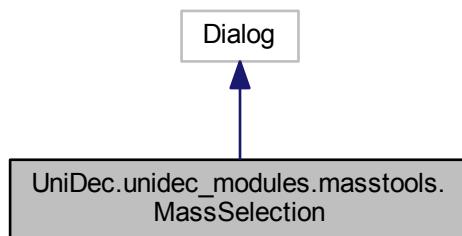
7.30.2.1 UniDec.unidec_modules.masstools.MassListCtrlPanel.list

The documentation for this class was generated from the following file:

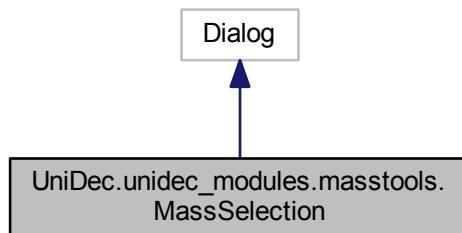
- C:/Python/UniDec/unidec_modules/masstools.py

7.31 UniDec.unidec_modules.masstools.MassSelection Class Reference

Inheritance diagram for UniDec.unidec_modules.masstools.MassSelection:



Collaboration diagram for UniDec.unidec_modules.masstools.MassSelection:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `init_dialog`
- def `on_simulate` (self, e)
- def `on_autocorr_window` (self, e)
- def `on_match_isolated` (self, e)
- def `on_match_all` (self, e)
- def `on_close` (self, e)
- def `on_close_cancel` (self, e)
- def `pop_from_peaks` (self, e)
- def `pop.oligo_iso` (self, e)
- def `pop.oligo_all` (self, e)
- def `on_clear_masslist` (self, e)
- def `on_clear_oligolist` (self, e)
- def `on_add_mass` (self, e)
- def `on_add_oligomer` (self, e)
- def `on_import_masses` (self, e)
- def `on_import_oligos` (self, e)

Public Attributes

- `pks`
- `config`
- `massdat`
- `masslistbox`
- `oligomerlistbox`
- `matchlistbox`
- `ctlmatcherror`

7.31.1 Constructor & Destructor Documentation

7.31.1.1 def UniDec.unidec_modules.masstools.MassSelection.`__init__` (`self, args, kwargs`)

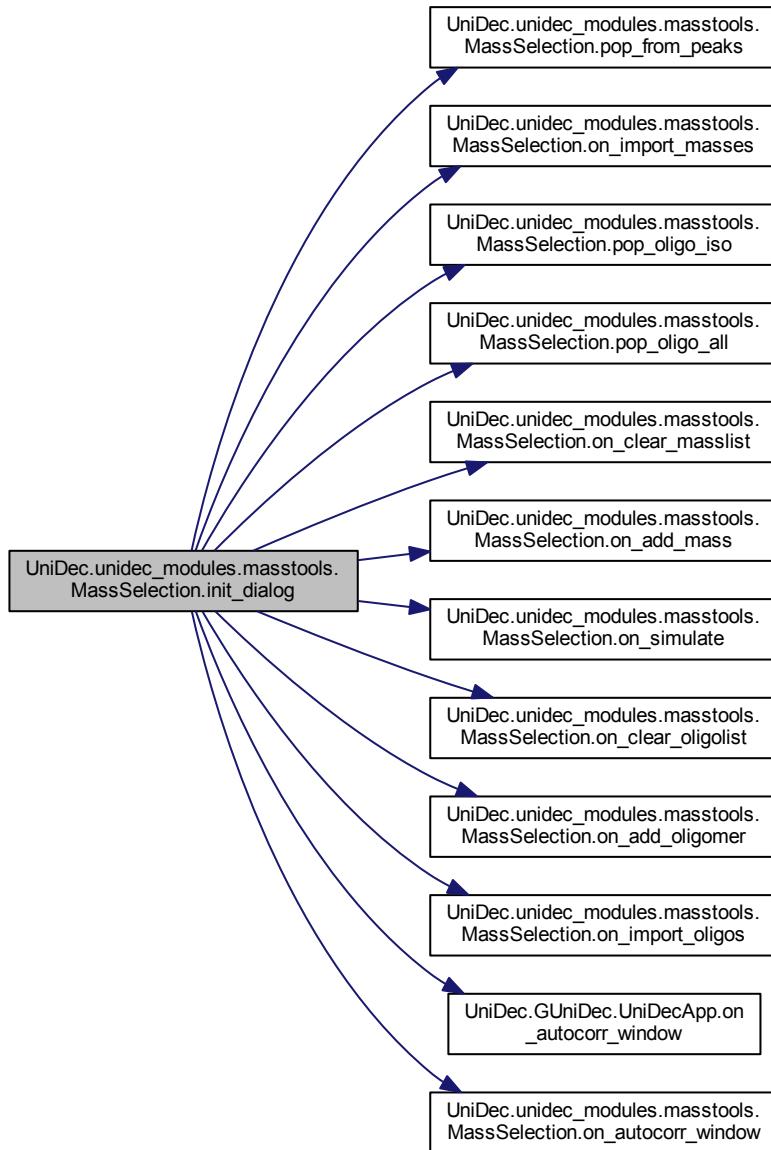
```
Initialize the dialog
:param args: Passed to wx.Dialog
:param kwargs: Passed to wx.Dialog
:return: None
```

7.31.2 Member Function Documentation

7.31.2.1 def UniDec.unidec_modules.masstools.MassSelection.`init_dialog` (`self, config, pks, massdat=None`)

```
Creates the dialog window and displays it.
:param config: UniDecConfig object
:param pks: Peaks object
:param massdat: Mass distribution
:return: None
```

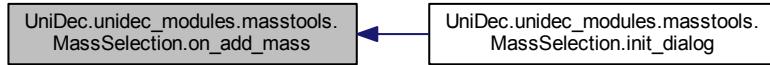
Here is the call graph for this function:



7.31.2.2 def UniDec.unidec_modules.masstools.MassSelection.on_add_mass (*self, e*)

Adds a blank line to the mass list.
:param e: Unused Event
:return: None

Here is the caller graph for this function:



7.31.2.3 def UniDec.unidec_modules.masstools.MassSelection.on_add_oligomer (self, e)

Adds a blank line to the oligomer list.
:param e: Unused event
:return: None

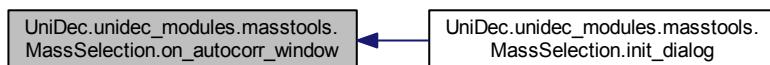
Here is the caller graph for this function:



7.31.2.4 def UniDec.unidec_modules.masstools.MassSelection.on_autocorr_window (self, e)

Opens up an autocorrelation window for the purpose of figuring out mass differences.
:param e: Unused event
:return: None

Here is the caller graph for this function:



7.31.2.5 def UniDec.unidec_modules.masstools.MassSelection.on_clear_masslist (self, e)

Clears the mass list.
:param e: Unused event
:return: None

Here is the caller graph for this function:



7.31.2.6 def UniDec.unidec_modules.masstools.MassSelection.on_clear_oligolist (self, e)

```
Clears the oligomer list.  
:param e: Unused Event  
:return: None
```

Here is the caller graph for this function:

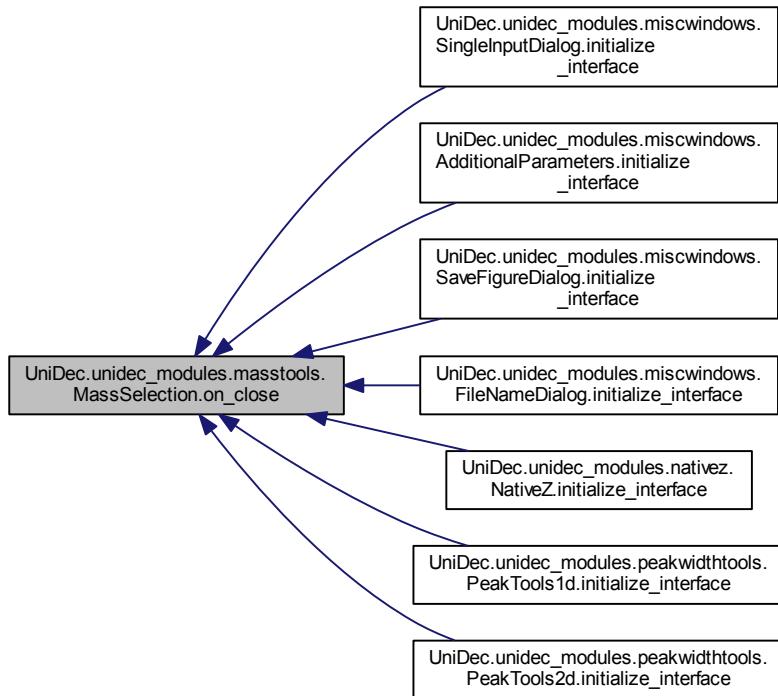


7.31.2.7 def UniDec.unidec_modules.masstools.MassSelection.on_close (self, e)

Close the dialog and apply the changes.

```
Sets self.config.masslist to the defined mass list.  
Sets self.config.oligomerlist to the defined oligomers.  
Sets self.config.matchlist to the matched values  
:param e: Unused event  
:return: None
```

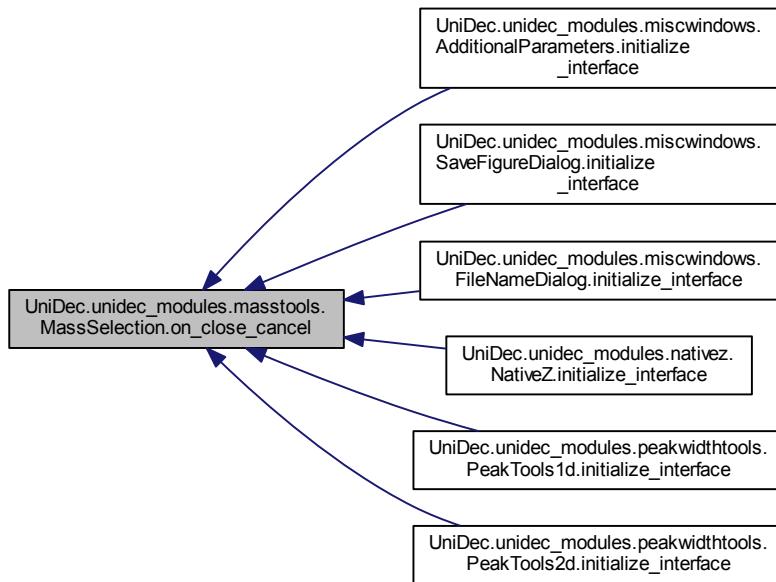
Here is the caller graph for this function:



7.31.2.8 def `UniDec.unidec_modules.masstools.MassSelection.on_close_cancel(self, e)`

Close the dialog but do not modify any of the values.
:param e: Unused event
:return: None

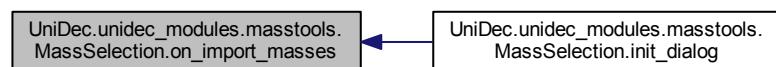
Here is the caller graph for this function:



7.31.2.9 def UniDec.unidec_modules.masstools.MassSelection.on_import_masses (self, e)

Opens a dialog to import mass list files.
:param e: Unused event
:return: None

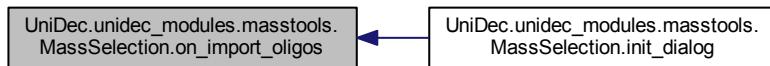
Here is the caller graph for this function:



7.31.2.10 def UniDec.unidec_modules.masstools.MassSelection.on_import_oligos (self, e)

Open a file dialog to import oligomer files.
:param e: Unused event
:return: None

Here is the caller graph for this function:



7.31.2.11 def UniDec.unidec_modules.masstools.MassSelection.on_match_all(self, e)

Match the peaks in self.pks to all possible combination of oligomers in the oligomerlist.
Uses ud.make_all_matches function.

Populated the matchlistbox with the results of the matching.

:param e: Unused event

:return: None

7.31.2.12 def UniDec.unidec_modules.masstools.MassSelection.on_match_isolated(self, e)

Match the peaks in self.pks to possible combination of isolated rows of oligomers in the oligomerlist.
Uses ud.make_isolated_match function.

Populated the matchlistbox with the results of the matching.

:param e: Unused event

:return: None

7.31.2.13 def UniDec.unidec_modules.masstools.MassSelection.on_simulate(self, e)

Replaces the peaks in self.pks with the masses defined in the self.masslistbox.

The intensity information comes from interpolating the mass distribution in self.massdat.

It flags self.pks.changes as 1, which is picked up downstream to say that these new peaks should be replotted.

:param e: Unused event

:return: None

Here is the caller graph for this function:



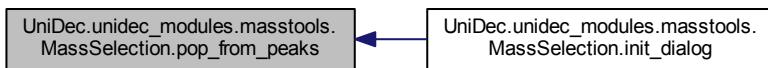
7.31.2.14 def UniDec.unidec_modules.masstools.MassSelection.pop_from_peaks(self, e)

Populate the mass list from the peak masses in self.pks

:param e: Unused event

:return: None

Here is the caller graph for this function:



7.31.2.15 def UniDec.unidec_modules.masstools.MassSelection.pop_oligo_all(self, e)

Populates the mass list with all possible oligomers.
:param e: Unused event
:return: None

Here is the caller graph for this function:



7.31.2.16 def UniDec.unidec_modules.masstools.MassSelection.pop_oligo_iso(self, e)

Populate the mass list with isolated oligomer rows.
:param e: Unused event
:return: None

Here is the caller graph for this function:



7.31.3 Member Data Documentation

7.31.3.1 UniDec.unidec_modules.masstools.MassSelection.config

7.31.3.2 UniDec.unidec_modules.masstools.MassSelection.ctlmatcherror

7.31.3.3 UniDec.unidec_modules.masstools.MassSelection.massdat

7.31.3.4 UniDec.unidec_modules.masstools.MassSelection.masslistbox

7.31.3.5 [UniDec.unidec_modules.masstools.MassSelection.matchlistbox](#)

7.31.3.6 [UniDec.unidec_modules.masstools.MassSelection.oligomerlistbox](#)

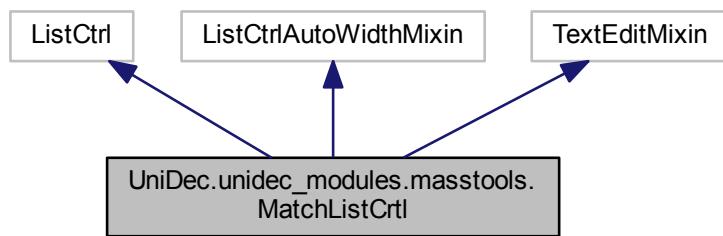
7.31.3.7 [UniDec.unidec_modules.masstools.MassSelection.pks](#)

The documentation for this class was generated from the following file:

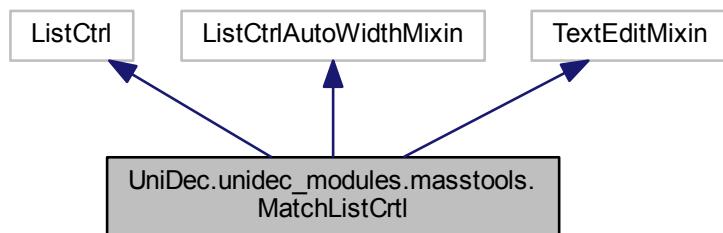
- C:/Python/UniDec/unidec_modules/[masstools.py](#)

7.32 UniDec.unidec_modules.masstools.MatchListCrtl Class Reference

Inheritance diagram for UniDec.unidec_modules.masstools.MatchListCrtl:



Collaboration diagram for UniDec.unidec_modules.masstools.MatchListCrtl:



Public Member Functions

- def [__init__](#)
- def [clear](#) (self)
- def [populate](#) (self, data1, data2, data3, data4)
- def [get_list](#) (self)

Public Attributes

- [index](#)

7.32.1 Constructor & Destructor Documentation

```
7.32.1.1 def UniDec.unidec_modules.masstools.MatchListCtrl.__init__ ( self, parent, id_value, pos =  
wx.DefaultPosition, size = wx.DefaultSize, style = 0 )
```

Create a four column uneditable list control.
:param parent: Parent panel or window
:param id_value: Passed to wx.ListCtrl
:param pos: Passed to wx.ListCtrl
:param size: Passed to wx.ListCtrl
:param style: Passed to wx.ListCtrl
:return: None

7.32.2 Member Function Documentation

```
7.32.2.1 def UniDec.unidec_modules.masstools.MatchListCtrl.clear ( self )
```

Clear the list
:return: None

```
7.32.2.2 def UniDec.unidec_modules.masstools.MatchListCtrl.get_list ( self )
```

:return: List items in a nested list

```
7.32.2.3 def UniDec.unidec_modules.masstools.MatchListCtrl.populate ( self, data1, data2, data3, data4 )
```

Populate the list of matches from four arrays
:param data1: The first column, the measured mass
:param data2: The second column, the simulated mass
:param data3: The third column, the error between measured and simulated.
:param data4: The fourth column, the match name.
:return: None

7.32.3 Member Data Documentation

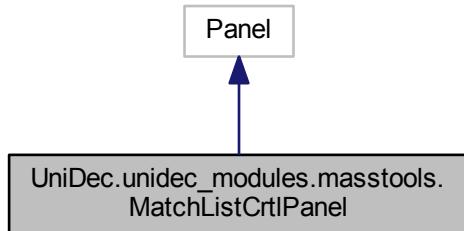
```
7.32.3.1 UniDec.unidec_modules.masstools.MatchListCtrl.index
```

The documentation for this class was generated from the following file:

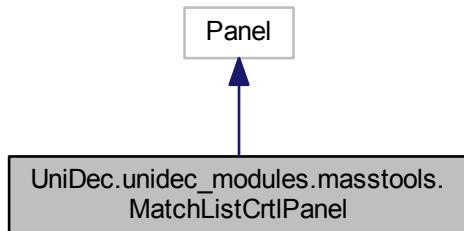
- C:/Python/UniDec/unidec_modules/[masstools.py](#)

7.33 UniDec.unidec_modules.masstools.MatchListCrtlPanel Class Reference

Inheritance diagram for UniDec.unidec_modules.masstools.MatchListCrtlPanel:



Collaboration diagram for UniDec.unidec_modules.masstools.MatchListCrtlPanel:



Public Member Functions

- def [__init__](#) (self, parent)

Public Attributes

- [list](#)

7.33.1 Constructor & Destructor Documentation

7.33.1.1 def UniDec.unidec_modules.masstools.MatchListCrtlPanel.[__init__](#) (self, parent)

```
ListCtrlPanel for the Match list
:param parent: Parent panel or window
:return: None
```

7.33.2 Member Data Documentation

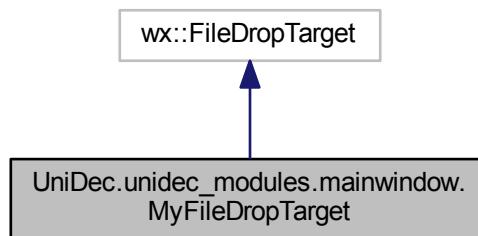
7.33.2.1 UniDec.unidec_modules.masstools.MatchListCtrlPanel.list

The documentation for this class was generated from the following file:

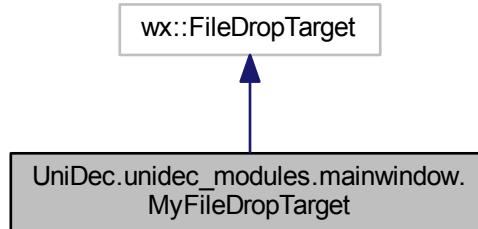
- C:/Python/UniDec/unidec_modules/[masstools.py](#)

7.34 UniDec.unidec_modules/mainwindow.MyFileDropTarget Class Reference

Inheritance diagram for UniDec.unidec_modules/mainwindow.MyFileDropTarget:



Collaboration diagram for UniDec.unidec_modules/mainwindow.MyFileDropTarget:



Public Member Functions

- def [__init__\(self, window\)](#)
- def [OnDropFiles\(self, x, y, filenames\)](#)

Public Attributes

- [window](#)

7.34.1 Detailed Description

7.34.2 Constructor & Destructor Documentation

7.34.2.1 def UniDec.unidec_modules/mainwindow.MyFileDropTarget.__init__(self, window)

Constructor

7.34.3 Member Function Documentation

7.34.3.1 def UniDec.unidec_modules/mainwindow.MyFileDropTarget.OnDropFiles(self, x, y, filenames)

When files are dropped, either open a single file or run in batch.

7.34.4 Member Data Documentation

7.34.4.1 UniDec.unidec_modules/mainwindow.MyFileDropTarget.window

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/mainwindow.py

7.35 UniDec.unidec_modules.mzMLimporter.mzMLimporter Class Reference

Public Member Functions

- def [__init__\(self, path, args, kwargs\)](#)
- def [get_data\(self\)](#)

Public Attributes

- [msrun](#)
- [data](#)

7.35.1 Detailed Description

Imports mzML data files.

7.35.2 Constructor & Destructor Documentation

7.35.2.1 def UniDec.unidec_modules.mzMLimporter.mzMLimporter.__init__(self, path, args, kwargs)

Imports mzML file, adds the chromatogram into a single spectrum.

```
:param path: .mzML file path
:param args: arguments (unused)
:param kwargs: keywords (unused)
:return: mzMLimporter object
```

7.35.3 Member Function Documentation

7.35.3.1 def UniDec.unidec_modules.mzMLimporter.mzMLimporter.get_data (self)

Returns merged 1D MS data from mzML import
:return: merged data

7.35.4 Member Data Documentation

7.35.4.1 UniDec.unidec_modules.mzMLimporter.mzMLimporter.data

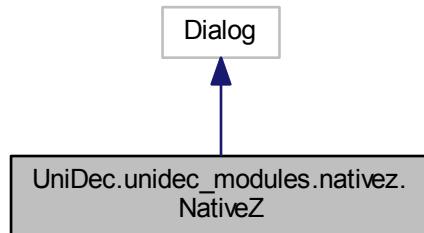
7.35.4.2 UniDec.unidec_modules.mzMLimporter.mzMLimporter.msrun

The documentation for this class was generated from the following file:

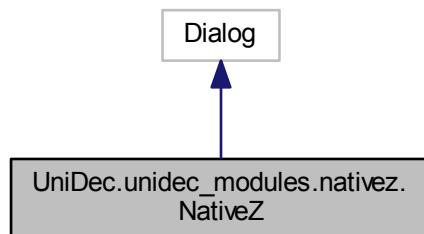
- C:/Python/UniDec/unidec_modules/[mzMLimporter.py](#)

7.36 UniDec.unidec_modules.nativez.NativeZ Class Reference

Inheritance diagram for UniDec.unidec_modules.nativez.NativeZ:



Collaboration diagram for UniDec.unidec_modules.nativez.NativeZ:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `initialize_interface` (self, massaxis, chargeaxis, igrd, config, pks)
- def `update` (self, e)
- def `on_replot` (self, e)
- def `plot_zoffs` (self)
- def `make_plot_7` (self, e)
- def `on_delete` (self, event)
- def `fit` (self, e)
- def `on_reset` (self, e)
- def `update_list` (self)
- def `populate_list` (self, e)
- def `on_add` (self, e)
- def `make_f_array`
- def `fast_extract` (self, f, width, eshape)
- def `get_maxima` (self)
- def `extract` (self, e)
- def `peak_extract` (self)
- def `save_figures` (self, e)
- def `on_close` (self, e)
- def `on_close_cancel` (self, e)

Public Attributes

- `figsize`
- `config`
- `pks`
- `zoffs`
- `massoffset`
- `massaxis`
- `chargeaxis`
- `igrd`
- `offset_totals`
- `offset_grid`
- `plot1`
- `plot2`
- `plot3`
- `plot4`
- `plot5`
- `plot6`
- `plot7`
- `zlistctrl`
- `ctlmassoffset`
- `ctlfilt`

7.36.1 Constructor & Destructor Documentation

7.36.1.1 def UniDec.unidec_modules.nativez.NativeZ.__init__ (`self, args, kwargs`)

Create a dialog for examining the native charge/mass relationship and extraction specific CID states.
Tries to create a big window, but will rescale to smaller if the screen is too small.

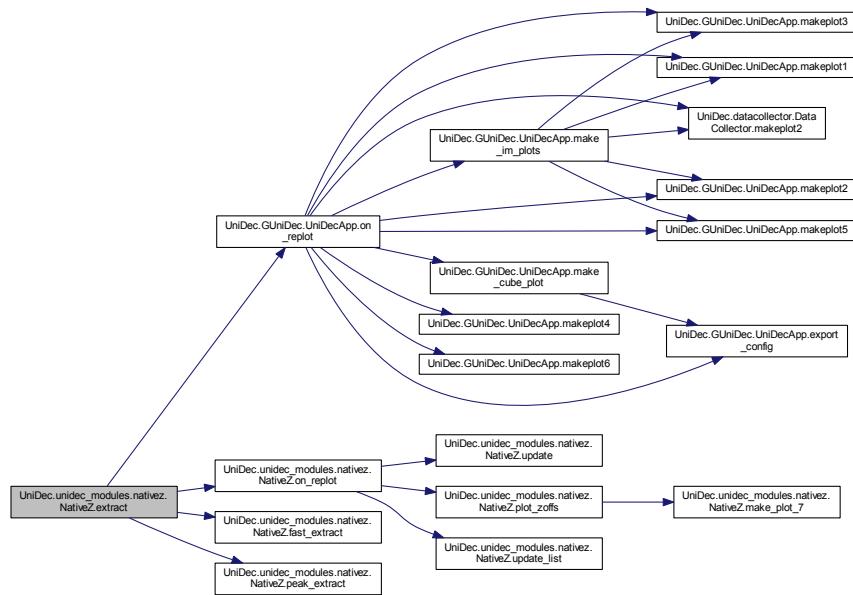
```
:param args: Passed to wx.Dialog
:param kwargs: Passed to wx.Dialog
:return: None
```

7.36.2 Member Function Documentation

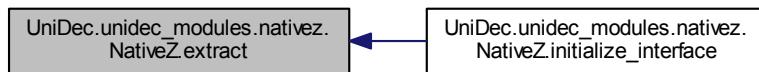
7.36.2.1 def UniDec.unidec_modules.nativez.NativeZ.extract(self, e)

Extract the mass distribution at each offset value, plot it, and write the outputs.
Call self.peak_extract
:param e: Unused event
:return: None

Here is the call graph for this function:



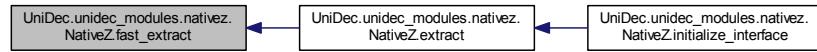
Here is the caller graph for this function:



7.36.2.2 def UniDec.unidec_modules.nativez.NativeZ.fast_extract(self, f, width, eshape)

Extract the intensity data for a specific charge offset from self.igrid. Mask all of the other data.
:param f: Charge offset
:param width: Width of the extraction (+/- from charge offset)
:param eshape: Shape of the extraction
0 = Box (+/- is a hard cutoff)
1 = Gaussian (+/- is std deviation of Gaussian)
:return: masked intensity values from self.igrid for a specific charge offset

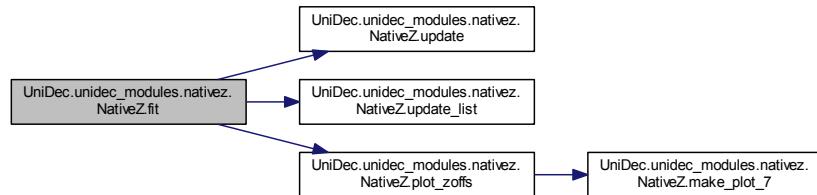
Here is the caller graph for this function:



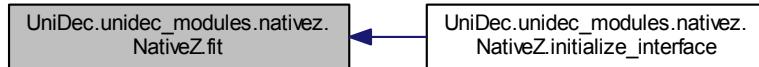
7.36.2.3 def UniDec.unidec_modules.nativez.NativeZ.fit (self, e)

Fit the offset totals to a series of overlapping Gaussians.
 Update the plots and listctrl from the result.
 :param e: Unused event
 :return: None

Here is the call graph for this function:



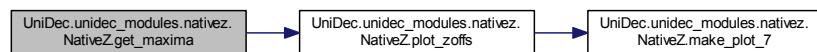
Here is the caller graph for this function:



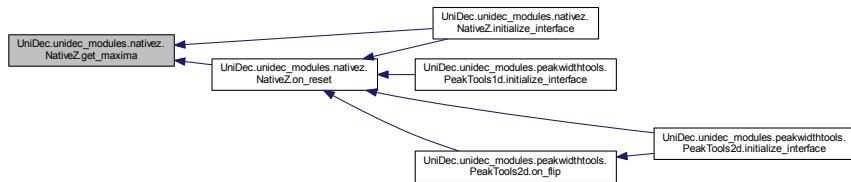
7.36.2.4 def UniDec.unidec_modules.nativez.NativeZ.get_maxima (self)

Detect peaks in self.offset_totals (the total extracted intensitites) and set default parameters.
 Plot the results.
 :return: None

Here is the call graph for this function:



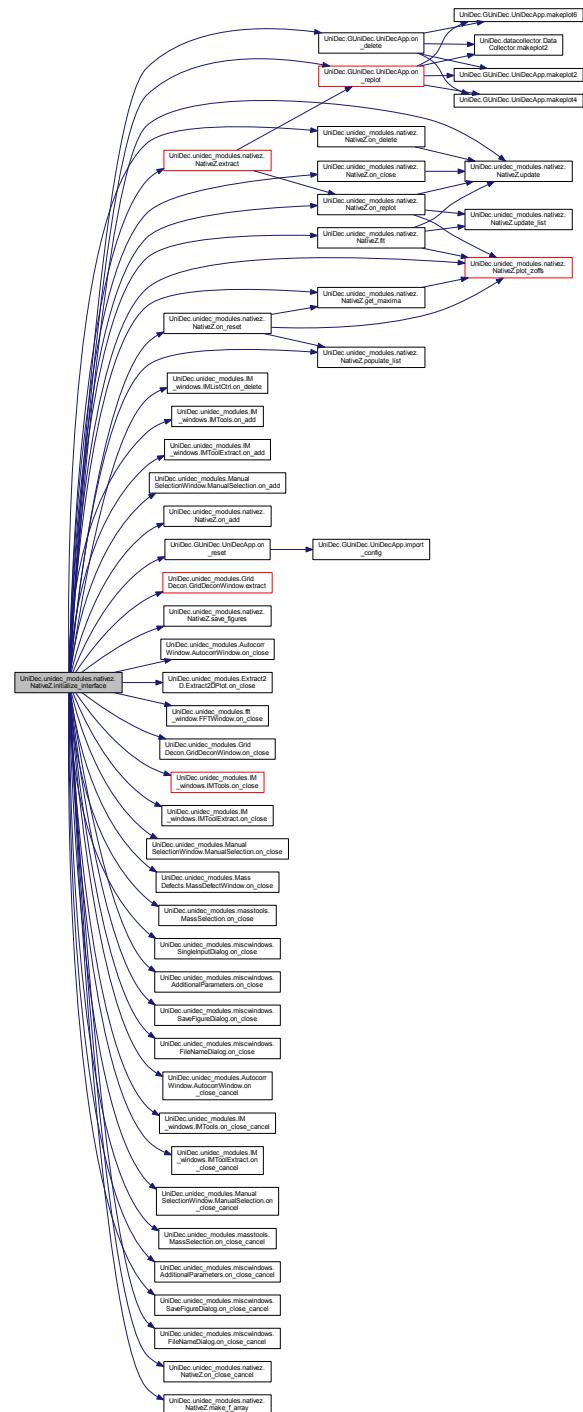
Here is the caller graph for this function:



7.36.2.5 def UniDec.unidec_modules.nativez.NativeZ.initialize_interface (*self*, *massaxis*, *chargeaxis*, *igrid*, *config*, *pks*)

Initialize the parameters, setup the GUI, and plot the intial results.
:param massaxis: Mass axis values
:param chargeaxis: Charge axis value
:param igrid: Intensities at each mass and charge point
:param config: UniDecConfig object
:param pks: Peaks object
:return: None

Here is the call graph for this function:



7.36.2.6 def UniDec.unidec.modules.nativez.NativeZ.make_f_array(self, minval, maxval, zwidth = 1)

Get the global offset parameters for the massaxis and chargeaxis.
Create a grid of mass and charge value.

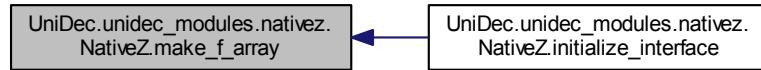
Create a grid of mass and charge value.
Calculate the charge offset at each point and store it at self.offset_grid.

Calculate the total intensity for each charge offset value +/- zwidth (default is 1).

```
:param minval: Minimum charge offset value  
:param maxval: Maximum charge offset value
```

```
:param zwidth: Tolerance window for the offset to be summed.
:return: None
```

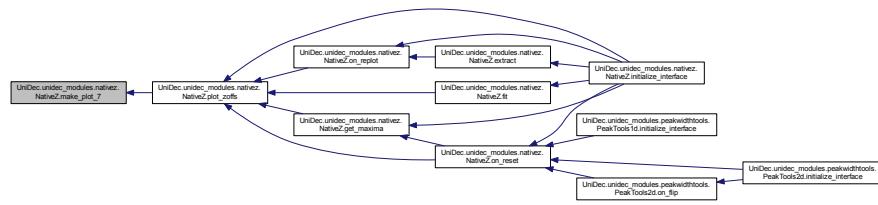
Here is the caller graph for this function:



7.36.2.7 def UniDec.unidec_modules.nativez.NativeZ.make_plot_7(self, e)

Plot the 2D mass v. charge plot.
 Add colored charge offset bands on top of the plot.
 :param e: Unused event
 :return: None

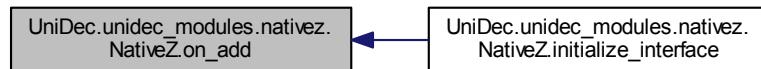
Here is the caller graph for this function:



7.36.2.8 def UniDec.unidec_modules.nativez.NativeZ.on_add(self, e)

Add a blank line to self.zlistctrl.
 :param e: Unused event
 :return: None

Here is the caller graph for this function:



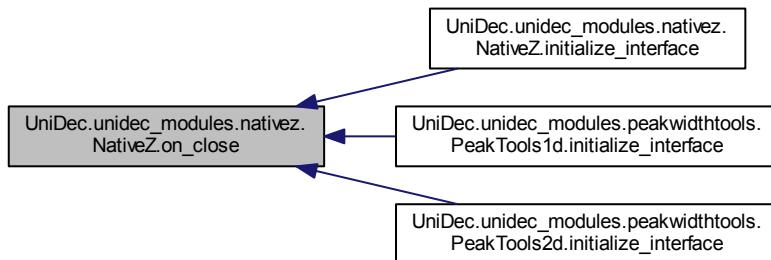
7.36.2.9 def UniDec.unidec_modules.nativez.NativeZ.on_close(self, e)

Close the window and update the parameters
 :param e:
 :return:

Here is the call graph for this function:



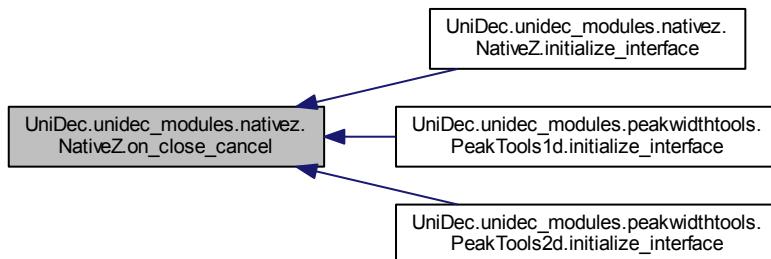
Here is the caller graph for this function:



7.36.2.10 def UniDec.unidec_modules.nativez.NativeZ.on_close_cancel (self, e)

Close the window but do not update the parameters.
:param e: Unused event
:return: None

Here is the caller graph for this function:

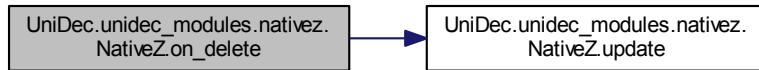


7.36.2.11 def UniDec.unidec_modules.nativez.NativeZ.on_delete (self, event)

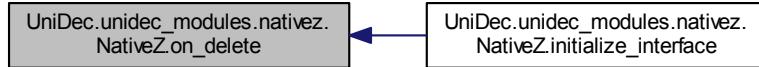
Delete item from the list ctrl.

```
:param event: wx.Button event
:return: None
```

Here is the call graph for this function:



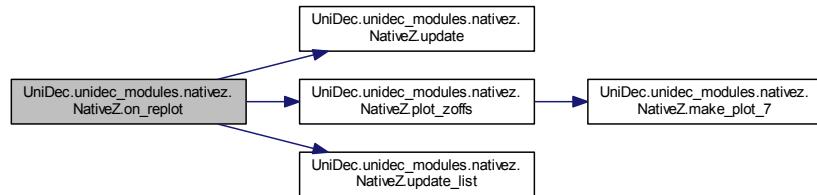
Here is the caller graph for this function:



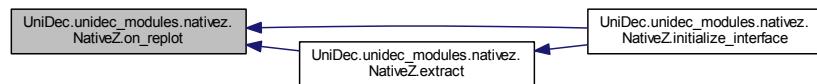
7.36.2.12 def UniDec.unidec_modules.nativez.NativeZ.on_replot(self, e)

Update the parameters and replot the results.
:param e: Unused event
:return: None

Here is the call graph for this function:



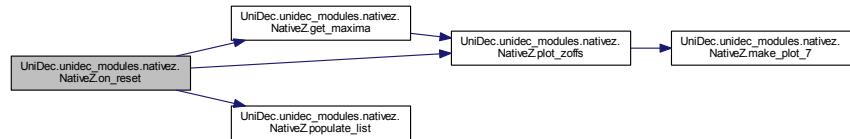
Here is the caller graph for this function:



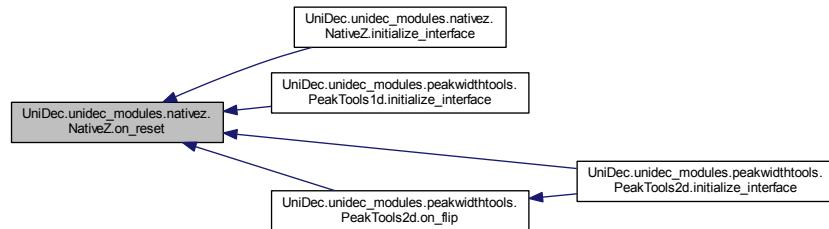
7.36.2.13 def UniDec.unidec_modules.nativez.NativeZ.on_reset(self, e)

Reset the listctrl and plots to the default states.
:param e: Unused event
:return: None

Here is the call graph for this function:



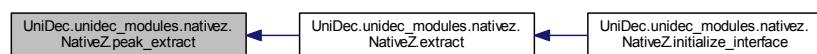
Here is the caller graph for this function:



7.36.2.14 def UniDec.unidec_modules.nativez.NativeZ.peak_extract(self)

Extract the values for local max (height) and area for peaks in pkls from each zoff.extract.
Plot the results.
Write the results to files.
:return: None

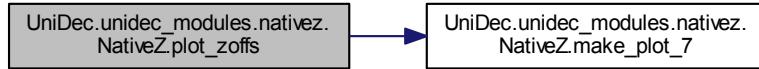
Here is the caller graph for this function:



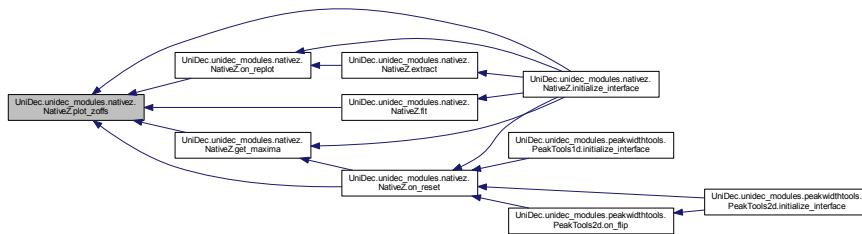
7.36.2.15 def UniDec.unidec_modules.nativez.NativeZ.plot_zoffs(self)

Plot the total charge offsets along with fits. Call self.make_plot_7.
:return: None

Here is the call graph for this function:



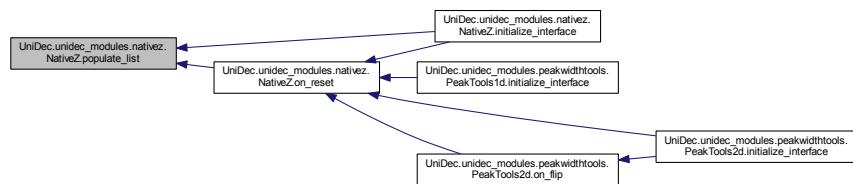
Here is the caller graph for this function:



7.36.2.16 def UniDec.unidec_modules.nativez.NativeZ.populate_list(self, e)

```
Add data from self.zoffs to self.zlistctrl.
:param e: Unused event
:return: None
```

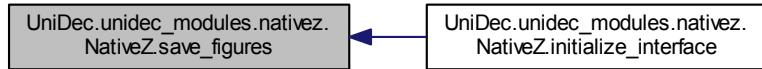
Here is the caller graph for this function:



7.36.2.17 def UniDec.unidec_modules.nativez.NativeZ.save_figures(self, e)

```
Save the figures as pdfs in the unidec folder.
:param e: Unused event
:return: None
```

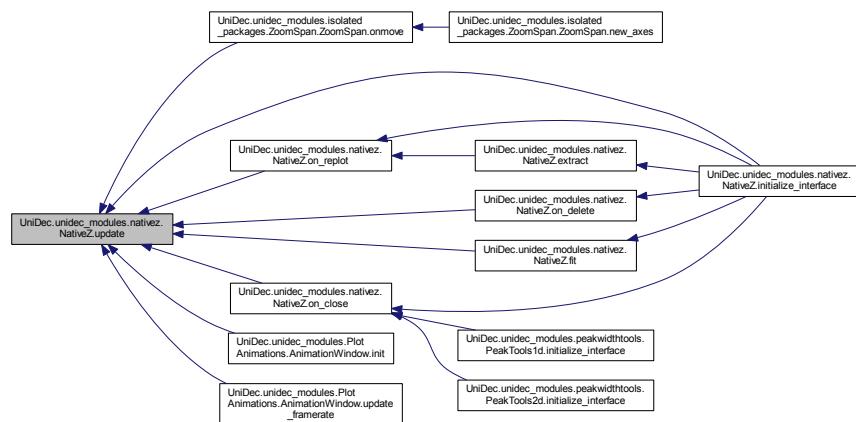
Here is the caller graph for this function:



7.36.2.18 def UniDec.unidec_modules.nativez.NativeZ.update (self, e)

```
Update self.zoffs from the self.zlistctrl. Update the intensities for each zoffset value.  
:param e:  
:return:
```

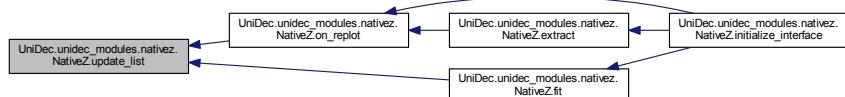
Here is the caller graph for this function:



7.36.2.19 def UniDec.unidec_modules.nativez.NativeZ.update_list(self)

```
Update self.zlistctrl from self.zoffs.  
:return: None
```

Here is the caller graph for this function:



7.36.3 Member Data Documentation

7.36.3.1 [UniDec.unidec_modules.nativez.NativeZ.chargeaxis](#)

7.36.3.2 [UniDec.unidec_modules.nativez.NativeZ.config](#)

7.36.3.3 [UniDec.unidec_modules.nativez.NativeZ.ctlfilt](#)

7.36.3.4 [UniDec.unidec_modules.nativez.NativeZ.ctlmassoffset](#)

7.36.3.5 [UniDec.unidec_modules.nativez.NativeZ.figsize](#)

7.36.3.6 [UniDec.unidec_modules.nativez.NativeZ.igrid](#)

7.36.3.7 [UniDec.unidec_modules.nativez.NativeZ.massaxis](#)

7.36.3.8 [UniDec.unidec_modules.nativez.NativeZ.massoffset](#)

7.36.3.9 [UniDec.unidec_modules.nativez.NativeZ.offset_grid](#)

7.36.3.10 [UniDec.unidec_modules.nativez.NativeZ.offset_totals](#)

7.36.3.11 [UniDec.unidec_modules.nativez.NativeZ.pks](#)

7.36.3.12 [UniDec.unidec_modules.nativez.NativeZ.plot1](#)

7.36.3.13 [UniDec.unidec_modules.nativez.NativeZ.plot2](#)

7.36.3.14 [UniDec.unidec_modules.nativez.NativeZ.plot3](#)

7.36.3.15 [UniDec.unidec_modules.nativez.NativeZ.plot4](#)

7.36.3.16 [UniDec.unidec_modules.nativez.NativeZ.plot5](#)

7.36.3.17 [UniDec.unidec_modules.nativez.NativeZ.plot6](#)

7.36.3.18 [UniDec.unidec_modules.nativez.NativeZ.plot7](#)

7.36.3.19 [UniDec.unidec_modules.nativez.NativeZ.zlistctrl](#)

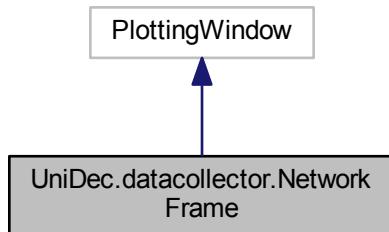
7.36.3.20 [UniDec.unidec_modules.nativez.NativeZ.zoffs](#)

The documentation for this class was generated from the following file:

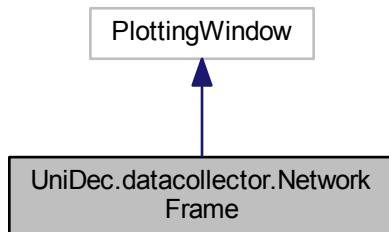
- C:/Python/UniDec/unidec_modules/[nativez.py](#)

7.37 UniDec.datacollector.NetworkFrame Class Reference

Inheritance diagram for UniDec.datacollector.NetworkFrame:



Collaboration diagram for UniDec.datacollector.NetworkFrame:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `clear_frame` (self)

Public Attributes

- `axes`
- `flag`

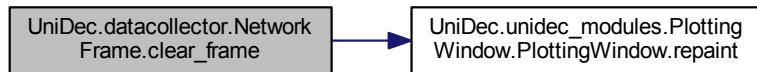
7.37.1 Constructor & Destructor Documentation

7.37.1.1 def `UniDec.datacollector.NetworkFrame.__init__ (self, args, kwargs)`

7.37.2 Member Function Documentation

7.37.2.1 def UniDec.datacollector.NetworkFrame.clear_frame (*self*)

Here is the call graph for this function:



7.37.3 Member Data Documentation

7.37.3.1 UniDec.datacollector.NetworkFrame.axes

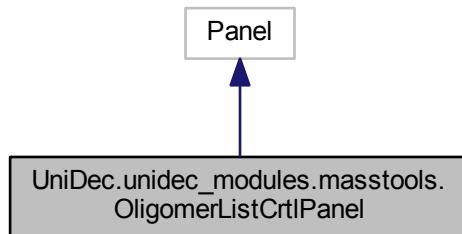
7.37.3.2 UniDec.datacollector.NetworkFrame.flag

The documentation for this class was generated from the following file:

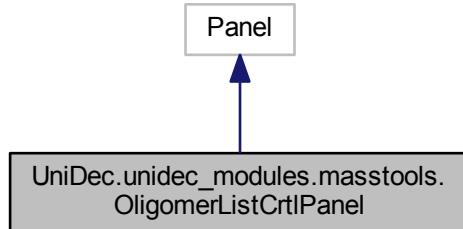
- C:/Python/UniDec/[datacollector.py](#)

7.38 UniDec.unidec_modules.masstools.OligomerListCrtlPanel Class Reference

Inheritance diagram for UniDec.unidec_modules.masstools.OligomerListCrtlPanel:



Collaboration diagram for UniDec.unidec_modules.masstools.OligomerListCtrlPanel:



Public Member Functions

- def [__init__](#) (self, parent)

Public Attributes

- [list](#)

7.38.1 Constructor & Destructor Documentation

7.38.1.1 def UniDec.unidec_modules.masstools.OligomerListCtrlPanel.[__init__](#) (self, parent)

```
ListCtrlPanel for the Oligomer list
:param parent: Parent panel or window
:return: None
```

7.38.2 Member Data Documentation

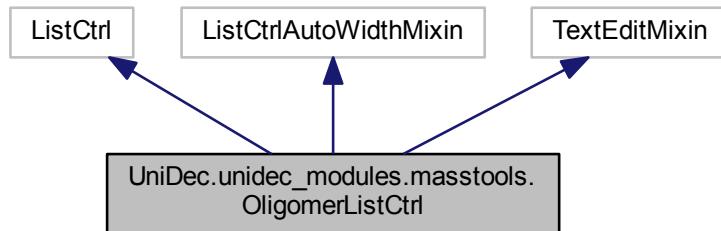
7.38.2.1 UniDec.unidec_modules.masstools.OligomerListCtrlPanel.list

The documentation for this class was generated from the following file:

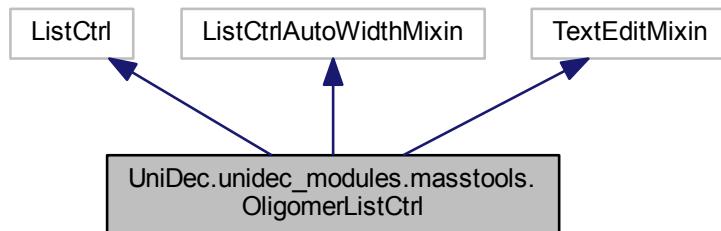
- C:/Python/UniDec/unidec_modules/[masstools.py](#)

7.39 UniDec.unidec_modules.masstools.OligomerListCtrl Class Reference

Inheritance diagram for UniDec.unidec_modules.masstools.OligomerListCtrl:



Collaboration diagram for UniDec.unidec_modules.masstools.OligomerListCtrl:



Public Member Functions

- def `__init__`
- def `clear (self)`
- def `add_line (self)`
- def `populate (self, data)`
- def `get_list (self)`
- def `on_right_click_oligolist (self, event)`
- def `on_oligo_delete (self, event)`

Public Attributes

- `index`
- `popupID2`

7.39.1 Constructor & Destructor Documentation

7.39.1.1 `def UniDec.unidec_modules.masstools.OligomerListCtrl.__init__(self, parent, id_value, pos = wx.DefaultPosition, size = wx.DefaultSize, style = 0)`

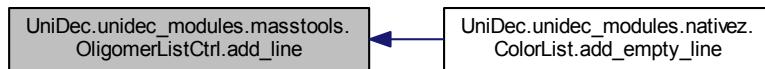
```
Create a 5 column list ctrl.
:param parent: Passed to wx.ListCtrl
:param id_value: Passed to wx.ListCtrl
:param pos: Passed to wx.ListCtrl
:param size: Passed to wx.ListCtrl
:param style: Passed to wx.ListCtrl
:return: None
```

7.39.2 Member Function Documentation

7.39.2.1 `def UniDec.unidec_modules.masstools.OligomerListCtrl.add_line(self)`

```
Add a blank line to the list.
:return: None
```

Here is the caller graph for this function:



7.39.2.2 `def UniDec.unidec_modules.masstools.OligomerListCtrl.clear(self)`

```
Clear the list.
:return: None
```

7.39.2.3 `def UniDec.unidec_modules.masstools.OligomerListCtrl.get_list(self)`

```
Return the values on the apanel as a nested list.
:return: List of values in N x 5 format.
```

7.39.2.4 `def UniDec.unidec_modules.masstools.OligomerListCtrl.on_oligo_delete(self, event)`

```
Delete the selected item.
:param event: Unused event
:return: None
```

7.39.2.5 `def UniDec.unidec_modules.masstools.OligomerListCtrl.on_right_click_oligolist(self, event)`

```
Open a right click menu
:param event: Unused event
:return: None
```

7.39.2.6 def UniDec.unidec_modules.masstools.OligomerListCtrl.populate(self, data)

```
Populate from an N x 4 or N x 5 array into the listctrl.  
:param data: Array  
:return: None
```

7.39.3 Member Data Documentation

7.39.3.1 UniDec.unidec_modules.masstools.OligomerListCtrl.index

7.39.3.2 UniDec.unidec_modules.masstools.OligomerListCtrl.popupID2

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/masstools.py

7.40 UniDec.unidec_modules.peakstructure.Peak Class Reference

Public Member Functions

- def [__init__](#)(self)

Public Attributes

- mass
- height
- ccs
- area
- color
- label
- marker
- textmarker
- ignore
- match
- matcherror
- integral
- integralrange
- mztab
- mztab2
- stickdat
- kendricknum
- kendrickdefect
- kmass
- score
- corrint
- correrr
- mztabi
- massavg
- masserr
- tval
- peakmasses
- fitmassavg
- fitmasserr
- fitarea
- fitareaerr
- diff

7.40.1 Detailed Description

Class for a single peak. Contains all key parameters for describing and plotting the peak.

