UniDec

Generated by Doxygen 1.8.10

Tue Sep 22 2015 16:47:44

Contents

1 Hierarchical Index **1**

1.1 Class Hierarchy 1

2 Class Index **3**

2.1 Class List 3

3 Class Documentation **5**

3.1 miscwindows.AdditionalParameters Class Reference 5

3.2 PlotAnimations.AnimationWindow Class Reference 6

3.3 masstools.AutocorrWindow Class Reference 7

3.4 plot1d.BarChart Class Reference 7

3.5 nativez.ColorList Class Reference 8

3.5.1 Detailed Description 8

3.5.2 Constructor & Destructor Documentation 9

3.5.2.1 __init__(self, parent) 9

3.6 ColorPlot.ColorPlot2D Class Reference 9

3.7 masstools.CorrListCtrl Class Reference 10

3.8 masstools.CorrListCtrlPanel Class Reference 10

3.9 plot3d.CubePlot Class Reference 10

3.10 datacollector.DataCollector Class Reference 12

3.11 unidec.DataContainer Class Reference 14

3.11.1 Constructor & Destructor Documentation 15

3.11.1.1 __init__(self) 15

3.12 Extract2D.Extract2DPlot Class Reference 15

3.13 miscwindows.FileNameDialog Class Reference 16

3.14 import_wizard.ImportWizard Class Reference 18

3.14.1 Member Function Documentation 18

3.14.1.1 export_file(self, evt) 18

3.14.1.2 export_then_load(self, evt) 18

3.14.1.3 get_folder_path(self, evt) 18

3.15 IM_windows.IMToolExtract Class Reference 19

3.16 IM_windows.IMTools Class Reference 20

3.17 UniFit.KDmodel Class Reference . . . 21
3.18 UniFit.kdstruct Class Reference . . . 22
3.19 datacollector.ListCtrlPanel Class Reference . . . 23
3.20 mainwindow.Mainwindow Class Reference . . . 23
3.20.1 Detailed Description . . . 27
3.20.2 Constructor & Destructor Documentation . . . 27
3.20.2.1 __init__(self, parent, title, config) . . . 27
3.20.3 Member Function Documentation . . . 27
3.20.3.1 clear_all_plots . . . 27
3.20.3.2 export_gui_to_config(self) . . . 27
3.20.3.3 import_config_to_