7.40.2 Constructor & Destructor Documentation

7.40.2.1 def UniDec.unidec_modules.peakstructure.Peak.__init__(self)

Initialize all parameters for the peak to defaults

7.40.3 Member Data Documentation

7.40.3.1 UniDec.unidec_modules.peakstructure.Peak.area

7.40.3.2 UniDec.unidec_modules.peakstructure.Peak.ccs

7.40.3.3 UniDec.unidec_modules.peakstructure.Peak.color

7.40.3.4 UniDec.unidec_modules.peakstructure.Peak.correrr

7.40.3.5 UniDec.unidec_modules.peakstructure.Peak.corrint

7.40.3.6 UniDec.unidec_modules.peakstructure.Peak.diff

7.40.3.7 UniDec.unidec_modules.peakstructure.Peak.fitarea

7.40.3.8 UniDec.unidec_modules.peakstructure.Peak.fitareaerr

7.40.3.9 UniDec.unidec_modules.peakstructure.Peak.fitmassavg

7.40.3.10 UniDec.unidec_modules.peakstructure.Peak.fitmasserr

7.40.3.11 UniDec.unidec_modules.peakstructure.Peak.height

7.40.3.12 UniDec.unidec_modules.peakstructure.Peak.ignore

7.40.3.13 UniDec.unidec_modules.peakstructure.Peak.integral

7.40.3.14 UniDec.unidec_modules.peakstructure.Peak.integralrange

7.40.3.15 UniDec.unidec_modules.peakstructure.Peak.kendrickdefect

7.40.3.16 UniDec.unidec_modules.peakstructure.Peak.kendricknum

7.40.3.17 UniDec.unidec_modules.peakstructure.Peak.kmass

7.40.3.18 UniDec.unidec_modules.peakstructure.Peak.label

7.40.3.19 UniDec.unidec_modules.peakstructure.Peak.marker

7.40.3.20 UniDec.unidec_modules.peakstructure.Peak.mass

7.40.3.21 UniDec.unidec_modules.peakstructure.Peak.massavg

7.40.3.22 UniDec.unidec_modules.peakstructure.Peak.masserr

7.40.3.23 UniDec.unidec_modules.peakstructure.Peak.match

7.40.3.24 UniDec.unidec_modules.peakstructure.Peak.matcherror

7.40.3.25 UniDec.unidec_modules.peakstructure.Peak.mztab

7.40.3.26 UniDec.unidec_modules.peakstructure.Peak.mztab2

7.40.3.27 UniDec.unidec_modules.peakstructure.Peak.mztabi

7.40.3.28 UniDec.unidec_modules.peakstructure.Peak.peakmasses

7.40.3.29 UniDec.unidec_modules.peakstructure.Peak.score

7.40.3.30 UniDec.unidec_modules.peakstructure.Peak.stickdat

7.40.3.31 UniDec.unidec_modules.peakstructure.Peak.textmarker

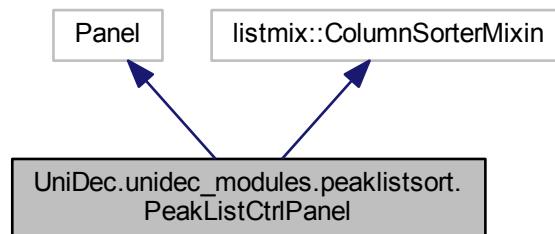
7.40.3.32 UniDec.unidec_modules.peakstructure.Peak.tval

The documentation for this class was generated from the following file:

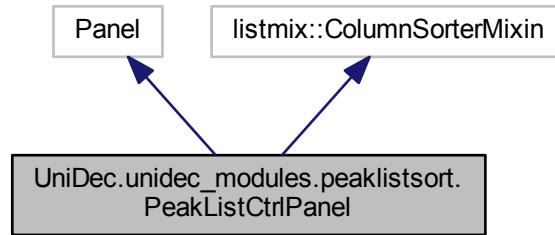
- C:/Python/UniDec/unidec_modules/peakstructure.py

7.41 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel Class Reference

Inheritance diagram for UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel:



Collaboration diagram for UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel:



Public Member Functions

- def `__init__` (self, parent)
- def `clear_list` (self)
- def `add_data`
- def `GetListCtrl` (self)
- def `on_column_click` (self, event)
- def `on_right_click`
- def `on_popup_one`
- def `on_popup_two`
- def `on_popup_six`
- def `on_popup_three`
- def `on_popup_four`
- def `on_popup_five`

Public Attributes

- `index`
- `list_ctrl`
- `EVT_DELETE_SELECTION_2`
- `EVT_CHARGE_STATE`
- `EVT_Differences`
- `remove`
- `selection`
- `selection2`
- `pks`
- `popupID1`
- `popupID2`
- `popupID3`
- `popupID4`
- `popupID5`
- `popupID6`

7.41.1 Detailed Description

Creates a list control panel for displaying and interacting with Peaks object

7.41.2 Constructor & Destructor Documentation

7.41.2.1 def UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.__init__(self, parent)

```
Initialize list_ctrl, bind events, and setup events to be broadcast back.
:param parent: Parent of panel that will be created
:return: None
```

7.41.3 Member Function Documentation

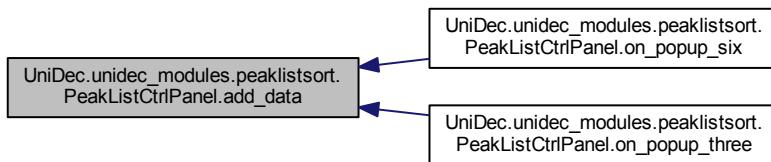
7.41.3.1 def UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.add_data(self, pks, show = "area", collab1 = "Mass (Da)")

```
Add data from a Peaks object to the list_ctrl
:param pks: Peaks object
:param show: Keyword describing what to show in column 1

area = p.area
integral = p.integral
diff = p.diff

:param collab1: Column 1 label
:return: None
```

Here is the caller graph for this function:



7.41.3.2 def UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.clear_list(self)

```
Remove all elements from list_ctrl
:return: None
```

7.41.3.3 def UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.GetListCtrl(self)

7.41.3.4 def UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.on_column_click(self, event)

7.41.3.5 def UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.on_popup_five(self, event = None)

```
Spawns a dialog for the first selected item to select the color.
Redraws the list control with the new colors and then triggers an EVT_DELETE_SELECTION_2.
:param event: Unused Event
:return: None
```

7.41.3.6 def UniDec.unidec_modules.peaklists.sort.PeakListCtrlPanel.on_popup_four (self, event=None)

Gets the selected items and adds it self.selection2. Triggers EVT_CHARGE_STATE.
 :param event:
 :return:

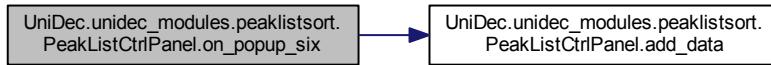
7.41.3.7 def UniDec.unidec_modules.peaklists.sort.PeakListCtrlPanel.on_popup_one (self, event=None)

The selected peaks are added to self.selection and deleted. For each delete peak, p.ignore is set to 1.
 Triggers EVT_DELETE_SELECTION_2.
 :param event: Unused Event
 :return: None

7.41.3.8 def UniDec.unidec_modules.peaklists.sort.PeakListCtrlPanel.on_popup_six (self, event=None)

Triggers EVT_DIFFERENCES. The first selected item becomes the reference mass. The difference between all masses and the reference mass is calculated and displayed in column 3.
 :param event: Unused Event
 :return: None

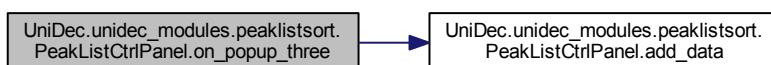
Here is the call graph for this function:



7.41.3.9 def UniDec.unidec_modules.peaklists.sort.PeakListCtrlPanel.on_popup_three (self, event=None)

Repopulates the list control with all elements in self.pks.peaks.
 :param event: Unused event
 :return: None

Here is the call graph for this function:



7.41.3.10 def UniDec.unidec_modules.peaklists.sort.PeakListCtrlPanel.on_popup_two (self, event=None)

The selected peaks are added to self.selection. All other peaks are deleted from list ctrl and p.ignore for each is set to 1.
 Triggers EVT_DELETE_SELECTION_2.
 :param event: Unused Event
 :return: None

7.41.3.11 def UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.on_right_click (self, event =None)

```
Spawn right click menu
:param event: Unused Event
:return: None
```

7.41.4 Member Data Documentation

7.41.4.1 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.EVT_CHARGE_STATE

7.41.4.2 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.EVT_DELETE_SELECTION_2

7.41.4.3 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.EVT_DIFFERENCES

7.41.4.4 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.index

7.41.4.5 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.list_ctrl

7.41.4.6 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.pks

7.41.4.7 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.popupID1

7.41.4.8 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.popupID2

7.41.4.9 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.popupID3

7.41.4.10 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.popupID4

7.41.4.11 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.popupID5

7.41.4.12 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.popupID6

7.41.4.13 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.remove

7.41.4.14 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.selection

7.41.4.15 UniDec.unidec_modules.peaklistsort.PeakListCtrlPanel.selection2

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/[peaklistsort.py](#)

7.42 UniDec.unidec_modules.peakstructure.Peaks Class Reference

Public Member Functions

- def [__init__](#) (self)
- def [add_peaks](#)
- def [default_params](#)
- def [get_mass_defects](#)
- def [score_peaks](#)

Public Attributes

- `peaks`
- `plen`
- `changed`
- `masses`
- `convolved`
- `composite`
- `peakcolors`
- `markers`
- `colormap`
- `textmarkers`
- `marklen`
- `massbins`

7.42.1 Detailed Description

Class containing all useful data about peaks.

The peaks themselves are of the `Peak` class and contained within the `self.peaks` list.

7.42.2 Constructor & Destructor Documentation

7.42.2.1 def UniDec.unidec_modules.peakstructure.Peaks.__init__(self)

Initialize Peaks class and set empty values
`:return:` None

7.42.3 Member Function Documentation

7.42.3.1 def UniDec.unidec_modules.peakstructure.Peaks.add_peaks(self, parray, massbins = 0)

Create peak objects from an array
`:param parray:` N x 2 array containing (mass, height) of each peak.
`:param massbins:` Describes the precision of the mass inputs by describing the bin size on the mass axis.
`:return:` None

7.42.3.2 def UniDec.unidec_modules.peakstructure.Peaks.default_params(self, cmap = "rainbow")

Set default parameters for peaks, such as color, label, and marker
`:param cmap:` Colormap from `matplotlib.cm`
`:return:` None

7.42.3.3 def UniDec.unidec_modules.peakstructure.Peaks.get_mass_defects(self, kendrickmass, mode = 0)

Get the mass defects and mass number for each peak
`:param kendrickmass:` Kendrick reference mass
`:param mode:` Select range of defects 1=(0,1), 0=(-0.5,0.5)
`:return:` None

7.42.3.4 def UniDec.unidec_modules.peakstructure.Peaks.score_peaks(self, thresh = 0, ci = 0.99)

For each peak, assign a score of the fractional number of charge states observed.
`:param thresh:` Optional threshold to define a noise floor.
`:return:` None

7.42.4 Member Data Documentation

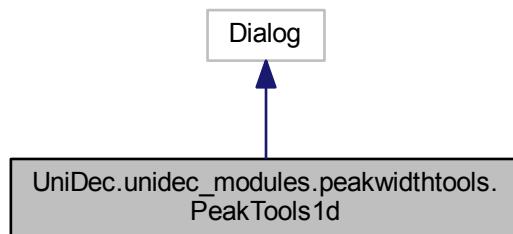
- 7.42.4.1 `UniDec.unidec_modules.peakstructure.Peaks.changed`
- 7.42.4.2 `UniDec.unidec_modules.peakstructure.Peaks.colormap`
- 7.42.4.3 `UniDec.unidec_modules.peakstructure.Peaks.composite`
- 7.42.4.4 `UniDec.unidec_modules.peakstructure.Peaks.convolved`
- 7.42.4.5 `UniDec.unidec_modules.peakstructure.Peaks.markers`
- 7.42.4.6 `UniDec.unidec_modules.peakstructure.Peaks.marklen`
- 7.42.4.7 `UniDec.unidec_modules.peakstructure.Peaks.massbins`
- 7.42.4.8 `UniDec.unidec_modules.peakstructure.Peaks.masses`
- 7.42.4.9 `UniDec.unidec_modules.peakstructure.Peaks.peakcolors`
- 7.42.4.10 `UniDec.unidec_modules.peakstructure.Peaks.peaks`
- 7.42.4.11 `UniDec.unidec_modules.peakstructure.Peaks.plen`
- 7.42.4.12 `UniDec.unidec_modules.peakstructure.Peaks.textmarkers`

The documentation for this class was generated from the following file:

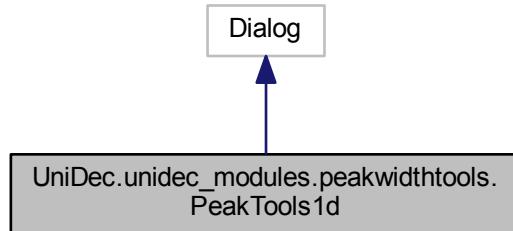
- C:/Python/UniDec/unidec_modules/[peakstructure.py](#)

7.43 UniDec.unidec_modules.peakwidthtools.PeakTools1d Class Reference

Inheritance diagram for UniDec.unidec_modules.peakwidthtools.PeakTools1d:



Collaboration diagram for UniDec.unidec_modules.peakwidthtools.PeakTools1d:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `initialize_interface` (self, config, data)
- def `on_close` (self, e)
- def `on_close_cancel` (self, e)
- def `on_reset` (self, e)
- def `on_center` (self, e)
- def `on_plot` (self, e)
- def `on_fit` (self, e)

Public Attributes

- `config`
- `data`
- `centdat`
- `psfun`
- `plot1`
- `resbox`
- `ctlpsfun`
- `ctlmzsig`
- `errorbox`

7.43.1 Constructor & Destructor Documentation

7.43.1.1 def UniDec.unidec_modules.peakwidthtools.PeakTools1d.__init__ (self, args, kwargs)

Create a dialog for fitting the peak shapes from the data.
:param args: Passed to wx.Dialog
:param kwargs: Passed to wx.Dialog
:return: None

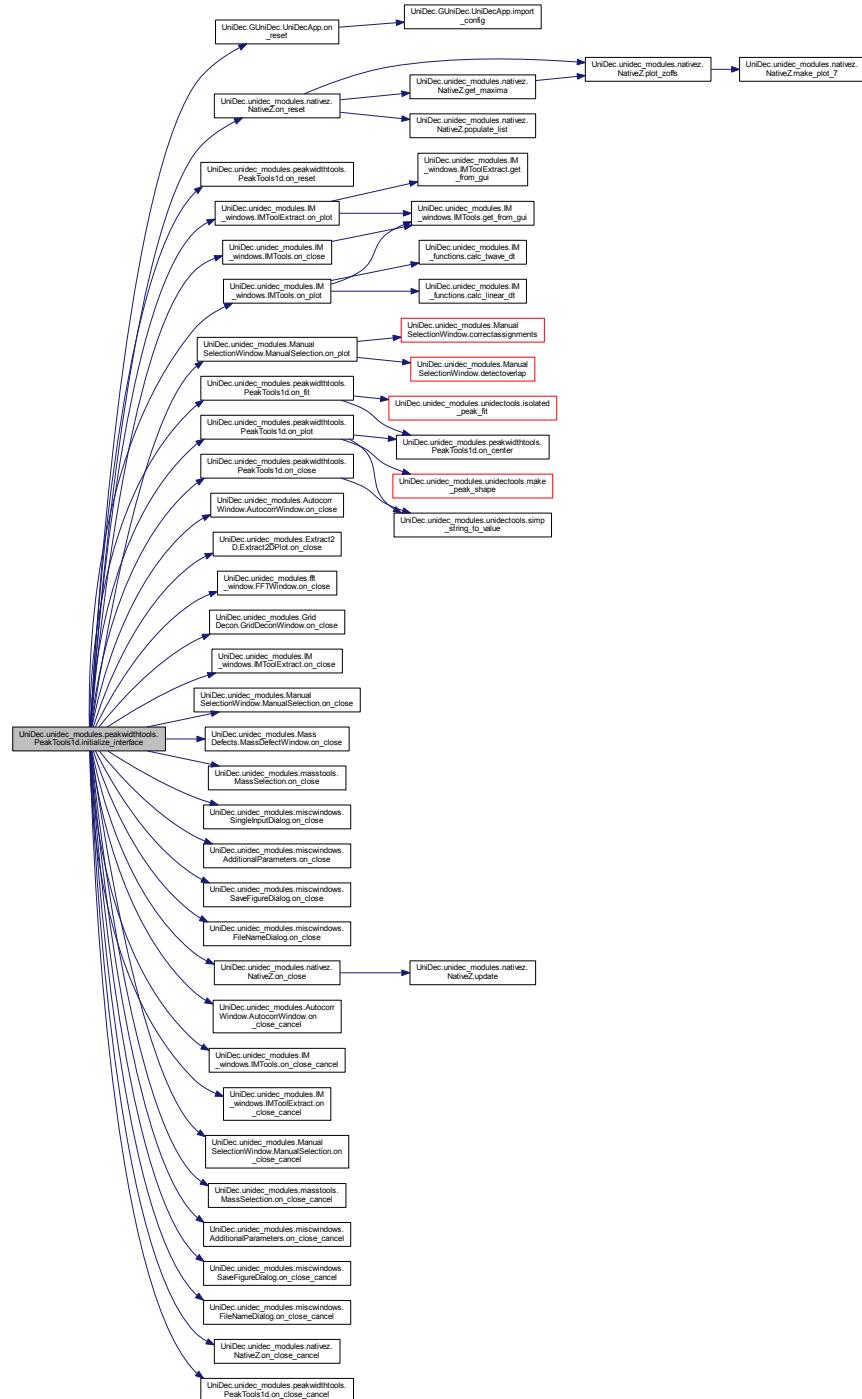
7.43.2 Member Function Documentation

7.43.2.1 def UniDec.unidec_modules.peakwidthtools.PeakTools1d.initialize_interface (self, config, data)

Create the GUI, import the paramters, and plot the intial data.

```
:param config: UniDecConfig Object
:param data: Data array (N x 2)
:return: None
```

Here is the call graph for this function:

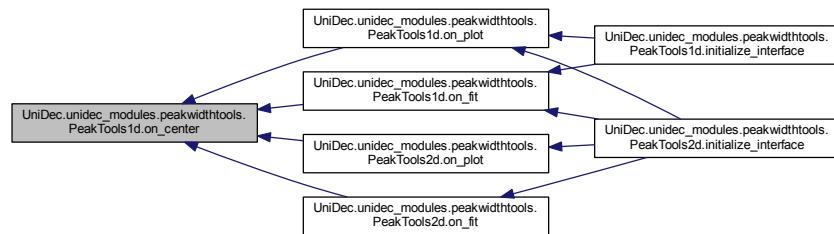


7.43.2.2 def UniDec.unidec_modules.peakwidthtools.PeakTools1d.on_center(self, e)

Crop the range to the values from the plot and replot the cropped data.

Note this is a bit clumsy. Hopefully someone will come along and make this more elegant someday...
:param e: Unused event
:return: None

Here is the caller graph for this function:



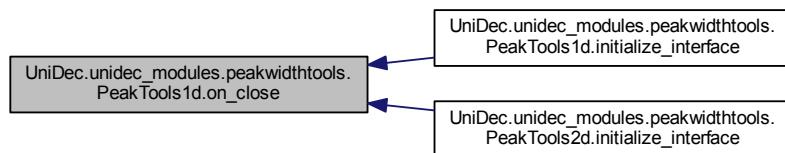
7.43.2.3 def UniDec.unidec_modules.peakwidthtools.PeakTools1d.on_close (self, e)

Close the window and update self.config.psfun and self.config.mzsig from the parameters in the GUI.
:param e: Unused event
:return: None

Here is the call graph for this function:



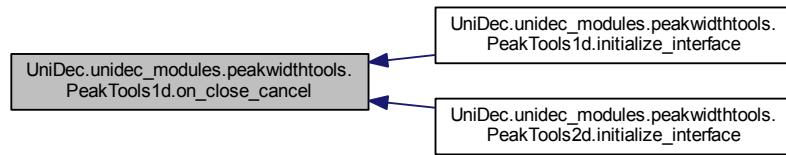
Here is the caller graph for this function:



7.43.2.4 def UniDec.unidec_modules.peakwidthtools.PeakTools1d.on_close_cancel (self, e)

Close the window but do not update the parameters.
:param e: Unused event
:return: None

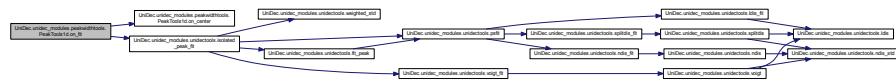
Here is the caller graph for this function:



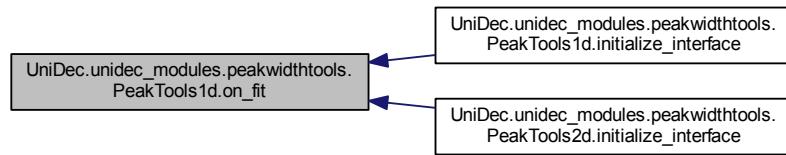
7.43.2.5 def UniDec.unidec_modules.peakwidthtools.PeakTools1d.on_fit(self, e)

```
Perform the fit, update the GUI, and plot the results.  
:param e: Unused event  
:return: None
```

Here is the call graph for this function:



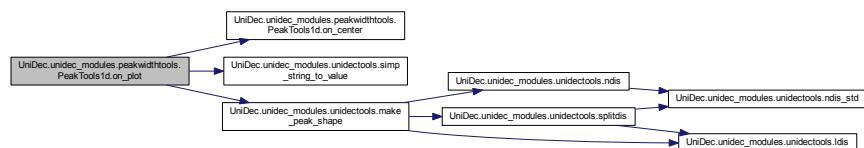
Here is the caller graph for this function:



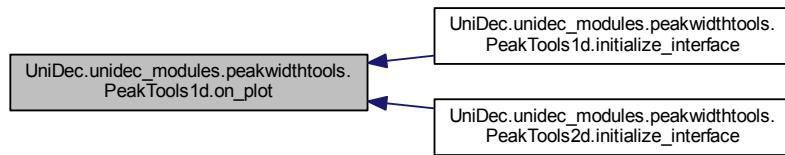
7.43.2.6 def UniDec.unidec_modules.peakwidthtools.PeakTools1d.on_plot(self, e)

```
For the sigma value in the self.ctrlmzsig, plot a simulated peak.  
:param e: Unused event  
:return: None
```

Here is the call graph for this function:



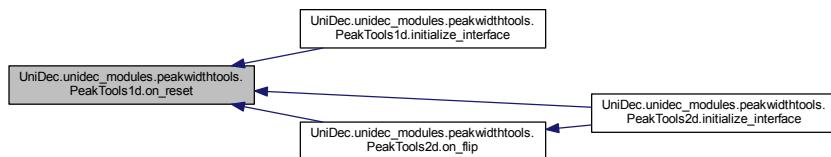
Here is the caller graph for this function:



7.43.2.7 def UniDec.unidec_modules.peakwidthtools.PeakTools1d.on_reset(self, e)

Reset the plot to the full range.
:param e: Unused event
:return:

Here is the caller graph for this function:



7.43.3 Member Data Documentation

7.43.3.1 UniDec.unidec_modules.peakwidthtools.PeakTools1d.centdat

7.43.3.2 UniDec.unidec_modules.peakwidthtools.PeakTools1d.config

7.43.3.3 UniDec.unidec_modules.peakwidthtools.PeakTools1d.ctlmzsig

7.43.3.4 UniDec.unidec_modules.peakwidthtools.PeakTools1d.ctlpsfun

7.43.3.5 UniDec.unidec_modules.peakwidthtools.PeakTools1d.data

7.43.3.6 UniDec.unidec_modules.peakwidthtools.PeakTools1d.errorbox

7.43.3.7 UniDec.unidec_modules.peakwidthtools.PeakTools1d.plot1

7.43.3.8 UniDec.unidec_modules.peakwidthtools.PeakTools1d.psfun

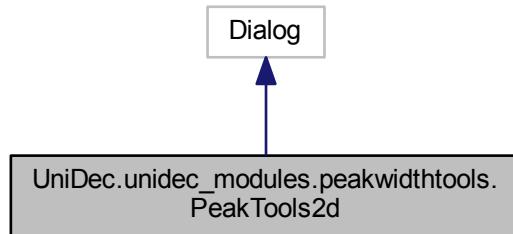
7.43.3.9 UniDec.unidec_modules.peakwidthtools.PeakTools1d.resbox

The documentation for this class was generated from the following file:

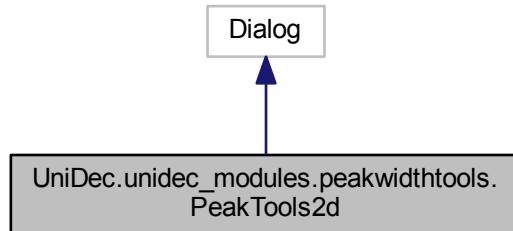
- C:/Python/UniDec/unidec_modules/[peakwidthtools.py](#)

7.44 UniDec.unidec_modules.peakwidthtools.PeakTools2d Class Reference

Inheritance diagram for UniDec.unidec_modules.peakwidthtools.PeakTools2d:



Collaboration diagram for UniDec.unidec_modules.peakwidthtools.PeakTools2d:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `initialize_interface` (self, data3, `data2`, `config`)
- def `on_close` (self, e)
- def `on_close_cancel` (self, e)
- def `on_flip` (self, e)
- def `on_reset` (self, e)
- def `on_center` (self, e)
- def `on_plot` (self, e)
- def `on_fit` (self, e)

Public Attributes

- `plot1`
- `flipbutton`
- `outmzsig`

- [outdtsig](#)
- [ctlpsfun](#)
- [ctlsigguess](#)
- [errorbox](#)
- [resbox](#)
- [config](#)
- [psfun](#)
- [flipflag](#)
- [centdat](#)
- [data](#)
- [data2](#)
- [mz](#)
- [dt](#)
- [C](#)
- [fitmid](#)
- [fitsig](#)

7.44.1 Constructor & Destructor Documentation

7.44.1.1 def UniDec.unidec_modules.peakwidthtools.PeakTools2d.__init__(self, args, kwargs)

Create a dialog for fitting peak shapes in 2D IM-MS data. Fits 1D first in MS then flips to other dimension.

```
:param args:
:param kwargs:
:return:
```

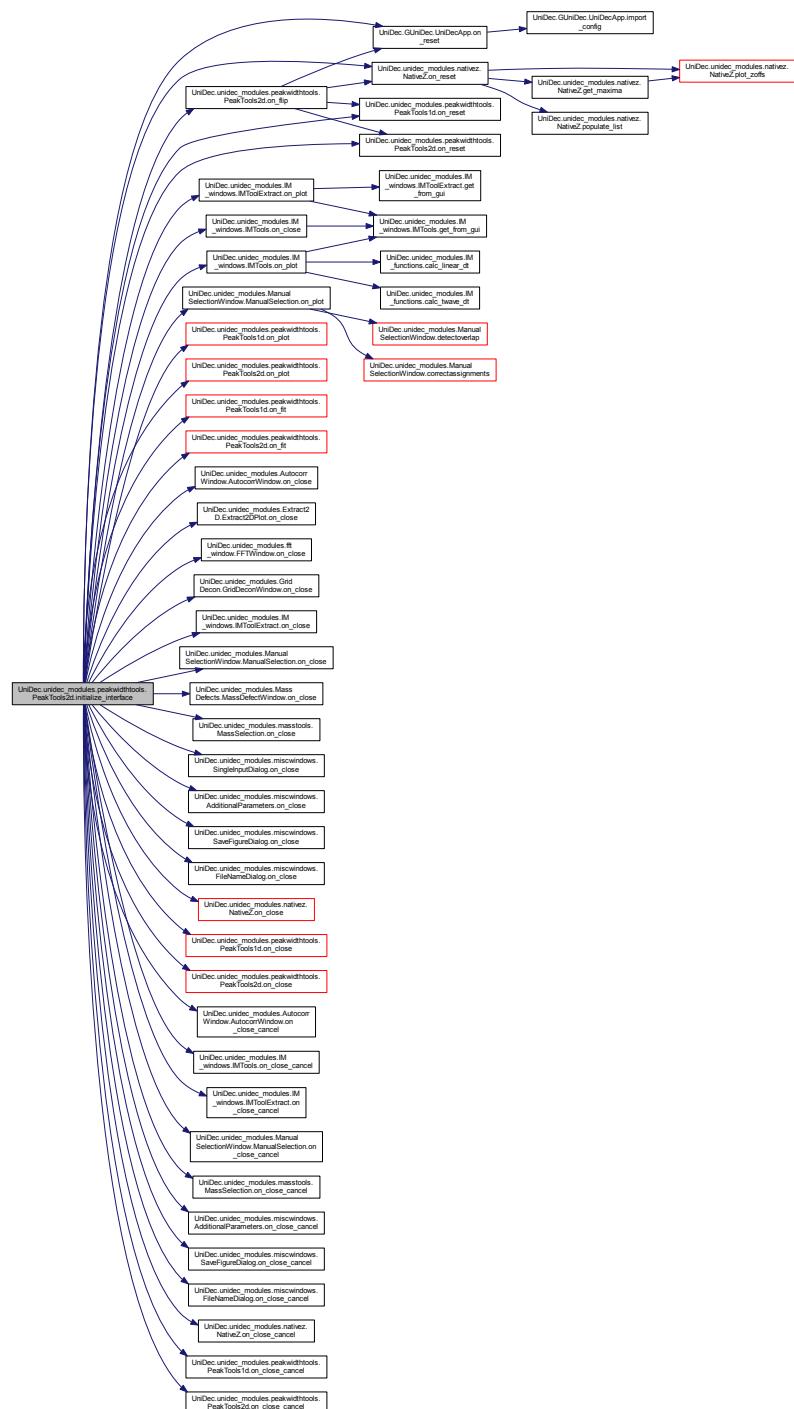
7.44.2 Member Function Documentation

7.44.2.1 def UniDec.unidec_modules.peakwidthtools.PeakTools2d.initialize_interface(self, data3, data2, config)

Initialize the parameters, create the interface, plot the initial data.

```
:param data3: 2D IM-MS data
:param data2: 1D MS data
:param config: UniDecConfig Object
:return: None
```

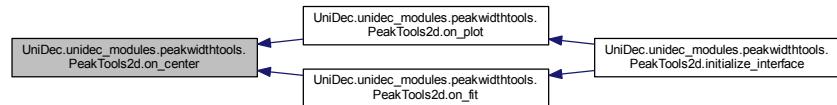
Here is the call graph for this function:



7.44.2.2 def UniDec.unidec_modules.peakwidthtools.PeakTools2d.on_center(self, e)

Gets the range from the current plot zoom, cuts the data, and plots the cut data.
:param e: Unused event
:returns: None

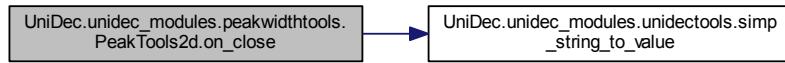
Here is the caller graph for this function:



7.44.2.3 def UniDec.unidec_modules.peakwidthtools.PeakTools2d.on_close (self, e)

```
Close the window and update self.config from the new values.
:param e: Unused event
:return: None
```

Here is the call graph for this function:



Here is the caller graph for this function:



7.44.2.4 def UniDec.unidec_modules.peakwidthtools.PeakTools2d.on_close_cancel (self, e)

```
Close the window but do not update self.config.
:param e: Unused event
:return: None
```

Here is the caller graph for this function:



7.44.2.5 def UniDec.unidec_modules.peakwidthtools.PeakTools2d.on_fit(self, e)

```
Fits the spectrum and outputs the results.  
:param e:  
:return:
```

Here is the call graph for this function:



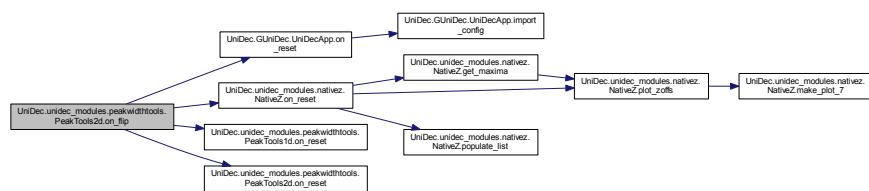
Here is the caller graph for this function:



7.44.2.6 def UniDec.unidec_modules.peakwidthtools.PeakTools2d.on_flip (self, e)

```
Flip from m/z to arrival time at the previously fit m/z value.  
:param e: Unused event  
:return: None
```

Here is the call graph for this function:



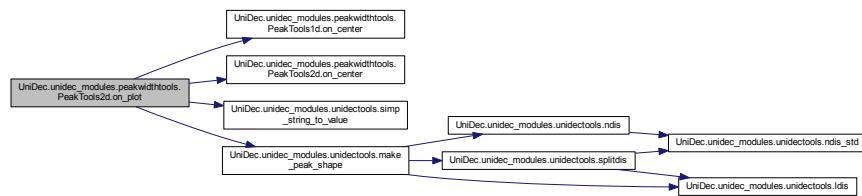
Here is the caller graph for this function:



7.44.2.7 def UniDec.unidec_modules.peakwidthtools.PeakTools2d.on_plot(self, e)

Plot a predicted peak shape based on the values input into the control.
:param e: Unused event
:return: None

Here is the call graph for this function:



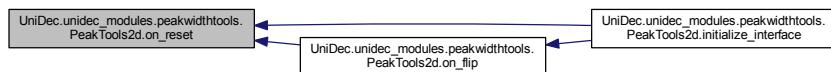
Here is the caller graph for this function:



7.44.2.8 def UniDec.unidec_modules.peakwidthtools.PeakTools2d.on_reset(self, e)

Resets the plot.
:param e: Unused event
:return: None

Here is the caller graph for this function:



7.44.3 Member Data Documentation

7.44.3.1 UniDec.unidec_modules.peakwidthtools.PeakTools2d.C

7.44.3.2 UniDec.unidec_modules.peakwidthtools.PeakTools2d.centdat

7.44.3.3 UniDec.unidec_modules.peakwidthtools.PeakTools2d.config

7.44.3.4 UniDec.unidec_modules.peakwidthtools.PeakTools2d.ctlpsfun

7.44.3.5 UniDec.unidec_modules.peakwidthtools.PeakTools2d.ctlsigguess

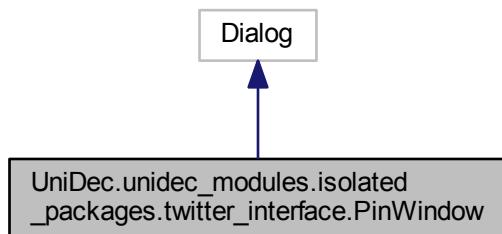
- 7.44.3.6 UniDec.unidec_modules.peakwidthtools.PeakTools2d.data
- 7.44.3.7 UniDec.unidec_modules.peakwidthtools.PeakTools2d.data2
- 7.44.3.8 UniDec.unidec_modules.peakwidthtools.PeakTools2d.dt
- 7.44.3.9 UniDec.unidec_modules.peakwidthtools.PeakTools2d.errorbox
- 7.44.3.10 UniDec.unidec_modules.peakwidthtools.PeakTools2d.fitmid
- 7.44.3.11 UniDec.unidec_modules.peakwidthtools.PeakTools2d.fitsig
- 7.44.3.12 UniDec.unidec_modules.peakwidthtools.PeakTools2d.flipbutton
- 7.44.3.13 UniDec.unidec_modules.peakwidthtools.PeakTools2d.flipflag
- 7.44.3.14 UniDec.unidec_modules.peakwidthtools.PeakTools2d.mz
- 7.44.3.15 UniDec.unidec_modules.peakwidthtools.PeakTools2d.outdtsig
- 7.44.3.16 UniDec.unidec_modules.peakwidthtools.PeakTools2d.outmzsig
- 7.44.3.17 UniDec.unidec_modules.peakwidthtools.PeakTools2d.plot1
- 7.44.3.18 UniDec.unidec_modules.peakwidthtools.PeakTools2d.psfun
- 7.44.3.19 UniDec.unidec_modules.peakwidthtools.PeakTools2d.resbox

The documentation for this class was generated from the following file:

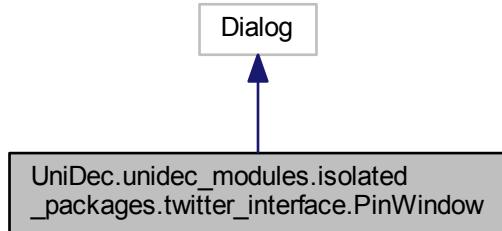
- C:/Python/UniDec/unidec_modules/[peakwidthtools.py](#)

7.45 UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow Class Reference

Inheritance diagram for UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow:



Collaboration diagram for UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow:



Public Member Functions

- def [__init__](#) (self, args, kwargs)
- def [OnClose](#) (self, e)
- def [OnCloseCancel](#) (self, e)

Public Attributes

- [pnl](#)
- [vbox](#)
- [sbs](#)
- [inputbox](#)
- [pin](#)

7.45.1 Constructor & Destructor Documentation

7.45.1.1 def UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow.[__init__](#) (self, args, kwargs)

7.45.2 Member Function Documentation

7.45.2.1 def UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow.[OnClose](#) (self, e)

7.45.2.2 def UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow.[OnCloseCancel](#) (self, e)

7.45.3 Member Data Documentation

7.45.3.1 UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow.[inputbox](#)

7.45.3.2 UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow.[pin](#)

7.45.3.3 UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow.[pnl](#)

7.45.3.4 UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow.[sbs](#)

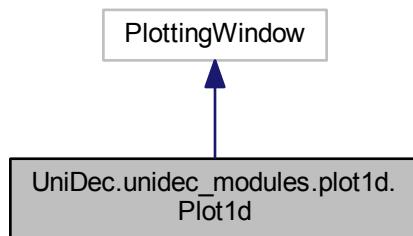
7.45.3.5 UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow.[vbox](#)

The documentation for this class was generated from the following file:

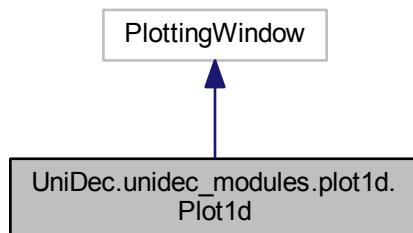
- C:/Python/UniDec/unidec_modules/isolated_packages/twitter_interface.py

7.46 UniDec.unidec_modules.plot1d.Plot1d Class Reference

Inheritance diagram for UniDec.unidec_modules.plot1d.Plot1d:



Collaboration diagram for UniDec.unidec_modules.plot1d.Plot1d:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `plotrefreshstop` (self, xvals, yvals, title="", xlabel="", ylabel="", label="", config=None, color="black", marker=None, zoom="box", nopaint=False, test_kda=False, integerticks=False, kwargs)
- def `plotadd`
- def `addtext` (self, txt, x, y, vlines=True, color="k", kwargs)
- def `texremove` (self)
- def `filledplot`
- def `histogram`
- def `barplottop`

Public Attributes

- `mlist`

- [x2](#)
- [colors](#)
- [xlabel](#)
- [ylabel](#)
- [zoomtype](#)
- [subplot1](#)
- [flag](#)
- [text](#)
- [lines](#)

7.46.1 Detailed Description

Class for 1D plots.

7.46.2 Constructor & Destructor Documentation

7.46.2.1 def UniDec.unidec_modules.plot1d.Plot1d.__init__(self, args, kwargs)

```
Inherit from PlottingWindow
:param args:
:param kwargs:
:return:
```

7.46.3 Member Function Documentation

7.46.3.1 def UniDec.unidec_modules.plot1d.Plot1d.addtext(self, txt, x, y, vlines=True, color="k", kwargs)

```
Adds text and lines. Puts things that have been added in self.lines and self.text lists.
:param txt: String of text to add
:param x: x position for where to add
:param y: y position for where to add
:param vlines: Whether to add vertical lines to the text as well.
:param color: Color of text and lines
:param kwargs: Keywords
If range=(a,b) is specified, adds a line from a to b and vertical lines at a and b.
:return: None
```

Here is the call graph for this function:

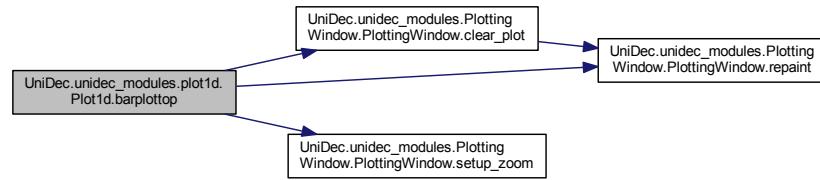


7.46.3.2 def UniDec.unidec_modules.plot1d.Plot1d.barplottop(self, xarr, yarr, peakval, colortab, xlabel = "", ylabel = "", title = "", zoom = "box", repaint = True)

```
Create a bar plot.
:param xarr: x value array
:param yarr: y value array
:param peakval: Bar labels to be listed below bars
:param colortab: List of colors for the various bars
```

```
:param xlabel: Label for x axis
:param ylabel: Label for y axis
:param title: Plot title
:param zoom: Type of zoom ('box' or 'span')
:param repaint: Boolean, whether to repaint or not when done.
:return: None
```

Here is the call graph for this function:



7.46.3.3 def UniDec.unidec_modules.plot1d.Plot1d.filledplot (*self*, *x*, *y*, *color* = "black")

Creates a plot filled between the y values and the y axis

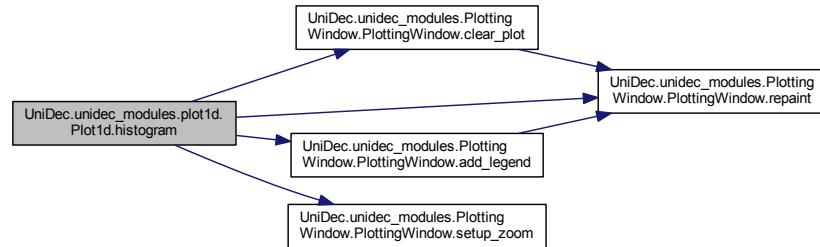
```
:param x: x values
:param y: y values
:param color: color
:return: None
```

7.46.3.4 def UniDec.unidec_modules.plot1d.Plot1d.histogram (*self*, *xarray*, *labels* = None, *xlab* = " ", *ylab* = " ", *title* = " ")

Creates a histogram plot.

```
:param xarray: Array of values in (N x M) array
:param labels: Labels for value
:param xlab: x axis label
:param ylab: y axis label
:param title: Plot Title
:return: None
```

Here is the call graph for this function:

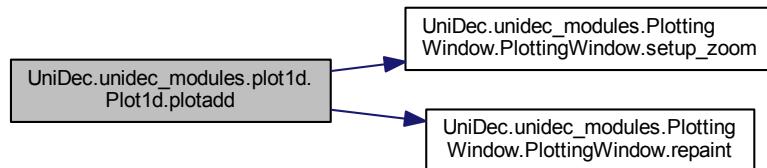


7.46.3.5 def UniDec.unidec_modules.plot1d.Plot1d.plotadd (*self*, *xvals*, *yvals*, *colval* = "black", *newlabel* = " ", *nopaint* = True)

Adds a plot.

```
:param xvals: x values
:param yvals: y values
:param colval: Color
:param newlabel: Label
:param nopaint: Boolean, whether to repaint or not
:return: None
```

Here is the call graph for this function:

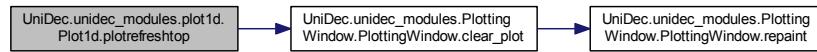


7.46.3.6 def UniDec.unidec_modules.plot1d.Plot1d.plotrefreshtop (self, xvals, yvals, title = "", xlabel = "", ylabel = "", label = "", config = None, color = "black", marker = None, zoom = "box", nopaint = False, test_kda = False, integerticks = False, kwargs)

Create a new 1D plot.

```
:param xvals: x values
:param yvals: y values
:param title: Plot title
:param xlabel: x axis label
:param ylabel: y axis label
:param label: label for legend
:param config: UniDecConfig object
:param color: Plot color
:param marker: Marker type
:param zoom: zoom type ('box' or 'span')
:param nopaint: Boolean, whether to repaint or not
:param test_kda: Boolean, whether to attempt to plot kDa rather than Da
:param integerticks: Boolean, whether to use inter tickmarks only
:param kwargs: Keywords
:return: None
```

Here is the call graph for this function:



7.46.3.7 def UniDec.unidec_modules.plot1d.Plot1d.textremove (self)

Remove text and lines previous placed in the self.text and self.lines containers

```
:return: None
```

7.46.4 Member Data Documentation

7.46.4.1 UniDec.unidec_modules.plot1d.Plot1d.colors

7.46.4.2 UniDec.unidec_modules.plot1d.Plot1d.flag

7.46.4.3 UniDec.unidec_modules.plot1d.Plot1d.lines

7.46.4.4 UniDec.unidec_modules.plot1d.Plot1d.mlist

7.46.4.5 UniDec.unidec_modules.plot1d.Plot1d.subplot1

7.46.4.6 UniDec.unidec_modules.plot1d.Plot1d.text

7.46.4.7 UniDec.unidec_modules.plot1d.Plot1d.x2

7.46.4.8 UniDec.unidec_modules.plot1d.Plot1d.xlabel

7.46.4.9 UniDec.unidec_modules.plot1d.Plot1d.ylabel

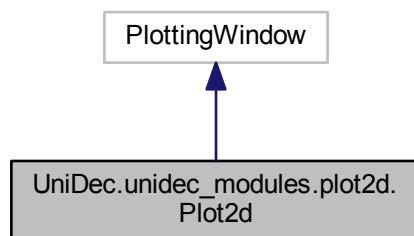
7.46.4.10 UniDec.unidec_modules.plot1d.Plot1d.zoomtype

The documentation for this class was generated from the following file:

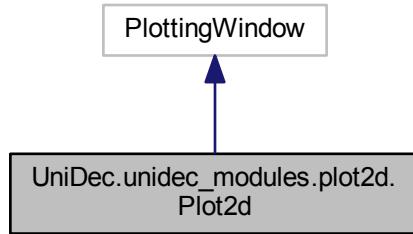
- C:/Python/UniDec/unidec_modules/[plot1d.py](#)

7.47 UniDec.unidec_modules.plot2d.Plot2d Class Reference

Inheritance diagram for UniDec.unidec_modules.plot2d.Plot2d:



Collaboration diagram for UniDec.unidec_modules.plot2d.Plot2d:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `contourplot`
- def `plot_native_z`

Public Attributes

- `xlabel`
- `ylabel`
- `cmap`
- `subplot1`
- `cbar`
- `flag`

7.47.1 Detailed Description

Plotting class for 2D contour plots

7.47.2 Constructor & Destructor Documentation

7.47.2.1 def UniDec.unidec_modules.plot2d.Plot2d.__init__(self, args, kwargs)

Initialize parameters for plotting window
:param args: Arguments passed to PlottingWindow
:param kwargs: Keywords passed to PlottingWindow
:return: Plot2d object

Here is the call graph for this function:



7.47.3 Member Function Documentation

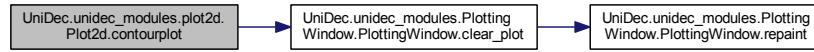
7.47.3.1 def UniDec.unidec_modules.plot2d.Plot2d.contourplot(self, dat =None, config =None, xvals =None, yvals =None, zgrid =None, xlab ='m/z (Th)', ylab ="Charge", title =' ', normflag =1, normrange =[0, repaint =True, nticks =None, test_kda =False)

Make 2D plot.

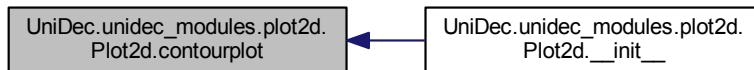
Data can be added using two methods:

```
1. If dat is specified, it will look for an N x 3 list of x,y,z values
2. If xvals, yvals, and zgrid are filled, it will plot zgrid assuming its shape is (len(xvals),len(yvals))
:param dat: N x 3 list in [x,y,z] format of data to be plotted
:param config: UniDecConfig object
:param xvals: x-axis values
:param yvals: y-axis values
:param zgrid: numpy array of shape (len(xvals),len(yvals))
:param xlab: Label for x-axis
:param ylab: Label for y-axis
:param title: Plot title
:param normflag: Set to 1 to normalize the plot range from min to max. If 0, will not normalize.
:param normrange: Range to normalize to if normflag is 0.
:param repaint: If true, will repaint the plot after it is done.
:param nticks: Number of ticks on the x-axis. If None, will use default.
:param test_kda: If true, will decide if the x-axis is better displayed in Da or kDa units.
:return: None
```

Here is the call graph for this function:



Here is the caller graph for this function:



7.47.3.2 def UniDec.unidec_modules.plot2d.Plot2d.plot_native_z(self, offset, col, xvals, width =0, alpha =1, shape =0)

Plots a showing the native charge offsets.

```
:param offset: Offset value
:param col: Color
:param xvals: x-axis (mass)
:param width: Width of charge distribution.
:param alpha: Transparency of plot overlay
:param shape: Indicates whether the width defines a step function of a Gaussian distribution
:return: None
```

Here is the call graph for this function:



7.47.4 Member Data Documentation

7.47.4.1 UniDec.unidec_modules.plot2d.Plot2d.cbar

7.47.4.2 UniDec.unidec_modules.plot2d.Plot2d.cmap

7.47.4.3 UniDec.unidec_modules.plot2d.Plot2d.flag

7.47.4.4 UniDec.unidec_modules.plot2d.Plot2d.subplot1

7.47.4.5 UniDec.unidec_modules.plot2d.Plot2d.xlabel

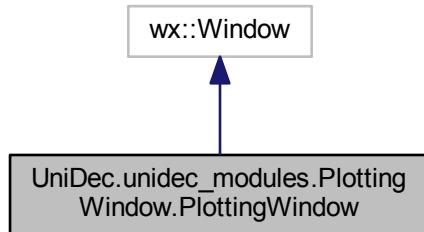
7.47.4.6 UniDec.unidec_modules.plot2d.Plot2d.ylabel

The documentation for this class was generated from the following file:

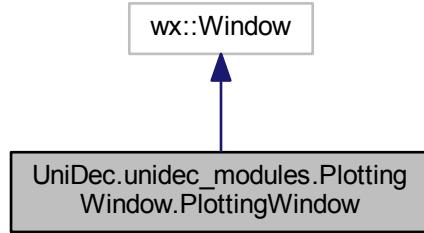
- C:/Python/UniDec/unidec_modules/[plot2d.py](#)

7.48 UniDec.unidec_modules.PlottingWindow.PlottingWindow Class Reference

Inheritance diagram for UniDec.unidec_modules.PlottingWindow.PlottingWindow:



Collaboration diagram for UniDec.unidec_modules.PlottingWindow.PlottingWindow:



Public Member Functions

- def [`__init__`](#) (self, args, kwargs)
- def [`on_release`](#) (self, event)
- def [`on_save_fig_dialog`](#) (self, evt)
- def [`on_save_fig`](#) (self, evt, path, kwargs)
- def [`save_figure`](#) (self, path, kwargs)
- def [`kda_test`](#) (self, xvals)
- def [`plotadddot`](#) (self, x, y, colval, markval)
- def [`repaint`](#) (self)
- def [`clear_plot`](#) (self, args)
- def [`set_nticks`](#) (self, bins)
- def [`add_legend`](#)
- def [`set_color`](#)
- def [`set_tickcolor`](#) (self)
- def [`size_handler`](#) (self, args, kwargs)
- def [`setup_zoom`](#)

Public Attributes

- [`figure`](#)
- [`int`](#)
- [`smash`](#)
- [`subplot1`](#)
- [`zoom`](#)
- [`canvas`](#)
- [`resize`](#)
- [`flag`](#)
- [`kda`](#)
- [`kdnorm`](#)
- [`normallicks`](#)
- [`nativez`](#)
- [`text`](#)
- [`lines`](#)
- [`cbar`](#)
- [`datalims`](#)
- [`cmap`](#)

- xlabel
- ylabel
- zoomtype
- tickcolor

7.48.1 Detailed Description

Class for wx window with embedded matplotlib plots

7.48.2 Constructor & Destructor Documentation

7.48.2.1 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.`__init__`(*self, args, kwargs*)

Initialize plot window parameters.

Optional keywords:

figsize: size of figure in inches

integrate: 0 or 1 of whether the plot should send the integrate pubsub when a right click is activated.

smash: 0 or 1 of whether the plot should send the integrate pubsub when a right click is activated.

```
:param args: Arguments
:param kwargs: Keywords
:return:
```

7.48.3 Member Function Documentation

7.48.3.1 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.`add_legend`(*self, location=1*)

Adds a legend to the plot.

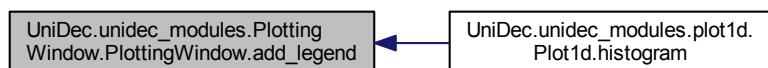
:param location: Integer code for location

:return: None

Here is the call graph for this function:



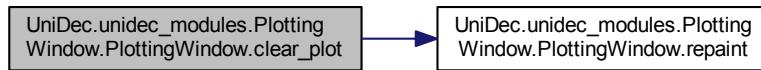
Here is the caller graph for this function:



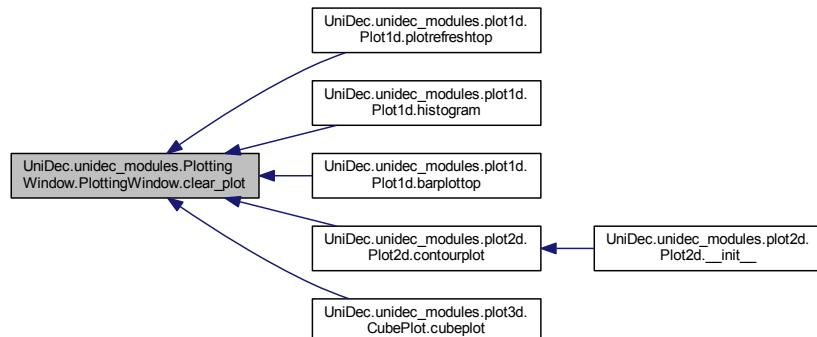
7.48.3.2 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.clear_plot (self, args)

Clear the plot and rest some of the parameters.
:param args: Arguments
:return:

Here is the call graph for this function:



Here is the caller graph for this function:



7.48.3.3 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.kda_test (self, xvals)

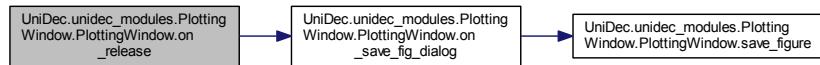
Test whether the axis should be normalized to convert mass units from Da to kDa.
Will use kDa if: $xvals[int(len(xvals) / 2)] > 100000$ or $xvals[len(xvals) - 1] > 1000000$

If kDa is used, self.kda=True and self.kdnorm=1000. Otherwise, self.kda=False and self.kdnorm=1.
:param xvals: mass axis
:return: None

7.48.3.4 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.on_release (self, event)

Function triggered on button release event from plot.
Currently wired to trigger on_save_figure_dialog on middle button.
:param event: wx.Event
:return: None

Here is the call graph for this function:

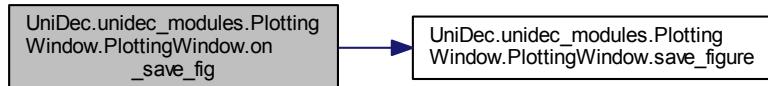


7.48.3.5 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.on_save_fig(self, evt, path, kwargs)

```

Save figure to path.
:param evt: wx.Event (unused)
:param path: Path to save figure to
:param kwargs: keywords passed to save_figure
:return: None
  
```

Here is the call graph for this function:

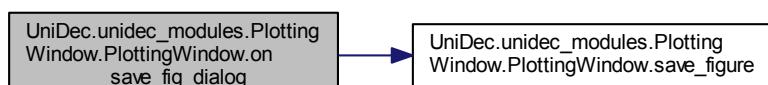


7.48.3.6 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.on_save_fig_dialog(self, evt)

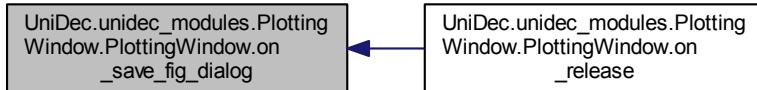
```

Open a save figure dialog for specified plot.
:param evt: wx.Event (unused)
:return: None
  
```

Here is the call graph for this function:



Here is the caller graph for this function:



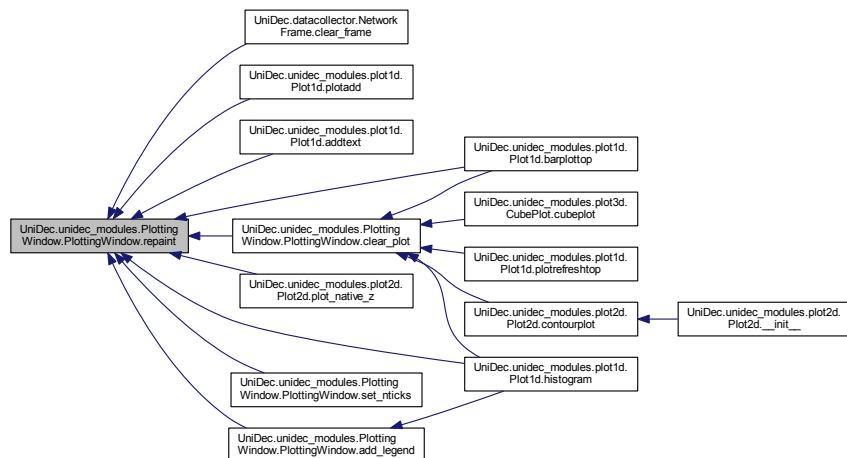
7.48.3.7 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.plotadddot (self, x, y, colval, markval)

Adds a scatter plot to the figure. May be one or more.
:param x: x values
:param y: y values
:param colval: Color
:param markval: Marker
:return: None

7.48.3.8 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.repaint (self)

Redraw and refresh the plot.
:return: None

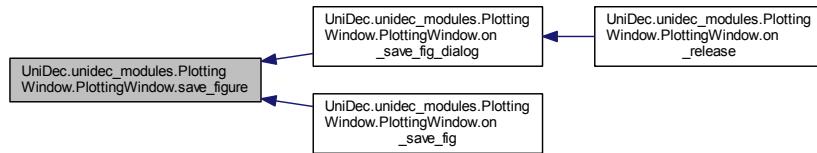
Here is the caller graph for this function:



7.48.3.9 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.save_figure (self, path, kwargs)

Saves Figure to path.
:param path: Path to save figure at.
:param kwargs: Keywords passed to matplotlib.figure.savefig
:return: None

Here is the caller graph for this function:



7.48.3.10 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.set_color (self, rgbtuple =None)

```
Sets background color
:param rgbtuple: background color
:return:
```

7.48.3.11 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.set_nticks (self, bins)

```
Set the number of ticks in the x-axis.
:param bins: Number of ticks in the x-axis
:return: None
```

Here is the call graph for this function:



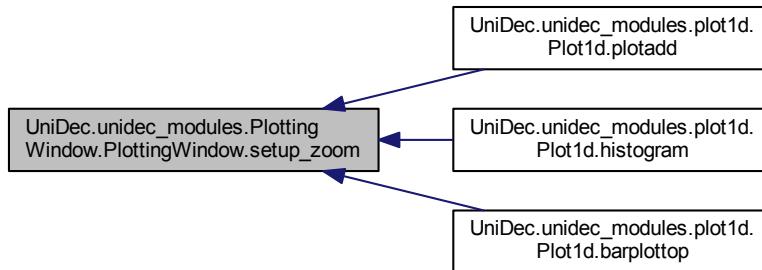
7.48.3.12 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.set_tickcolor (self)

```
Sets tick colors based on the colormap set at self.cmap
:return: None
```

7.48.3.13 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.setup_zoom (self, plots, zoom, data_lims =None)

```
Set up zoom on axes.
:param plots: Axes objects to setup
:param zoom: Type of zoom ('span' or 'box')
:param data_lims: Optional manual description of the data limits (where to go when fully zoomed out)
:return: None
```

Here is the caller graph for this function:



7.48.3.14 def UniDec.unidec_modules.PlottingWindow.PlottingWindow.size_handler (self, args, kwargs)

```
Resizes the plots
:param args:
:param kwargs:
:return: None
```

7.48.4 Member Data Documentation

[7.48.4.1 UniDec.unidec_modules.PlottingWindow.PlottingWindow.canvas](#)

[7.48.4.2 UniDec.unidec_modules.PlottingWindow.PlottingWindow.cbar](#)

[7.48.4.3 UniDec.unidec_modules.PlottingWindow.PlottingWindow.cmap](#)

[7.48.4.4 UniDec.unidec_modules.PlottingWindow.PlottingWindow.datalims](#)

[7.48.4.5 UniDec.unidec_modules.PlottingWindow.PlottingWindow.figure](#)

[7.48.4.6 UniDec.unidec_modules.PlottingWindow.PlottingWindow.flag](#)

[7.48.4.7 UniDec.unidec_modules.PlottingWindow.PlottingWindow.int](#)

[7.48.4.8 UniDec.unidec_modules.PlottingWindow.PlottingWindow.kda](#)

[7.48.4.9 UniDec.unidec_modules.PlottingWindow.PlottingWindow.kdnorm](#)

[7.48.4.10 UniDec.unidec_modules.PlottingWindow.PlottingWindow.lines](#)

[7.48.4.11 UniDec.unidec_modules.PlottingWindow.PlottingWindow.nativez](#)

[7.48.4.12 UniDec.unidec_modules.PlottingWindow.PlottingWindow.normallicks](#)

[7.48.4.13 UniDec.unidec_modules.PlottingWindow.PlottingWindow.resize](#)

[7.48.4.14 UniDec.unidec_modules.PlottingWindow.PlottingWindow.smash](#)

7.48.4.15 UniDec.unidec_modules.PlottingWindow.PlottingWindow.subplot1

7.48.4.16 UniDec.unidec_modules.PlottingWindow.PlottingWindow.text

7.48.4.17 UniDec.unidec_modules.PlottingWindow.PlottingWindow.tickcolor

7.48.4.18 UniDec.unidec_modules.PlottingWindow.PlottingWindow.xlabel

7.48.4.19 UniDec.unidec_modules.PlottingWindow.PlottingWindow.ylabel

7.48.4.20 UniDec.unidec_modules.PlottingWindow.PlottingWindow.zoom

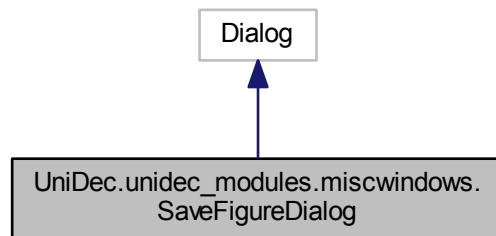
7.48.4.21 UniDec.unidec_modules.PlottingWindow.PlottingWindow.zoomtype

The documentation for this class was generated from the following file:

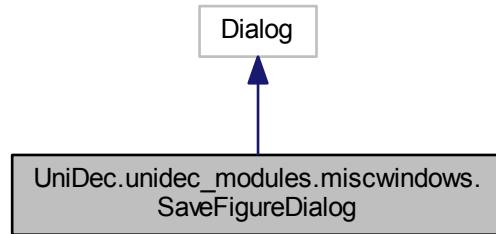
- C:/Python/UniDec/unidec_modules/[PlottingWindow.py](#)

7.49 UniDec.unidec_modules.miscwindows.SaveFileDialog Class Reference

Inheritance diagram for UniDec.unidec_modules.miscwindows.SaveFileDialog:



Collaboration diagram for UniDec.unidec_modules.miscwindows.SaveFileDialog:



Public Member Functions

- def `__init__` (`self, args, kwargs`)
- def `initialize_interface` (`self, config`)
- def `on_close` (`self, e`)
- def `on_close_cancel` (`self, e`)
- def `on_choose_dir` (`self, e`)

Public Attributes

- `config`
- `headerbox`
- `dirinput`
- `extbox`
- `widebox`
- `tallbox`
- `tbox`
- `b1`
- `b2`
- `b3`
- `b4`
- `directory`
- `header`
- `extension`
- `transparent`
- `rect`
- `figsize`

7.49.1 Constructor & Destructor Documentation

7.49.1.1 def UniDec.unidec_modules.mscwindows.SaveFileDialog.__init__ (`self, args, kwargs`)

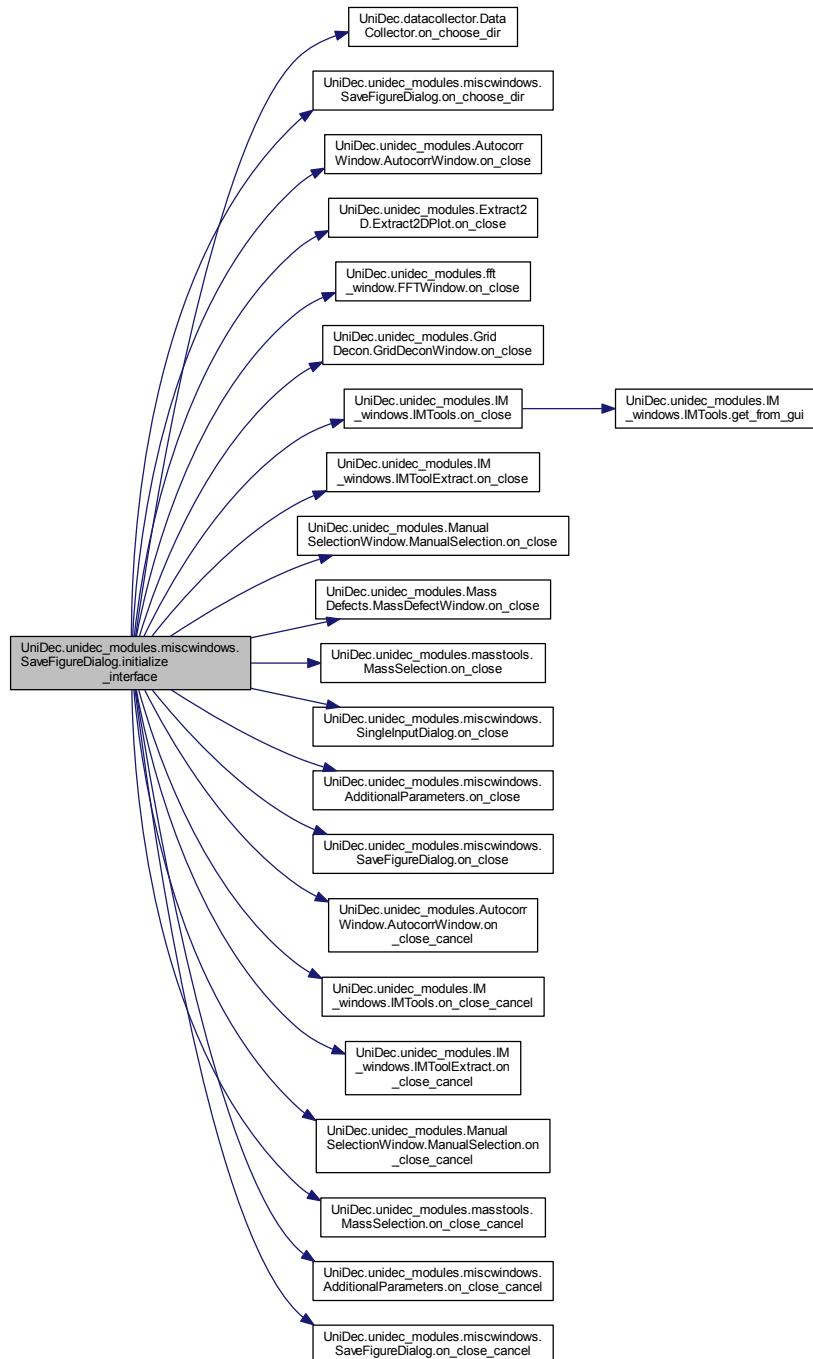
```
Window for setting save figure parameters.  
:param args: Passed to wx.Dialog  
:param kwargs: Passed to wx.Dialog  
:return: None
```

7.49.2 Member Function Documentation

7.49.2.1 def UniDec.unidec_modules.mscwindows.SaveFileDialog.initialize_interface (`self, config`)

```
Initialize the GUI.  
:param config: UniDecConfig  
:return:
```

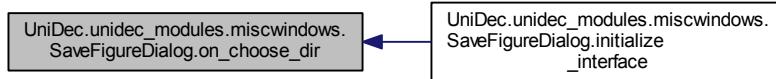
Here is the call graph for this function:



7.49.2.2 def UniDec.unidec_modules.misctools.SaveFileDialog.on_choose_dir (self, e)

Open a dialog to choose the directory.
:param e: Unused event
:return: None

Here is the caller graph for this function:



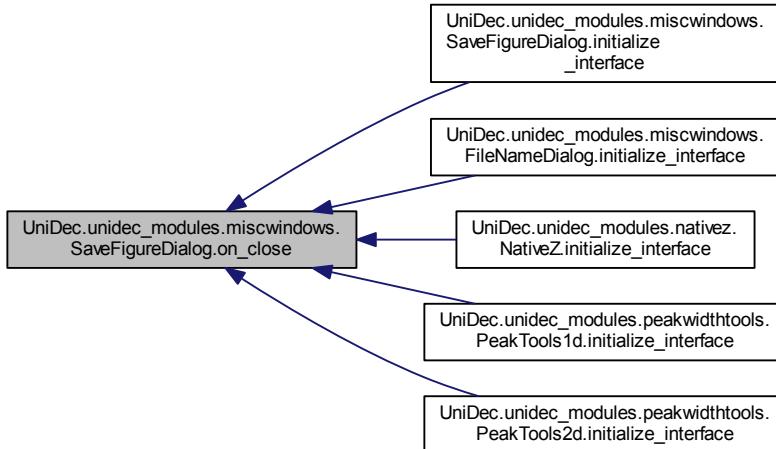
7.49.2.3 def UniDec.unidec_modules.mscwindows.SaveFileDialog.on_close (self, e)

Close the window and save the parameters to the class.

:param e: Unused event

:return: None

Here is the caller graph for this function:



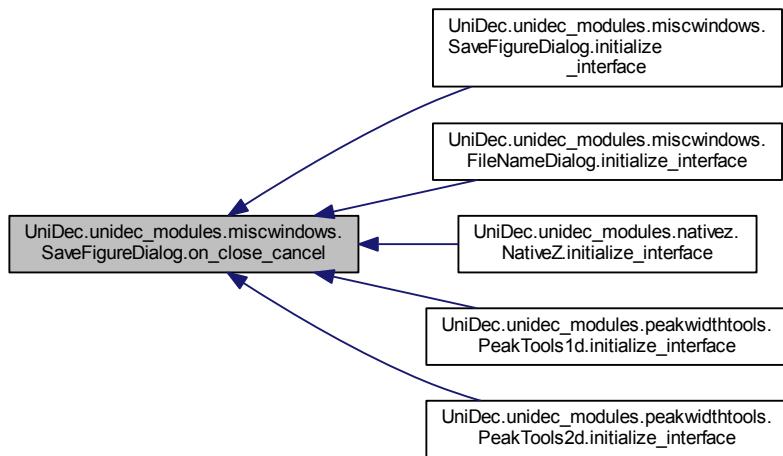
7.49.2.4 def UniDec.unidec_modules.mscwindows.SaveFileDialog.on_close_cancel (self, e)

Destroy the window without setting anything.

:param e: Unused event

:return: None

Here is the caller graph for this function:



7.49.3 Member Data Documentation

- 7.49.3.1 [UniDec.unidec_modules.mscwindows.SaveFileDialog.b1](#)
- 7.49.3.2 [UniDec.unidec_modules.mscwindows.SaveFileDialog.b2](#)
- 7.49.3.3 [UniDec.unidec_modules.mscwindows.SaveFileDialog.b3](#)
- 7.49.3.4 [UniDec.unidec_modules.mscwindows.SaveFileDialog.b4](#)
- 7.49.3.5 [UniDec.unidec_modules.mscwindows.SaveFileDialog.config](#)
- 7.49.3.6 [UniDec.unidec_modules.mscwindows.SaveFileDialog.directory](#)
- 7.49.3.7 [UniDec.unidec_modules.mscwindows.SaveFileDialog.dirinput](#)
- 7.49.3.8 [UniDec.unidec_modules.mscwindows.SaveFileDialog.extbox](#)
- 7.49.3.9 [UniDec.unidec_modules.mscwindows.SaveFileDialog.extension](#)
- 7.49.3.10 [UniDec.unidec_modules.mscwindows.SaveFileDialog.figsize](#)
- 7.49.3.11 [UniDec.unidec_modules.mscwindows.SaveFileDialog.header](#)
- 7.49.3.12 [UniDec.unidec_modules.mscwindows.SaveFileDialog.headerbox](#)
- 7.49.3.13 [UniDec.unidec_modules.mscwindows.SaveFileDialog.rect](#)
- 7.49.3.14 [UniDec.unidec_modules.mscwindows.SaveFileDialog.tallbox](#)
- 7.49.3.15 [UniDec.unidec_modules.mscwindows.SaveFileDialog.tbox](#)
- 7.49.3.16 [UniDec.unidec_modules.mscwindows.SaveFileDialog.transparent](#)

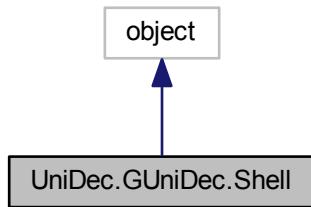
7.49.3.17 UniDec.unidec_modules.miscwindows.SaveFigureDialog.widebox

The documentation for this class was generated from the following file:

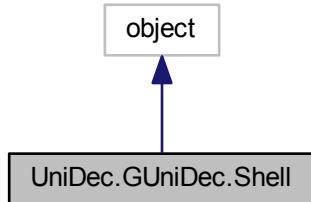
- C:/Python/UniDec/unidec_modules/[miscwindows.py](#)

7.50 UniDec.GUniDec.Shell Class Reference

Inheritance diagram for UniDec.GUniDec.Shell:



Collaboration diagram for UniDec.GUniDec.Shell:



Public Member Functions

- def [__init__](#) (self, args, kwargs)

Public Attributes

- [shell](#)
- [shellwindow](#)

7.50.1 Constructor & Destructor Documentation

7.50.1.1 def UniDec.GUniDec.Shell.__init__(self, args, kwargs)

7.50.2 Member Data Documentation

7.50.2.1 UniDec.GUniDec.Shell.shell

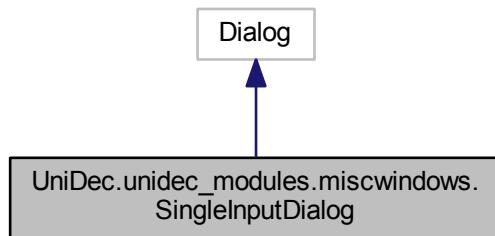
7.50.2.2 UniDec.GUniDec.Shell.shellwindow

The documentation for this class was generated from the following file:

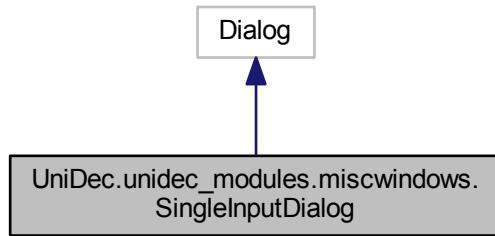
- C:/Python/UniDec/GUniDec.py

7.51 UniDec.unidec_modules.miscwindows.SingleInputDialog Class Reference

Inheritance diagram for UniDec.unidec_modules.miscwindows.SingleInputDialog:



Collaboration diagram for UniDec.unidec_modules.miscwindows.SingleInputDialog:



Public Member Functions

- def `__init__`(self, args, kwargs)
- def `initialize_interface`
- def `on_close`(self, e)

Public Attributes

- `value`
- `inputbox`

7.51.1 Constructor & Destructor Documentation

7.51.1.1 def UniDec.unidec_modules.misctools.SingleInputDialog.__init__(self, args, kwargs)

Simple dialog for a single textctrl input.

:param args: Passed to wx.Dialog.

:param kwargs: Passed to wx.Dialog.

:return: None

7.51.2 Member Function Documentation

7.51.2.1 def UniDec.unidec_modules.misctools.SingleInputDialog.initialize_interface(self, title = "", message = "", defaultvalue = "")

Create a simple dialog window interface.

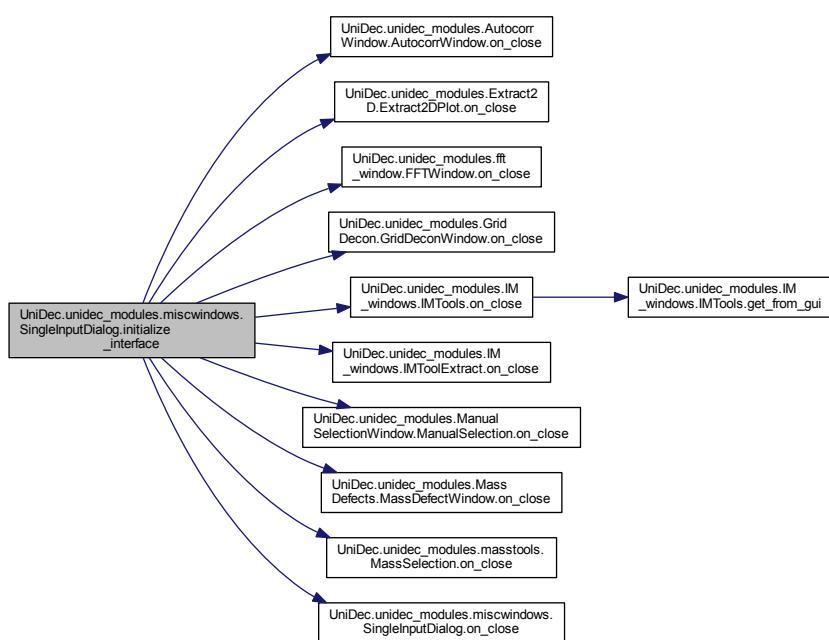
:param title: Title for the frame.

:param message: Message inside the window.

:param defaultvalue: String default value for the window.

:return: None

Here is the call graph for this function:



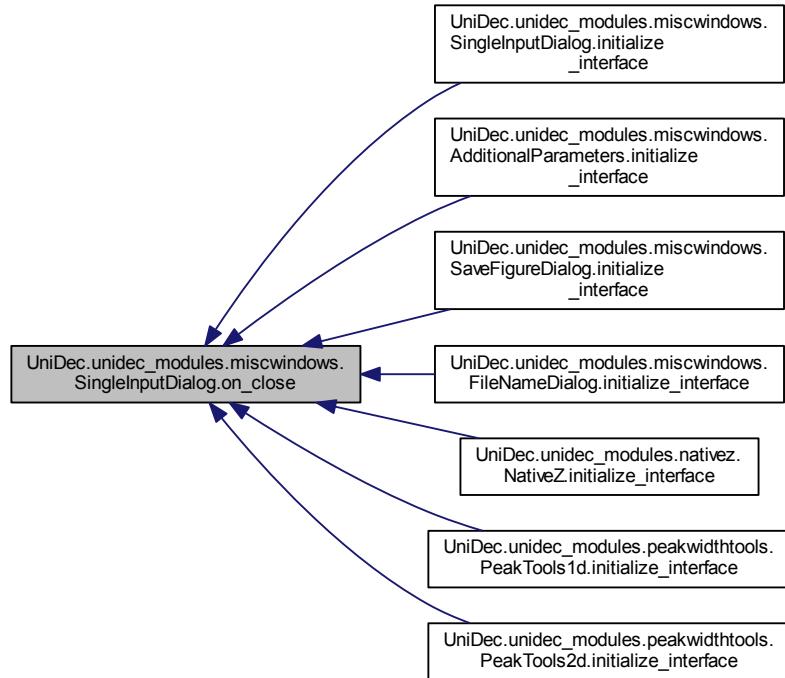
7.51.2.2 def UniDec.unidec_modules.misctools.SingleInputDialog.on_close(self, e)

Close the window and set `self.value` to the value returned by the `inputbox`.

:param e: Unused event

:return: `self.value`

Here is the caller graph for this function:



7.51.3 Member Data Documentation

7.51.3.1 `UniDec.unidec_modules.miscwindows.SingleInputDialog.inputbox`

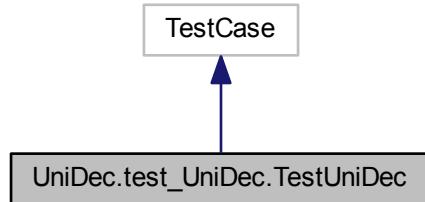
7.51.3.2 `UniDec.unidec_modules.miscwindows.SingleInputDialog.value`

The documentation for this class was generated from the following file:

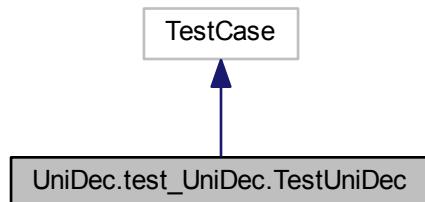
- C:/Python/UniDec/unidec_modules/[miscwindows.py](#)

7.52 UniDec.test_UniDec.TestUniDec Class Reference

Inheritance diagram for UniDec.test_UniDec.TestUniDec:



Collaboration diagram for UniDec.test_UniDec.TestUniDec:



Public Member Functions

- def `setUpClass` (`cls`)
- def `test_unidec_paths` (`self`)
- def `test_reset_config` (`self`)
- def `test_export_import_config` (`self`)
- def `test_open_file` (`self`)
- def `test_auto_MS` (`self`)
- def `test_auto_IMMS` (`self`)
- def `test_save_load` (`self`)

7.52.1 Member Function Documentation

7.52.1.1 def UniDec.test_UniDec.TestUniDec.setUpClass (`cls`)

7.52.1.2 def UniDec.test_UniDec.TestUniDec.test_auto_IMMS (`self`)

Open a file, process the data, and pick the peaks.
Check that the maximum peak is what is expected.
:return:

7.52.1.3 def UniDec.test_UniDec.TestUniDec.test_auto_MS (self)

Open a file, process the data, and pick the peaks.
Check that the maximum peak is what is expected.
:return:

7.52.1.4 def UniDec.test_UniDec.TestUniDec.test_export_import_config (self)

Write the default config to the default config file.
Switch a value.
Import the default back.
Check if the value has switched.
:return:

7.52.1.5 def UniDec.test_UniDec.TestUniDec.test_open_file (self)

Open several test spectra from various data types in self.testdir.
Check the that dimensions are the same as expected.
Check that it fails on a file that isn't there.
:return:

7.52.1.6 def UniDec.test_UniDec.TestUniDec.test_reset_config (self)

Check whether a specific value is being reset while another is not.
:return:

7.52.1.7 def UniDec.test_UniDec.TestUniDec.test_save_load (self)**7.52.1.8 def UniDec.test_UniDec.TestUniDec.test_unidec_paths (self)**

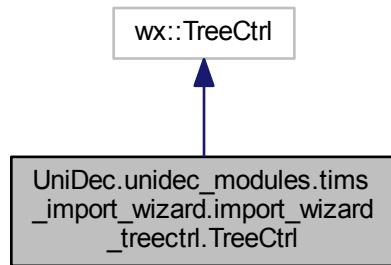
Test whether the paths specified actually have the correct files there.
:return:

The documentation for this class was generated from the following file:

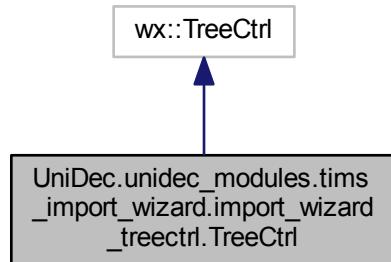
- C:/Python/UniDec/test_UniDec.py

7.53 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrl Class Reference

Inheritance diagram for UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrl:



Collaboration diagram for UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrl:



Public Member Functions

- def [__init__](#) (self, parent, id, pos, size, style)

7.53.1 Constructor & Destructor Documentation

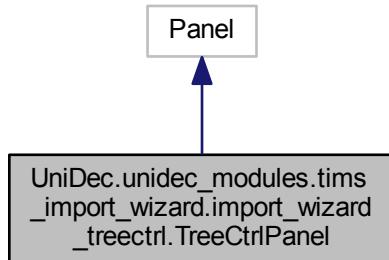
7.53.1.1 def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrl.[__init__](#) (self, parent, id, pos, size, style)

The documentation for this class was generated from the following file:

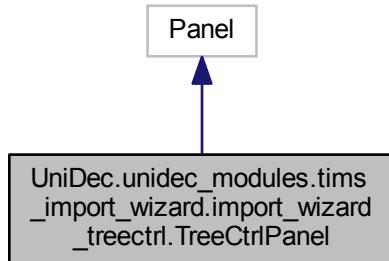
- C:/Python/UniDec/unidec_modules/tims_import_wizard/[import_wizard_treectrl.py](#)

7.54 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel Class Reference

Inheritance diagram for UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel:



Collaboration diagram for UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel:



Public Member Functions

- def [__init__](#) (self, parent, [link](#))
- def [populate_tree](#) (self)
- def [add_root](#)
- def [add_children](#)
- def [raw_file_info](#) (self, [path](#))
- def [OnSize](#) (self, event)
- def [on_selected_changed](#) (self, event)
- def [on_activate](#) (self, event)
- def [on_item_expanded](#) (self, event)

Public Attributes

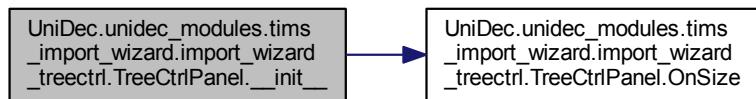
- [link](#)

- [tree](#)
- [fldridx](#)
- [fldropenidx](#)
- [fileidx](#)
- [il](#)
- [path](#)
- [raw](#)
- [item](#)

7.54.1 Constructor & Destructor Documentation

7.54.1.1 `def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.__init__ (self, parent, link)`

Here is the call graph for this function:

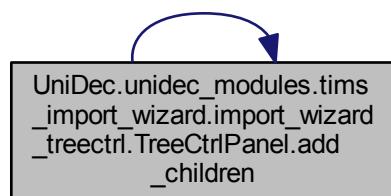


7.54.2 Member Function Documentation

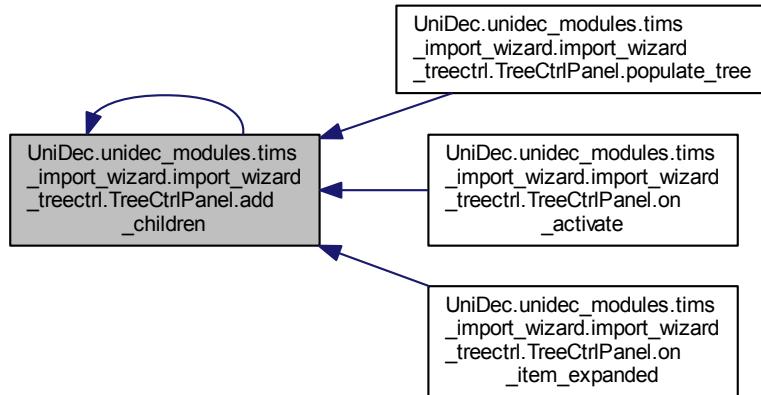
7.54.2.1 `def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.add_children (self, parent, path, depth_limit = 1)`

Recursively adds children up to the depth specified

Here is the call graph for this function:



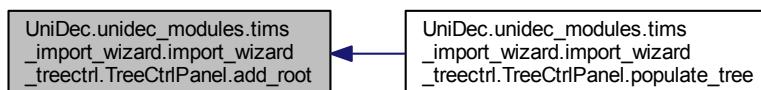
Here is the caller graph for this function:



7.54.2.2 `def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.add_root(self, name, data = None)`

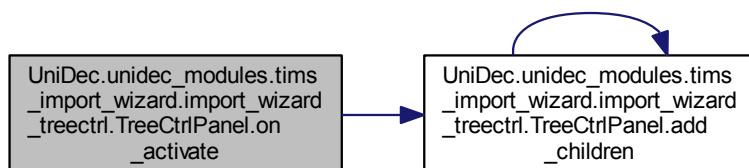
Add root folder to tree
returns root object

Here is the caller graph for this function:



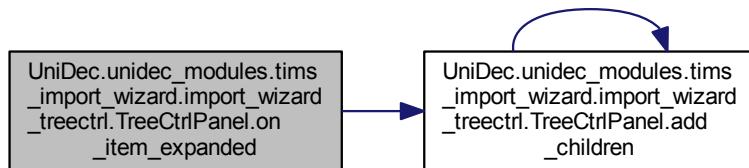
7.54.2.3 `def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.on_activate(self, event)`

Here is the call graph for this function:



7.54.2.4 def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.on_item_expanded (self, event)

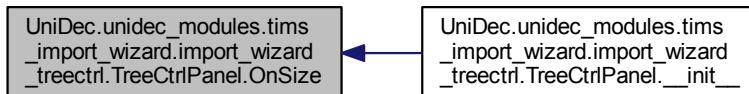
Here is the call graph for this function:



7.54.2.5 def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.on_selected_changed (self, event)

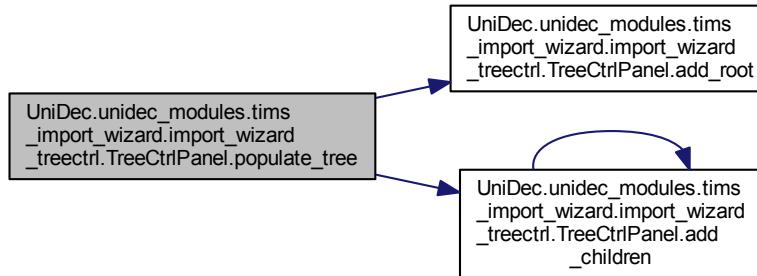
7.54.2.6 def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.OnSize (self, event)

Here is the caller graph for this function:



7.54.2.7 def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.populate_tree (self)

Here is the call graph for this function:



7.54.2.8 def UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.raw_file_info (self, path)

7.54.3 Member Data Documentation

7.54.3.1 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.fileidx

7.54.3.2 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.fldridx

7.54.3.3 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.fldropenidx

7.54.3.4 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.il

7.54.3.5 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.item

7.54.3.6 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.link

7.54.3.7 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.path

7.54.3.8 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.raw

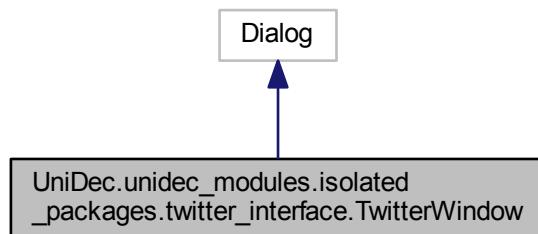
7.54.3.9 UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel.tree

The documentation for this class was generated from the following file:

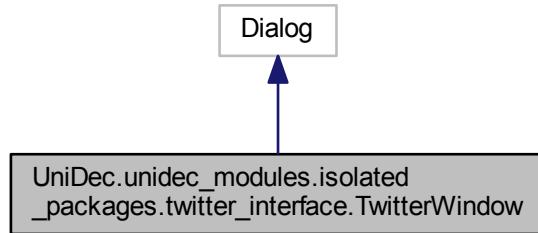
- C:/Python/UniDec/unidec_modules/tims_import_wizard/[import_wizard_treectrl.py](#)

7.55 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow Class Reference

Inheritance diagram for UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow:



Collaboration diagram for UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `LoadScreenName` (self)
- def `OnClose` (self, e)
- def `OnCloseCancel` (self, e)
- def `OnPreview` (self, e)
- def `OnCharacterCount` (self, e)
- def `OnLaunchWeb` (self, e)
- def `Tweet` (self, e)

Public Attributes

- `pngs`
- `codes`
- `imflag`
- `previewsize`
- `APP_KEY`
- `APP_SECRET`
- `pnl`
- `vbox`
- `sb`
- `sbs`
- `hbox1`
- `loginbutton`
- `userbox`
- `hbox2`
- `inputbox2`
- `countbox`
- `hbox3`
- `imagechoice`
- `previewbutton`
- `hbox4`
- `emptyimg`
- `imageCtrl`
- `hbox5`
- `tweetbutton`

- [OAUTH_TOKEN](#)
- [OAUTH_TOKEN_SECRET](#)
- [screen_name](#)
- [imageFile](#)
- [url](#)
- [pinwindow](#)
- [pin](#)

7.55.1 Constructor & Destructor Documentation

7.55.1.1 `def UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.__init__ (self, args, kwargs)`

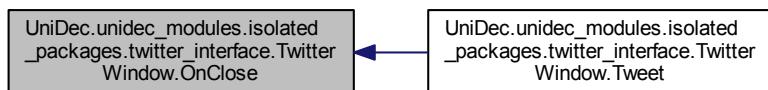
7.55.2 Member Function Documentation

7.55.2.1 `def UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.LoadScreenName (self)`

7.55.2.2 `def UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.OnCharacterCount (self, e)`

7.55.2.3 `def UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.OnClose (self, e)`

Here is the caller graph for this function:

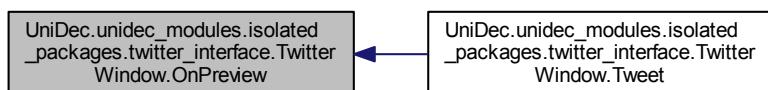


7.55.2.4 `def UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.OnCloseCancel (self, e)`

7.55.2.5 `def UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.OnLaunchWeb (self, e)`

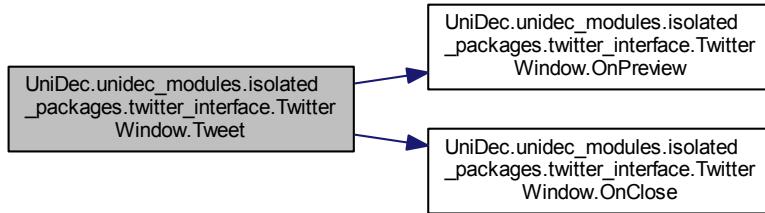
7.55.2.6 `def UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.OnPreview (self, e)`

Here is the caller graph for this function:



7.55.2.7 def UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.Tweet (self, e)

Here is the call graph for this function:



7.55.3 Member Data Documentation

7.55.3.1 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.APP_KEY

7.55.3.2 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.APP_SECRET

7.55.3.3 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.codes

7.55.3.4 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.countbox

7.55.3.5 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.emptyimg

7.55.3.6 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.hbox1

7.55.3.7 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.hbox2

7.55.3.8 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.hbox3

7.55.3.9 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.hbox4

7.55.3.10 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.hbox5

7.55.3.11 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.imagechoice

7.55.3.12 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.imageCtrl

7.55.3.13 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.imageFile

7.55.3.14 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.imflag

7.55.3.15 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.inputbox2

7.55.3.16 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.loginbutton

7.55.3.17 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.OAUTH_TOKEN

7.55.3.18 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.OAUTH_TOKEN_SECRET

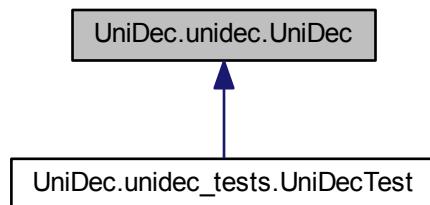
- 7.55.3.19 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.pin
- 7.55.3.20 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.pinwindow
- 7.55.3.21 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.pngs
- 7.55.3.22 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.pnl
- 7.55.3.23 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.previewbutton
- 7.55.3.24 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.previewsize
- 7.55.3.25 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.sb
- 7.55.3.26 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.sbs
- 7.55.3.27 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.screen_name
- 7.55.3.28 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.tweetbutton
- 7.55.3.29 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.url
- 7.55.3.30 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.userbox
- 7.55.3.31 UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow.vbox

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/isolated_packages/twitter_interface.py

7.56 UniDec.unidec.UniDec Class Reference

Inheritance diagram for UniDec.unidec.UniDec:



Public Member Functions

- def [__init__](#) (self)
- def [initialize](#) (self)
- def [reset_config](#) (self)
- def [load_config](#) (self, f_name)

- def `export_config`
- def `open_file` (self, file_name, file_directory, kwargs)
- def `raw_process`
- def `process_data` (self, kwargs)
- def `run_unidec`
- def `unidec_imports`
- def `pick_peaks` (self)
- def `convolve_peaks` (self)
- def `autorun` (self)
- def `check_badness` (self)
- def `autocorrelation`
- def `kendrick_peaks`
- def `kendrick_continuous`
- def `save_default` (self)
- def `load_default` (self)
- def `mass_grid_to_f_grid` (self)
- def `integrate`
- def `autointegrate`
- def `get_auto_peak_width` (self)
- def `export_params` (self, e)
- def `process_mass_data` (self)
- def `center_of_mass`
- def `fit_all_masses` (self)
- def `get_charge_peaks` (self)
- def `save_state` (self, file_name)
- def `load_state` (self, load_path)
- def `cross_validate`
- def `normalize_peaks` (self)
- def `align_peaks`
- def `correlate_intensities` (self, pmasses=None, x_range=None, window=None, ci=0.99, kwargs)
- def `get_peaks_scores` (self, window=None, x_range=None, ci=0.99, kwargs)
- def `fit_isolated_peaks` (self, pmasses=None, x_range=None, window=None, norm=False, plot_fits=False, kwargs)
- def `get_errors` (self, kwargs)
- def `open_test_spectrum` (self, masslist=None, n=1, kwargs)
- def `make_plot`

Public Attributes

- `version`
- `config`
- `data`
- `pks`
- `autopeaks`
- `peakparams`
- `massfit`
- `massfitdat`
- `errorgrid`

7.56.1 Constructor & Destructor Documentation

7.56.1.1 def UniDec.unidec.UniDec.__init__(self)

```
UniDec Engine

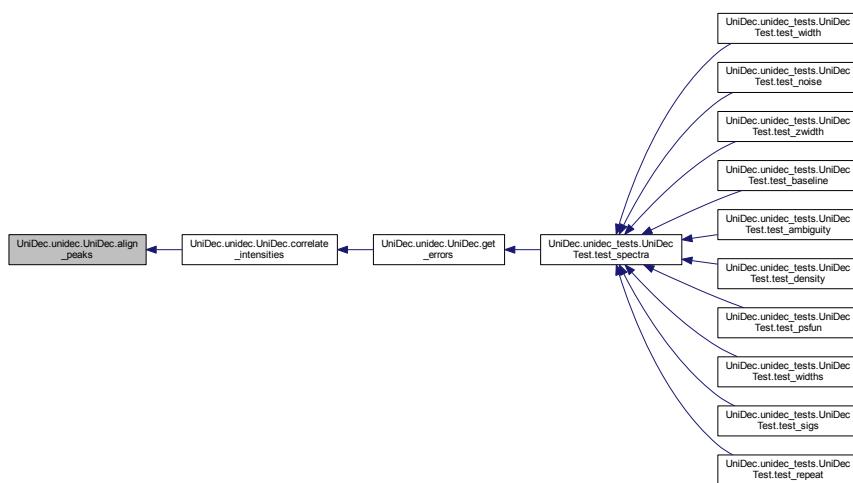
Consists of three main subclasses: Config, DataContainer, Peaks

:returns: None
```

7.56.2 Member Function Documentation

7.56.2.1 def UniDec.unidec.UniDec.align_peaks(self, pmasses =None, x_range =None, window =None, norm = False)

Here is the caller graph for this function:



7.56.2.2 def UniDec.unidec.UniDec.autocorrelation(self, massdat =None)

```
Performs autocorrelation on mass data. Result is stored as self.data.autocorr.
Picks peaks greater than 0 using peak detection parameters in config file.
Peaks are stored as a peak structure at self.autopeaks
:param massdat: Data on which to run autocorrelation. Default is None, in which case self.data.massdat is used
:returns: float. First peak in autocorrelation.
```

7.56.2.3 def UniDec.unidec.UniDec.autointegrate(self, ztab =None)

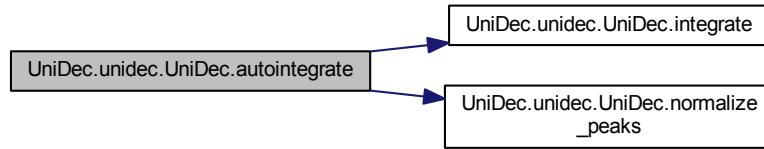
Perform automatic integration of peaks.

If self.config.integrateup is empty, the upperbound becomes self.config.peakwindow.
If self.config.integratelb is empty, the lowerbound becomes -self.config.peakwindow.

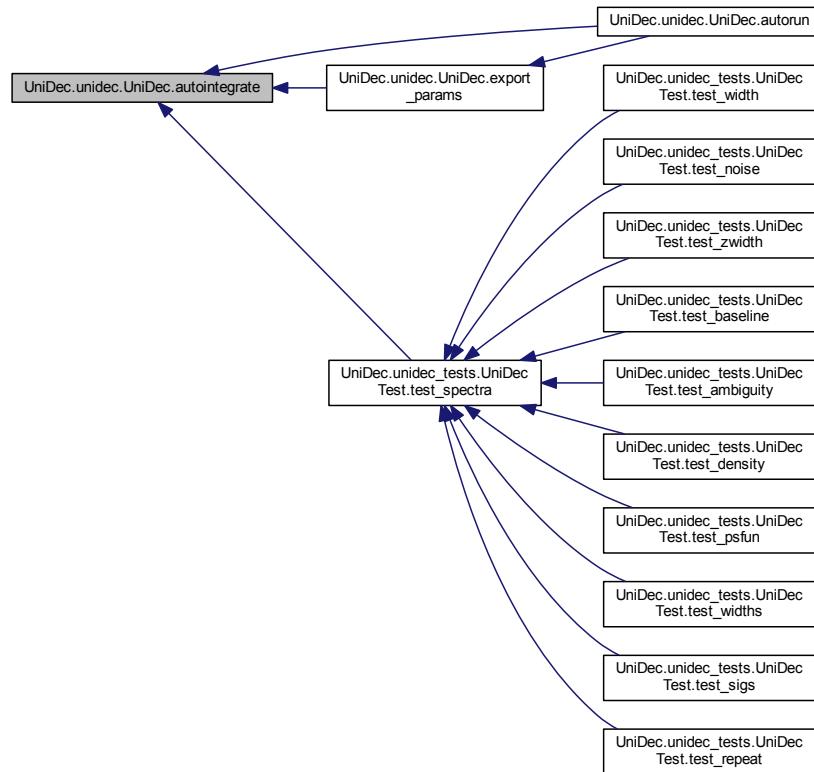
Integral range for each peak is set to peak.integralrange.
Integral value is set to peak.integral.

If ztab parameter is set to a list of charge states, it will integrate the mass vs charge grid at each individual charge state. Otherwise, this is ignored.
:param ztab: List of charge states (default = None)
:return: zarea: P x Z array where P is the number of peaks and Z is the number of charge states.
Each value of the array is the integral of peak P at charge state Z.

Here is the call graph for this function:

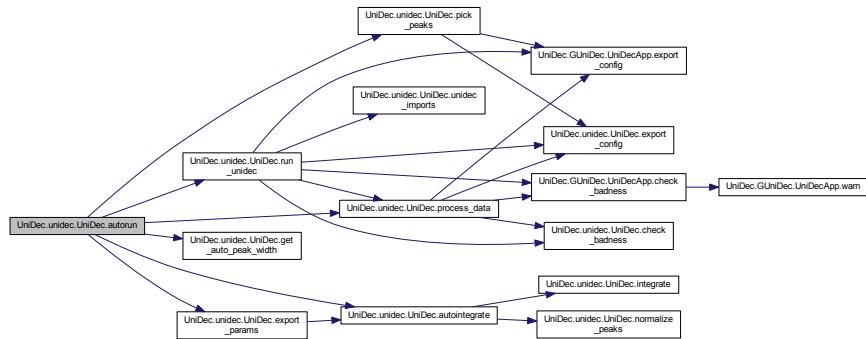


Here is the caller graph for this function:



7.56.2.4 def UniDec.unidec.UniDec.autorun (self)

Here is the call graph for this function:



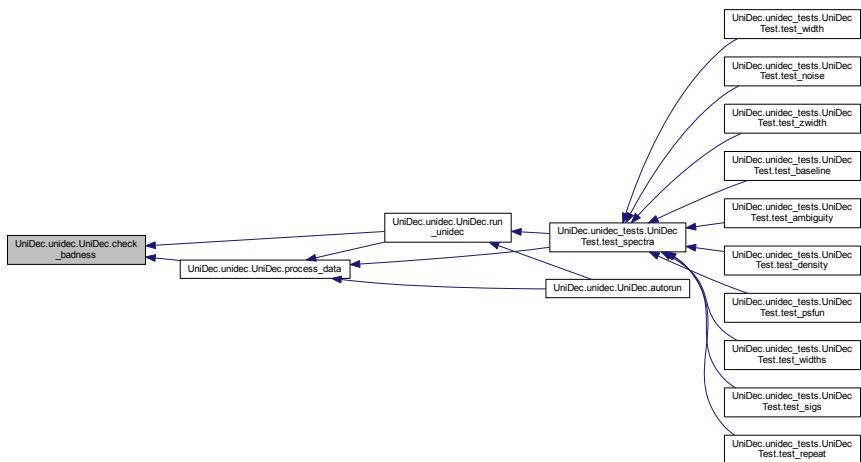
7.56.2.5 def UniDec.unidec.UniDec.center_of_mass (self, data=None, limits=None)

Return the center of mass and weighted standard deviation for data within some limits. If data is None, self.data.massdat is used. If limits is None, the whole range is used.
:param data: mass data to determine center of mass
:param limits: limits to restrict the calculation
:return: com, std (center of mass, weighted standard deviation)

7.56.2.6 def UniDec.unidec.UniDec.check_badness (self)

Check for problematic variables, such as upper bounds less than lower bounds and raise warning if found.
:return:

Here is the caller graph for this function:



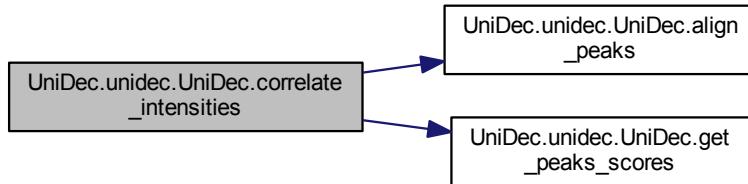
7.56.2.7 def UniDec.unidec.UniDec.convolve_peaks (self)

Convolve Peaks with Peak Shape

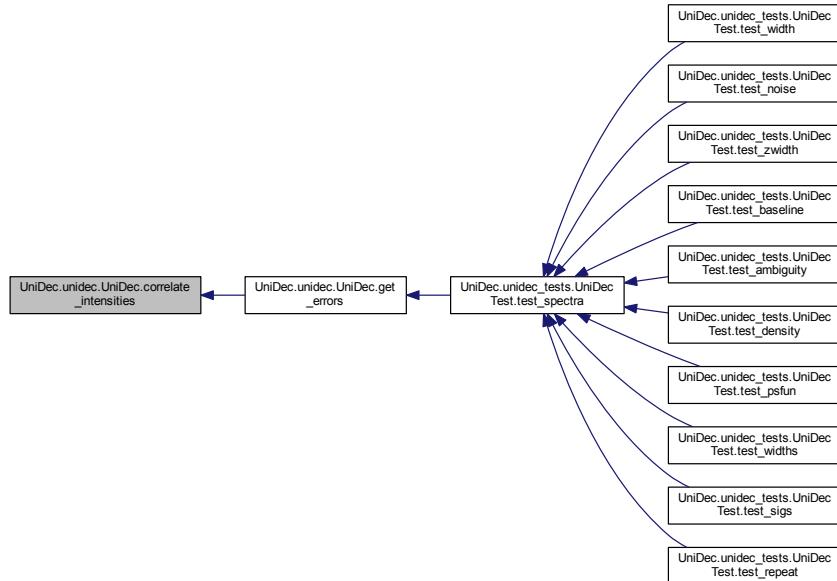
```
:return: None
```

7.56.2.8 def UniDec.unidec.UniDec.correlate_intensities (self, pmasses =None, x_range =None, window =None, ci = 0.99, kwargs)

Here is the call graph for this function:



Here is the caller graph for this function:



7.56.2.9 def UniDec.unidec.UniDec.cross_validate (self, numcrosstot = 5)

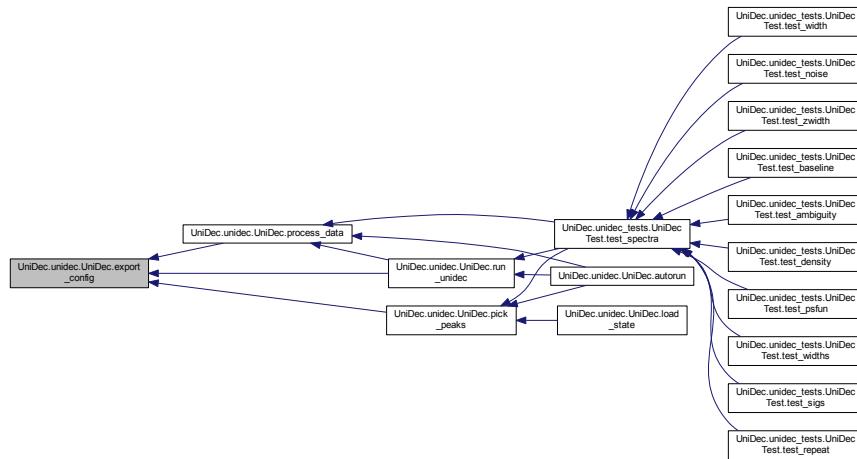
Experimental function to perform cross validation
:param numcrosstot: Number of cross validation routines to perform
:return: mean, stddev (mean and standard deviation of mass distribution following cross validation)

7.56.2.10 def UniDec.unidec.UniDec.export_config (self, f_name =None)

Export UniDec Configuration File

```
:param f_name: File name, Default of None will using config.confname
:return: None
```

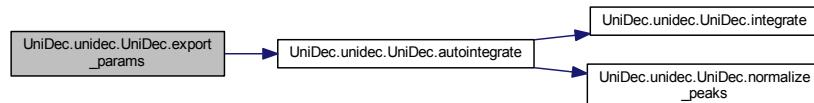
Here is the caller graph for this function:



7.56.2.11 def UniDec.unidec.UniDec.export_params (self, e)

Export a number of different parameters about the peaks into different text files.
:param e: if e is "PostFit", it will output mass fit parameters as well
:return: None

Here is the call graph for this function:



Here is the caller graph for this function:

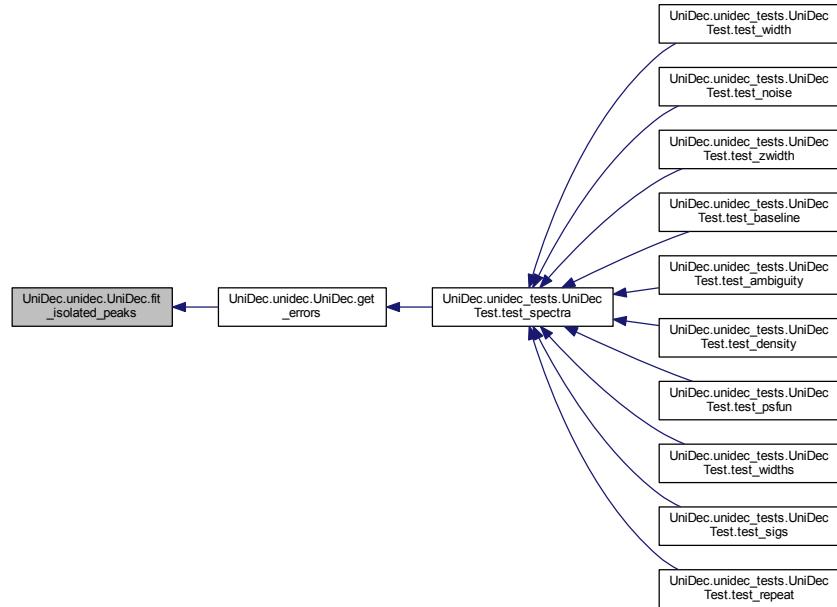


7.56.2.12 def UniDec.unidec.UniDec.fit_all_masses (self)

Fit all masses to a series of peaks, with initial guesses defined by the peak parameters.
:return: self.massfitdat, self.massfit (fit to data, fit parameters)

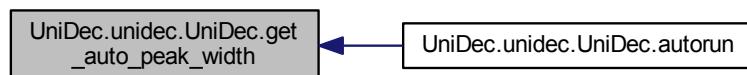
```
7.56.2.13 def UniDec.unidec.UniDec.fit_isolated_peaks( self, pmasses =None, x_range =None, window =None, norm =False, plot_fits =False, kwargs )
```

Here is the caller graph for this function:



```
7.56.2.14 def UniDec.unidec.UniDec.get_auto_peak_width( self )
```

Here is the caller graph for this function:

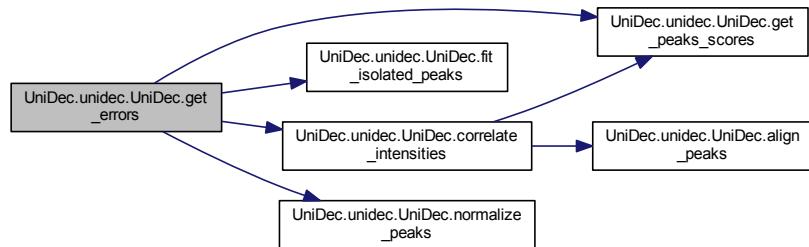


```
7.56.2.15 def UniDec.unidec.UniDec.get_charge_peaks( self )
```

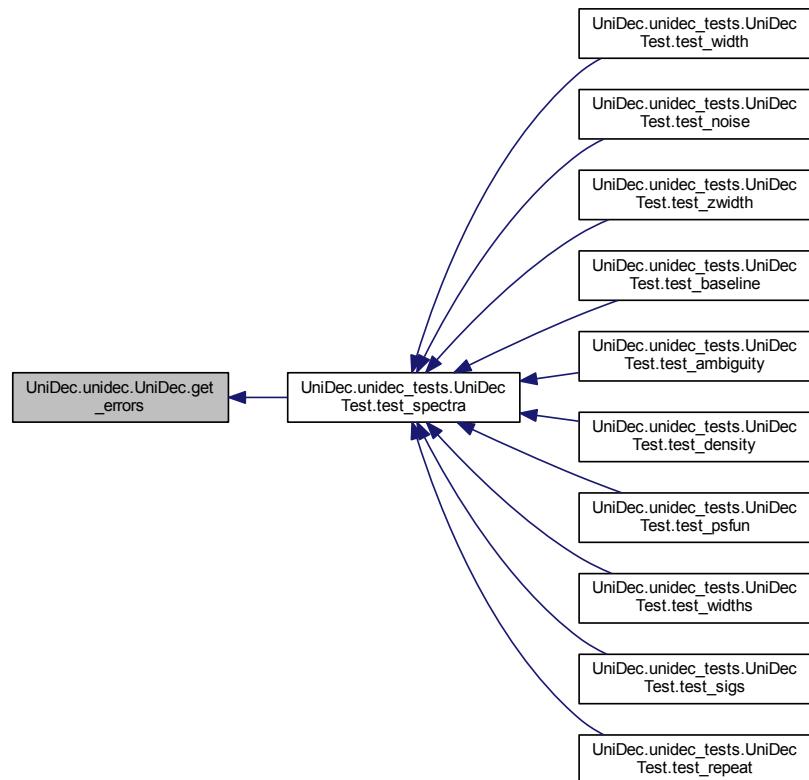
Determines total charge distribution. Imports each charge state as a peak in `self.pks`. Will overwrite mass peaks.
:return: `cpeaks` (Z x 2 array of (charge state, intensity))

7.56.2.16 def UniDec.unidec.UniDec.get_errors (self, kwargs)

Here is the call graph for this function:

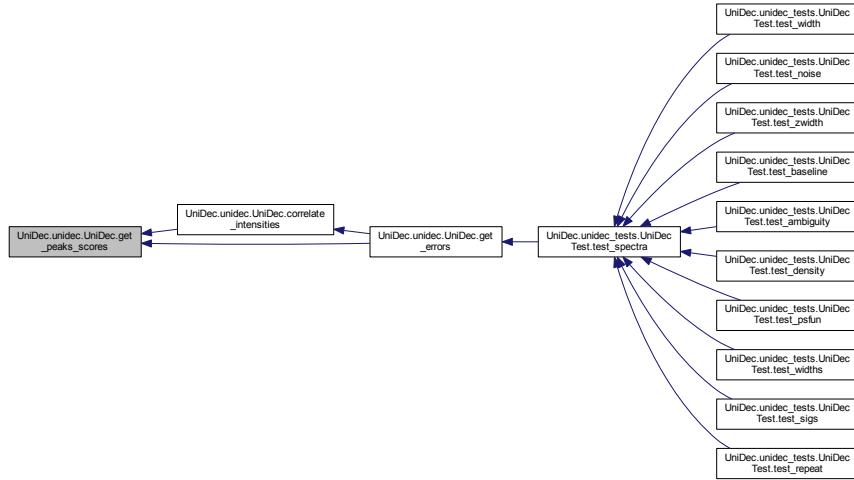


Here is the caller graph for this function:



7.56.2.17 def UniDec.uniDec.UniDec.get_peaks_scores (self, window =None, x_range =None, ci =0.99, kwargs)

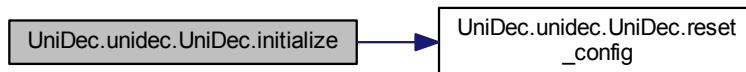
Here is the caller graph for this function:



7.56.2.18 def UniDec.uniDec.UniDec.initialize (self)

```
Initialize Config, DataContainer, and Peaks
:returns: None
```

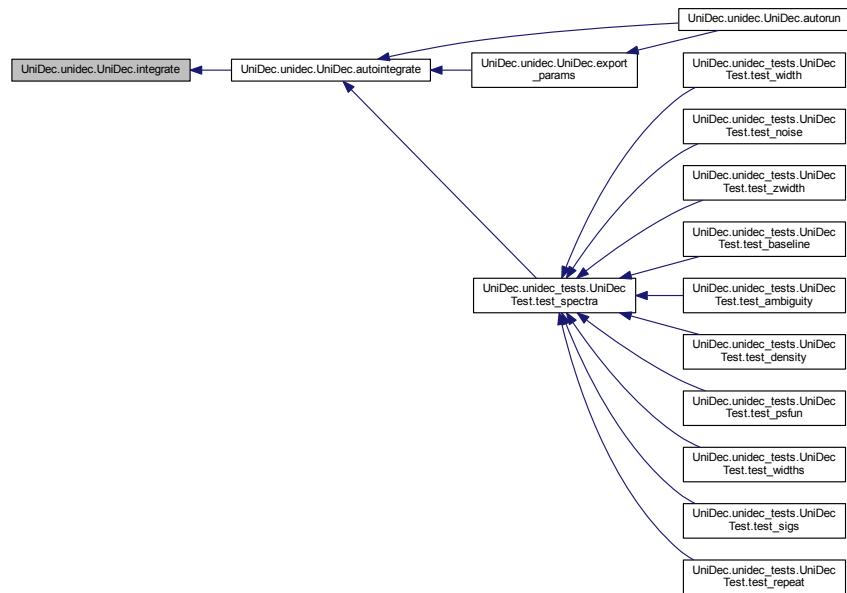
Here is the call graph for this function:



7.56.2.19 def UniDec.uniDec.UniDec.integrate (self, limits, data =None)

```
Trapezoid integrate data between limits[0] and limits[1]
:param limits: [min,max] list of lower and upper bounds on integration
:param data: N x 2 array of data (mass, intensity)
If data is None (default), self.data.massdat is used.
:returns: None
```

Here is the caller graph for this function:



7.56.2.20 def UniDec.unidec.UniDec.kendrick_continuous (self, ref_mass = None, centermode = 0, nbins = 50, transformmode = 0, xaxistype = 1)

```

Runs continuous Kendrick analysis on self.data.massdat
:param ref_mass: Kendrick mass. Default is self.config.kendrickmass if it is already set and >0.
Otherwise, default is oligomer mass (self.config.molig)
:param centermode: Set range for normalization 0=(0,1),1=(-0.5,0.5). Default is 0.
:param nbins: Set mass defect axis density. Default is 50 bins.
:param transformmode: Set type of transformation. 0=Interpolation. 1=Integration. Default is 0.
:param xaxistype: Set x-axis dimensions. 0=Kendrick Mass Number, 1=Mass Number * Kendrick Mass. Default is 1.
:return: mass grid, mass defect grid, intensity grid. All with shape (len(self.data.massdat),nbins)
  
```

7.56.2.21 def UniDec.unidec.UniDec.kendrick_peaks (self, kmass = None, centermode = 1)

```

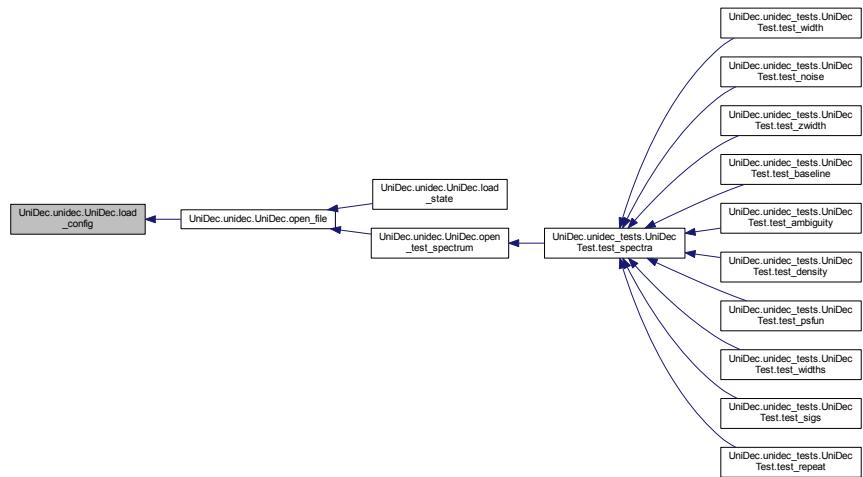
Run Kendrick analysis on peaks (self.pks object)
:param kmass: Kendrick mass. Default is prior kendrick mass if it exists and is >0.
Otherwise, default is oligomer mass (self.config.molig)
:param centermode: Set range for normalization 1=(0,1),0=(-0.5,0.5)
:return: Array of [mass,defect] for each peak in self.pks.
  
```

7.56.2.22 def UniDec.unidec.UniDec.load_config (self, f_name)

```

Import UniDec Configuration File
:param f_name: File name
:return: None
  
```

Here is the caller graph for this function:



7.56.2.23 def UniDec.unidec.UniDec.load_default (self)

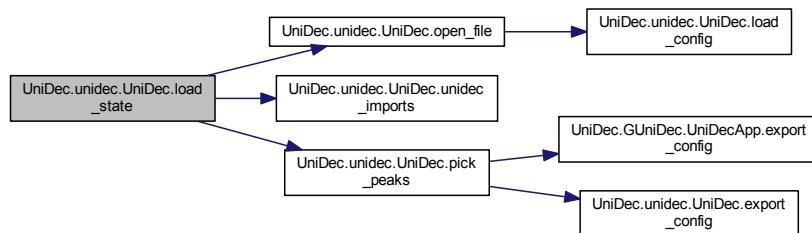
Loads config from default location set at self.config.defaultconfig
 :return: None

7.56.2.24 def UniDec.unidec.UniDec.load_state (self, load_path)

Load UniDec state from a zip save file.

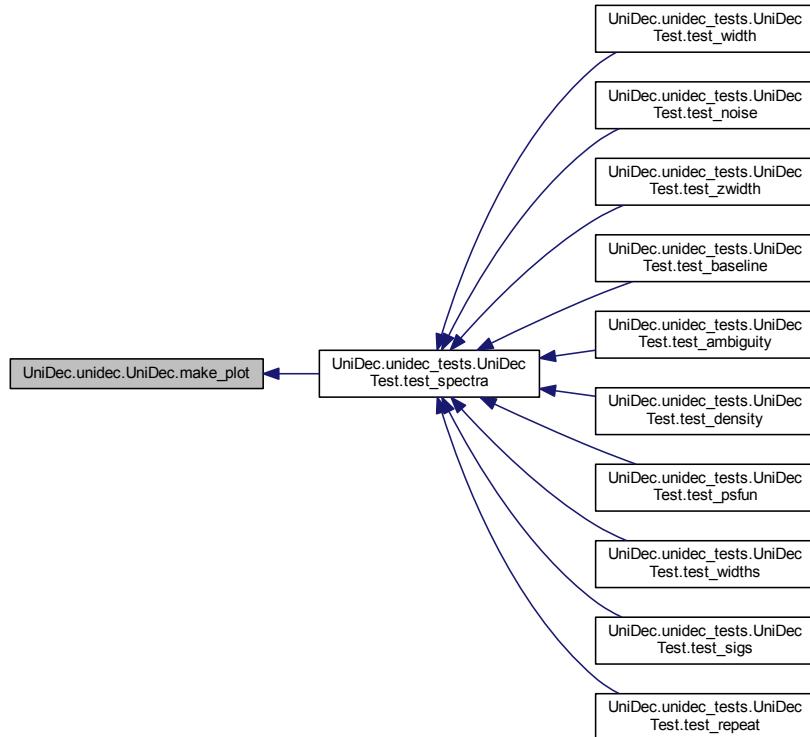
Note: save_state is located under unidectools (ud.savestate)
 :param load_path: .zip file to load
 :return: True is successful, False if failed

Here is the call graph for this function:



7.56.2.25 def UniDec.unidec.UniDec.make_plot(self, massrange =None)

Here is the caller graph for this function:



7.56.2.26 def UniDec.unidec.UniDec.mass_grid_to_f_grid(self)

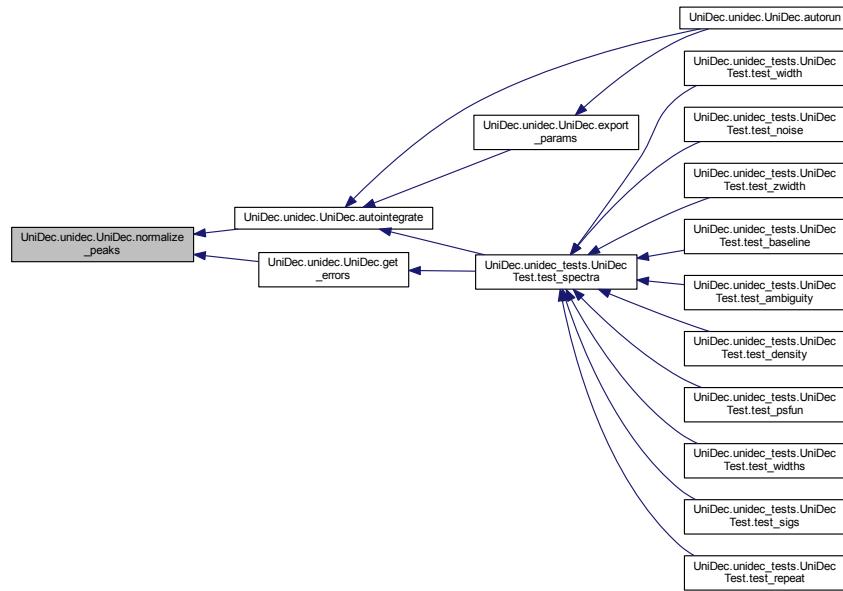
Convert the mass vs charge grid to a mass vs charge offset grid.

Calculates the charge offset for each (mass,charge) point, creates a new axis of regularly spaced charge offsets (oaxis), and the interpolates a new grid of (mass, offset) from oaxis, which is output as outgrid.
:return: oxais, outgrid: offset axis (N) and offset grid (M x N)

7.56.2.27 def UniDec.unidec.UniDec.normalize_peaks(self)

```
Noamlize everything in the peaks accoring to the type set in self.config.peaknorm
0 = No normalization
1 = Normalize the max value to 1
2 = Normalize the sum to 1
:return: None
```

Here is the caller graph for this function:



7.56.2.28 def UniDec.uniDec.UniDec.open_file(self, file_name, file_directory, kwargs)

Open text or mzML file. Will create _unidecfiles directory if it does not exist.

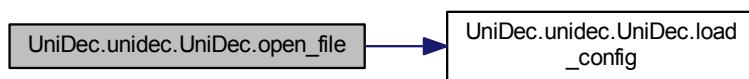
If it finds a _conf.dat file in _unidecfiles, it will import the old configuration. Otherwise, it keeps the existing configuration but resets file names.

If silent=True is passed in **kwargs, prints are suppressed.

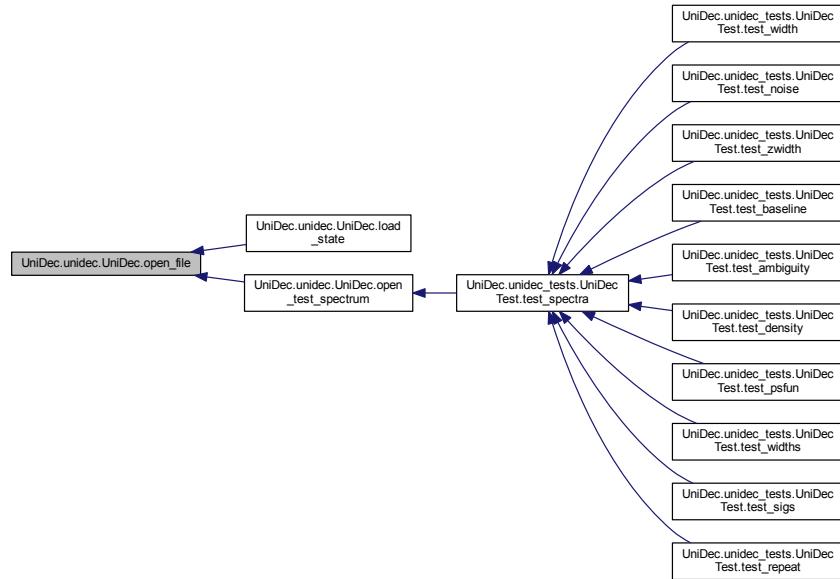
```

:param file_name: Name of file to open. May be in x y or x y z text format or in mzML format.
May be tab or space delimited
:param file_directory: Directory in which filename is located
:returns: None
  
```

Here is the call graph for this function:

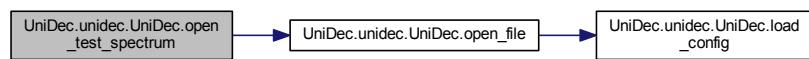


Here is the caller graph for this function:

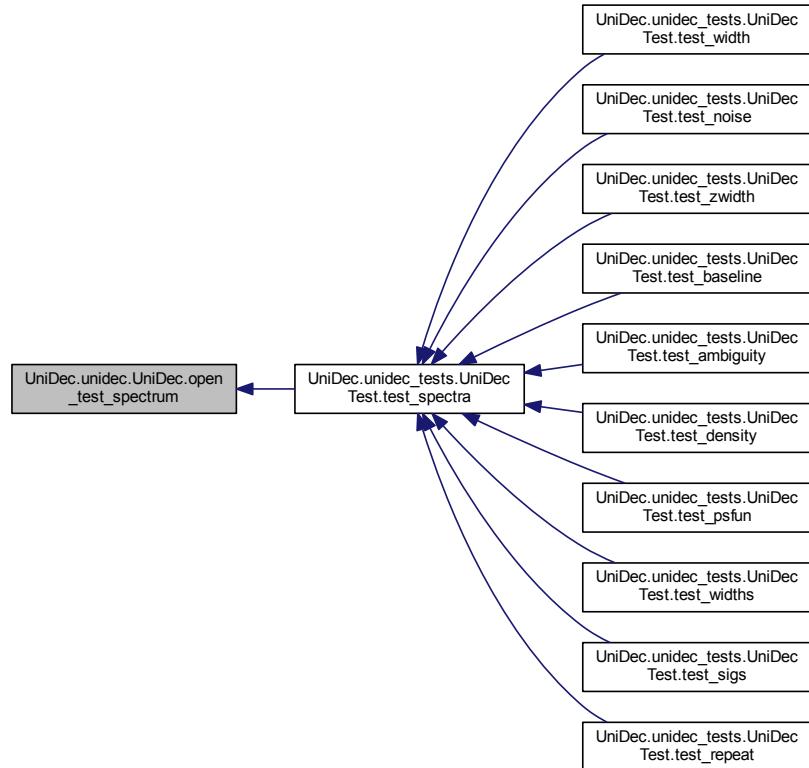


7.56.2.29 `def UniDec.unidec.UniDec.open_test_spectrum(self, masslist=None, n=1, kwargs)`

Here is the call graph for this function:



Here is the caller graph for this function:

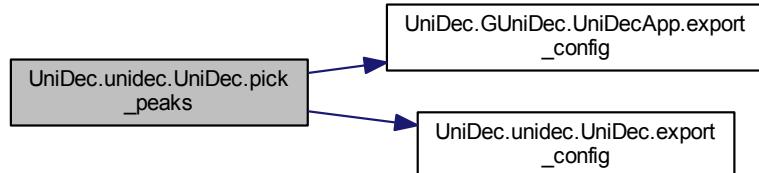


7.56.2.30 def UniDec.unidec.UniDec.pick_peaks (self)

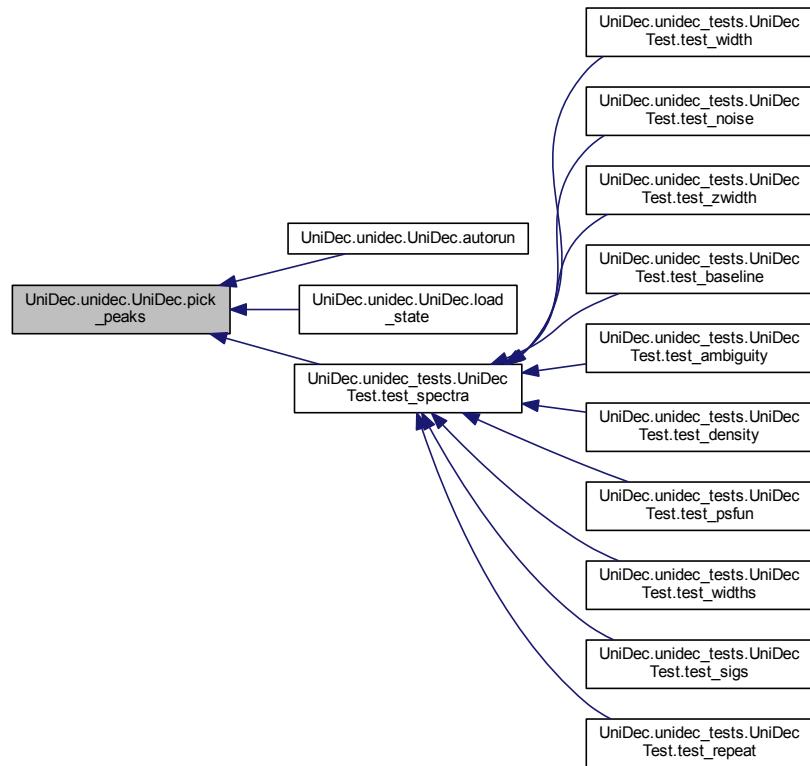
```

Detect, Normalize, and Output Peaks
:returns: None
  
```

Here is the call graph for this function:



Here is the caller graph for this function:

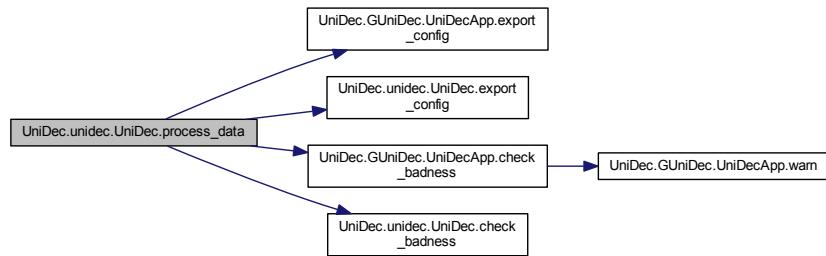


7.56.2.31 def UniDec.unidec.UniDec.process_data(self, kwargs)

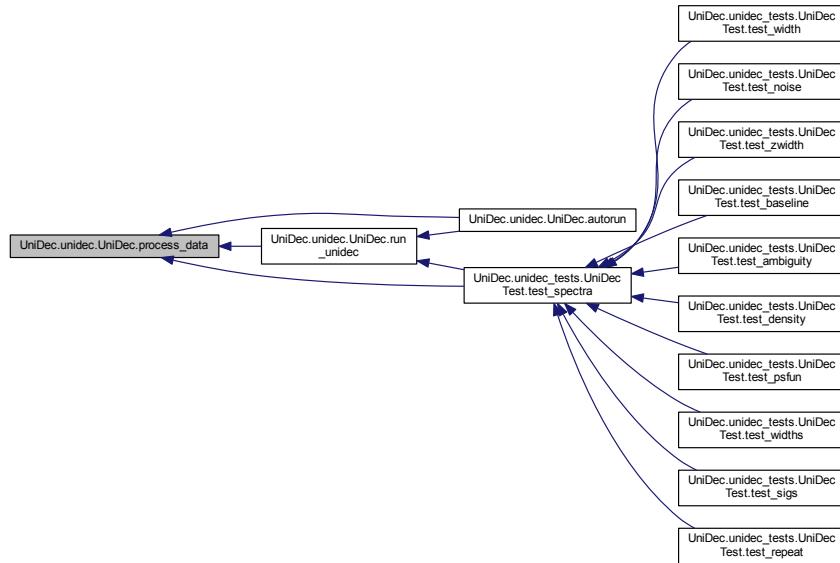
Process data according to parameters in config.

Checks certain parameters to make sure the limits make sense.
Will accept silent=True kwarg to suppress printing.
:return: None

Here is the call graph for this function:



Here is the caller graph for this function:



7.56.2.32 def UniDec.unidec.UniDec.process_mass_data (self)

Apply the same parameters used to process the data to process the mass distribution. Linearization parameters are ignored, but smoothing, baseline subtraction, normalization, and intensity threshold all apply.
:return: None

7.56.2.33 def UniDec.unidec.UniDec.raw_process (self, dirname, inflag = False, binsize = 1)

Processes Water's Raw files into .txt using external calls to:
self.config.rawreaderpath for MS
self.config.cdcreaderpath for IM-MS

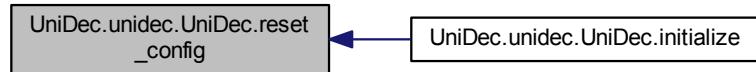
Default files are created with the header of the .raw file plus:
_rawdata.txt for MS
_imraw.txt for IM-MS

:param dirname: .raw directory name
:param inflag: If True, it will put the output .txt file inside the existing .raw directory. If False, it will put the file in the same directory that contains the .raw directory
:param binsize: Parameter for IM-MS to specify the m/z bin size for conversion. If binsize=0, the conversion will be at full resolution (which is huge), so the default is every 1 m/z.
:return: self.config.filename, self.config.dirname (name and location of created file)

7.56.2.34 def UniDec.unidec.UniDec.reset_config (self)

Resets UniDec config to default. Should not reset paths or filenames.
:return: None

Here is the caller graph for this function:



7.56.2.35 def UniDec.unidec.UniDec.run_unidec (self, silent=False, efficiency=False)

Runs UniDec.

Checks that everything is set to go and then places external call to:
`self.config.UniDecPath` for MS
`self.config.UniDecIMPath` for IM-MS

If successful, calls `self.unidec_imports()`

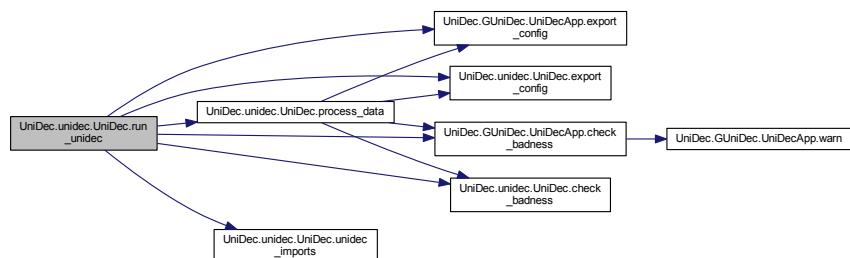
If not, prints the error code.

:param silent: If True, it will suppress printing the output from UniDec

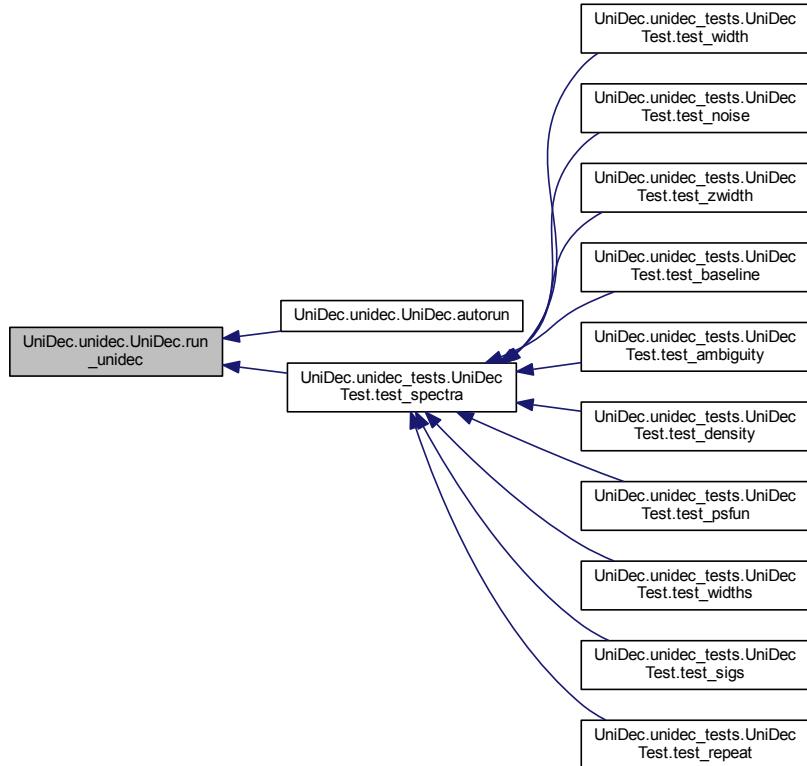
:param efficiency: Passed to `self.unidec_imports()`

:return: out (stdout from external UniDec call)

Here is the call graph for this function:



Here is the caller graph for this function:



7.56.2.36 def UniDec.unidec.UniDec.save_default(self)

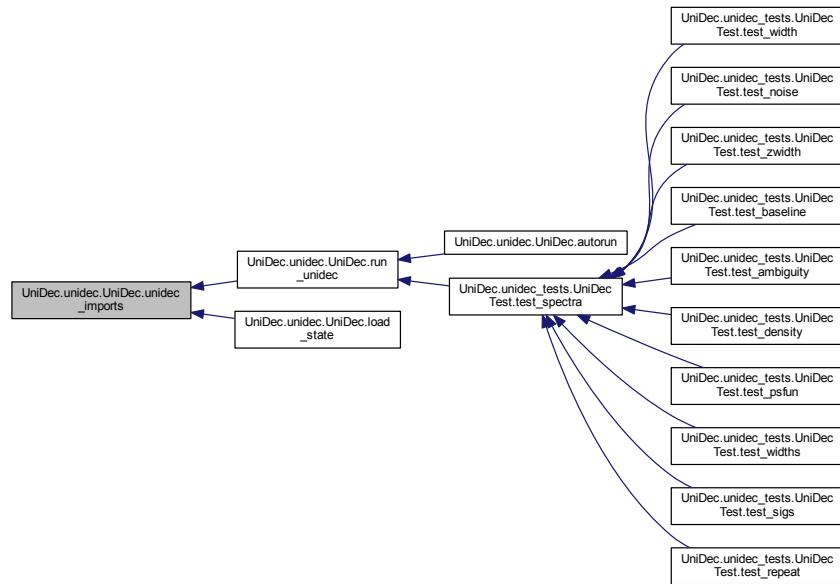
Saves existing config in default location set at self.config.defaultconfig
 :return: None

7.56.2.37 def UniDec.unidec.UniDec.save_state(self, file_name)

7.56.2.38 def UniDec.unidec.UniDec.unidec_imports(self, efficiency=False)

Imports files output from the UniDec core executable into self.data.
 :param efficiency: If True, it will ignore the larger files to speed up the run.
 :return: None

Here is the caller graph for this function:



7.56.3 Member Data Documentation

7.56.3.1 UniDec.unidec.UniDec.autopeaks

7.56.3.2 UniDec.unidec.UniDec.config

7.56.3.3 UniDec.unidec.UniDec.data

7.56.3.4 UniDec.unidec.UniDec.errorgrid

7.56.3.5 UniDec.unidec.UniDec.massfit

7.56.3.6 UniDec.unidec.UniDec.massfitdat

7.56.3.7 UniDec.unidec.UniDec.peakparams

7.56.3.8 UniDec.unidec.UniDec.pks

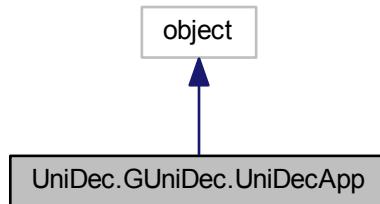
7.56.3.9 UniDec.unidec.UniDec.version

The documentation for this class was generated from the following file:

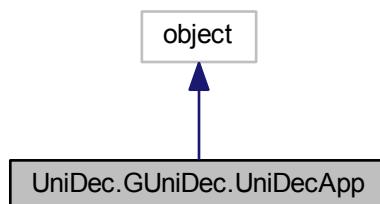
- C:/Python/UniDec/unidec.py

7.57 UniDec.GUniDec.UniDecApp Class Reference

Inheritance diagram for UniDec.GUniDec.UniDecApp:



Collaboration diagram for UniDec.GUniDec.UniDecApp:



Public Member Functions

- def `__init__` (self, args, kwargs)
- def `start` (self)
- def `on_end_session` (self)
- def `quit_application` (self)
- def `init` (self, args, kwargs)
- def `import_config`
- def `export_config`
- def `on_open`
- def `on_open_file`
- def `on_save_state`
- def `on_load_state`
- def `on_raw_open`
- def `on_load_conf_file`
- def `on_save_default`
- def `on_load_default`
- def `on_paste_spectrum`
- def `on_reset`

- def `on_dataprep_button`
- def `on_unidec_button`
- def `after_unidec_run` (self)
- def `on_pick_peaks`
- def `on_plot_peaks`
- def `on_peak_errors`
- def `check_badness` (self)
- def `warn`
- def `on_auto`
- def `makeplot1`
- def `makeplot2`
- def `makeplot3`
- def `makeplot4`
- def `makeplot5`
- def `makeplot6`
- def `on_plot_composite`
- def `make_im_plots` (self)
- def `on_plot_nativeccs`
- def `on_replot`
- def `make_cube_plot`
- def `on_delete`
- def `on_charge_states`
- def `on_differences`
- def `on_plot_offsets`
- def `on_color_plot1d`
- def `plot_integral`
- def `on_integrate`
- def `on_smash` (self)
- def `on_get_mzlimits` (self)
- def `on_charge_plot`
- def `on_batch_raw`
- def `on_manual`
- def `on_match`
- def `on_mass_tools`
- def `on_auto_peak_width`
- def `on_peak_width_tool`
- def `on_additional_parameters`
- def `on_autocorr_window`
- def `on_unidec_path`
- def `on_file_name`
- def `on_data_collector`
- def `on_import_wizard`
- def `on_im_tools`
- def `on_im_extract`
- def `on_tweet`
- def `on_kendrick`
- def `on_2d_grid`
- def `on_nativez_tools`
- def `on_export_params`
- def `on_mass_process`
- def `on_calibrate`
- def `on_center_of_mass`
- def `on_zerocharge_mass`
- def `on_fit_masses`
- def `on_batch`

- def `on_batch2`
- def `on_super_batch`
- def `on_cross_validate`
- def `on_pdf_report`
- def `on_fft_window` (self, e)
- def `on_left_click` (self, xpos, ypos)
- def `on_grid_decon` (self, e)
- def `on_flip_mode` (self, e)
- def `on_flip_tabbed` (self, e)
- def `on_flip_twave` (self, e)
- def `remake_mainwindow`

Public Attributes

- `eng`
- `view`
- `twittercodes`

7.57.1 Detailed Description

Main UniDec GUI Application.

Presenter contains UniDec engine at `self.eng` and main GUI window at `self.view`

7.57.2 Constructor & Destructor Documentation

7.57.2.1 def UniDec.GUniDec.UniDecApp.`__init__` (`self, args, kwargs`)

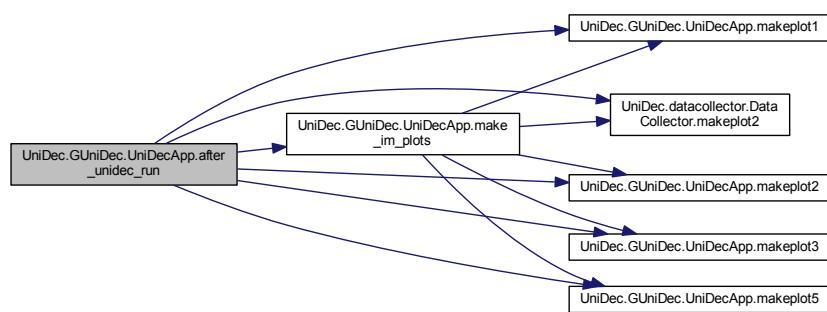
```
Initialize App
:param args:
:param kwargs:
:return: UniDecApp object
```

7.57.3 Member Function Documentation

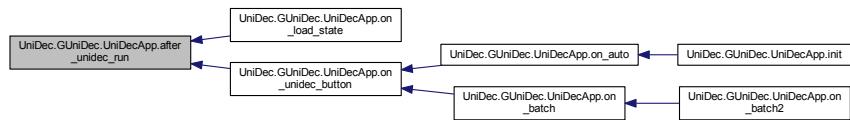
7.57.3.1 def UniDec.GUniDec.UniDecApp.`after_unidec_run` (`self`)

```
Plots to make after running UniDec.
:return: None
```

Here is the call graph for this function:



Here is the caller graph for this function:



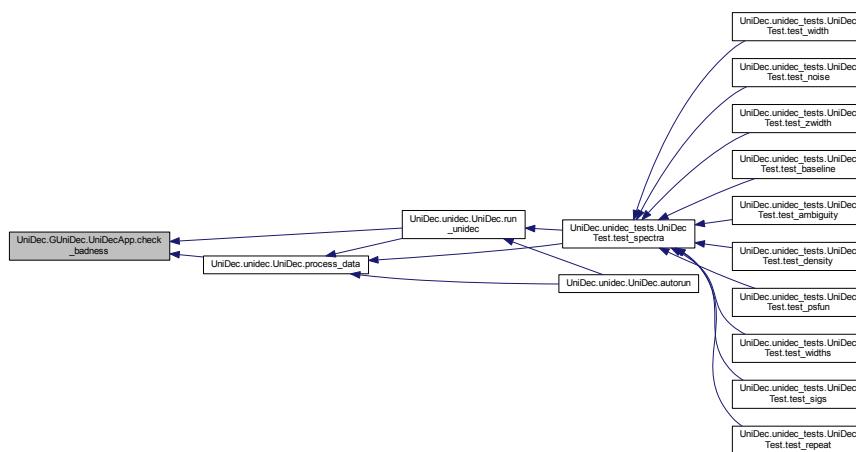
7.57.3.2 def UniDec.GUniDec.UniDecApp.check_badness (self)

Check for any bad parameters and warn the user if something is off.
:returns: code (see unidecstructure.check_badness)

Here is the call graph for this function:



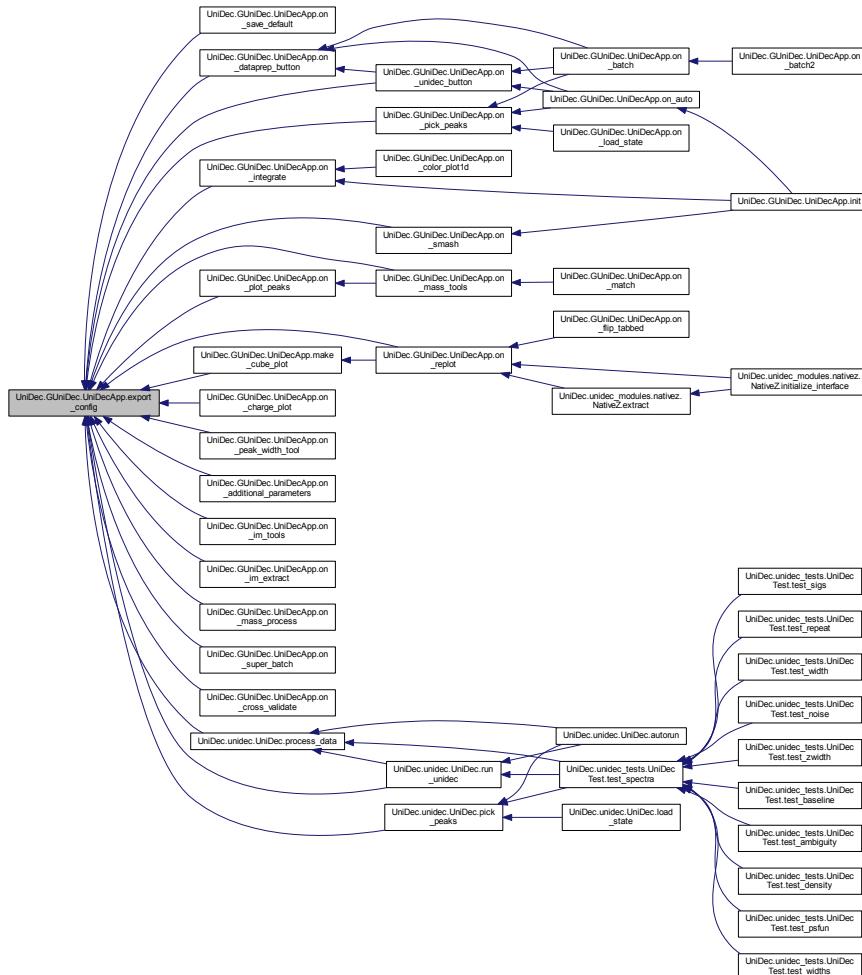
Here is the caller graph for this function:



7.57.3.3 def UniDec.GUniDec.UniDecApp.export_config (self, file_name = None)

Get configuration from GUI and (if file_name is specified) write from engine to file_name
:param file_name: Path of file to save config to
:returns: None

Here is the caller graph for this function:

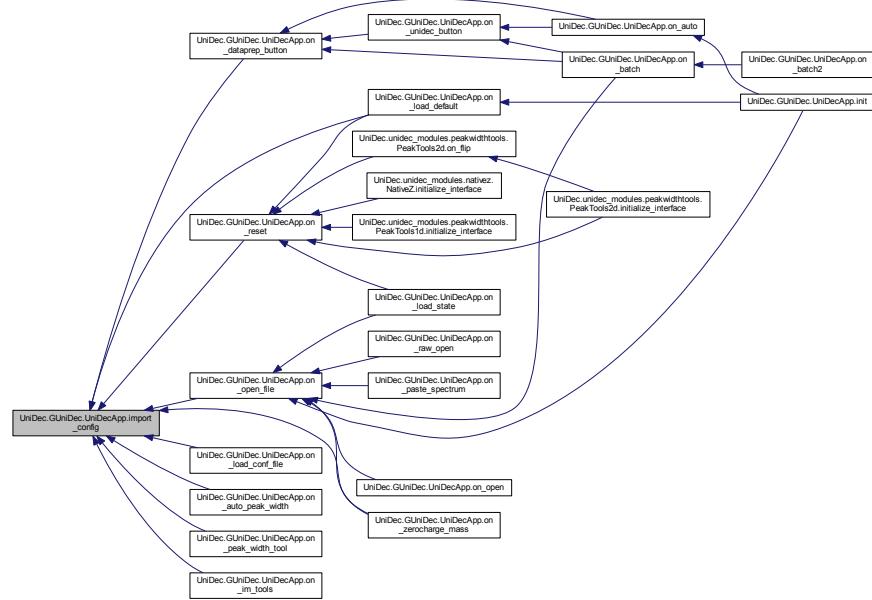


7.57.3.4 def UniDec.GUniDec.UniDecApp.import_config (self, file_name = None)

```

Import configuration from file to engine (if file_name is specified) and from engine to GUI.
:param file_name: Path of file to import
:return: None
  
```

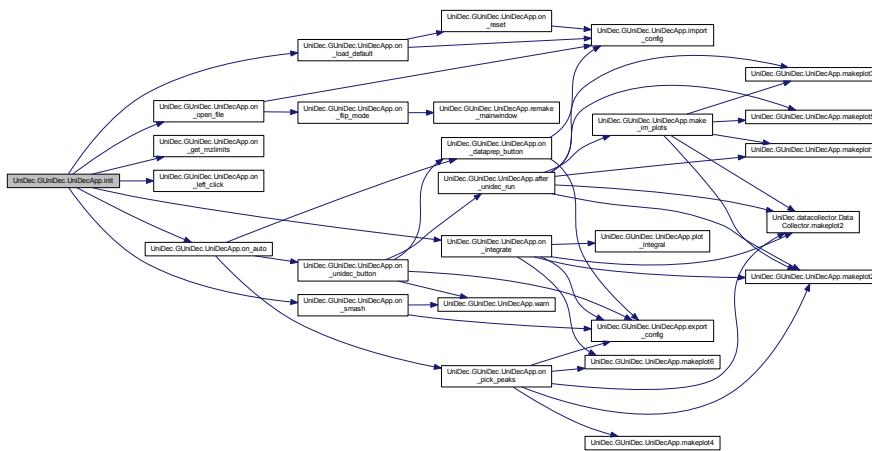
Here is the caller graph for this function:



7.57.3.5 def UniDec.GUniDec.UniDecApp.init (self, args, kwargs)

```
Initialize Engine and View. Load defaults.  
:param args:  
:param kwargs:  
:return:
```

Here is the call graph for this function:



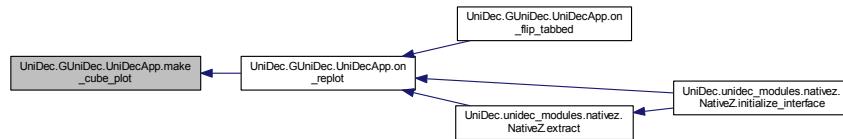
7.57.3.6 def UniDec.GUniDec.UniDecApp.make_cube_plot(self, e = None)

```
Make cube plots for IMMS.  
:param e: unused event  
:return: None
```

Here is the call graph for this function:



Here is the caller graph for this function:

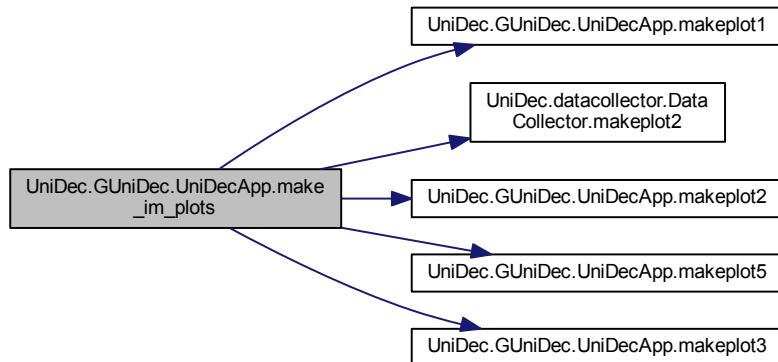


7.57.3.7 def UniDec.GUniDec.UniDecApp.make_im_plots (self)

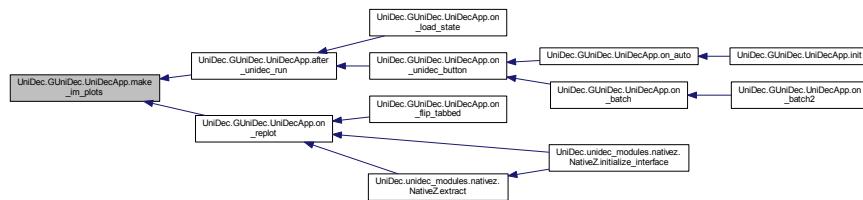
```

Make Ion Mobility plots (but not cube plots)
:returns: None
  
```

Here is the call graph for this function:



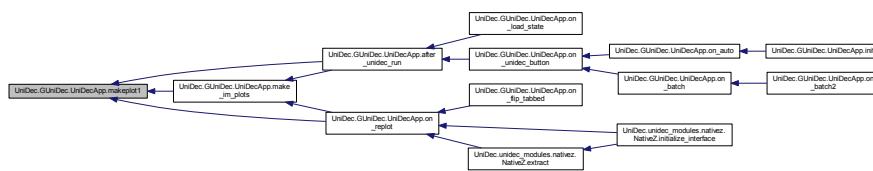
Here is the caller graph for this function:



7.57.3.8 def UniDec.GUniDec.UniDecApp.makeplot1 (self, e=None)

Plot data and fit in self.view.plot1 and optionally in plot1fit
:param e: unused event
:return: None

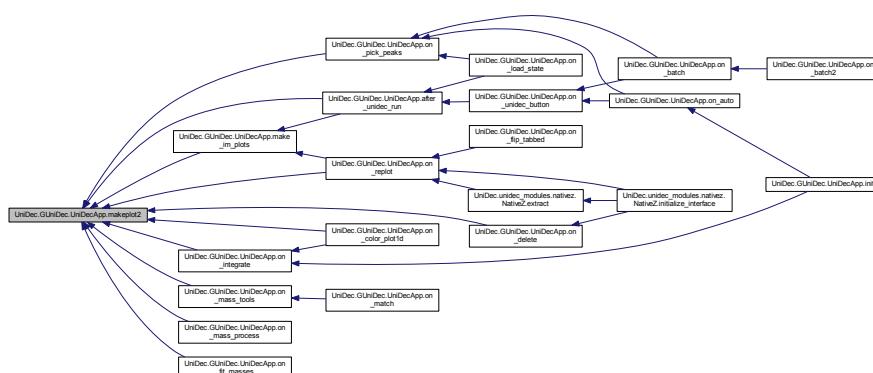
Here is the caller graph for this function:



7.57.3.9 def UniDec.GUniDec.UniDecApp.makeplot2 (self, e=None)

Plot mass data and peaks if possible in self.view.plot2
:param e: unused event
:return: None

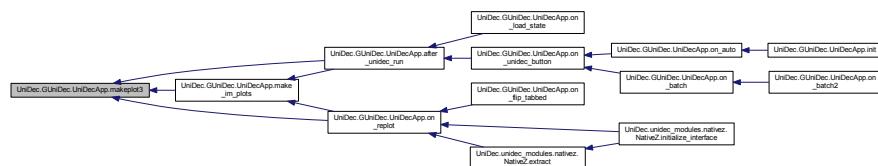
Here is the caller graph for this function:



7.57.3.10 def UniDec.GUniDec.UniDecApp.makeplot3 (self, e=None)

```
Plot m/z vs charge grid.
:param e: unused event
:return: None
```

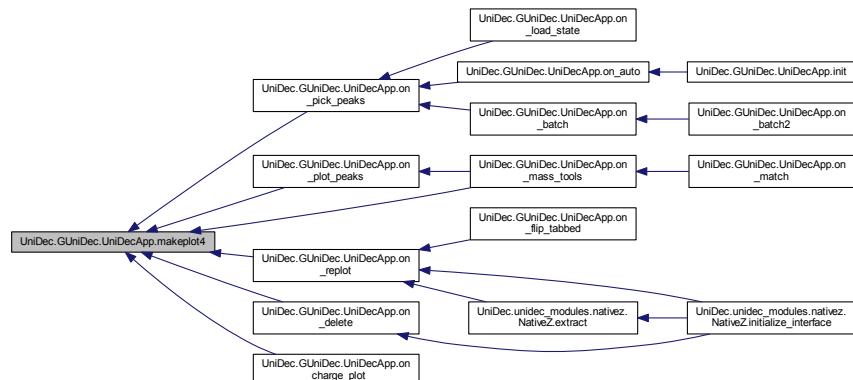
Here is the caller graph for this function:



7.57.3.11 def UniDec.GUniDec.UniDecApp.makeplot4 (self, e=None)

```
Plots isolated peaks against the data in self.view.plot4.
Will plot dots at peak positions.
If possible, will plot full isolated spectra.
:param e: unused event
:return: None
```

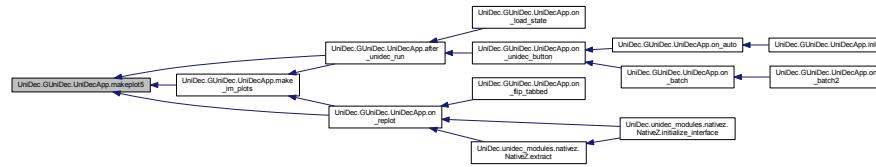
Here is the caller graph for this function:



7.57.3.12 def UniDec.GUniDec.UniDecApp.makeplot5 (self, e=None)

```
Plot mass vs charge grid
:param e: unused event
:return: None
```

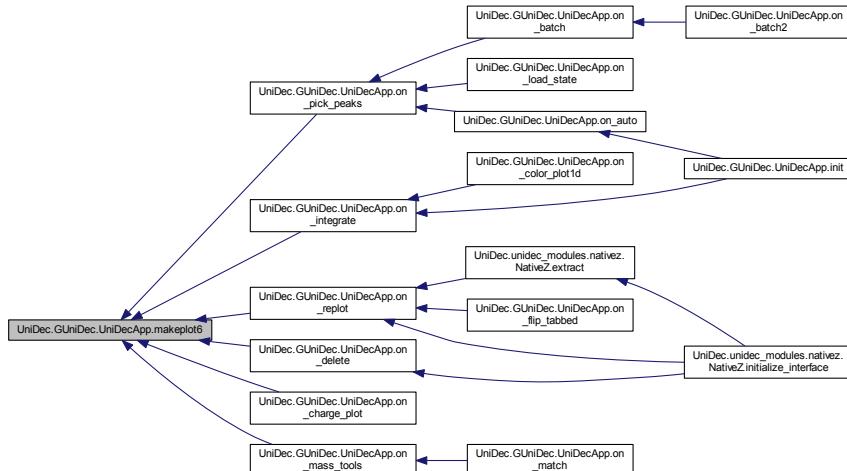
Here is the caller graph for this function:



7.57.3.13 def UniDec.GUniDec.UniDecApp.makeplot6(self, e=None, show="height")

Plots bar chart of peak heights or areas in self.view.plot6.
:param e: unused event
:param show: What parameter to plot
"height" will plot p.height for p in self.eng.pks.peaks
"integral" will plot p.integral
:return: None

Here is the caller graph for this function:



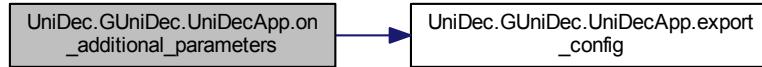
7.57.3.14 def UniDec.GUniDec.UniDecApp.on_2d_grid(self, e=None)

Opens 2D grid extraction window. Grid extraction parameters are stored at self.eng.config.gridparams.
:param e: unused event
:return: None

7.57.3.15 def UniDec.GUniDec.UniDecApp.on_additional_parameters(self, e=None)

Open additional data parameter window, which has some of the experimental and obscure variables.
Window directly modifies self.eng.config.
Saves config to file after window is closed.
:param e: unused event
:return: None

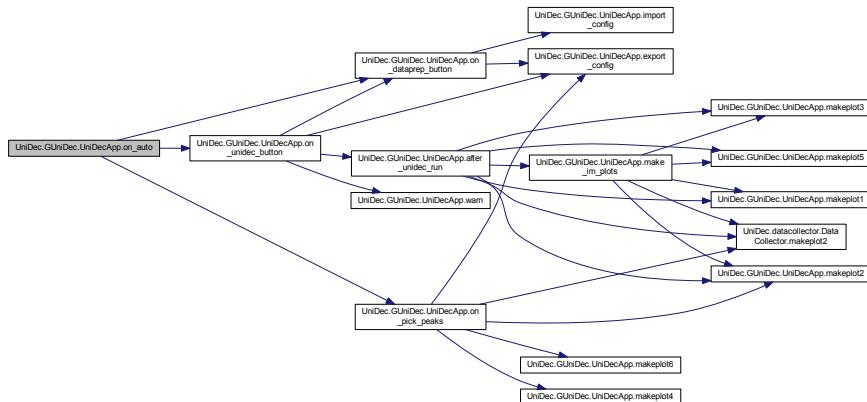
Here is the call graph for this function:



7.57.3.16 def UniDec.GUniDec.UniDecApp.on_auto(self, e=None)

Prepare data, run UniDec, and pick peaks.
:param e: unused space for event
:return: None

Here is the call graph for this function:

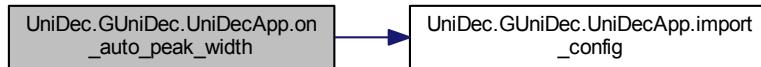


Here is the caller graph for this function:



7.57.3.17 def UniDec.GUniDec.UniDecApp.on_auto_peak_width (self, e=None)

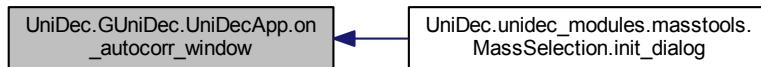
Here is the call graph for this function:



7.57.3.18 def UniDec.GUniDec.UniDecApp.on_autocorr_window (self, e=None)

Opens the autocorrelation window. Feed the config and massdat from the engine.
:param e: Unused event
:return: None

Here is the caller graph for this function:



7.57.3.19 def UniDec.GUniDec.UniDecApp.on_batch (self, e=None, flag=0, batchfiles=None)

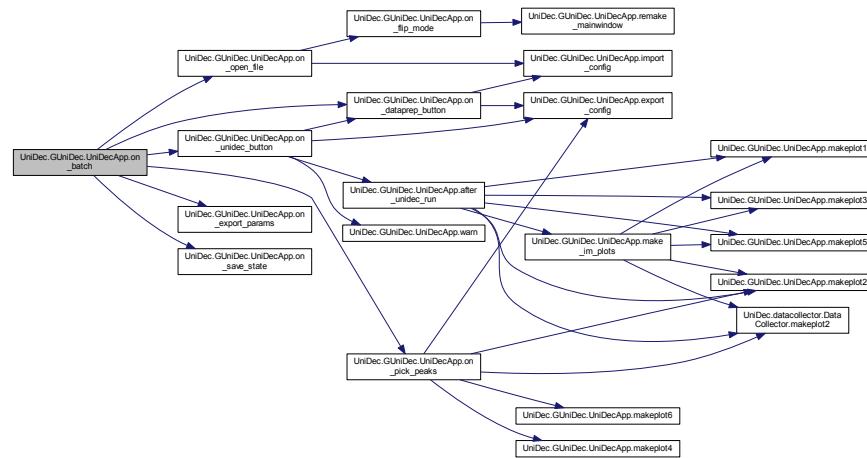
Batch processing!

Spawns a directory to select multiple files.
Feeds the file names into a loop that:

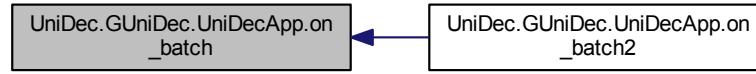
Opens the file (self.on_open_file)
Prepares the data (self.on_dataprep_button)
Runs UniDec (self.unidec_button)
Picks Peaks (self.on_pick_peaks)
Exports Peak Parameters (self.on_export_params)
Saves State (self.on_save_state)

If uses self.eng.config.batchflag to prevent certain things from plotting and all key parameters from changing.
If batchflag is 2 (flag=1),
 all key paramters are kept, but the data ranges are refreshed from the individual files.
:param e: event passed to some function (unused)
:param flag: flag added to self.eng.config.batchflag
:param batchfiles: List of files to run in batch. If None, will open dialog.
:return:

Here is the call graph for this function:



Here is the caller graph for this function:

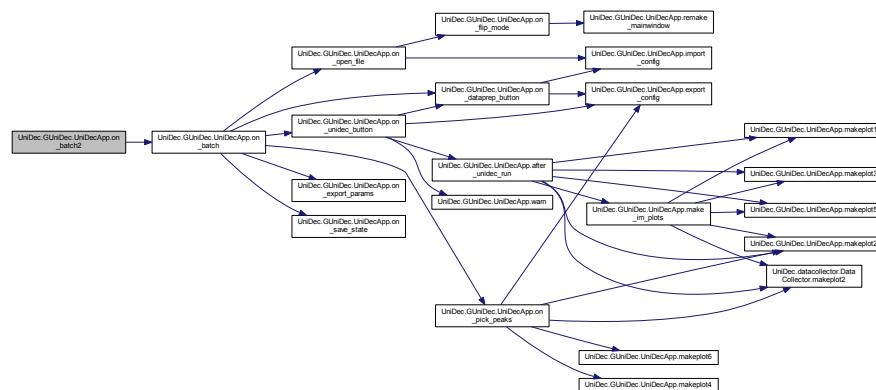


7.57.3.20 def UniDec.GUniDec.UniDecApp.on_batch2(self, e=None)

Runs batch processing without restricting the data ranges.

The date range can be set ahead of time and will update independently for each file.
 Other parameters are fixed for the whole batch.
`:param e: unused event passed to self.on_batch`
`:return: None`

Here is the call graph for this function:



7.57.3.21 def UniDec.GUniDec.UniDecApp.on_batch_raw (self, e=None, dirs=None, clip=True)

Batch process Waters .Raw files into .txt files.
 Opens a multiple directory dialog and then sends the results to self.eng.raw_process
 :param e: unused event
 :return: None

7.57.3.22 def UniDec.GUniDec.UniDecApp.on_calibrate (self, e=None)

7.57.3.23 def UniDec.GUniDec.UniDecApp.on_center_of_mass (self, e=None)

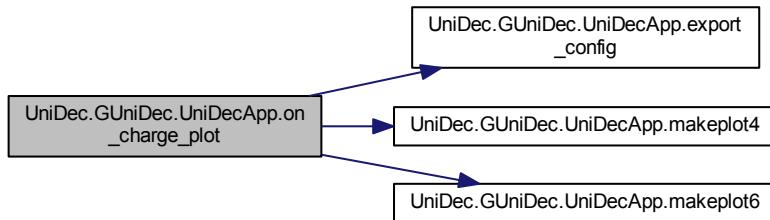
Determines the center of mass for the region zoomed on plot2.

Get limits from plot2.
 Get Center of Mass from self.eng.center_of_mass
 Reports these as text on plot2.
 :param e:
 :return:

7.57.3.24 def UniDec.GUniDec.UniDecApp.on_charge_plot (self, e=None)

Change peaks and plots so that the total charge distribution is plotted in plot2.
 Picks new peaks as each charge state and updates peakpanel.
 :param e: unused event
 :return: None

Here is the call graph for this function:

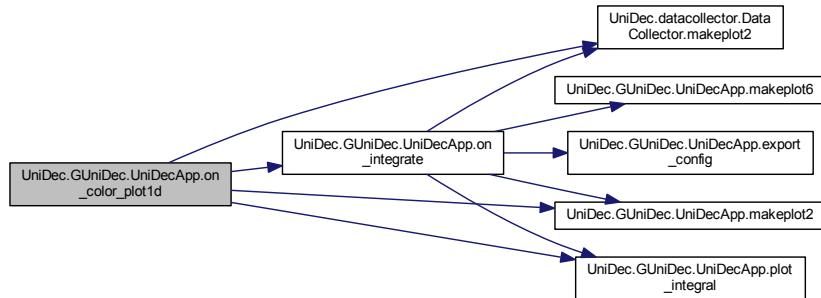


7.57.3.25 def UniDec.GUniDec.UniDecApp.on_charge_states (self, e=None)

Triggered by right click "plot charge states" on self.view.peakpanel.
 Plots a line with text listing the charge states of a specific peak.
 :param e: unused event
 :return: None

7.57.3.26 def UniDec.GUniDec.UniDecApp.on_color_plot1d (*self*, *e*=None, *filled*=False)

Here is the call graph for this function:



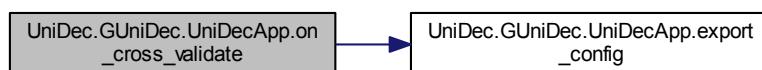
7.57.3.27 def UniDec.GUniDec.UniDecApp.on_cross_validate (*self*, *e*=None)

Experimental...

Run cross validation on spectrum by splitting the spectrum into subspectra and fitting each independently.

Runs `self.eng.cross_validate()`
 Adds plots of mean and std deviation to `plot2`
`:param e: unused event`
`:return: None`

Here is the call graph for this function:



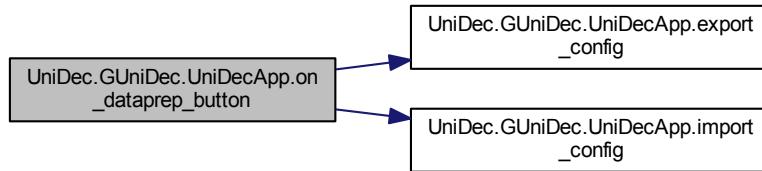
7.57.3.28 def UniDec.GUniDec.UniDecApp.on_data_collector (*self*, *e*=None)

Spawns separate DataCollector window.
`:param e: unused event`
`:return: None`

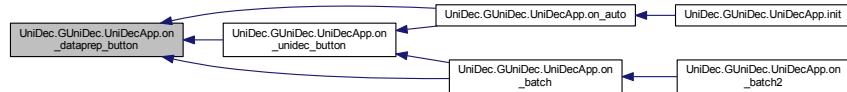
7.57.3.29 def UniDec.GUniDec.UniDecApp.on_dataprep_button (*self*, *e*=None)

Prepares data. Runs `eng.process_data()` and then updates and plots in view
`:param e: unused space for event`
`:return: None`

Here is the call graph for this function:



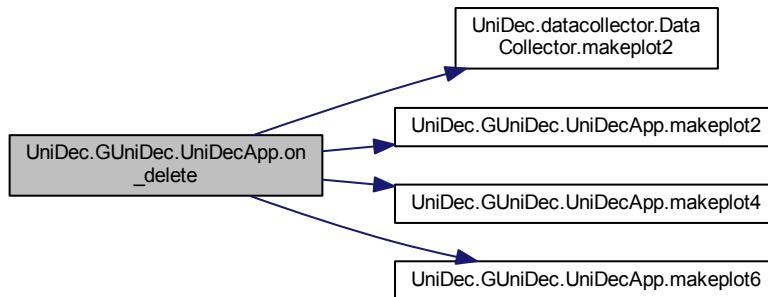
Here is the caller graph for this function:



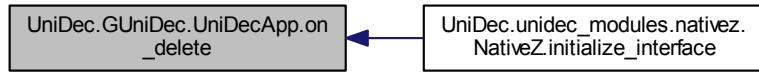
7.57.3.30 def UniDec.GUniDec.UniDecApp.on_delete(self, e=None)

Triggered on deletion or modification of selection in self.view.peakpanel.
Replots everything with peaks involved to reflect ignored peaks.
:param e: unused event
:return: None

Here is the call graph for this function:



Here is the caller graph for this function:



7.57.3.31 def UniDec.GUniDec.UniDecApp.on_differences(self, e=None)

Triggered by right click "Display Differences" on self.view.peakpanel.
 Plots a line with text listing the difference between each mass and a specific peak.
 Updates the peakpanel to show the differences.
 :param e: unused event
 :return: None

7.57.3.32 def UniDec.GUniDec.UniDecApp.on_end_session(self)

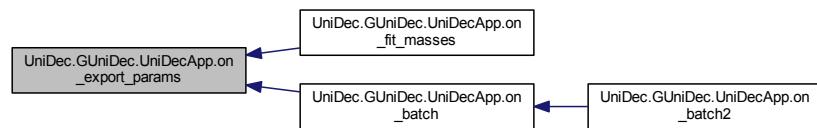
Here is the call graph for this function:



7.57.3.33 def UniDec.GUniDec.UniDecApp.on_export_params(self, e=None)

Runs self.eng.export_params(), which gets critical peak parameters and writes them to a file.
 :param e: event or arguments passed to self.eng.export_params()
 :return: None

Here is the caller graph for this function:



7.57.3.34 def UniDec.GUniDec.UniDecApp.on_fft_window(self, e)

7.57.3.35 def UniDec.GUniDec.UniDecApp.on_file_name(self, e=None)

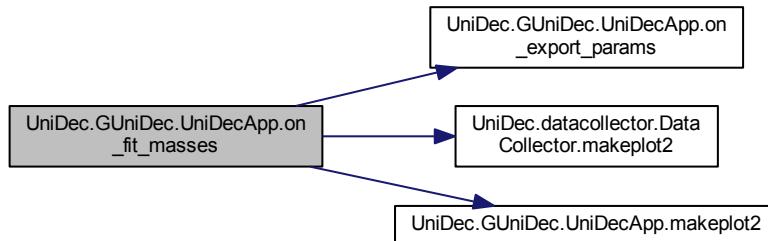
Opens window with default file names in it.
 Possible to tweak default paths here, but probably dangerous.
 :param e: unused event
 :return: None

7.57.3.36 def UniDec.GUniDec.UniDecApp.on_fit_masses(self, e=None)

Using the peaks as a starting guess, it will fit the zero-charge mass spectrum to a set of overlapping peaks.

Gets guesses using self.on_export_params()
 Calls self.eng.fit_all_masses()
 Then, plots resulting fit.
 Updates peakpanel to reflect normalized peak area based on fits.
 Export parameters from fit using self.on_export_params() and sending the "PostFit" argument
 :param e: event or argument passed to self.on_export_params
 :return: None

Here is the call graph for this function:



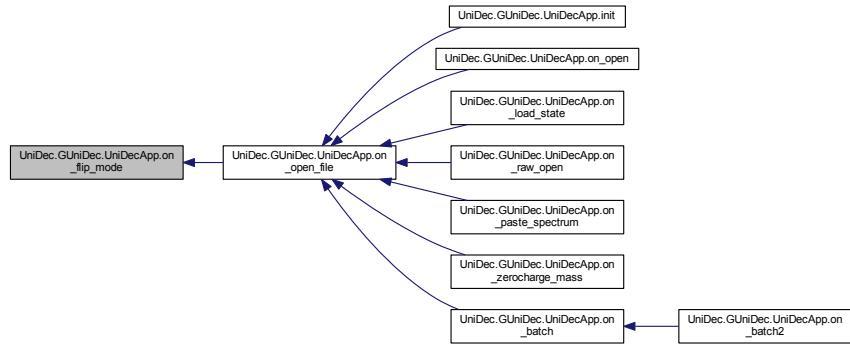
7.57.3.37 def UniDec.GUniDec.UniDecApp.on_flip_mode(self, e)

Flips between MS and IM-MS mode
 :param e: wx event or anything (will flip if not 0)
 :return: None

Here is the call graph for this function:



Here is the caller graph for this function:

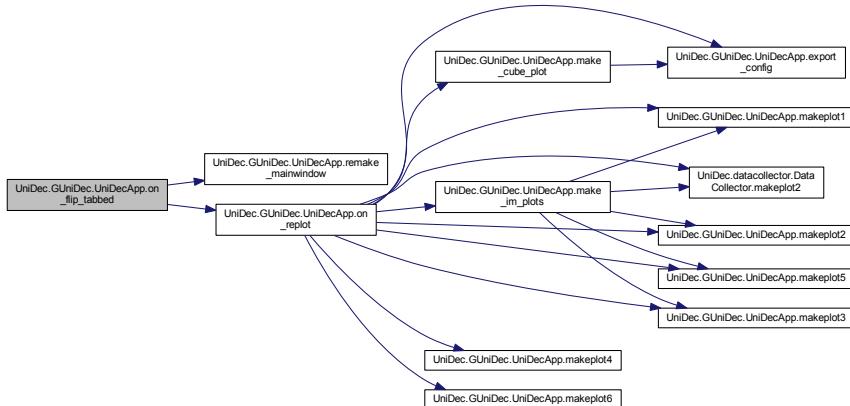


7.57.3.38 def UniDec.GUniDec.UniDecApp.on_flip_tabbed(self, e)

```

Flips between tabbed plots and a single window of plots
:param e: wx Event or anything (will flip if not 0)
:return: None
  
```

Here is the call graph for this function:

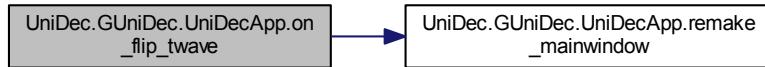


7.57.3.39 def UniDec.GUniDec.UniDecApp.on_flip_twave(self, e)

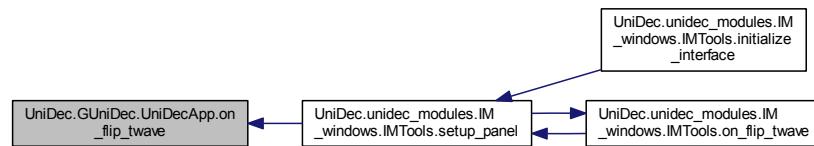
```

Flips between T-Wave and Linear IM-MS
:param e: wx Event or anything (will get value from Selection if not 0)
:return: None
  
```

Here is the call graph for this function:



Here is the caller graph for this function:



7.57.3.40 def UniDec.GUniDec.UniDecApp.on_get_mzlimits (self)

Here is the caller graph for this function:

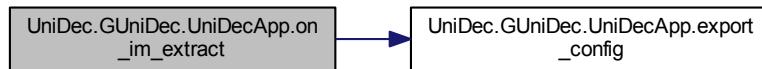


7.57.3.41 def UniDec.GUniDec.UniDecApp.on_grid_decon (self, e)

7.57.3.42 def UniDec.GUniDec.UniDecApp.on_im_extract (self, e =None)

Open IM extraction window for extracting data from IM plots.
 Has to run UniDec again with self.eng.config.zout=-1,
 which causes the export of all charge state slices of mass vs ccs plots.
 Normally only the faces of the mass vs ccs vs charge cube are output.
 :param e: unused event
 :return: None

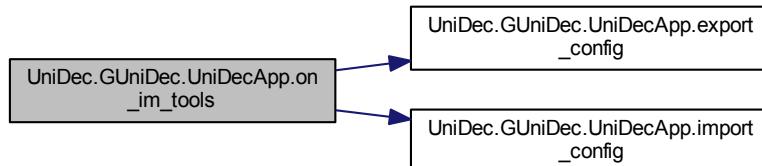
Here is the call graph for this function:



7.57.3.43 def UniDec.GUniDec.UniDecApp.on_im_tools(self, e=None)

Open IM Parameters tool window for guessing at IM parameters.
:param e: unused event
:return: None

Here is the call graph for this function:



7.57.3.44 def UniDec.GUniDec.UniDecApp.on_import_wizard(self, e=None)

Opens Import Wizard for extreme file conversion.
:param e: unused event
:return: None

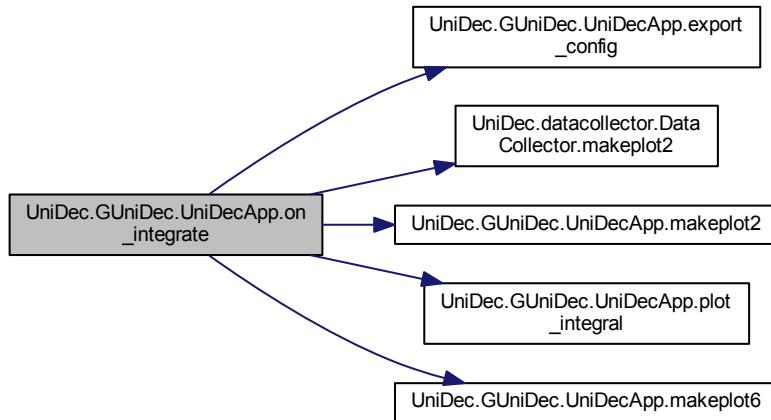
7.57.3.45 def UniDec.GUniDec.UniDecApp.on_integrate(self, plot=True, filled=True)

Triggered by right click on plot2. Integrates peaks.

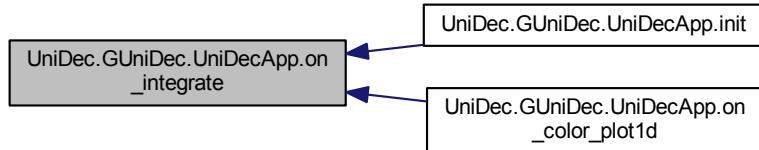
If plot2 is zoomed out, it will use self.eng.autointegrate() to integrate the peaks.
If plot2 is zoomed in to a single peak, the integral for that peak is recalculated from the plot limits.
If plot2 is zoomed in to more than one peak, the integral is not set for a single peak but simply printed on the plot

:param plot: Boolean, whether to add filled areas to plot.
:return: None

Here is the call graph for this function:



Here is the caller graph for this function:



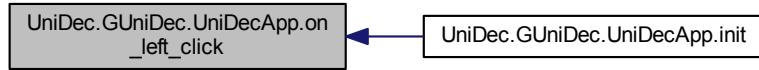
7.57.3.46 def UniDec.GUniDec.UniDecApp.on_kendrick(self, e=None)

Opens Kendrick Mass Defect Analysis window.
:param e: unused event
:return: None

7.57.3.47 def UniDec.GUniDec.UniDecApp.on_left_click(self, xpos, ypos)

Triggered by pubsub from plot windows.
Gets a m/z peak near the click, stores it, and waits for another click.
When two clicks has been performed, it tries to calculate the mass from their m/z value.
:param xpos: x position fed from event
:param ypos: y position fed from event
:return: None

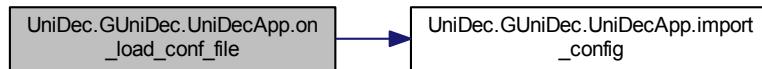
Here is the caller graph for this function:



7.57.3.48 def UniDec.GUniDec.UniDecApp.on_load_conf_file(self, e=None)

Opens a file dialog and then imports a new _conf.dat config file
:param e: unused space for event
:return: None

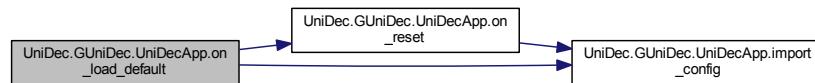
Here is the call graph for this function:



7.57.3.49 def UniDec.GUniDec.UniDecApp.on_load_default(self, e=None)

Resets the configuration then loads the default config file from self.eng.config.defaultconfig.
Ignores min and max data cutoffs.
:param e: unused space for event
:return: None

Here is the call graph for this function:



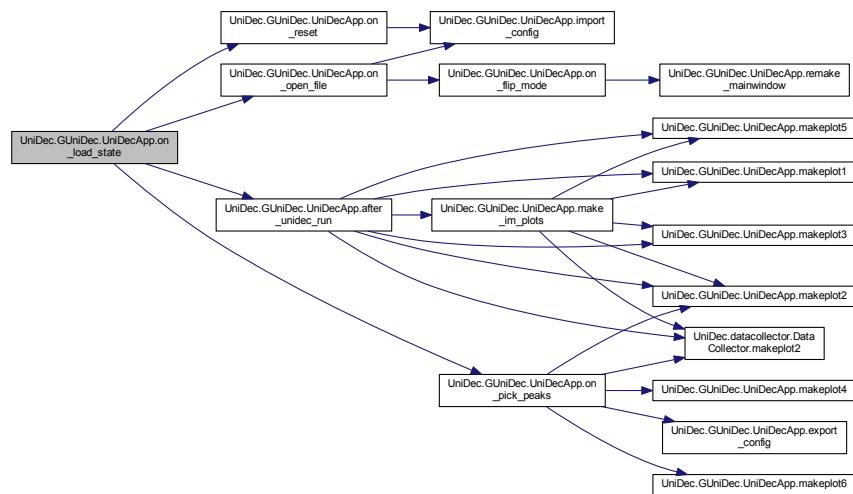
Here is the caller graph for this function:



7.57.3.50 def UniDec.GUniDec.UniDecApp.on_load_state(self, e=None)

Loads a saved file state by running self.eng.load_state and then updating self.view.
Runs several engine components rather than importing.
:param e: unused space for event
:return: None

Here is the call graph for this function:



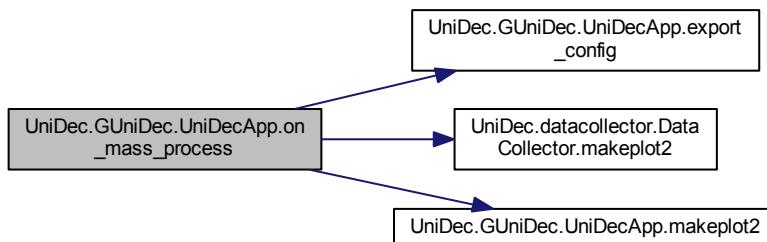
7.57.3.51 def UniDec.GUniDec.UniDecApp.on_manual(self, e=None)

Opens window for setting manual assignments. Window directly modifies self.eng.config.
:param e: unused event
:return: None

7.57.3.52 def UniDec.GUniDec.UniDecApp.on_mass_process(self, e=None)

Updates config from the GUI, processes the zero-charge mass spectrum with the same parameters used for the raw data, then replots the zero-charge mass spectrum.
:param e: unused event
:return: None

Here is the call graph for this function:

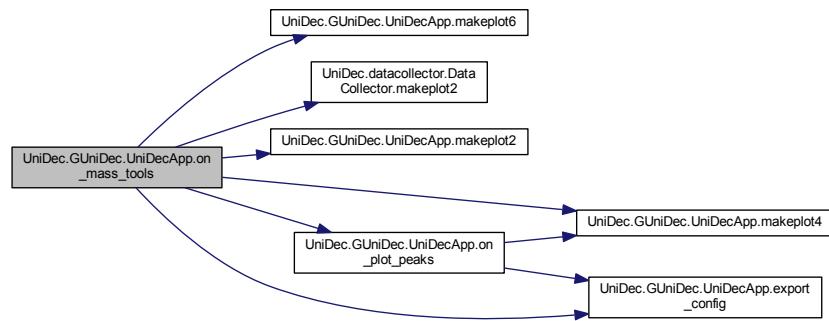


7.57.3.53 def UniDec.GUniDec.UniDecApp.on_mass_tools(self, e=None, show=True)

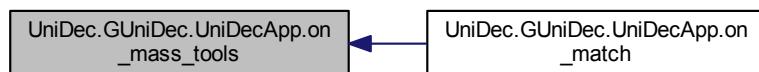
Opens masstools window.

If a match was performed, it will update plot 6 and the peak panel.
 If the user decides to use simulated masses, it will make plot these new peaks.
 :param e: unused event
 :param show: Whether to show the window (True) or simply match and return (False)
 :return: None

Here is the call graph for this function:



Here is the caller graph for this function:



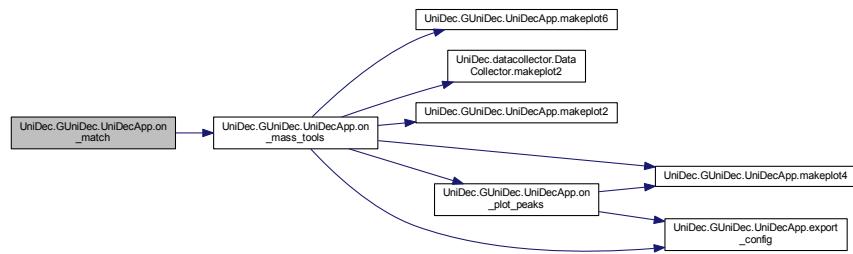
7.57.3.54 def UniDec.GUniDec.UniDecApp.on_match(self, e=None)

Automatic matching to present oligomer list.

Opens masstools window but doesn't make it visible.
 Matches results to any combination of oligomers.
 Hits ok and plots results.

```
:param e:  
:return:
```

Here is the call graph for this function:



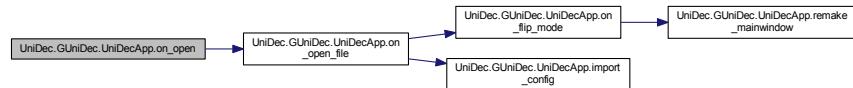
7.57.3.55 def UniDec.GUniDec.UniDecApp.on_nativez_tools (self, e=None)

Opens Native Charge State analysis tools window. Parameters are stored in self.eng.config.zoffs.
:param e: unused event
:return: None

7.57.3.56 def UniDec.GUniDec.UniDecApp.on_open (self, e=None)

Open dialog for file opening
:param e: unused space for event
:return: None

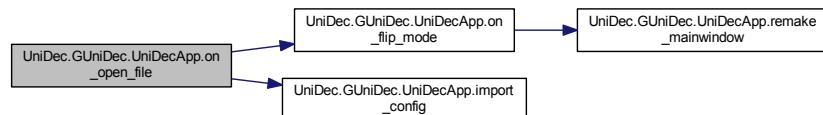
Here is the call graph for this function:



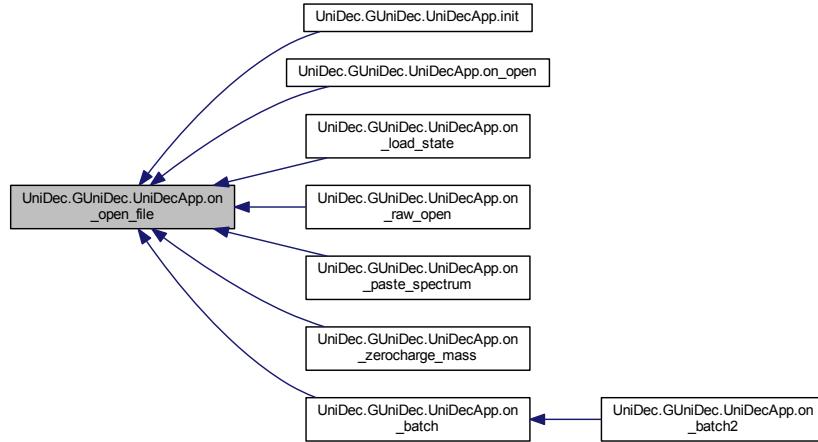
7.57.3.57 def UniDec.GUniDec.UniDecApp.on_open_file (self, filename, directory, skipengine=False)

Opens a file. Run self.eng.open_file.
:param filename: File name
:param directory: Directory containing file
:param skipengine: Boolean, Whether to skip running the engine (used when loading state)
:return: None

Here is the call graph for this function:



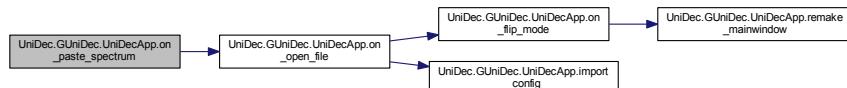
Here is the caller graph for this function:



7.57.3.58 def UniDec.GUniDec.UniDecApp.on_paste_spectrum (self, e=None)

Gets spectrum from the clipboard, writes it to a new file, and then opens that new file.
:param e: unused space for event
:return: None

Here is the call graph for this function:



7.57.3.59 def UniDec.GUniDec.UniDecApp.on_pdf_report (self, e=None)

Creates PDF report.

First, writes figures to PDF.
Then sends results to texmaker, which creates a .tex file.
Finally, runs pdflatex as commandline subprocess to convert .tex to PDF.

:param e: event passed to `self.view.on_save_figur_pdf`
:return: None

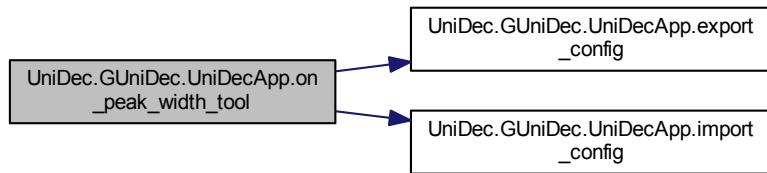
7.57.3.60 def UniDec.GUniDec.UniDecApp.on_peak_errors (self, e=None)

Get peak errors and plot on Plot2.
:param e: unused space for event
:return: None

7.57.3.61 def UniDec.GUniDec.UniDecApp.on_peak_width_tool (self, e=None)

Open peak width tool window. After it has returned, update the GUI to reflect the new peak widths.
:param e: unused event
:return: None

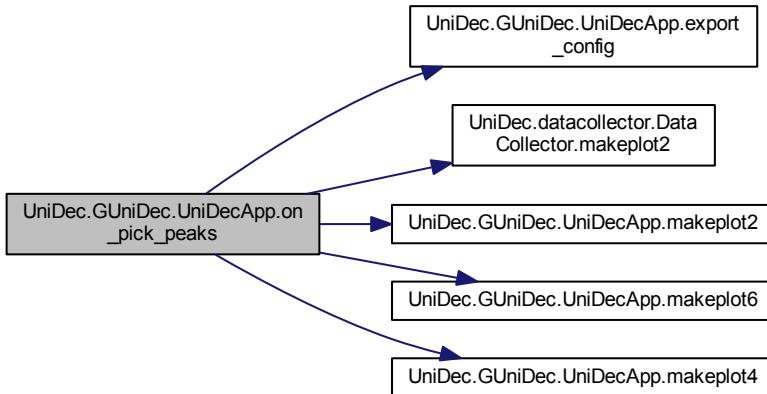
Here is the call graph for this function:



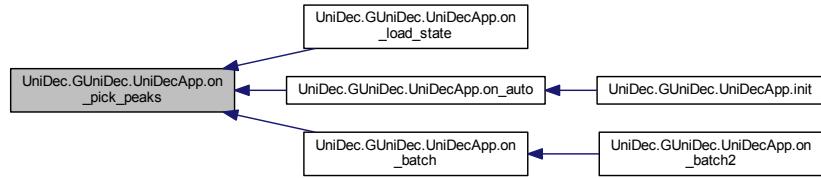
7.57.3.62 def UniDec.GUniDec.UniDecApp.on_pick_peaks (self, e=None)

Pick peaks and perform initial plots on them.
:param e: unused space for event
:return: None

Here is the call graph for this function:



Here is the caller graph for this function:



7.57.3.63 def UniDec.GUniDec.UniDecApp.on_plot_composite(self, e=None)

Plots a composite of isolated peaks that are selected.
:param e: unused event
:return: None

7.57.3.64 def UniDec.GUniDec.UniDecApp.on_plot_nativeccs(self, e=None)

Plot native CCS as a red line on `self.view.plot5mccs` (mass vs ccs) plot.
:param e: unused event
:return: None

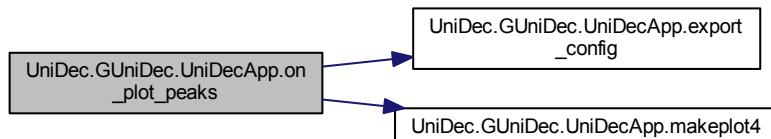
7.57.3.65 def UniDec.GUniDec.UniDecApp.on_plot_offsets(self, e=None)

Transform the mass vs charge grid to a mass vs charge offset grid. Plot in `self.view.plot5`.
:param e: unused event
:return: None

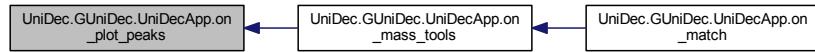
7.57.3.66 def UniDec.GUniDec.UniDecApp.on_plot_peaks(self, e=None)

Plots individual peaks as simulated spectra in plot 4.
:param e: unused space for event
:return: None

Here is the call graph for this function:



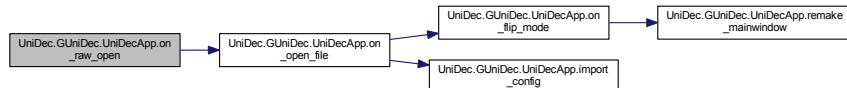
Here is the caller graph for this function:



7.57.3.67 def UniDec.GUniDec.UniDecApp.on_raw_open(self, e=None, dirname=None)

Opens a file dialog for opening a raw file. Runs self.eng.raw_process and then opens the processed file.
:param e: unused space for event
:return:

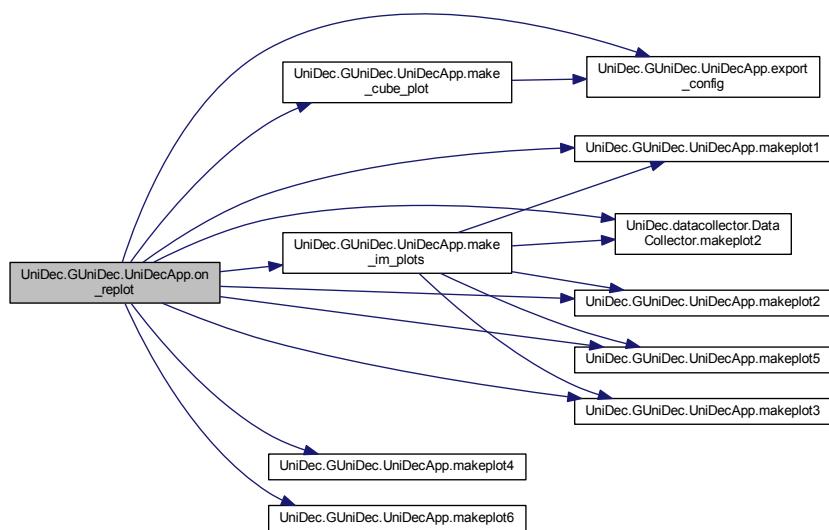
Here is the call graph for this function:



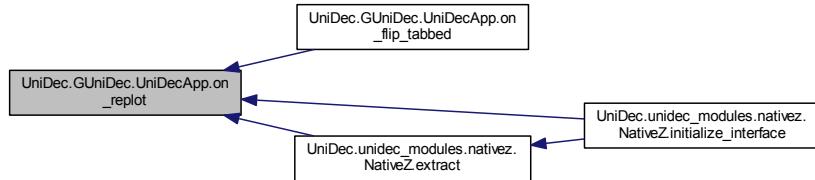
7.57.3.68 def UniDec.GUniDec.UniDecApp.on_replot(self, e=None)

Refresh the parameters from the GUI and plot everything again with the new parameters.
:param e: unused event
:return: None

Here is the call graph for this function:



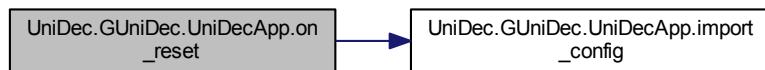
Here is the caller graph for this function:



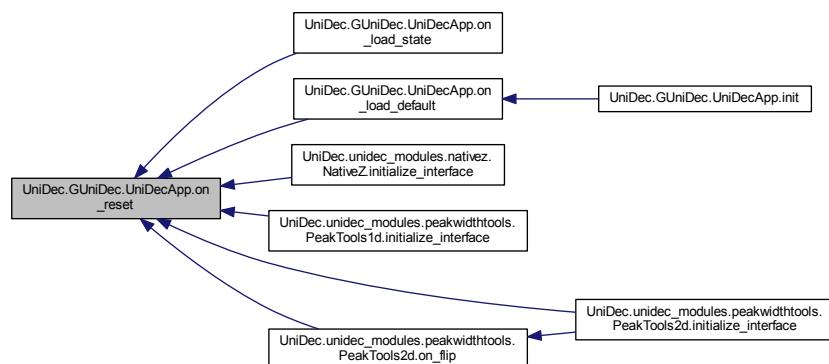
7.57.3.69 def UniDec.GUniDec.UniDecApp.on_reset(self, e=None)

Resets UniDecConfig to default and then loads to `self.view`.
:param e: unused space for event
:return:

Here is the call graph for this function:



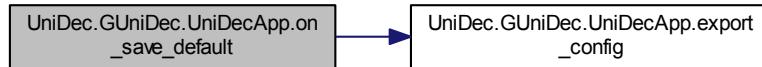
Here is the caller graph for this function:



7.57.3.70 def UniDec.GUniDec.UniDecApp.on_save_default(self, e=None)

Saves the default config file to `self.eng.config.defaultconfig`
:param e: unused space for event
:return: None

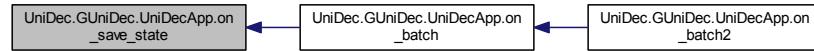
Here is the call graph for this function:



7.57.3.71 def UniDec.GUniDec.UniDecApp.on_save_state (self, e=None, filenew=None)

Saves the state by running `self.eng.save_state`. If no file is specified, opens a file dialog.
:param e: unused space for event
:param filenew: Save state zip file name
:return: None

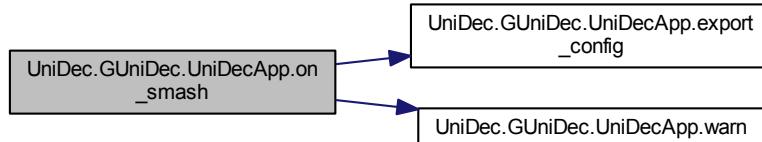
Here is the caller graph for this function:



7.57.3.72 def UniDec.GUniDec.UniDecApp.on_smash (self)

Triggered by right click on plot1.
Smashes the zoomed region to 0. Used to eliminate unwanted peaks.
:return: None

Here is the call graph for this function:



Here is the caller graph for this function:



7.57.3.73 def UniDec.GUniDec.UniDecApp.on_super_batch(self, e=None)

Speedy, minimal batch processing. Data must be processed in advance.

Does not load file or process data.

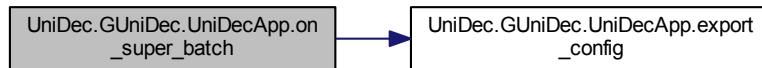
Simply writes the configuration with updated defaults to a conf.dat file.
Then runs the conf.dat file with UniDec binary.

Does not do any post processing.

This function is useful for largee data sets where you are using DataCollector or some other program to analyze the results outside of UniDec. It allows new parameters to be run with the maximum speed.

```
:param e: unused event
:return: None
```

Here is the call graph for this function:



7.57.3.74 def UniDec.GUniDec.UniDecApp.on_tweet(self, e=None)

Opens Twitter Extension Window.

First makes PNG files of all the figures it can. Those are fed to the window.

self.twittercodes is modified if the person has logged in, so that the person only has to log in once.

Note: don't mess with self.twittercodes. It DOES NOT contain log in information such as user name or password, but it shouldn't be printed, which is why it lives in the memory only.

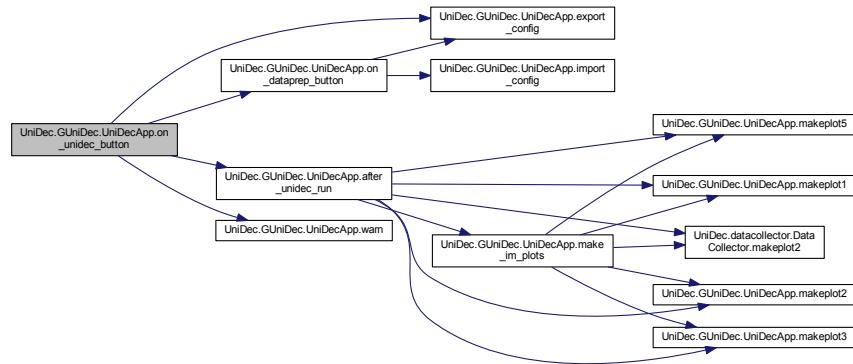
```
:param e: event
:return: None
```

7.57.3.75 def UniDec.GUniDec.UniDecApp.on_unidec_button(self, e=None)

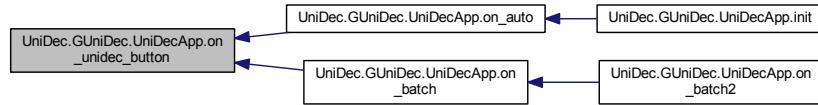
Runs UniDec, imports the results, and plots the output.

```
:param e: unused space for event
:return: None
```

Here is the call graph for this function:



Here is the caller graph for this function:



7.57.3.76 def UniDec.GUniDec.UniDecApp.on_unidec_path(self, e=None)

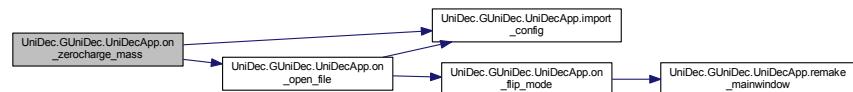
Opens file dialog to specify new UniDec binary.
 Only useful for advanced users or if something has gone horribly wrong.
 Modifies self.eng.config.UniDecPath and others.
 :param e: unused event
 :return: None

7.57.3.77 def UniDec.GUniDec.UniDecApp.on_zerocharge_mass(self, e=None)

The old switcheroo. Takes the mass output and makes it the m/z input.
 Then changes some of the deconvolution parameters to reflect this.

The reason for this type of function is to separate deconvolution from deisotoping when isotope mode is on.
 Deconvolution can be performed to generate a zero-charge mass spectrum, which can then be loaded as a new spectrum and deisotoped with isotope mode. Still a bit experimental...
 :param e: unused event
 :return: None

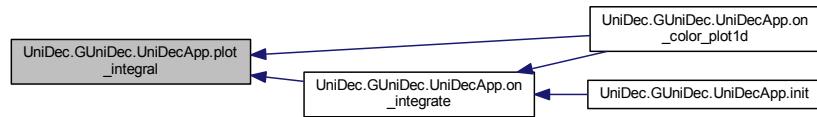
Here is the call graph for this function:



7.57.3.78 def UniDec.GUniDec.UniDecApp.plot_integral (self, limits, color=None, filled=True)

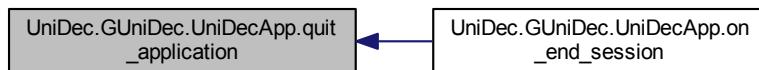
Plot a filled integral under a peak.
:param limits: Limits of integration
:param color: Color of fill and plot
:return: None

Here is the caller graph for this function:



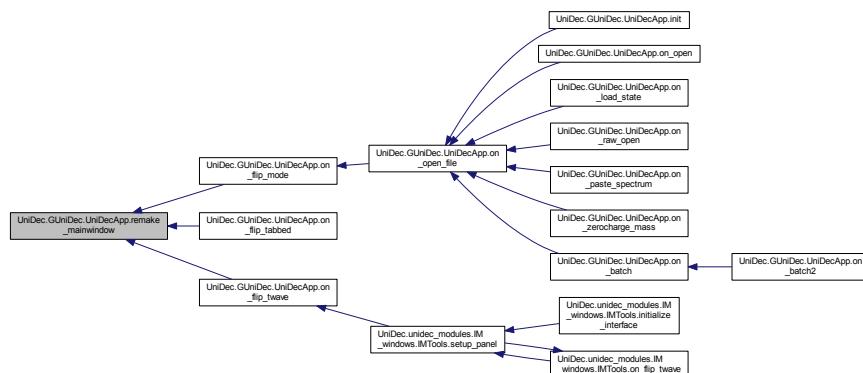
7.57.3.79 def UniDec.GUniDec.UniDecApp.quit_application (self)

Here is the caller graph for this function:



7.57.3.80 def UniDec.GUniDec.UniDecApp.remake_mainwindow (self, tabbed=None)

Here is the caller graph for this function:



7.57.3.81 def UniDec.GUniDec.UniDecApp.start (self)

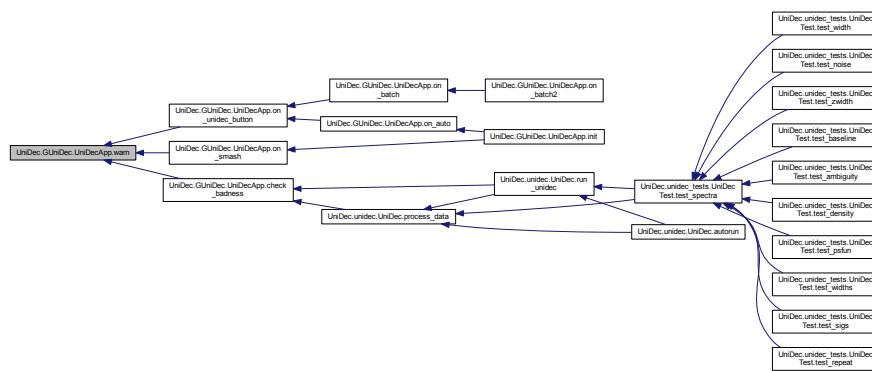
Launch view and start MainLoop

:return:

7.57.3.82 def UniDec.GUniDec.UniDecApp.warn (self, message, caption = 'Warning!')

Send the user a message box.
:param message: Message string
:param caption: Caption string
:return: None

Here is the caller graph for this function:



7.57.4 Member Data Documentation

7.57.4.1 UniDec.GUniDec.UniDecApp.eng

7.57.4.2 UniDec.GUniDec.UniDecApp.twittercodes

7.57.4.3 UniDec.GUniDec.UniDecApp.view

The documentation for this class was generated from the following file:

- C:/Python/UniDec/GUniDec.py

7.58 UniDec.unidec_modules.unidecstructure.UniDecConfig Class Reference

Public Member Functions

- def [__init__](#) (self)
- def [initialize](#) (self)
- def [default_colormaps](#) (self)
- def [config_export](#) (self, name)
- def [config_import](#) (self, name)
- def [print_config](#) (self)
- def [default_file_names](#) (self)
- def [check_badness](#) (self)
- def [default_high_res](#) (self)
- def [default_isotopic_res](#) (self)
- def [default_zero_charge](#) (self)
- def [initialize_system_paths](#) (self)

Public Attributes

- `infname`
- `outfname`
- `mfile`
- `manualfile`
- `confname`
- `ofile`
- `matchfile`
- `peaksfile`
- `dirname`
- `filename`
- `extension`
- `imflag`
- `publicationmode`
- `discreteplot`
- `cmap`
- `peakcmap`
- `rawflag`
- `detectoreffva`
- `mzbins`
- `smooth`
- `subbuff`
- `subtype`
- `inthresh`
- `minmz`
- `maxmz`
- `numit`
- `zzsig`
- `startz`
- `endz`
- `numz`
- `mzsиг`
- `psfun`
- `massub`
- `masslb`
- `msig`
- `molig`
- `massbins`
- `adductmass`
- `damp`
- `aggressiveflag`
- `suppression`
- `isotopemode`
- `peakwindow`
- `peakthresh`
- `peakplotthresh`
- `separation`
- `peaknorm`
- `error`
- `mtabsig`
- `poolflag`
- `nativezub`
- `nativezlб`
- `inflate`

- linflag
- integratelb
- integrateub
- mindt
- maxdt
- smoothdt
- subbufdt
- ccslb
- ccsub
- nativeccsub
- nativeccslb
- dtsig
- ccsbins
- csig
- pusher
- zout
- temp
- pressure
- volt
- to
- driftlength
- tcal1
- tcal2
- edc
- gasmass
- twaveflag
- batchflag
- procflag
- runtime
- massdatnormtop
- mfileflag
- manualfileflag
- kendrickmass
- masslist
- matchlist
- oligomerlist
- manuallist
- zoffs
- massoffset
- extractshape
- gridparams
- griddecon
- matchtolerance
- cmaps
- cmaps2
- badtest
- warning
- system
- defaultUnidecDir
- defaultUnidecName
- defaultIMName
- UniDecPath
- UniDecName
- UniDecIMName
- UniDecDir

- [UniDecIMPath](#)
- [rawreaderpath](#)
- [cdcreaderpath](#)
- [defaultconfig](#)

7.58.1 Detailed Description

Class containing all options and configurations for UniDec GUI and Program. Contains methods to export and import config to text file for running UniDec core binaries and for storing parameters for GUI.

7.58.2 Constructor & Destructor Documentation

7.58.2.1 def UniDec.unidec_modules.unidecstructure.UniDecConfig.__init__(self)

Initialize Everything. Set default paths and run self.initialize
 :return: UniDecConfig object

7.58.3 Member Function Documentation

7.58.3.1 def UniDec.unidec_modules.unidecstructure.UniDecConfig.check_badness(self)

Test for a few things that will crash the program:
 Min is greater than Max for m/z, charge, mass, native charge, ccs, native ccs, dt
 Bad IM-MS calibration values.
 Peak width is zero
 m/z resolution is really small.
 :return: None

7.58.3.2 def UniDec.unidec_modules.unidecstructure.UniDecConfig.config_export(self, name)

Writes config to file give in name. Typically in format: name value.

Also exports manuallist, masslist, and oligomerlist to text files.
 :param name: File name to write to.
 :return: None

7.58.3.3 def UniDec.unidec_modules.unidecstructure.UniDecConfig.config_import(self, name)

Imports configuration from txt file. Also imports masslist, manuallist, and oligomerlist.
 :param name: File to import from.
 :return: None

7.58.3.4 def UniDec.unidec_modules.unidecstructure.UniDecConfig.default_colormaps(self)

Get default matplotlib colormaps and set names to self.cmaps.
 A more list is set as self.cmaps2. For some reason, matplotlib v.1.5.0 allows viridis and other new colormaps with the colormaps() but not cm.datad. Even weirder, they work for some things and not others. Solution, two lists, one for the 2D plots and the other for the linear colors.
 :return: None

7.58.3.5 def UniDec.unidec_modules.unidecstructure.UniDecConfig.default_file_names(self)

Sets the default file names. For things comming into and out of the program. In theory these can be modified, but it might be risky.
 :return: None

7.58.3.6 def UniDec.unidec_modules.unidecstructure.UniDecConfig.default_high_res (self)

Sets some defaults for high resolution spectra. Leaves other values unchanged.
:return: None

7.58.3.7 def UniDec.unidec_modules.unidecstructure.UniDecConfig.default_isotopic_res (self)

Sets some defaults for isotopic resolution spectra. Leaves other values unchanged.
:return: None

7.58.3.8 def UniDec.unidec_modules.unidecstructure.UniDecConfig.default_zero_charge (self)

Sets some defaults for when the zero-charge mass spectrum itself is to be deisotoped. Leaves other values unchanged.
:return: None

7.58.3.9 def UniDec.unidec_modules.unidecstructure.UniDecConfig.initialize (self)

Initialize configuration parameters but not paths. Runs self.default_colormaps
:return: None

7.58.3.10 def UniDec.unidec_modules.unidecstructure.UniDecConfig.initialize_system_paths (self)

Initialize initial paths for UniDec directories
:return: None

7.58.3.11 def UniDec.unidec_modules.unidecstructure.UniDecConfig.print_config (self)

Simple debugging command to read in the config file and print out its contents.
:return: None

7.58.4 Member Data Documentation

7.58.4.1 UniDec.unidec_modules.unidecstructure.UniDecConfig.adductmass

7.58.4.2 UniDec.unidec_modules.unidecstructure.UniDecConfig.aggressiveflag

7.58.4.3 UniDec.unidec_modules.unidecstructure.UniDecConfig.badtest

7.58.4.4 UniDec.unidec_modules.unidecstructure.UniDecConfig.batchflag

7.58.4.5 UniDec.unidec_modules.unidecstructure.UniDecConfig.ccsbins

7.58.4.6 UniDec.unidec_modules.unidecstructure.UniDecConfig.ccslb

7.58.4.7 UniDec.unidec_modules.unidecstructure.UniDecConfig.ccsub

7.58.4.8 UniDec.unidec_modules.unidecstructure.UniDecConfig.cdcreaderpath

7.58.4.9 UniDec.unidec_modules.unidecstructure.UniDecConfig.cmap

- 7.58.4.10 [UniDec.unidec_modules.unidecstructure.UniDecConfig.cmmaps](#)
- 7.58.4.11 [UniDec.unidec_modules.unidecstructure.UniDecConfig.cmmaps2](#)
- 7.58.4.12 [UniDec.unidec_modules.unidecstructure.UniDecConfig.confname](#)
- 7.58.4.13 [UniDec.unidec_modules.unidecstructure.UniDecConfig.csig](#)
- 7.58.4.14 [UniDec.unidec_modules.unidecstructure.UniDecConfig.damp](#)
- 7.58.4.15 [UniDec.unidec_modules.unidecstructure.UniDecConfig.defaultconfig](#)
- 7.58.4.16 [UniDec.unidec_modules.unidecstructure.UniDecConfig.defaultIMName](#)
- 7.58.4.17 [UniDec.unidec_modules.unidecstructure.UniDecConfig.defaultUnidecDir](#)
- 7.58.4.18 [UniDec.unidec_modules.unidecstructure.UniDecConfig.defaultUnidecName](#)
- 7.58.4.19 [UniDec.unidec_modules.unidecstructure.UniDecConfig.detectoreffva](#)
- 7.58.4.20 [UniDec.unidec_modules.unidecstructure.UniDecConfig.dirname](#)
- 7.58.4.21 [UniDec.unidec_modules.unidecstructure.UniDecConfig.discreteplot](#)
- 7.58.4.22 [UniDec.unidec_modules.unidecstructure.UniDecConfig.driftlength](#)
- 7.58.4.23 [UniDec.unidec_modules.unidecstructure.UniDecConfig.dtsig](#)
- 7.58.4.24 [UniDec.unidec_modules.unidecstructure.UniDecConfig.edc](#)
- 7.58.4.25 [UniDec.unidec_modules.unidecstructure.UniDecConfig.endz](#)
- 7.58.4.26 [UniDec.unidec_modules.unidecstructure.UniDecConfig.error](#)
- 7.58.4.27 [UniDec.unidec_modules.unidecstructure.UniDecConfig.extension](#)
- 7.58.4.28 [UniDec.unidec_modules.unidecstructure.UniDecConfig.extractshape](#)
- 7.58.4.29 [UniDec.unidec_modules.unidecstructure.UniDecConfig.filename](#)
- 7.58.4.30 [UniDec.unidec_modules.unidecstructure.UniDecConfig.gasmass](#)
- 7.58.4.31 [UniDec.unidec_modules.unidecstructure.UniDecConfig.gridddecon](#)
- 7.58.4.32 [UniDec.unidec_modules.unidecstructure.UniDecConfig.gridparams](#)
- 7.58.4.33 [UniDec.unidec_modules.unidecstructure.UniDecConfig.imflag](#)
- 7.58.4.34 [UniDec.unidec_modules.unidecstructure.UniDecConfig.inflate](#)
- 7.58.4.35 [UniDec.unidec_modules.unidecstructure.UniDecConfig.infname](#)
- 7.58.4.36 [UniDec.unidec_modules.unidecstructure.UniDecConfig.integratelb](#)
- 7.58.4.37 [UniDec.unidec_modules.unidecstructure.UniDecConfig.integrateub](#)

- 7.58.4.38 UniDec.unidec_modules.unidecstructure.UniDecConfig.intthresh
- 7.58.4.39 UniDec.unidec_modules.unidecstructure.UniDecConfig.isotopemode
- 7.58.4.40 UniDec.unidec_modules.unidecstructure.UniDecConfig.kendrickmass
- 7.58.4.41 UniDec.unidec_modules.unidecstructure.UniDecConfig.linflag
- 7.58.4.42 UniDec.unidec_modules.unidecstructure.UniDecConfig.manualfile
- 7.58.4.43 UniDec.unidec_modules.unidecstructure.UniDecConfig.manualfileflag
- 7.58.4.44 UniDec.unidec_modules.unidecstructure.UniDecConfig.manuallist
- 7.58.4.45 UniDec.unidec_modules.unidecstructure.UniDecConfig.massbins
- 7.58.4.46 UniDec.unidec_modules.unidecstructure.UniDecConfig.massdatnormtop
- 7.58.4.47 UniDec.unidec_modules.unidecstructure.UniDecConfig.masslb
- 7.58.4.48 UniDec.unidec_modules.unidecstructure.UniDecConfig.masslist
- 7.58.4.49 UniDec.unidec_modules.unidecstructure.UniDecConfig.massoffset
- 7.58.4.50 UniDec.unidec_modules.unidecstructure.UniDecConfig.massub
- 7.58.4.51 UniDec.unidec_modules.unidecstructure.UniDecConfig.matchfile
- 7.58.4.52 UniDec.unidec_modules.unidecstructure.UniDecConfig.matchlist
- 7.58.4.53 UniDec.unidec_modules.unidecstructure.UniDecConfig.matchtolerance
- 7.58.4.54 UniDec.unidec_modules.unidecstructure.UniDecConfig.maxdt
- 7.58.4.55 UniDec.unidec_modules.unidecstructure.UniDecConfig.maxmz
- 7.58.4.56 UniDec.unidec_modules.unidecstructure.UniDecConfig.mfile
- 7.58.4.57 UniDec.unidec_modules.unidecstructure.UniDecConfig.mfileflag
- 7.58.4.58 UniDec.unidec_modules.unidecstructure.UniDecConfig.mindt
- 7.58.4.59 UniDec.unidec_modules.unidecstructure.UniDecConfig.minmz
- 7.58.4.60 UniDec.unidec_modules.unidecstructure.UniDecConfig.molig
- 7.58.4.61 UniDec.unidec_modules.unidecstructure.UniDecConfig.msig
- 7.58.4.62 UniDec.unidec_modules.unidecstructure.UniDecConfig.mtabsig
- 7.58.4.63 UniDec.unidec_modules.unidecstructure.UniDecConfig.mzbins
- 7.58.4.64 UniDec.unidec_modules.unidecstructure.UniDecConfig.mzsig
- 7.58.4.65 UniDec.unidec_modules.unidecstructure.UniDecConfig.nativeccslb

- 7.58.4.66 UniDec.unidec_modules.unidecstructure.UniDecConfig.nativeccsub
- 7.58.4.67 UniDec.unidec_modules.unidecstructure.UniDecConfig.nativezlb
- 7.58.4.68 UniDec.unidec_modules.unidecstructure.UniDecConfig.nativezub
- 7.58.4.69 UniDec.unidec_modules.unidecstructure.UniDecConfig.numit
- 7.58.4.70 UniDec.unidec_modules.unidecstructure.UniDecConfig.numz
- 7.58.4.71 UniDec.unidec_modules.unidecstructure.UniDecConfig.ofile
- 7.58.4.72 UniDec.unidec_modules.unidecstructure.UniDecConfig.oligomerlist
- 7.58.4.73 UniDec.unidec_modules.unidecstructure.UniDecConfig.outfname
- 7.58.4.74 UniDec.unidec_modules.unidecstructure.UniDecConfig.peakcmap
- 7.58.4.75 UniDec.unidec_modules.unidecstructure.UniDecConfig.peaknorm
- 7.58.4.76 UniDec.unidec_modules.unidecstructure.UniDecConfig.peakplotthresh
- 7.58.4.77 UniDec.unidec_modules.unidecstructure.UniDecConfig.peaksfile
- 7.58.4.78 UniDec.unidec_modules.unidecstructure.UniDecConfig.peakthresh
- 7.58.4.79 UniDec.unidec_modules.unidecstructure.UniDecConfig.peakwindow
- 7.58.4.80 UniDec.unidec_modules.unidecstructure.UniDecConfig.poolflag
- 7.58.4.81 UniDec.unidec_modules.unidecstructure.UniDecConfig.pressure
- 7.58.4.82 UniDec.unidec_modules.unidecstructure.UniDecConfig.procflag
- 7.58.4.83 UniDec.unidec_modules.unidecstructure.UniDecConfig.psfun
- 7.58.4.84 UniDec.unidec_modules.unidecstructure.UniDecConfig.publicationmode
- 7.58.4.85 UniDec.unidec_modules.unidecstructure.UniDecConfig.pusher
- 7.58.4.86 UniDec.unidec_modules.unidecstructure.UniDecConfig.rawflag
- 7.58.4.87 UniDec.unidec_modules.unidecstructure.UniDecConfig.rawreaderpath
- 7.58.4.88 UniDec.unidec_modules.unidecstructure.UniDecConfig.runtime
- 7.58.4.89 UniDec.unidec_modules.unidecstructure.UniDecConfig.separation
- 7.58.4.90 UniDec.unidec_modules.unidecstructure.UniDecConfig.smooth
- 7.58.4.91 UniDec.unidec_modules.unidecstructure.UniDecConfig.smoothhdt
- 7.58.4.92 UniDec.unidec_modules.unidecstructure.UniDecConfig.startz
- 7.58.4.93 UniDec.unidec_modules.unidecstructure.UniDecConfig.subbufdt

7.58.4.94 UniDec.unidec_modules.unidecstructure.UniDecConfig.subbuff

7.58.4.95 UniDec.unidec_modules.unidecstructure.UniDecConfig.subtype

7.58.4.96 UniDec.unidec_modules.unidecstructure.UniDecConfig.suppression

7.58.4.97 UniDec.unidec_modules.unidecstructure.UniDecConfig.system

7.58.4.98 UniDec.unidec_modules.unidecstructure.UniDecConfig.tcal1

7.58.4.99 UniDec.unidec_modules.unidecstructure.UniDecConfig.tcal2

7.58.4.100 UniDec.unidec_modules.unidecstructure.UniDecConfig.temp

7.58.4.101 UniDec.unidec_modules.unidecstructure.UniDecConfig.to

7.58.4.102 UniDec.unidec_modules.unidecstructure.UniDecConfig.twaveflag

7.58.4.103 UniDec.unidec_modules.unidecstructure.UniDecConfig.UniDecDir

7.58.4.104 UniDec.unidec_modules.unidecstructure.UniDecConfig.UniDecIMName

7.58.4.105 UniDec.unidec_modules.unidecstructure.UniDecConfig.UniDecIMPath

7.58.4.106 UniDec.unidec_modules.unidecstructure.UniDecConfig.UniDecName

7.58.4.107 UniDec.unidec_modules.unidecstructure.UniDecConfig.UniDecPath

7.58.4.108 UniDec.unidec_modules.unidecstructure.UniDecConfig.volt

7.58.4.109 UniDec.unidec_modules.unidecstructure.UniDecConfig.warning

7.58.4.110 UniDec.unidec_modules.unidecstructure.UniDecConfig.zoffs

7.58.4.111 UniDec.unidec_modules.unidecstructure.UniDecConfig.zout

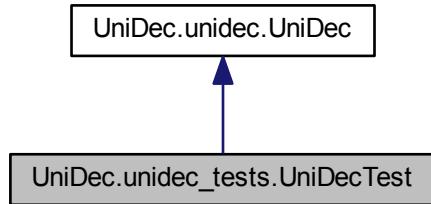
7.58.4.112 UniDec.unidec_modules.unidecstructure.UniDecConfig.zzsig

The documentation for this class was generated from the following file:

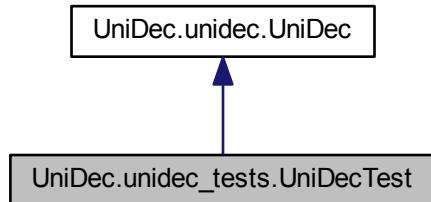
- C:/Python/UniDec/unidec_modules/[unidecstructure.py](#)

7.59 UniDec.unidec_tests.UniDecTest Class Reference

Inheritance diagram for UniDec.unidec_tests.UniDecTest:



Collaboration diagram for UniDec.unidec_tests.UniDecTest:



Public Member Functions

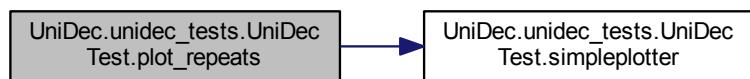
- def [test_spectra](#) (self, mlist=None, ilist=None, res=1000, noise=0.0, pad=2000, window=None, plot=False, restricted=True, massbins=10, psfun=0, mzsig=None, kwargs)
- def [simpleplotter](#) (self, m1, m2, e1, e2, i)
- def [plot_repeats](#) (self, peaks)
- def [plot_test](#) (self, tests, vals, testdat, testmdat, peaks)
- def [test_width](#) (self, kwargs)
- def [test_noise](#) (self, kwargs)
- def [test_zwidth](#) (self, kwargs)
- def [test_baseline](#) (self, kwargs)
- def [test_ambiguity](#) (self, kwargs)
- def [test_density](#) (self, kwargs)
- def [test_psfun](#) (self, kwargs)
- def [test_widths](#) (self, kwargs)
- def [test_sigs](#) (self, kwargs)
- def [test_repeat](#) (self, kwargs)

Additional Inherited Members

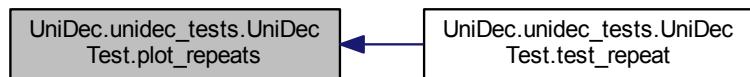
7.59.1 Member Function Documentation

7.59.1.1 def UniDec.unidec_tests.UniDecTest.plot_repeats(*self*, *peaks*)

Here is the call graph for this function:

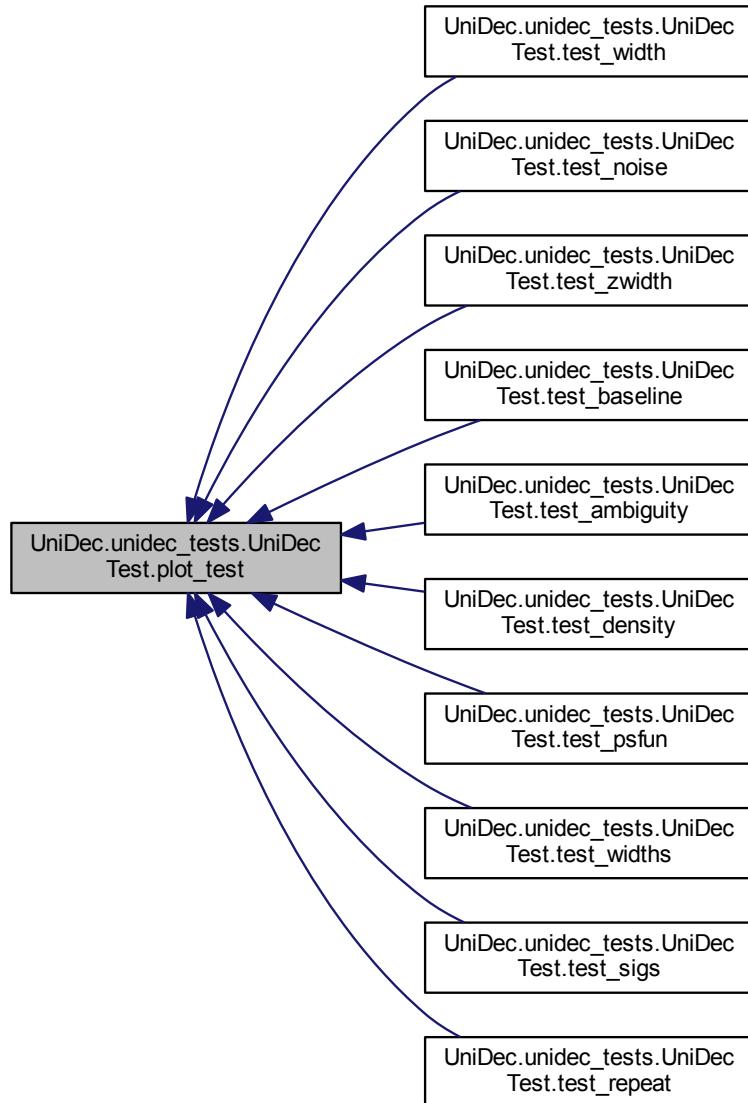


Here is the caller graph for this function:



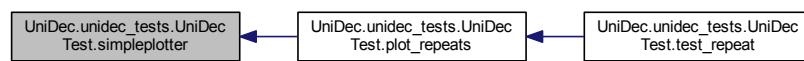
```
7.59.1.2 def UniDec.unidec_tests.UniDecTest.plot_test( self, tests, vals, testdat, testmdat, peaks )
```

Here is the caller graph for this function:



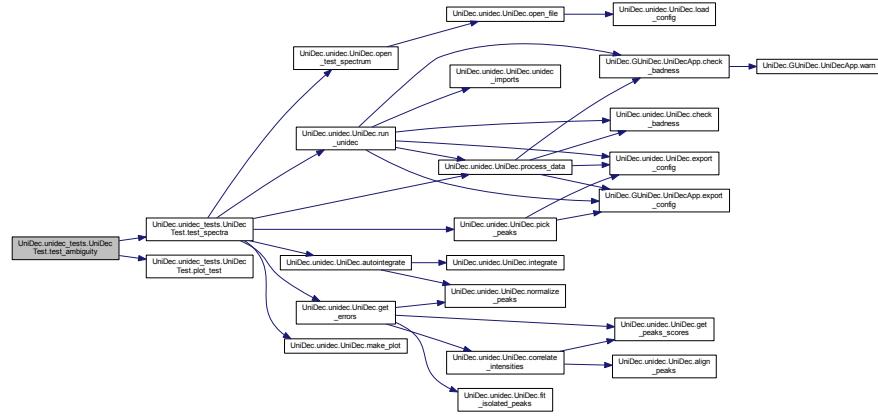
```
7.59.1.3 def UniDec.unidec_tests.UniDecTest.simpleplotter( self, m1, m2, e1, e2, i )
```

Here is the caller graph for this function:



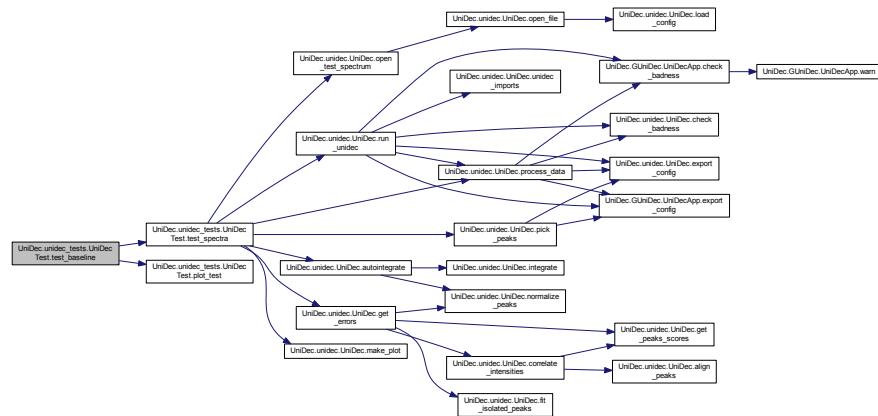
7.59.1.4 def UniDec.unidec_tests.UniDecTest.test_ambiguity (self, kwargs)

Here is the call graph for this function:



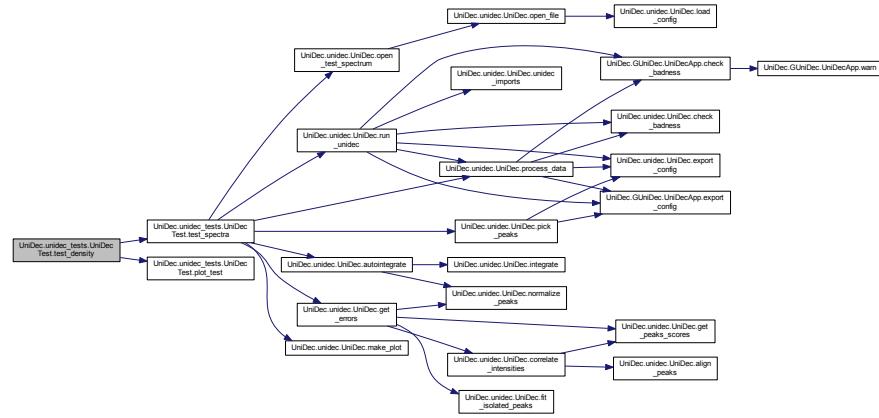
7.59.1.5 def UniDec.unidec_tests.UniDecTest.test_baseline (self, kwargs)

Here is the call graph for this function:



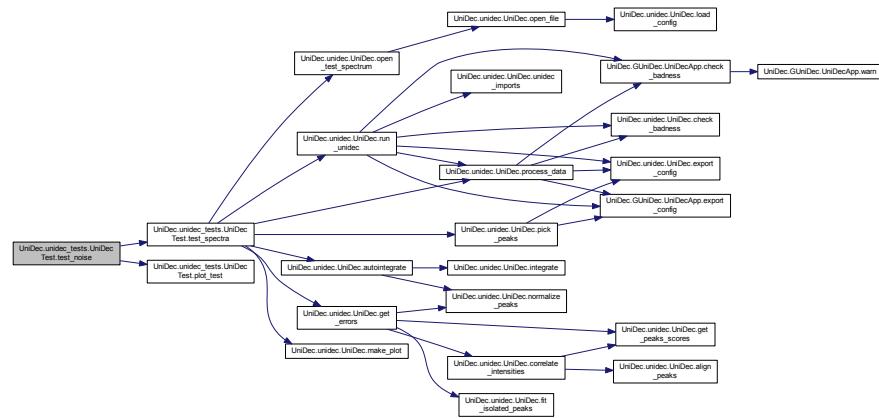
7.59.1.6 def UniDec.unidec_tests.UniDecTest.test_density (self, kwargs)

Here is the call graph for this function:



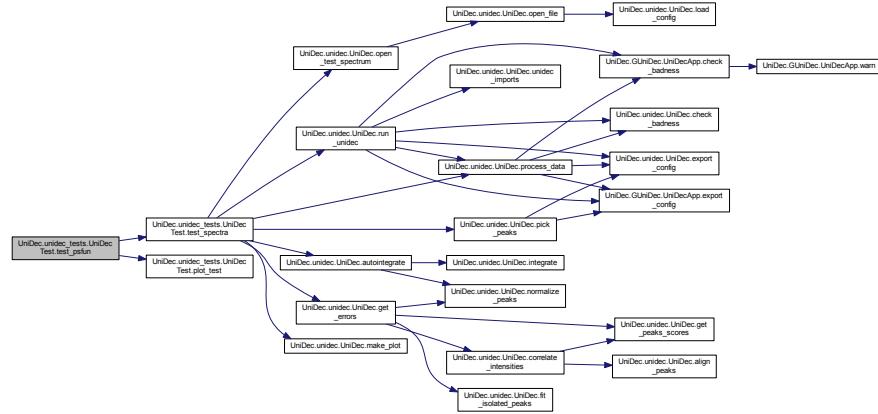
7.59.1.7 def UniDec.unidec_tests.UniDecTest.test_noise (self, kwargs)

Here is the call graph for this function:



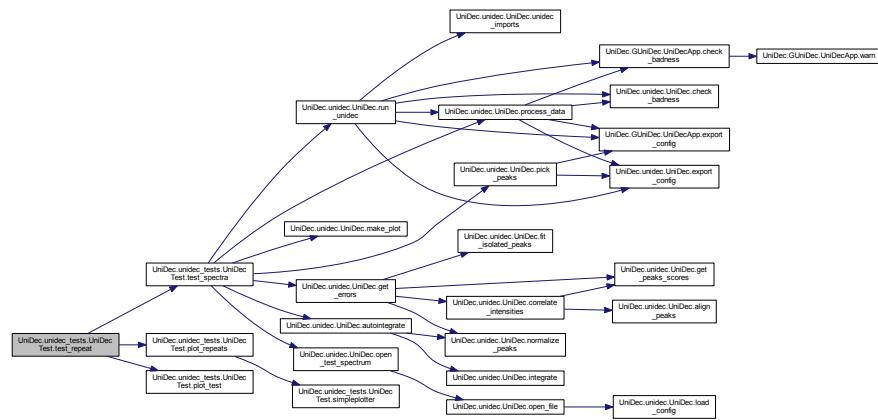
7.59.1.8 def UniDec.unidec_tests.UniDecTest.test_psfun (self, kwargs)

Here is the call graph for this function:



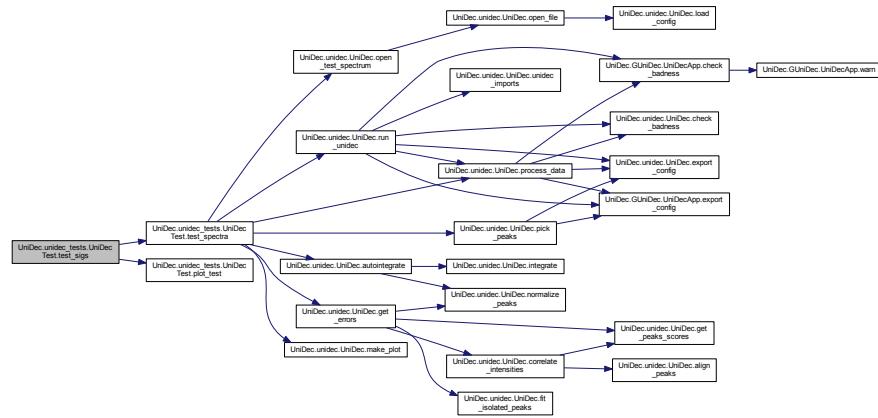
7.59.1.9 def UniDec.unidec_tests.UniDecTest.test_repeat (self, kwargs)

Here is the call graph for this function:



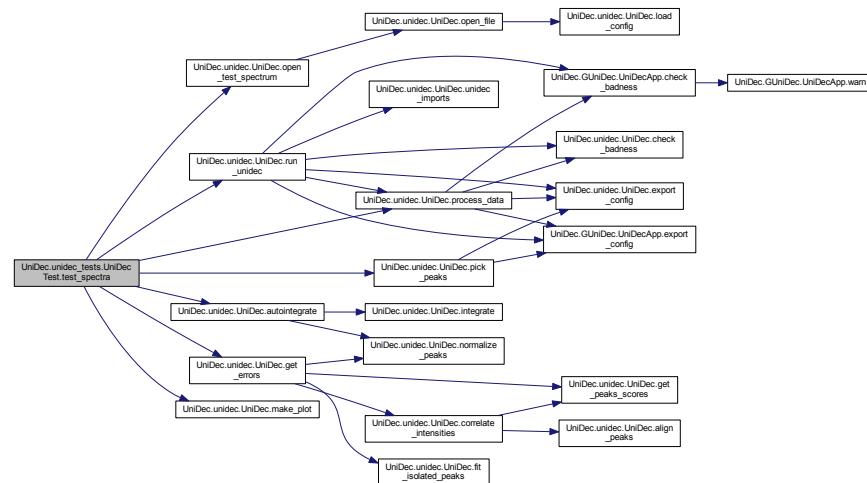
7.59.1.10 def UniDec.unidec_tests.UniDecTest.test_sigs (self, kwargs)

Here is the call graph for this function:

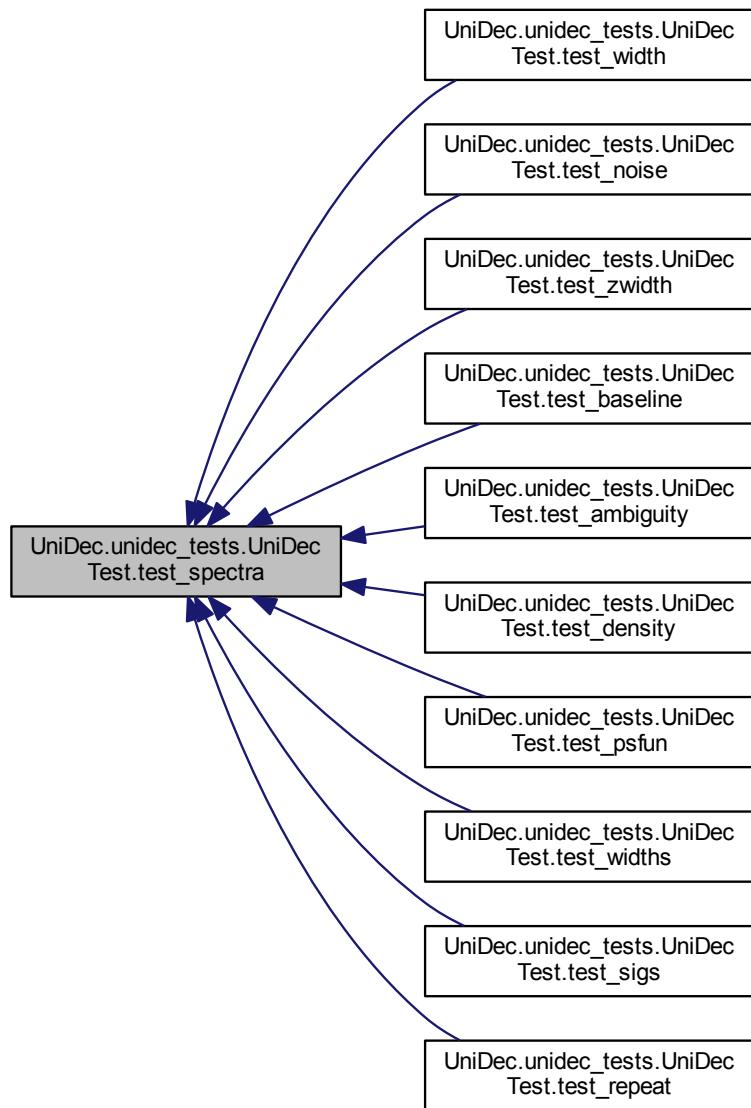


7.59.1.11 def UniDec.unidec_tests.UniDecTest.test_spectra (self, mlist=None, ilist=None, res=1000, noise=0.0, pad=2000, window=None, plot=False, restricted=True, massbins=10, psfun=0, mzsig=None, kwargs)

Here is the call graph for this function:

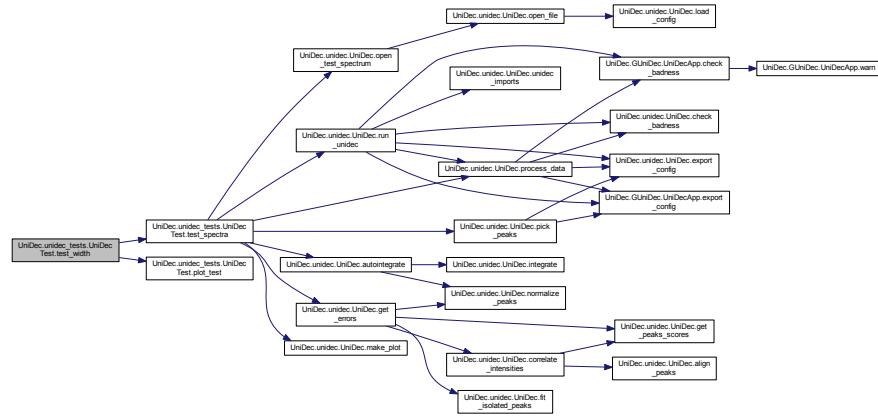


Here is the caller graph for this function:



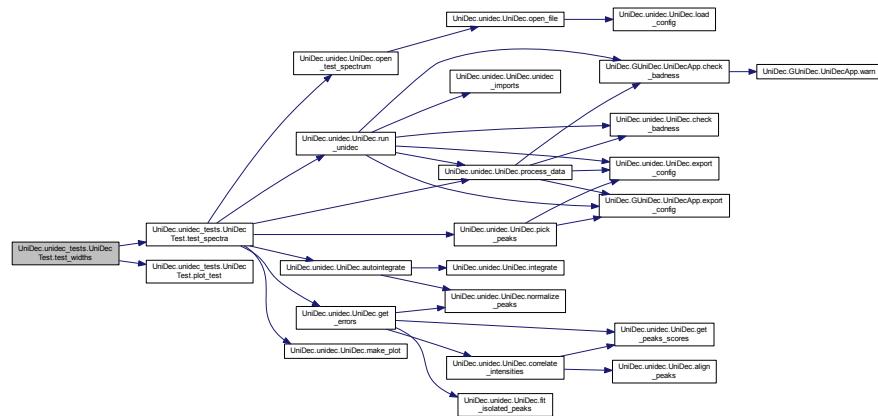
7.59.1.12 def UniDec.unidec_tests.UniDecTest.test_width (self, kwargs)

Here is the call graph for this function:



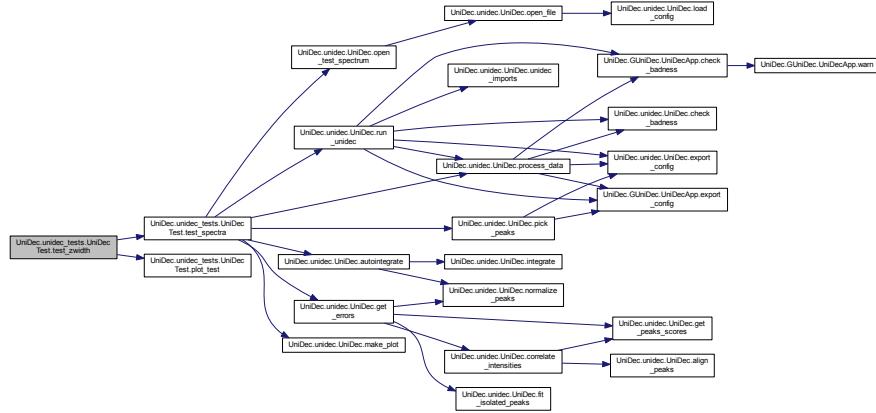
7.59.1.13 def UniDec.unidec_tests.UniDecTest.test_widths (self, kwargs)

Here is the call graph for this function:



7.59.1.14 def UniDec.unidec_tests.UniDecTest.test_zwidth (self, kwargs)

Here is the call graph for this function:

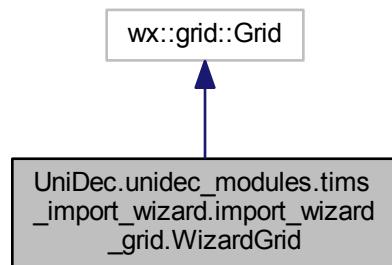


The documentation for this class was generated from the following file:

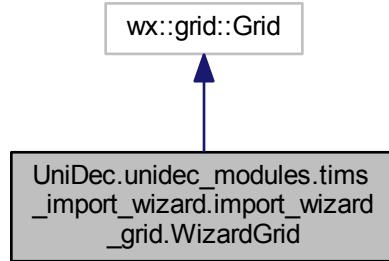
- C:/Python/UniDec/unidec_tests.py

7.60 UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid Class Reference

Inheritance diagram for UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid:



Collaboration diagram for UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid:



Public Member Functions

- def [__init__](#)
- def [sneaky_resize](#) (self, panel_width)
- def [showPopupMenu](#) (self, evt)
- def [set_labels](#) (self, mode)
- def [EvtDriftType](#) (self, evt)
- def [clear_all](#) (self, evt)
- def [add_dataset](#) (self, out)
- def [next_free_row](#)
- def [column_labels](#) (self)
- def [fill_down](#) (self, evt)
- def [remove_row](#) (self, evt)

Public Attributes

- [col_header](#)
- [col_conv](#)
- [col](#)
- [popupID1](#)

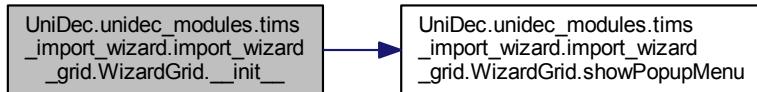
7.60.1 Detailed Description

Grid for data import wizard

7.60.2 Constructor & Destructor Documentation

```
7.60.2.1 def UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.__init__ ( self, parent, link,
grid_size = ( 0, 14, labels = 0 )
```

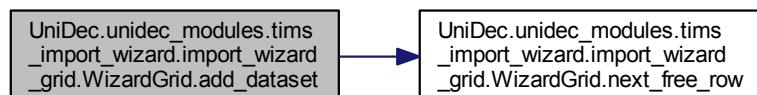
Here is the call graph for this function:



7.60.3 Member Function Documentation

```
7.60.3.1 def UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.add_dataset ( self, out )
```

Here is the call graph for this function:

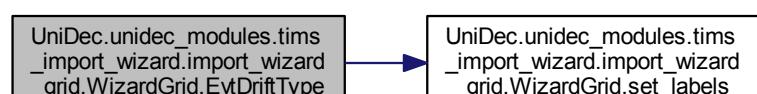


```
7.60.3.2 def UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.clear_all ( self, evt )
```

```
7.60.3.3 def UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.column_labels ( self )
```

```
7.60.3.4 def UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.EvtDriftType ( self, evt )
```

Here is the call graph for this function:

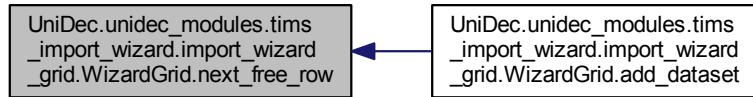


```
7.60.3.5 def UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.fill_down ( self, evt )
```

Try to fill down the columnn

7.60.3.6 def UniDec.unidec_modules.tims_import_wizard.import_wizard.WizardGrid.next_free_row (self, column = 0)

Here is the caller graph for this function:

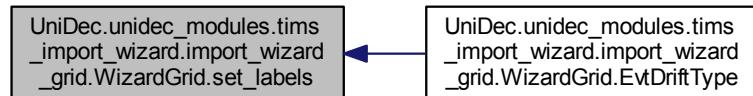


7.60.3.7 def UniDec.unidec_modules.tims_import_wizard.import_wizard.WizardGrid.remove_row (self, evt)

7.60.3.8 def UniDec.unidec_modules.tims_import_wizard.import_wizard.WizardGrid.set_labels (self, mode)

Set initial column headers based on mode
0 - Linear
1 - T-wave

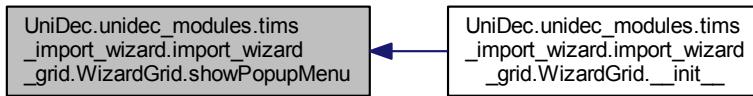
Here is the caller graph for this function:



7.60.3.9 def UniDec.unidec_modules.tims_import_wizard.import_wizard.WizardGrid.showPopupMenu (self, evt)

Create and display a popup menu on right-click event

Here is the caller graph for this function:



7.60.3.10 def UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.sneaky_resize(self, panel_width)

7.60.4 Member Data Documentation

7.60.4.1 UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.col

7.60.4.2 UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.col_conv

7.60.4.3 UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.col_header

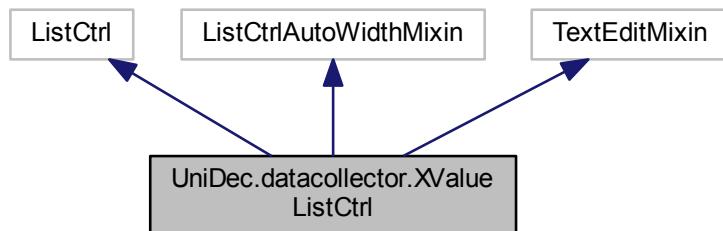
7.60.4.4 UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid.popupID1

The documentation for this class was generated from the following file:

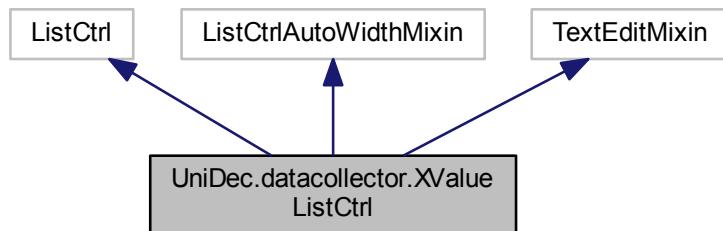
- C:/Python/UniDec/unidec_modules/tims_import_wizard/[import_wizard_grid.py](#)

7.61 UniDec.datacollector.XValueListCtrl Class Reference

Inheritance diagram for UniDec.datacollector.XValueListCtrl:



Collaboration diagram for UniDec.datacollector.XValueListCtrl:



Public Member Functions

- def [__init__](#)
- def [populate](#)
- def [clear_list](#) (*self*)
- def [add_line](#)
- def [get_list](#) (*self*)
- def [get_maxes](#) (*self*)

Public Attributes

- [currentItem](#)

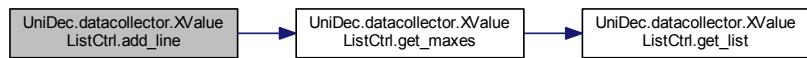
7.61.1 Constructor & Destructor Documentation

7.61.1.1 def [UniDec.datacollector.XValueListCtrl.__init__](#) (*self*, *parent*, *id_value*, *pos*=wx.DefaultPosition, *size*=wx.DefaultSize, *style*=0)

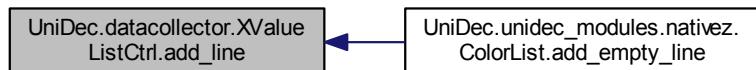
7.61.2 Member Function Documentation

7.61.2.1 def [UniDec.datacollector.XValueListCtrl.add_line](#) (*self*, *val*=0)

Here is the call graph for this function:

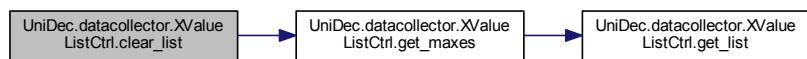


Here is the caller graph for this function:



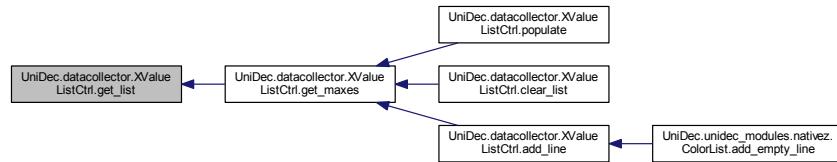
7.61.2.2 def [UniDec.datacollector.XValueListCtrl.clear_list](#) (*self*)

Here is the call graph for this function:



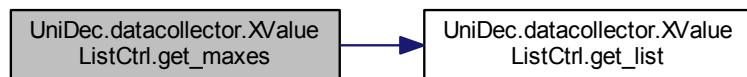
7.61.2.3 def UniDec.datacollector.XValueListCtrl.get_list (self)

Here is the caller graph for this function:

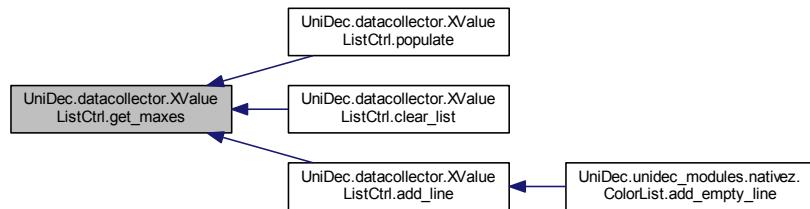


7.61.2.4 def UniDec.datacollector.XValueListCtrl.get_maxes (self)

Here is the call graph for this function:

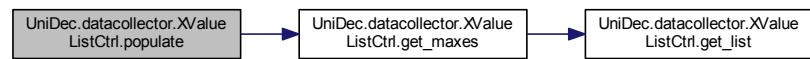


Here is the caller graph for this function:



7.61.2.5 def UniDec.datacollector.XValueListCtrl.populate (self, listctrldata, colors = None)

Here is the call graph for this function:



7.61.3 Member Data Documentation

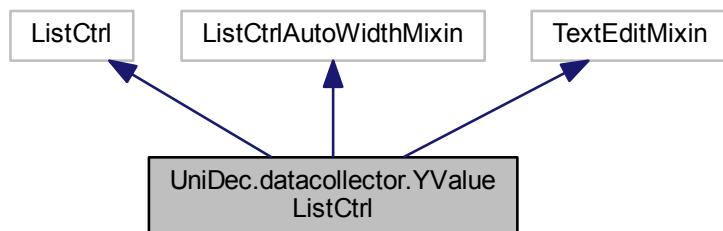
7.61.3.1 UniDec.datacollector.XValueListCtrl.currentItem

The documentation for this class was generated from the following file:

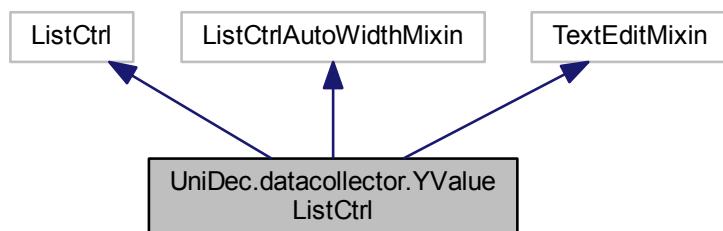
- C:/Python/UniDec/[datacollector.py](#)

7.62 UniDec.datacollector.YValueListCtrl Class Reference

Inheritance diagram for UniDec.datacollector.YValueListCtrl:



Collaboration diagram for UniDec.datacollector.YValueListCtrl:



Public Member Functions

- def [`__init__`](#)
- def [`populate`](#)
- def [`clear_list`](#) (`self`)
- def [`add_line`](#)
- def [`get_list`](#) (`self`)

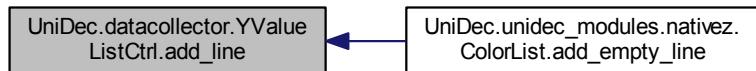
7.62.1 Constructor & Destructor Documentation

```
7.62.1.1 def UniDec.datacollector.YValueListCtrl.__init__ ( self, parent, id_value, pos=wx.DefaultPosition, size =wx.DefaultSize, style=0 )
```

7.62.2 Member Function Documentation

```
7.62.2.1 def UniDec.datacollector.YValueListCtrl.add_line ( self, file_name = "file.txt", var1 = "count", var2 = 0 )
```

Here is the caller graph for this function:



```
7.62.2.2 def UniDec.datacollector.YValueListCtrl.clear_list ( self )
```

```
7.62.2.3 def UniDec.datacollector.YValueListCtrl.get_list ( self )
```

```
7.62.2.4 def UniDec.datacollector.YValueListCtrl.populate ( self, listctrldata, colors=None )
```

The documentation for this class was generated from the following file:

- C:/Python/UniDec/[datacollector.py](#)

7.63 UniDec.unidec_modules.nativez.Zoffset Class Reference

Public Member Functions

- def [__init__](#) (self)
- def [make](#) (self, offset, intensity, index, color, marker)

Public Attributes

- [offset](#)
- [intensity](#)
- [index](#)
- [color](#)
- [marker](#)
- [id](#)
- [width](#)
- [nstate](#)
- [extractwidth](#)
- [extract](#)

7.63.1 Constructor & Destructor Documentation

7.63.1.1 def UniDec.unidec_modules.nativez.Zoffset.__init__(self)

```
A simple class for defining a charge offset species.  
:return: None
```

7.63.2 Member Function Documentation

7.63.2.1 def UniDec.unidec_modules.nativez.Zoffset.make(self, offset, intensity, index, color, marker)

```
Add details to the charge offset species.  
:param offset: Charge offset value  
:param intensity: Intensity  
:param index: Index in the list  
:param color: Color  
:param marker: Marker for the plot  
:return: None
```

7.63.3 Member Data Documentation

7.63.3.1 UniDec.unidec_modules.nativez.Zoffset.color

7.63.3.2 UniDec.unidec_modules.nativez.Zoffset.extract

7.63.3.3 UniDec.unidec_modules.nativez.Zoffset.extractwidth

7.63.3.4 UniDec.unidec_modules.nativez.Zoffset.id

7.63.3.5 UniDec.unidec_modules.nativez.Zoffset.index

7.63.3.6 UniDec.unidec_modules.nativez.Zoffset.intensity

7.63.3.7 UniDec.unidec_modules.nativez.Zoffset.marker

7.63.3.8 UniDec.unidec_modules.nativez.Zoffset.nstate

7.63.3.9 UniDec.unidec_modules.nativez.Zoffset.offset

7.63.3.10 UniDec.unidec_modules.nativez.Zoffset.width

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/nativez.py

7.64 UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox Class Reference

Public Member Functions

- def __init__
- def new_axes
- def update_background (self, event)
- def ignore (self, event)
- def press (self, event)
- def release (self, event)

- def `update` (`self`)
- def `onmove` (`self, event`)
- def `set_active` (`self, active`)
- def `get_active` (`self`)

Public Attributes

- `crossoverpercent`
- `axes`
- `canvas`
- `visible`
- `cids`
- `active`
- `to_draw`
- `background`
- `onselect`
- `onmove_callback`
- `useblit`
- `minspanx`
- `minspany`
- `integrate`
- `smash`
- `validButtons`
- `spancoords`
- `eventpress`
- `eventrelease`
- `data_lims`
- `rectprops`
- `buttonDown`
- `prev`

7.64.1 Detailed Description

Select a min/max range of the x axes for a matplotlib Axes

Example usage::

```
from matplotlib.widgets import RectangleSelector
from pylab import *

def onselect(xmin, xmax, value, ymin, ymax):
    'eclick and erelease are matplotlib events at press and release'
    print ' x,y min position : (%f, %f)' % (xmin, ymin)
    print ' x,y max position : (%f, %f)' % (xmax, ymax)
    print ' used button : ', eclick.button

def toggle_selector(event):
    print ' Key pressed.'
    if event.key in ['Q', 'q'] and toggle_selector.RS.active:
        print ' RectangleSelector deactivated.'
        toggle_selector.RS.set_active(False)
    if event.key in ['A', 'a'] and not toggle_selector.RS.active:
        print ' RectangleSelector activated.'
        toggle_selector.RS.set_active(True)

x = arange(100)/(99.0)
y = sin(x)
fig = figure
axes = subplot(111)
axes.plot(x,y)
```

```

toggle_selector.RS = ZoomBox(axes, onselect, drawtype='line')
connect('key_press_event', toggle_selector)
show()

```

7.64.2 Constructor & Destructor Documentation

7.64.2.1 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.__init__ (*self*, *axes*, *onselect*, *drawtype* = 'box', *minspanx* = None, *minspany* = None, *useblit* = False, *lineprops* = None, *rectprops* = None, *onmove_callback* = None, *spancoords* = 'data', *button* = None, *data_lims* = None, *integrate* = 0, *smash* = 0)

Create a selector in axes. When a selection is made, clear the span and call onselect with

```
onselect(pos_1, pos_2)
```

and clear the drawn box/line. There pos_i are arrays of length 2 containing the x- and y-coordinate.

If minspanx is not None then events smaller than minspanx in x direction are ignored(it's the same for y).

The rect is drawn with rectprops; default
`rectprops = dict(facecolor='red', edgecolor = 'black', alpha=0.5, fill=False)`

The line is drawn with lineprops; default
`lineprops = dict(color='black', linestyle='-', linewidth = 2, alpha=0.5)`

Use type if you want the mouse to draw a line, a box or nothing between click and actual position ny setting

`drawtype = 'line', drawtype='box' or drawtype = 'none'.`

`spancoords` is one of 'data' or 'pixels'. If 'data', minspanx and minspanx will be interpreted in the same coordinates as the x and y axis, if 'pixels', they are in pixels

`button` is a list of integers indicating which mouse buttons should be used for rectangle selection. You can also specify a single integer if only a single button is desired. Default is None, which does not limit which button can be used.

Note, typically:

```
1 = left mouse button
2 = center mouse button (scroll wheel)
3 = right mouse button
```

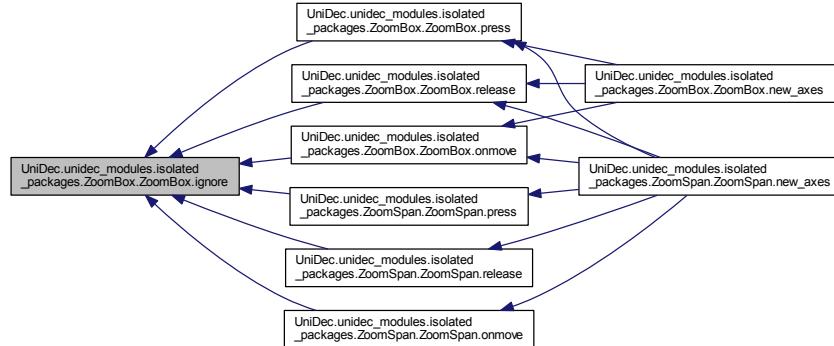
7.64.3 Member Function Documentation

7.64.3.1 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.get_active (*self*)

to get status of active mode (boolean variable)

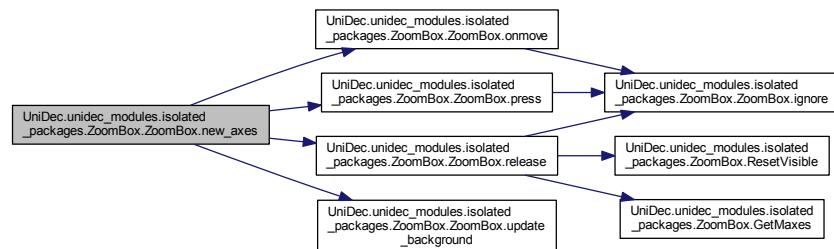
7.64.3.2 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.ignore (self, event)

Here is the caller graph for this function:



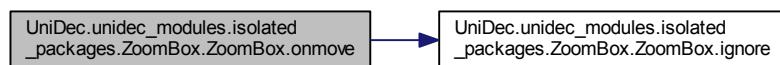
7.64.3.3 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.new_axes (self, axes, rectprops=None)

Here is the call graph for this function:

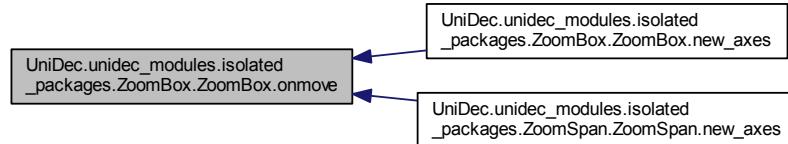


7.64.3.4 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.onmove (self, event)

Here is the call graph for this function:



Here is the caller graph for this function:

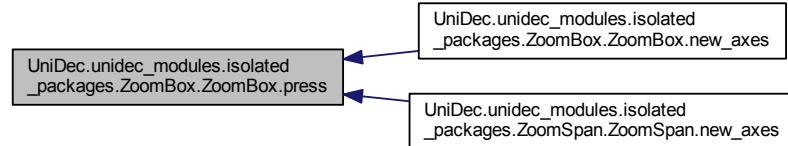


7.64.3.5 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.press (self, event)

Here is the call graph for this function:

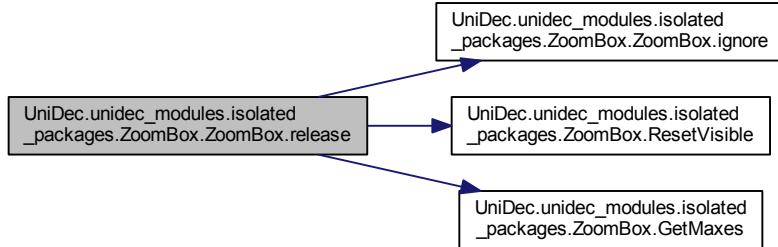


Here is the caller graph for this function:

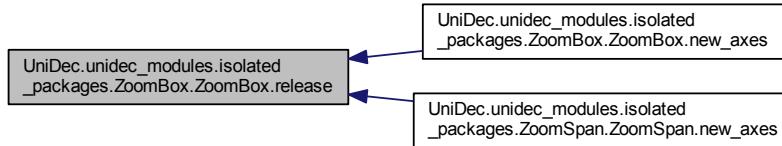


7.64.3.6 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.release (self, event)

Here is the call graph for this function:



Here is the caller graph for this function:



7.64.3.7 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.set_active (self, active)

Use this to activate / deactivate the RectangleSelector

from your program with an boolean variable 'active'.

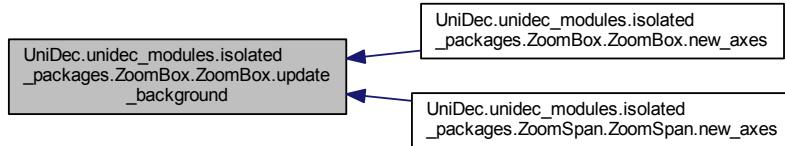
7.64.3.8 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.update (self)

Here is the caller graph for this function:



7.64.3.9 def UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.update_background (*self*, *event*)

Here is the caller graph for this function:



7.64.4 Member Data Documentation

- 7.64.4.1 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.active`
- 7.64.4.2 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.axes`
- 7.64.4.3 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.background`
- 7.64.4.4 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.buttonDown`
- 7.64.4.5 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.canvas`
- 7.64.4.6 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.cids`
- 7.64.4.7 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.crossoverpercent`
- 7.64.4.8 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.data_lims`
- 7.64.4.9 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.eventpress`
- 7.64.4.10 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.eventrelease`
- 7.64.4.11 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.integrate`
- 7.64.4.12 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.minspanx`
- 7.64.4.13 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.minspany`
- 7.64.4.14 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.onmove_callback`
- 7.64.4.15 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.onselect`
- 7.64.4.16 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.prev`
- 7.64.4.17 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.rectprops`
- 7.64.4.18 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.smash`
- 7.64.4.19 `UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.spancoords`

7.64.4.20 UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.to_draw

7.64.4.21 UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.useblit

7.64.4.22 UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.validButtons

7.64.4.23 UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox.visible

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/isolated_packages/ZoomBox.py

7.65 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan Class Reference

Public Member Functions

- def `__init__`
- def `new_axes` (self, axes)
- def `update_background` (self, event)
- def `ignore` (self, event)
- def `press` (self, event)
- def `release` (self, event)
- def `update` (self)
- def `onmove` (self, event)

Public Attributes

- axes
- canvas
- visible
- cids
- rect
- background
- pressv
- rectprops
- onselect
- onmove_callback
- useblit
- minspan
- buttonDown
- prev
- data_lims

7.65.1 Detailed Description

Expansion of matplotlib embed in wx example by John Bender and Edward Abraham, see http://www.scipy.org/Matplotlib_figure_in_a_wx_panel

This version allows the user to zoom in on the figure using either a span selector or a box selector. You can also set a persistent span selector that acts as cursor references on top of whatever is plotted

ZoomSpan based on matplotlib.widgets.SpanSelector
 CursorSpan based on matplotlib.widgets.SpanSelector
 BoxZoom based on matplotlib.widgets.RectangleSelector

Brian J. Soher, Duke University, 20 October, 2010

Select a min/max range of the x or y axes for a matplotlib Axes

Example usage:

```
axes = subplot(111)
axes.plot(x,y)

def onselect(vmin, vmax):
    print vmin, vmax
span = ZoomSpan(axes, onselect, 'horizontal')

onmove_callback is an optional callback that will be called on mouse move
with the span range
```

7.65.2 Constructor & Destructor Documentation

7.65.2.1 def UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.__init__(self, axes, onselect, minspan = None, useblit = False, rectprops = None, onmove_callback = None)

Create a span selector in axes. When a selection is made, clear the span and call onselect with

```
onselect(vmin, vmax)
```

If minspan is not None, ignore events smaller than minspan

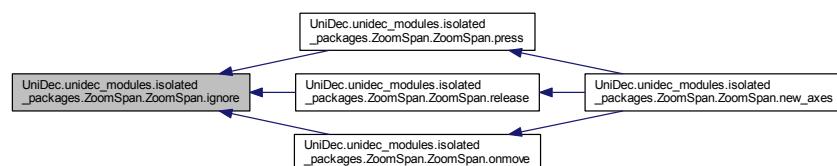
The span rect is drawn with rectprops; default
`rectprops = dict(facecolor='red', alpha=0.5)`

set the visible attribute to False if you want to turn off the functionality of the span selector

7.65.3 Member Function Documentation

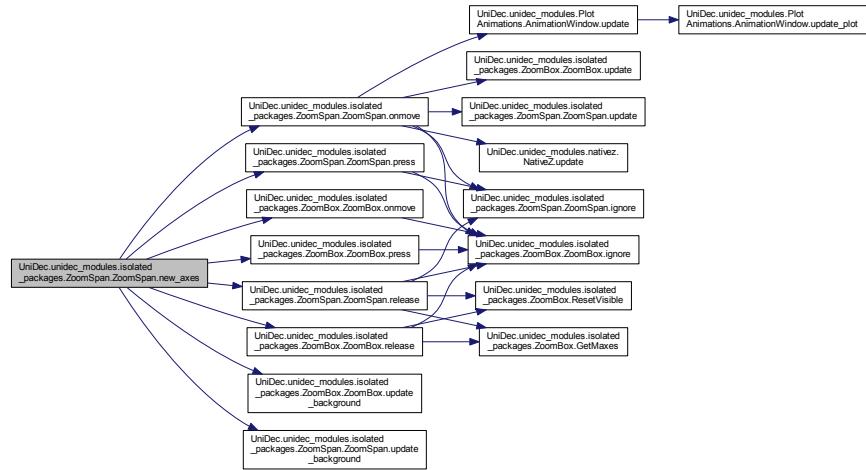
7.65.3.1 def UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.ignore(self, event)

Here is the caller graph for this function:



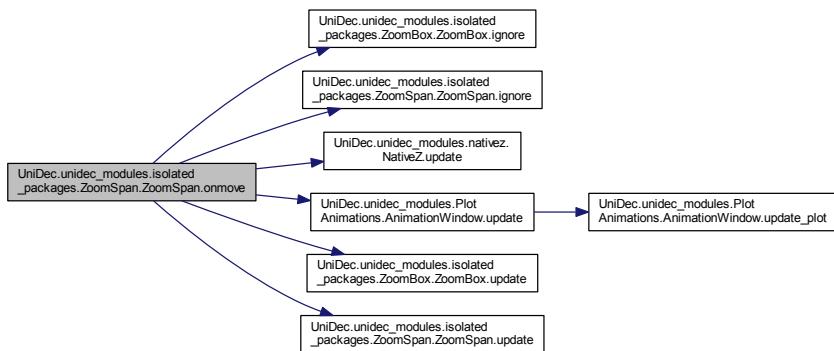
7.65.3.2 def UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.new_axes (self, axes)

Here is the call graph for this function:



7.65.3.3 def UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.onmove (self, event)

Here is the call graph for this function:

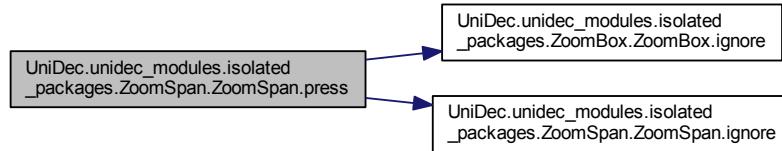


Here is the caller graph for this function:

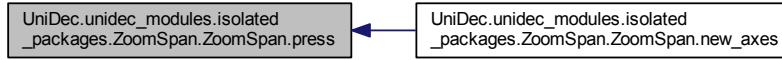


7.65.3.4 def UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.press (self, event)

Here is the call graph for this function:

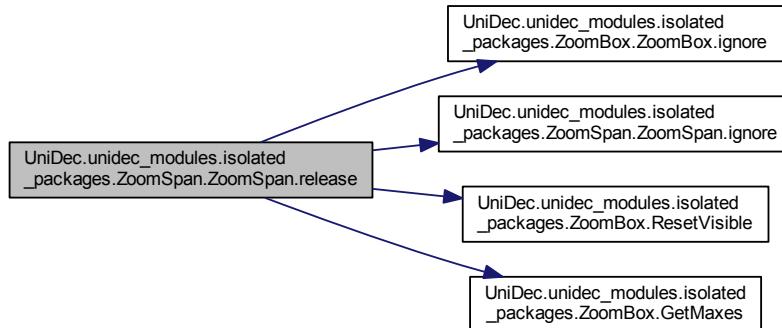


Here is the caller graph for this function:



7.65.3.5 def UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.release (self, event)

Here is the call graph for this function:



Here is the caller graph for this function:



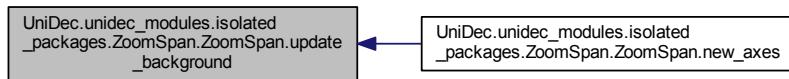
7.65.3.6 def UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.update (self)

Here is the caller graph for this function:



7.65.3.7 def UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.update_background (self, event)

Here is the caller graph for this function:



7.65.4 Member Data Documentation

- 7.65.4.1 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.axes
- 7.65.4.2 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.background
- 7.65.4.3 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.buttonDown
- 7.65.4.4 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.canvas
- 7.65.4.5 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.cids
- 7.65.4.6 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.data_lims
- 7.65.4.7 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.minspan
- 7.65.4.8 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.onmove_callback
- 7.65.4.9 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.onselect
- 7.65.4.10 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.pressv
- 7.65.4.11 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.prev
- 7.65.4.12 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.rect
- 7.65.4.13 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.rectprops
- 7.65.4.14 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.useblit

7.65.4.15 UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan.visible

The documentation for this class was generated from the following file:

- C:/Python/UniDec/unidec_modules/isolated_packages/[ZoomSpan.py](#)

Chapter 8

File Documentation

8.1 C:/Python/UniDec/__init__.py File Reference

Namespaces

- [UniDec](#)

Variables

- string [UniDec.__author__](#) = 'Michael.Marty'

8.2 C:/Python/UniDec/unidec_modules/__init__.py File Reference

Namespaces

- [UniDec.unidec_modules](#)

Variables

- string [UniDec.unidec_modules.__author__](#) = 'michael.marty'

8.3 C:/Python/UniDec/unidec_modules/isolated_packages/__init__.py File Reference

Namespaces

- [UniDec.unidec_modules.isolated_packages](#)

Variables

- string [UniDec.unidec_modules.isolated_packages.__author__](#) = 'Michael.Marty'

8.4 C:/Python/UniDec/unidec_modules/tims_import_wizard/__init__.py File Reference

Namespaces

- [UniDec.unidec_modules.tims_import_wizard](#)

Variables

- string [UniDec.unidec_modules.tims_import_wizard.__author__](#) = 'michael.marty'

8.5 C:/Python/UniDec/datacollector.py File Reference

Classes

- class [UniDec.datacollector.XValueListCtrl](#)
- class [UniDec.datacollector.YValueListCtrl](#)
- class [UniDec.datacollector.ListCtrlPanel](#)
- class [UniDec.datacollector.NetworkFrame](#)
- class [UniDec.datacollector.DataCollector](#)

Namespaces

- [UniDec.datacollector](#)

Variables

- string [UniDec.datacollector.__author__](#) = 'michael.marty'
- dictionary [UniDec.datacollector.datachoices](#) = {0: "Raw Data", 1: "Processed Data", 2: "Zero Charge Mass Spectrum"}
- dictionary [UniDec.datacollector.extractchoices](#) = {0: "Height", 1: "Local Max", 2: "Area", 3: "Center of Mass", 4: "Local Max Position"}
- dictionary [UniDec.datacollector.extractlabels](#) = {0: "Intensity", 1: "Intensity", 2: "Area", 3: "mass", 4: "mass"}
- dictionary [UniDec.datacollector.modelchoices](#)
- tuple [UniDec.datacollector.app](#) = wx.App(False)
- tuple [UniDec.datacollector.frame](#) = DataCollector(None, "Collect Data")

8.6 C:/Python/UniDec/GUniDec.py File Reference

Classes

- class [UniDec.GUniDec.Shell](#)
- class [UniDec.GUniDec.UniDecApp](#)

Namespaces

- [UniDec.GUniDec](#)

Variables

- string [UniDec.GUniDec.__author__](#) = 'Michael.Marty'
- tuple [UniDec.GUniDec.app](#) = UniDecApp()

8.7 C:/Python/UniDec/import_wizard.py File Reference

Classes

- class [UniDec.import_wizard.ImportWizard](#)

Namespaces

- [UniDec.import_wizard](#)

Variables

- tuple [UniDec.import_wizard.app](#) = wx.App(False)
- tuple [UniDec.import_wizard.frame](#) = ImportWizard(None)

8.8 C:/Python/UniDec/readme.md File Reference

8.9 C:/Python/UniDec/test_UniDec.py File Reference

Classes

- class [UniDec.test_UniDec.TestUniDec](#)

Namespaces

- [UniDec.test_UniDec](#)

8.10 C:/Python/UniDec/unidec.py File Reference

Classes

- class [UniDec.unidec.DataContainer](#)
- class [UniDec.unidec.UniDec](#)

Namespaces

- [UniDec.unidec](#)

Variables

- string [UniDec.unidec.__author__](#) = 'Michael.Marty'
- tuple [UniDec.unidec.eng](#) = UniDec()
- string [UniDec.unidec.filename](#) = "0.txt"
- string [UniDec.unidec.path](#) = "C:\\cprog\\UniDecDemo"
- list [UniDec.unidec.files](#) = ["0.txt"]

8.11 C:/Python/UniDec/unidec_modules/auto_peak.py File Reference

Namespaces

- [UniDec.unidec_modules.auto_peak](#)

Variables

- string [UniDec.unidec_modules.auto_peak.__author__](#) = 'Michael.Marty'
- string [UniDec.unidec_modules.auto_peak.file](#) = "C:\\cprog\\UniDecDemo\\MTM_ADH_5_rawdata.txt"
- tuple [UniDec.unidec_modules.auto_peak.data](#) = np.loadtxt(file, skiprows=10)
- tuple [UniDec.unidec_modules.auto_peak.thresh](#) = auto_noise_level(data)
- tuple [UniDec.unidec_modules.auto_peak.avgb](#)s = average_bin_size(data)
- int [UniDec.unidec_modules.auto_peak.window](#) = fwhm/avgb/4
- tuple [UniDec.unidec_modules.auto_peak.cwt](#)dat = np.transpose([data[:, 0], cwt])
- tuple [UniDec.unidec_modules.auto_peak.peaks](#) = peakdetect(cwt, None, window * 2., thresh)
- int [UniDec.unidec_modules.auto_peak.zm](#) = 1
- list [UniDec.unidec_modules.auto_peak.ivals](#) = peaks[:, 1]
- tuple [UniDec.unidec_modules.auto_peak.maxpos](#) = np.argmax(ivals)
- list [UniDec.unidec_modules.auto_peak.mins](#) = []
- tuple [UniDec.unidec_modules.auto_peak.x](#) = np.abs(zm - zm[maxpos])
- tuple [UniDec.unidec_modules.auto_peak.diffs](#) = np.diff(x)
- tuple [UniDec.unidec_modules.auto_peak.minpos](#) = np.argmin(diffs)
- tuple [UniDec.unidec_modules.auto_peak.minval](#) = np.average(x[minpos:minpos + 2])
- int [UniDec.unidec_modules.auto_peak.mass](#) = 1
- list [UniDec.unidec_modules.auto_peak.mz](#) = peaks[maxpos, 0]
- tuple [UniDec.unidec_modules.auto_peak.charge](#) = np.round(mass / mz)
- [UniDec.unidec_modules.auto_peak.tolerance](#) = charge*fwhm
- tuple [UniDec.unidec_modules.auto_peak.vec](#) = np.array([mass, ival[s[maxpos]], mz, charge, diff[minpos], tolerance, zm[maxpos], False])
- tuple [UniDec.unidec_modules.auto_peak.sindex](#) = np.argsort(mins[:, 4])
- list [UniDec.unidec_modules.auto_peak.peakassignments](#) = []
- list [UniDec.unidec_modules.auto_peak.row](#) = mins[i]
- list [UniDec.unidec_modules.auto_peak.swaps](#) = []
- list [UniDec.unidec_modules.auto_peak.topmass](#) = row[0]
- list [UniDec.unidec_modules.auto_peak.topcharge](#) = row[3]
- tuple [UniDec.unidec_modules.auto_peak.zms](#) = np.abs(row[6] - mins[:, 6])
- list [UniDec.unidec_modules.auto_peak.newmass](#) = mins[j, 2]
- int [UniDec.unidec_modules.auto_peak.newspot](#) = 0
- tuple [UniDec.unidec_modules.auto_peak.swaprows](#) = deepcopy(mins[newspot:j])
- list [UniDec.unidec_modules.auto_peak.boo1](#) = mins[:, 7]
- list [UniDec.unidec_modules.auto_peak.y](#) = mins[boo1, 4]
- tuple [UniDec.unidec_modules.auto_peak.m](#) = np.array(m)

8.12 C:/Python/UniDec/unidec_modules/AutocorrWindow.py File Reference

Classes

- class [UniDec.unidec_modules.AutocorrWindow.CorrListCtrl](#)
- class [UniDec.unidec_modules.AutocorrWindow.CorrListCtrlPanel](#)
- class [UniDec.unidec_modules.AutocorrWindow.AutocorrWindow](#)

Namespaces

- [UniDec.unidec_modules.AutocorrWindow](#)

Variables

- string [UniDec.unidec_modules.AutocorrWindow.__author__](#) = 'Michael.Marty'

8.13 C:/Python/UniDec/unidec_modules/ColorPlot.py File Reference

Classes

- class [UniDec.unidec_modules.ColorPlot2D](#)

Namespaces

- [UniDec.unidec_modules.ColorPlot](#)

Variables

- string [UniDec.unidec_modules.ColorPlot.__author__](#) = 'Michael.Marty'

8.14 C:/Python/UniDec/unidec_modules/Extract2D.py File Reference

Classes

- class [UniDec.unidec_modules.Extract2D.Extract2DPlot](#)

Namespaces

- [UniDec.unidec_modules.Extract2D](#)

Variables

- string [UniDec.unidec_modules.Extract2D.__author__](#) = 'Michael.Marty'
- string [UniDec.unidec_modules.Extract2D.dir_name](#) = "C:\\MassLynx\\Mike.PRO\\Data\\150521\\mzML\\AqpZ_05_Ramp3\\MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_unidecfiles"
- string [UniDec.unidec_modules.Extract2D.file_name](#) = "MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_mass.txt"
- tuple [UniDec.unidec_modules.Extract2D.path](#) = os.path.join(dir_name, file_name)
- tuple [UniDec.unidec_modules.Extract2D.data](#) = np.loadtxt(path)
- tuple [UniDec.unidec_modules.Extract2D.data2](#) = np.loadtxt(path)
- tuple [UniDec.unidec_modules.Extract2D.data3](#) = np.loadtxt(path)
- list [UniDec.unidec_modules.Extract2D.datalist](#) = [data, data2, data3]
- tuple [UniDec.unidec_modules.Extract2D.app](#) = wx.App(False)
- tuple [UniDec.unidec_modules.Extract2D.frame](#) = Extract2DPlot(None, datalist, yvals=np.array([100., 120., 180.]))

8.15 C:/Python/UniDec/unidec_modules/fft_test.py File Reference

Namespaces

- [UniDec.unidec_modules.fft_test](#)

Functions

- def [UniDec.unidec_modules.fft_test.MALDI_baseline](#) (data, w)
- def [UniDec.unidec_modules.fft_test.calc_medians](#) (data, start, stop, w)
- def [UniDec.unidec_modules.fft_test.fit_medians](#) (data, start, stop, w)
- def [UniDec.unidec_modules.fft_test.old_cwt_2d](#)
- def [UniDec.unidec_modules.fft_test.cwt_2d](#)
- def [UniDec.unidec_modules.fft_test.ifitfun](#) (x, data, recon)
- def [UniDec.unidec_modules.fft_test.optimize_overlap](#) (data, recon)

Variables

- string [UniDec.unidec_modules.fft_test.__author__](#) = 'michael.marty'
- string [UniDec.unidec_modules.fft_test.datfile](#) = "C:\\NDData\\PG25\\CG_07\\150820(CG_07_ramp90.txt"
- tuple [UniDec.unidec_modules.fft_test.data](#) = np.loadtxt(datfile)
- float [UniDec.unidec_modules.fft_test.mzbinsize](#) = 1.0
- int [UniDec.unidec_modules.fft_test.baseline](#) = 30
- tuple [UniDec.unidec_modules.fft_test.background](#) = np.sin((data[:, 0] - data[0, 0]) / (data[len(data) - 1, 0] - data[0, 0]) * np.pi)
- int [UniDec.unidec_modules.fft_test.width](#) = 20
- int [UniDec.unidec_modules.fft_test.num](#) = 10
- int [UniDec.unidec_modules.fft_test.cutoff](#) = 5000
- string [UniDec.unidec_modules.fft_test.wf](#) = "dog"
- int [UniDec.unidec_modules.fft_test.param](#) = 2
- int [UniDec.unidec_modules.fft_test.hpfilt](#) = 1
- tuple [UniDec.unidec_modules.fft_test.lpfilt](#) = stats.norm.cdf(widths, cutoff, cutoff * 0.01)
- [UniDec.unidec_modules.fft_test.filt](#) = lpfilt
- tuple [UniDec.unidec_modules.fft_testfiltmat](#) = np.transpose([filt for d in data])
- tuple [UniDec.unidec_modules.fft_test.recon](#) = mlpy.wavelet.icwt(cwt * filtmat, mzbinsize, widths, wf=wf, p=param)
- tuple [UniDec.unidec_modules.fft_test.reconscale](#) = optimize_overlap(data, recon)
- tuple [UniDec.unidec_modules.fft_test.fdat](#) = np.average(cwt, axis=1)
- list [UniDec.unidec_modules.fft_test.boo1](#) = data[:, 0]
- tuple [UniDec.unidec_modules.fft_test.mindat](#) = min(data[:, 0])
- tuple [UniDec.unidec_modules.fft_test.maxdat](#) = max(data[:, 0])
- tuple [UniDec.unidec_modules.fft_test.mzdata](#) = linearize(data, 0.05, 3)
- tuple [UniDec.unidec_modules.fft_test.xvals](#) = np.arange(mindat, maxdat, 500)
- tuple [UniDec.unidec_modules.fft_test.results](#) = np.array([windowed_fft(mzdata, x, 2000) for x in xvals])
- list [UniDec.unidec_modules.fft_test.intdat](#) = results[:, :, 1]
- tuple [UniDec.unidec_modules.fft_test.yvals](#) = np.unique(results[:, :, 0])

8.16 C:/Python/UniDec/unidec_modules/fft_window.py File Reference

Classes

- class [UniDec.unidec_modules.fft_window.FFTWindow](#)

Namespaces

- [UniDec.unidec_modules.fft_window](#)

Variables

- string [UniDec.unidec_modules.fft_window.__author__](#) = 'Michael.Marty'
- string [UniDec.unidec_modules.fft_window.datfile](#) = "C:\\NDData\\PG25\\CG_07\\150820(CG_07_ramp90.txt"
- tuple [UniDec.unidec_modules.fft_window.data2](#) = np.loadtxt(datfile)
- tuple [UniDec.unidec_modules.fft_window.app](#) = wx.App(False)
- tuple [UniDec.unidec_modules.fft_window.frame](#) = FFTWindow(None, data2)

8.17 C:/Python/UniDec/unidec_modules/GridDecon.py File Reference

Classes

- class [UniDec.unidec_modules.GridDecon.GridDeconWindow](#)

Namespaces

- [UniDec.unidec_modules.GridDecon](#)

Functions

- def [UniDec.unidec_modules.GridDecon.make_pmat](#) (mzgrid, fwhm)
- def [UniDec.unidec_modules.GridDecon.conv](#) (b, pmat)
- def [UniDec.unidec_modules.GridDecon.blur](#) (b, msig, zsig)
- def [UniDec.unidec_modules.GridDecon.grid_unidec](#)

Variables

- string [UniDec.unidec_modules.GridDecon.__author__](#) = 'Michael.Marty'
- string [UniDec.unidec_modules.GridDecon.dir_name](#) = "C:\\MassLynx\\Mike.PRO\\Data\\150521\\mzML\\AqpZ_05_Ramp3\\"
- string [UniDec.unidec_modules.GridDecon.file_name](#) = "MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100.txt"
- tuple [UniDec.unidec_modules.GridDecon.path](#) = os.path.join(dir_name, file_name)
- tuple [UniDec.unidec_modules.GridDecon.data](#) = np.loadtxt(path)
- tuple [UniDec.unidec_modules.GridDecon.app](#) = wx.App(False)
- tuple [UniDec.unidec_modules.GridDecon.frame](#) = GridDeconWindow(None, data)

8.18 C:/Python/UniDec/unidec_modules/IM_functions.py File Reference

Namespaces

- [UniDec.unidec_modules.IM_functions](#)

Functions

- def [UniDec.unidec_modules.IM_functions.smooth_2d](#) (igrid, smooth, smoothdt)
- def [UniDec.unidec_modules.IM_functions.min_array](#) (igrid, xwidth, ywidth)
- def [UniDec.unidec_modules.IM_functions.intensitythresh](#) (igrid, thresh)
- def [UniDec.unidec_modules.IM_functions.subtract_complex_2d](#) (igrid, config)
- def [UniDec.unidec_modules.IM_functions.compress_2d](#) (xgrid, ygrid, zgrid, num)
- def [UniDec.unidec_modules.IM_functions.linearize_2d](#) (xvals, yvals, igrid, binsize)
- def [UniDec.unidec_modules.IM_functions.detectoreff_2d](#) (igrid, xgrid, va)
- def [UniDec.unidec_modules.IM_functions.process_data_2d](#) (xgrid, ygrid, igrid, config)
- def [UniDec.unidec_modules.IM_functions.calc_twave_dt](#) (mass, z, ccs, config)
- def [UniDec.unidec_modules.IM_functions.calc_linear_dt](#) (mass, z, ccs, config)
- def [UniDec.unidec_modules.IM_functions.calc_native_ccs](#) (mass, gasmass)

Variables

- string [UniDec.unidec_modules.IM_functions.__author__](#) = 'Michael.Marty'

8.19 C:/Python/UniDec/unidec_modules/IM_windows.py File Reference

Classes

- class [UniDec.unidec_modules.IM_windows.ILMListCtrl](#)
- class [UniDec.unidec_modules.IM_windows.ILMListCtrlPanel](#)
- class [UniDec.unidec_modules.IM_windows.ILMTools](#)
- class [UniDec.unidec_modules.IM_windows.ILMToolExtract](#)

Namespaces

- [UniDec.unidec_modules.IM_windows](#)

Variables

- string [UniDec.unidec_modules.IM_windows.__author__](#) = 'Michael.Marty'

8.20 C:/Python/UniDec/unidec_modules/isolated_packages/FileDialogs.py File Reference

Namespaces

- [UniDec.unidec_modules.isolated_packages.FileDialogs](#)

Functions

- def [UniDec.unidec_modules.isolated_packages.FileDialogs.save_file_dialog](#)
- def [UniDec.unidec_modules.isolated_packages.FileDialogs.open_file_dialog](#)
- def [UniDec.unidec_modules.isolated_packages.FileDialogs.open_multiple_files_dialog](#)
- def [UniDec.unidec_modules.isolated_packages.FileDialogs.open_dir_dialog](#)
- def [UniDec.unidec_modules.isolated_packages.FileDialogs.open_multiple_dir_dialog](#) (message, default)
- def [UniDec.unidec_modules.isolated_packages.FileDialogs.open_single_dir_dialog](#) (message, default)

Variables

- tuple `UniDec.unidec_modules.isolated_packages.FileDialogs.default_dir` = `os.path.abspath(os.path.join(os.getcwd(), os.path.pardir, 'data/'))`

8.21 C:/Python/UniDec/unidec_modules/isolated_packages/option_d.py File Reference

Namespaces

- `UniDec.unidec_modules.isolated_packages.option_d`

Variables

- dictionary `UniDec.unidec_modules.isolated_packages.option_d.parameters`
- list `UniDec.unidec_modules.isolated_packages.option_d.cm_data`
- tuple `UniDec.unidec_modules.isolated_packages.option_d.viridis` = `LinearSegmentedColormap.from_list(__file__, cm_data)`
- list `UniDec.unidec_modules.isolated_packages.option_d.cm_data2`
- tuple `UniDec.unidec_modules.isolated_packages.option_d.parula_map` = `LinearSegmentedColormap.from_list('parula', cm_data2)`
- list `UniDec.unidec_modules.isolated_packages.option_d.cm_data3`
- tuple `UniDec.unidec_modules.isolated_packages.option_d.fake_parula_map` = `LinearSegmentedColormap.from_list(__file__, cm_data3)`

8.22 C:/Python/UniDec/unidec_modules/isolated_packages/texmaker.py File Reference

Namespaces

- `UniDec.unidec_modules.isolated_packages.texmaker`

Functions

- def `UniDec.unidec_modules.isolated_packages.texmaker.MakeTexReport` (fname, config, path, peaks, labels, names, color, figureflags)
- def `UniDec.unidec_modules.isolated_packages.texmaker.PDFTexReport` (fname)

8.23 C:/Python/UniDec/unidec_modules/isolated_packages/twitter_interface.py File Reference

Classes

- class `UniDec.unidec_modules.isolated_packages.twitter_interface.TwitterWindow`
- class `UniDec.unidec_modules.isolated_packages.twitter_interface.PinWindow`

Namespaces

- `UniDec.unidec_modules.isolated_packages.twitter_interface`

Variables

- string [UniDec.unidec_modules.isolated_packages.twitter_interface.__author__](#) = 'Michael'

8.24 C:/Python/UniDec/unidec_modules/isolated_packages/ZoomBox.py File Reference

Classes

- class [UniDec.unidec_modules.isolated_packages.ZoomBox.ZoomBox](#)

Namespaces

- [UniDec.unidec_modules.isolated_packages.ZoomBox](#)

Functions

- def [UniDec.unidec_modules.isolated_packages.ZoomBox.GetMaxes](#)
- def [UniDec.unidec_modules.isolated_packages.ZoomBox.ResetVisible](#) (axes)
- def [UniDec.unidec_modules.isolated_packages.ZoomBox.GetStart](#) (axes)

8.25 C:/Python/UniDec/unidec_modules/isolated_packages/ZoomSpan.py File Reference

Classes

- class [UniDec.unidec_modules.isolated_packages.ZoomSpan.ZoomSpan](#)

Namespaces

- [UniDec.unidec_modules.isolated_packages.ZoomSpan](#)

8.26 C:/Python/UniDec/unidec_modules/mainwindow.py File Reference

Classes

- class [UniDec.unidec_modules/mainwindow.Mainwindow](#)
- class [UniDec.unidec_modules/mainwindow.MyFileDropTarget](#)

Namespaces

- [UniDec.unidec_modules/mainwindow](#)

Variables

- string [UniDec.unidec_modules/mainwindow.__author__](#) = 'Michael.Marty'

8.27 C:/Python/UniDec/unidec_modules/ManualSelectionWindow.py File Reference

Classes

- class [UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrl](#)
- class [UniDec.unidec_modules.ManualSelectionWindow.ManagedListCtrlPanel](#)
- class [UniDec.unidec_modules.ManualSelectionWindow.ManualSelection](#)

Namespaces

- [UniDec.unidec_modules.ManualSelectionWindow](#)

Functions

- def [UniDec.unidec_modules.ManualSelectionWindow.closest](#) (x, y, manlist)
- def [UniDec.unidec_modules.ManualSelectionWindow.correctassignments](#) (manlist, xdat, ydat)
- def [UniDec.unidec_modules.ManualSelectionWindow.range_overlap](#) (a_min, a_max, b_min, b_max)
- def [UniDec.unidec_modules.ManualSelectionWindow.checkoverlap](#) (l1, l2)
- def [UniDec.unidec_modules.ManualSelectionWindow.detectoverlap](#) (manlist)

Variables

- string [UniDec.unidec_modules.ManualSelectionWindow.__author__](#) = 'Michael.Marty'

8.28 C:/Python/UniDec/unidec_modules/MassDefects.py File Reference

Classes

- class [UniDec.unidec_modules.MassDefects.MassDefectWindow](#)

Namespaces

- [UniDec.unidec_modules.MassDefects](#)

Variables

- string [UniDec.unidec_modules.MassDefects.__author__](#) = 'Michael.Marty'
- string [UniDec.unidec_modules.MassDefects.dir](#) = "C:\\MassLynx\\Mike.PRO\\Data\\150521\\mzML\\AqpZ_←
05_Ramp3\\MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_20mit100_unidecfiles"
- string [UniDec.unidec_modules.MassDefects.file](#) = "MTM_150521_AqpZ_05_POPC_Ramp_1-5pbar_←
20mit100_mass.txt"
- tuple [UniDec.unidec_modules.MassDefects.path](#) = os.path.join(dir, file)
- tuple [UniDec.unidec_modules.MassDefects.data](#) = np.loadtxt(path)
- tuple [UniDec.unidec_modules.MassDefects.data2](#) = np.loadtxt(path)
- list [UniDec.unidec_modules.MassDefects.datalist](#) = [data, data2]
- tuple [UniDec.unidec_modules.MassDefects.app](#) = wx.App(False)
- tuple [UniDec.unidec_modules.MassDefects.frame](#) = MassDefectWindow(None, datalist)

8.29 C:/Python/UniDec/unidec_modules/MassFitter.py File Reference

Classes

- class [UniDec.unidec_modules.MassFitter.MassFitter](#)

Namespaces

- [UniDec.unidec_modules.MassFitter](#)

Functions

- def [UniDec.unidec_modules.MassFitter.make_mass_list](#) (massdat, arrayin, psfun, startarray, args)
- def [UniDec.unidec_modules.MassFitter.error_function](#) (array, massdat, psfun, startarray, args)
- def [UniDec.unidec_modules.MassFitter.least_squares_minimize](#) (massdat, array, psfun, args)

Variables

- string [UniDec.unidec_modules.MassFitter.__author__](#) = 'Michael.Marty'

8.30 C:/Python/UniDec/unidec_modules/MassSpecBuilder.py File Reference

Namespaces

- [UniDec.unidec_modules.MassSpecBuilder](#)

Functions

- def [UniDec.unidec_modules.MassSpecBuilder.make_mass_spectrum](#) (array, zrange=(10, 50, mzrange=(2000, 10000, mz_bin_size=1, adductmass=1.00727647, psfun=0, noise=0, baseline=0, kwargs))
- def [UniDec.unidec_modules.MassSpecBuilder.get_zrange](#) (params)
- def [UniDec.unidec_modules.MassSpecBuilder.get_mzrange](#) (params)
- def [UniDec.unidec_modules.MassSpecBuilder.simple_params](#) (masslist, intlist=None, resolution=1000, zwidth=2, rlist=None, kwargs)
- def [UniDec.unidec_modules.MassSpecBuilder.simple_spectrum](#) (masslist, kwargs)

Variables

- string [UniDec.unidec_modules.MassSpecBuilder.__author__](#) = 'Michael.Marty'

8.31 C:/Python/UniDec/unidec_modules/masstools.py File Reference

Classes

- class [UniDec.unidec_modules.masstools.MassListCtrl](#)
- class [UniDec.unidec_modules.masstools.MassListCtrlPanel](#)
- class [UniDec.unidec_modules.masstools.OligomerListCtrl](#)
- class [UniDec.unidec_modules.masstools.OligomerListCtrlPanel](#)
- class [UniDec.unidec_modules.masstools.MatchListCtrl](#)
- class [UniDec.unidec_modules.masstools.MatchListCtrlPanel](#)
- class [UniDec.unidec_modules.masstools.MassSelection](#)

Namespaces

- [UniDec.unidec_modules.masstools](#)

8.32 C:/Python/UniDec/unidec_modules/miscwindows.py File Reference

Classes

- class [UniDec.unidec_modules.misctools.SingleInputDialog](#)
- class [UniDec.unidec_modules.misctools.AdditionalParameters](#)
- class [UniDec.unidec_modules.misctools.SaveFigureDialog](#)
- class [UniDec.unidec_modules.misctools.FileNameDialog](#)

Namespaces

- [UniDec.unidec_modules.misctools](#)

Functions

- def [UniDec.unidec_modules.misctools.setup_tab_box](#) (tab, plot)

Variables

- string [UniDec.unidec_modules.misctools.__author__](#) = 'Michael.Marty'

8.33 C:/Python/UniDec/unidec_modules/mzMLimporter.py File Reference

Classes

- class [UniDec.unidec_modules.mzMLimporter.mzMLimporter](#)

Namespaces

- [UniDec.unidec_modules.mzMLimporter](#)

Functions

- def [UniDec.unidec_modules.mzMLimporter.get_resolution](#) (testdata)
- def [UniDec.unidec_modules.mzMLimporter.merge_spectra](#) (datalist)

Variables

- string [UniDec.unidec_modules.mzMLimporter.__author__](#) = 'Michael.Marty'
- string [UniDec.unidec_modules.mzMLimporter.dir](#) = "C:\\cprog\\Joe"
- string [UniDec.unidec_modules.mzMLimporter.file](#) = "20150304_myo_70r_5u_full-ALL.mzML"
- tuple [UniDec.unidec_modules.mzMLimporter.tstart](#) = time.time()
- tuple [UniDec.unidec_modules.mzMLimporter.data](#) = mzMLimporter(os.path.join(dir, file))
- tuple [UniDec.unidec_modules.mzMLimporter.tend](#) = time.time()

8.34 C:/Python/UniDec/unidec_modules/nativez.py File Reference

Classes

- class [UniDec.unidec_modules.nativez.Zoffset](#)
- class [UniDec.unidec_modules.nativez.NativeZ](#)
- class [UniDec.unidec_modules.nativez.ColorList](#)

Namespaces

- [UniDec.unidec_modules.nativez](#)

Variables

- string [UniDec.unidec_modules.nativez.__author__](#) = 'Michael.Marty'

8.35 C:/Python/UniDec/unidec_modules/peaklistsorth.py File Reference

Classes

- class [UniDec.unidec_modules.peaklistsorth.PeakListCtrlPanel](#)

Namespaces

- [UniDec.unidec_modules.peaklistsorth](#)

8.36 C:/Python/UniDec/unidec_modules/peakstructure.py File Reference

Classes

- class [UniDec.unidec_modules.peakstructure.Peak](#)
- class [UniDec.unidec_modules.peakstructure.Peaks](#)

Namespaces

- [UniDec.unidec_modules.peakstructure](#)

Variables

- string [UniDec.unidec_modules.peakstructure.__author__](#) = 'Michael.Marty'

8.37 C:/Python/UniDec/unidec_modules/peakwidthtools.py File Reference

Classes

- class [UniDec.unidec_modules.peakwidthtools.PeakTools1d](#)
- class [UniDec.unidec_modules.peakwidthtools.PeakTools2d](#)

Namespaces

- [UniDec.unidec_modules.peakwidthtools](#)

Variables

- string [UniDec.unidec_modules.peakwidthtools.__author__](#) = 'Michael.Marty'

8.38 C:/Python/UniDec/unidec_modules/plot1d.py File Reference

Classes

- class [UniDec.unidec_modules.plot1d.Plot1d](#)

Namespaces

- [UniDec.unidec_modules.plot1d](#)

8.39 C:/Python/UniDec/unidec_modules/plot2d.py File Reference

Classes

- class [UniDec.unidec_modules.plot2d.Plot2d](#)

Namespaces

- [UniDec.unidec_modules.plot2d](#)

Variables

- string [UniDec.unidec_modules.plot2d.__author__](#) = 'Michael.Marty'

8.40 C:/Python/UniDec/unidec_modules/plot3d.py File Reference

Classes

- class [UniDec.unidec_modules.plot3d.CubePlot](#)

Namespaces

- [UniDec.unidec_modules.plot3d](#)

Variables

- string [UniDec.unidec_modules.plot3d.__author__](#) = 'Michael.Marty'

8.41 C:/Python/UniDec/unidec_modules/PlotAnimations.py File Reference

Classes

- class [UniDec.unidec_modules.PlotAnimations.AnimationWindow](#)

Namespaces

- [UniDec.unidec_modules.PlotAnimations](#)

Variables

- string [UniDec.unidec_modules.PlotAnimations.__author__](#) = 'Michael.Marty'
- tuple [UniDec.unidec_modules.PlotAnimations.x](#) = np.arange(0.0, 10.0)
- tuple [UniDec.unidec_modules.PlotAnimations.datalist](#) = np.array([np.transpose([x, x]), np.transpose([x, x * x]), np.transpose([x, x * x * x])])
- tuple [UniDec.unidec_modules.PlotAnimations.app](#) = wx.App(False)
- tuple [UniDec.unidec_modules.PlotAnimations.frame](#) = AnimationWindow(None, datalist)

8.42 C:/Python/UniDec/unidec_modules/PlottingWindow.py File Reference

Classes

- class [UniDec.unidec_modules.PlottingWindow.PlottingWindow](#)

Namespaces

- [UniDec.unidec_modules.PlottingWindow](#)

8.43 C:/Python/UniDec/unidec_modules/tims_import_wizard/data_importer.py File Reference

Namespaces

- [UniDec.unidec_modules.tims_import_wizard.data_importer](#)

Functions

- def [UniDec.unidec_modules.tims_import_wizard.data_importer.auto_from_wizard](#) (lines, exedir)
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.run_get_data](#) (job_kwargs)
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.MakeUniDecConfig](#) (job_kwargs)
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.process_from_wizard](#) (kwargs)
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.mp_process_from_wizard](#) (job_list)
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.data_import_worker](#) (worker_queue, result←_queue)
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.split_and_strip](#) (line, delimiter=')
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.parse_file](#)
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.GetLines](#) (InputFileName)
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.GetStartEndMass](#) (RawFile)
- def [UniDec.unidec_modules.tims_import_wizard.data_importer.get_stat_code](#)

- def `UniDec.unidec_modules.tims_import_wizard.data_importer.header_desc` (file_path)
- def `UniDec.unidec_modules.tims_import_wizard.data_importer.search_extern`

Variables

- `UniDec.unidec_modules.tims_import_wizard.data_importer.use_mp_import = True`
- dictionary `UniDec.unidec_modules.tims_import_wizard.data_importer.param_file_cache = {}`

8.44 C:/Python/UniDec/unidec_modules/tims_import_wizard/get_data_wrapper.py File Reference

Namespaces

- `UniDec.unidec_modules.tims_import_wizard.get_data_wrapper`

Functions

- def `UniDec.unidec_modules.tims_import_wizard.get_data_wrapper.new_get_data`
- def `UniDec.unidec_modules.tims_import_wizard.get_data_wrapper.new_get_data_MS`

8.45 C:/Python/UniDec/unidec_modules/tims_import_wizard/import_wizard_grid.py File Reference

Classes

- class `UniDec.unidec_modules.tims_import_wizard.import_wizard_grid.WizardGrid`

Namespaces

- `UniDec.unidec_modules.tims_import_wizard.import_wizard_grid`

8.46 C:/Python/UniDec/unidec_modules/tims_import_wizard/import_wizard_treectrl.py File Reference

Classes

- class `UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrl`
- class `UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl.TreeCtrlPanel`

Namespaces

- `UniDec.unidec_modules.tims_import_wizard.import_wizard_treectrl`

8.47 C:/Python/UniDec/unidec_modules/tims_import_wizard/ImporterProgressGauge.py File Reference

Namespaces

- [UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge](#)

Functions

- def [UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.progress_dialog](#)
- def [UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.on_callback \(\)](#)

Variables

- [UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.dlg](#) = None
- int [UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.counter](#) = 1
- int [UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.maximum](#) = 1
- [UniDec.unidec_modules.tims_import_wizard.ImporterProgressGauge.pub_message](#) = None

8.48 C:/Python/UniDec/unidec_modules/tims_import_wizard/TagTypes.py File Reference

Namespaces

- [UniDec.unidec_modules.tims_import_wizard.TagTypes](#)

Functions

- def [UniDec.unidec_modules.tims_import_wizard.TagTypes.format_tag_name \(tag_type\)](#)

Variables

- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.SAMPLE](#) = 'sample'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.DESCRIPTION](#) = 'description'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.DRIFT_V](#) = 'dv'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.COLLISION_V](#) = 'cv'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.FILE_PATH](#) = 'file_path'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.FILE_NAME](#) = 'file_name'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.DRIFT_PRESSURE](#) = 'drift_pressure'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.TEMP](#) = 'temp'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.ATOM](#) = 'atom'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.WAVE_VELOCITY](#) = 'wave_velocity'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.WAVE_HEIGHT](#) = 'wave_height'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.EDC](#) = 'edc'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.CONE](#) = 'cone'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.EXTRACT](#) = 'extract'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.START](#) = 'start'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.END](#) = 'end'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.BIN](#) = 'bin'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.RANGE](#) = 'range'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.TYPE](#) = 'type'
- string [UniDec.unidec_modules.tims_import_wizard.TagTypes.PUSHER](#) = 'pusher'

- string `UniDec.unidec_modules.tims_import_wizard.TagTypes.FUNCTION` = 'function'
- string `UniDec.unidec_modules.tims_import_wizard.TagTypes.SCAN_START` = 'scan_start'
- string `UniDec.unidec_modules.tims_import_wizard.TagTypes.SCAN_END` = 'scan_end'
- string `UniDec.unidec_modules.tims_import_wizard.TagTypes.TCAL1` = "tcal1"
- string `UniDec.unidec_modules.tims_import_wizard.TagTypes.TCAL2` = "tcal2"
- dictionary `UniDec.unidec_modules.tims_import_wizard.TagTypes.tag_type_formatting`

8.49 C:/Python/UniDec/unidec_modules/unidecstructure.py File Reference

Classes

- class `UniDec.unidec_modules.unidecstructure.UniDecConfig`

Namespaces

- `UniDec.unidec_modules.unidecstructure`

Variables

- string `UniDec.unidec_modules.unidecstructure.__author__` = 'Michael.Marty'

8.50 C:/Python/UniDec/unidec_modules/unidectools.py File Reference

Namespaces

- `UniDec.unidec_modules.unidectools`

Functions

- def `UniDec.unidec_modules.unidectoolsisempty (thing)`
- def `UniDec.unidec_modules.unidectools.string_to_value (s)`
- def `UniDec.unidec_modules.unidectools.simp_string_to_value (s)`
- def `UniDec.unidec_modules.unidectools.string_to_int`
- def `UniDec.unidec_modules.unidectools.safedivide (a, b)`
- def `UniDec.unidec_modules.unidectools.weighted_std (values, weights)`
- def `UniDec.unidec_modules.unidectools.interp_pos (array, target)`
- def `UniDec.unidec_modules.unidectools.interp_val (data, target)`
- def `UniDec.unidec_modules.unidectools.nearestunsorted (array, target)`
- def `UniDec.unidec_modules.unidectools.nearest (array, target)`
- def `UniDec.unidec_modules.unidectools.get_z_offset (mass, charge)`
- def `UniDec.unidec_modules.unidectools.predict_charge (mass)`
- def `UniDec.unidec_modules.unidectools.simchargefit (x2)`
- def `UniDec.unidec_modules.unidectools.get_tvalue`
- def `UniDec.unidec_modules.unidectools.get_zvalue`
- def `UniDec.unidec_modules.unidectools.integrate (data, start, end)`
- def `UniDec.unidec_modules.unidectools.center_of_mass`
- def `UniDec.unidec_modules.unidectools.stepmax (array, index)`
- def `UniDec.unidec_modules.unidectools.localmax (array, start, end)`
- def `UniDec.unidec_modules.unidectools.localmaxpos (data, start, end)`
- def `UniDec.unidec_modules.unidectools.localmax2 (array, index, window)`

- def `UniDec.unidec_modules.unidectools.simple_extract`
- def `UniDec.unidec_modules.unidectools.data_extract` (data, x, extract_method, window=None, kwargs)
- def `UniDec.unidec_modules.unidectools.data_extract_grid`
- def `UniDec.unidec_modules.unidectools.kendrick_analysis`
- def `UniDec.unidec_modules.unidectools.solve_for_mass`
- def `UniDec.unidec_modules.unidectools.header_test` (path)
- def `UniDec.unidec_modules.unidectools.load_mz_file` (path, config)
- def `UniDec.unidec_modules.unidectools.zipdir` (path, zip_handle)
- def `UniDec.unidec_modules.unidectools.zip_folder` (save_path)
- def `UniDec.unidec_modules.unidectools.dataexport` (datatop, fname)
- def `UniDec.unidec_modules.unidectools.mergedata` (data1, data2)
- def `UniDec.unidec_modules.unidectools.mergedata2d` (x1, y1, x2, y2, z2)
- def `UniDec.unidec_modules.unidectools.auto_peak_width` (datatop)
- def `UniDec.unidec_modules.unidectools.auto_noise_level`
- def `UniDec.unidec_modules.unidectools.average_bin_size` (datatop)
- def `UniDec.unidec_modules.unidectools.cal_data`
- def `UniDec.unidec_modules.unidectools.datachop` (datatop, newmin, newmax)
- def `UniDec.unidec_modules.unidectools.datasimpsub` (datatop, buff)
- def `UniDec.unidec_modules.unidectools.datacompsub` (datatop, buff)
- def `UniDec.unidec_modules.unidectools.calc_local_mins` (data, w)
- def `UniDec.unidec_modules.unidectools.polynomial_background_subtract`
- def `UniDec.unidec_modules.unidectools.savgol`
- def `UniDec.unidec_modules.unidectools.savgol_background_subtract`
- def `UniDec.unidec_modules.unidectools.intensitythresh` (datatop, thresh)
- def `UniDec.unidec_modules.unidectools.gsmooth` (datatop, sig)
- def `UniDec.unidec_modules.unidectools.nonlinear_axis` (start, end, res)
- def `UniDec.unidec_modules.unidectools.linear_interpolation` (x1, x2, x)
- def `UniDec.unidec_modules.unidectools.integrate` (datatop, intx)
- def `UniDec.unidec_modules.unidectools.interpolate` (datatop, intx)
- def `UniDec.unidec_modules.unidectools.linearize` (datatop, binsize, linflag)
- def `UniDec.unidec_modules.unidectools.nonlinearize` (datatop, num_compressed)
- def `UniDec.unidec_modules.unidectools.removeduplicates` (datatop)
- def `UniDec.unidec_modules.unidectools.normalize` (datatop)
- def `UniDec.unidec_modules.unidectools.detectoreff` (datatop, va)
- def `UniDec.unidec_modules.unidectools.dataprep` (datatop, config)
- def `UniDec.unidec_modules.unidectools.unidec_call` (exepath, configfile, silent=False, kwargs)
- def `UniDec.unidec_modules.unidectools.peakdetect`
- def `UniDec.unidec_modules.unidectools.mergepeaks` (peaks1, peaks2, window)
- def `UniDec.unidec_modules.unidectools.make_peaks_mztab` (mzgrid, pks, adductmass)
- def `UniDec.unidec_modules.unidectools.makespecfun` (i, k, peaks_masses, adductmass, charges, xvals, ftab, xmax, xmin)
- def `UniDec.unidec_modules.unidectools.make_peaks_mztab_spectrum` (mzgrid, pks, data2, mztab)
- def `UniDec.unidec_modules.unidectools.makeconvspecies` (processed_data, pks, config)
- def `UniDec.unidec_modules.unidectools.nonlinstickconv` (xvals, mztab, fwhm, psfun)
- def `UniDec.unidec_modules.unidectools.stickconv` (mztab, kernel)
- def `UniDec.unidec_modules.unidectools.make_alpha_cmap` (rgb_tuple, alpha)
- def `UniDec.unidec_modules.unidectools.color_map_array` (array, cmap, alpha)
- def `UniDec.unidec_modules.unidectools.lengths` (array)
- def `UniDec.unidec_modules.unidectools.combine` (array2)
- def `UniDec.unidec_modules.unidectools.combine_all` (array2)
- def `UniDec.unidec_modules.unidectools.make_isolated_match` (oligos)
- def `UniDec.unidec_modules.unidectools.make_all_matches` (oligos)
- def `UniDec.unidec_modules.unidectools.match`
- def `UniDec.unidec_modules.unidectools.ndis_std`
- def `UniDec.unidec_modules.unidectools.ndis` (x, mid, fwhm, kwargs)

- def `UniDec.unidec_modules.unidectools.ndis_fit` (`x, s, m, a, b`)
- def `UniDec.unidec_modules.unidectools.ldis`
- def `UniDec.unidec_modules.unidectools.ldis_fit` (`x, s, m, a, b`)
- def `UniDec.unidec_modules.unidectools.splitdis`
- def `UniDec.unidec_modules.unidectools.splitdis_fit` (`x, s, m, a, b`)
- def `UniDec.unidec_modules.unidectools.voigt`
- def `UniDec.unidec_modules.unidectools.cconv` (`a, b`)
- def `UniDec.unidec_modules.unidectools.single_cwt`
- def `UniDec.unidec_modules.unidectools.continuous_wavelet_transform`
- def `UniDec.unidec_modules.unidectools.autocorr`
- def `UniDec.unidec_modules.unidectools.cconvolve` (`xvals, mztab, fwhm, psfun`)
- def `UniDec.unidec_modules.unidectools.conv_peak_shape_kernel` (`xaxis, psfun, fwhm`)
- def `UniDec.unidec_modules.unidectools.make_peak_shape`
- def `UniDec.unidec_modules.unidectools.gaussfit`
- def `UniDec.unidec_modules.unidectools.psfit` (`x, s, m, a, b, psfun`)
- def `UniDec.unidec_modules.unidectools.voigt_fit`
- def `UniDec.unidec_modules.unidectools.fit_peak` (`xvals, yvals, psfun, midguess, fwhmguess, aguess, bguess`)
- def `UniDec.unidec_modules.unidectools.isolated_peak_fit` (`xvals, yvals, psfun, kwargs`)
- def `UniDec.unidec_modules.unidectools.fft` (`data`)
- def `UniDec.unidec_modules.unidectools.fft_diff` (`data, diffrange=[500.]`)
- def `UniDec.unidec_modules.unidectools.pad_data`
- def `UniDec.unidec_modules.unidectools.pad_two_power` (`data`)
- def `UniDec.unidec_modules.unidectools.double_fft_diff`
- def `UniDec.unidec_modules.unidectools.windowed_fft`
- def `UniDec.unidec_modules.unidectools.win_fft_grid` (`rawdata, binsize, wbin, window_fwhm, diffrange`)
- def `UniDec.unidec_modules.unidectools.win_fft_diff`
- def `UniDec.unidec_modules.unidectools.correlation_integration` (`dat1, dat2, alpha=0.01, plot_corr=False, kwargs`)
- def `UniDec.unidec_modules.unidectools.wide_sse` (`dat1, dat2, sig`)
- def `UniDec.unidec_modules.unidectools.broaden` (`aligned`)

Variables

- int `UniDec.unidec_modules.unidectools.is_64bits` = `sys.maxsize>2`
- string `UniDec.unidec_modules.unidectools.dllname` = "libmypfunc"
- `UniDec.unidec_modules.unidectools.testpath` = `dllname`
- `UniDec.unidec_modules.unidectools.dllpath` = `testpath`
- tuple `UniDec.unidec_modules.unidectools.pathoffile` = `os.path.dirname(os.path.abspath(__file__))`
- tuple `UniDec.unidec_modules.unidectools.libs` = `cdll.LoadLibrary(dllpath)`

8.51 C:/Python/UniDec/unidec_modules/UniFit.py File Reference

Classes

- class `UniDec.unidec_modules.UniFit.kdstruct`
- class `UniDec.unidec_modules.UniFit.KDmodel`

Namespaces

- `UniDec.unidec_modules.UniFit`

Functions

- def `UniDec.unidec_modules.UniFit.safedivide` (a, b)
- def `UniDec.unidec_modules.UniFit.fixlists` (list1, list2)
- def `UniDec.unidec_modules.UniFit.sortarray` (a)
- def `UniDec.unidec_modules.UniFit.CompareModels` (e1, e2, p1, p2, n, thresh)
- def `UniDec.unidec_modules.UniFit.Ftest` (e1, e2, p1, p2, n)
- def `UniDec.unidec_modules.UniFit.findend` (reactions, end)
- def `UniDec.unidec_modules.UniFit.findpaths` (reactions)
- def `UniDec.unidec_modules.UniFit.GetError` (data, pfree, lfree, ureact, prottab, ligtab, paths, kds, weights, nodelist, nfactors)
- def `UniDec.unidec_modules.UniFit.MinFree` (ptot, ltot, ureact, prottab, ligtab, paths, kds, pguess, lguess, nfactors)
- def `UniDec.unidec_modules.UniFit.GetFree` (pO, ptot, ltot, ureact, prottab, ligtab, paths, kds, nfactors)
- def `UniDec.unidec_modules.UniFit.MakeGrid` (pfree, lfree, ureact, prottab, ligtab, paths, kds, nfactors)
- def `UniDec.unidec_modules.UniFit.draw_graph_structure`
- def `UniDec.unidec_modules.UniFit.draw_graph`
- def `UniDec.unidec_modules.UniFit.MinFreeError` (kds, data, weights, kdargs)
- def `UniDec.unidec_modules.UniFit.GetDegenKD` (kds, kdargs)
- def `UniDec.unidec_modules.UniFit.Minimize` (data, kdargs, kwargs)
- def `UniDec.unidec_modules.UniFit.BootMin` (data, kdargs, weights)
- def `UniDec.unidec_modules.UniFit.BootMinWorker` (queue, results_queue)

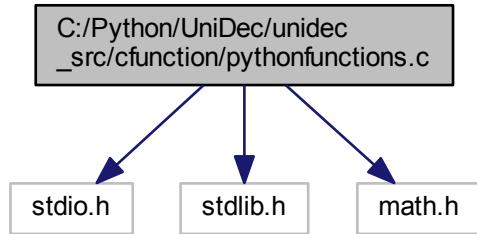
Variables

- string `UniDec.unidec_modules.UniFit.__author__` = 'Michael.Marty'
- int `UniDec.unidec_modules.UniFit.switch` = 3
- string `UniDec.unidec_modules.UniFit.path` = "C:\\cprog\\Tim\\raw"
- string `UniDec.unidec_modules.UniFit.file_name` = "man7.inp"
- tuple `UniDec.unidec_modules.UniFit.data` = np.loadtxt(file_name)
- list `UniDec.unidec_modules.UniFit.pcconc` = data[0]
- list `UniDec.unidec_modules.UniFit.lconc` = data[1]
- tuple `UniDec.unidec_modules.UniFit.header` = string.split(file_name, ".")
- int `UniDec.unidec_modules.UniFit.nprot` = 1
- int `UniDec.unidec_modules.UniFit.nlig` = 4
- int `UniDec.unidec_modules.UniFit.maxsites` = 4
- list `UniDec.unidec_modules.UniFit.nodelist` = [[1, j] for j in xrange(0, nlig + 1)]
- `UniDec.unidec_modules.UniFit.dims` = data.shape
- tuple `UniDec.unidec_modules.UniFit.fit`

8.52 C:/Python/UniDec/unidec_src/cfunction/pythonfunctions.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
```

Include dependency graph for pythonfunctions.c:



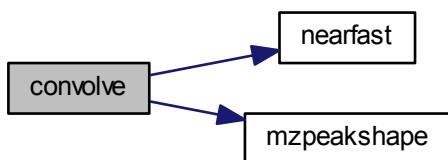
Functions

- double [mzpeakshape](#) (double x, double y, double sig, int psfun)
- int [nearfast](#) (double *dataMZ, double point, int numdat)
- void [convolve](#) (double *xvals, double *input, double *output, int psfun, double sig, int len)
- void [distance](#) (double *points, double *output, int len)
- void [inversemask](#) (double *mzgrid, double *massgrid, double *rands, double *totals, double peakwidth, int psfun, int bnum, int gdim1, int gdim2)

8.52.1 Function Documentation

8.52.1.1 void convolve (double * *xvals*, double * *input*, double * *output*, int *psfun*, double *sig*, int *len*)

Here is the call graph for this function:



8.52.1.2 void distance (double * *points*, double * *output*, int *len*)

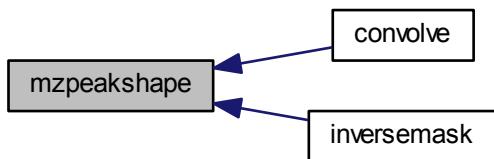
```
8.52.1.3 void inversemask ( double * mzgrid, double * massgrid, double * rands, double * totals, double peakwidth, int psfun, int bnum, int gdim1, int gdim2 )
```

Here is the call graph for this function:



```
8.52.1.4 double mzpeakshape ( double x, double y, double sig, int psfun )
```

Here is the caller graph for this function:



```
8.52.1.5 int nearfast ( double * dataMZ, double point, int numdat )
```

Here is the caller graph for this function:



8.53 C:/Python/UniDec/unidec_tests.py File Reference

Classes

- class [UniDec.unidec_tests.UniDecTest](#)

Namespaces

- [UniDec.unidec_tests](#)

Variables

- string [UniDec.unidec_tests.__author__](#) = 'Michael.Marty'
- tuple [UniDec.unidec_tests.eng](#) = UniDecTest()

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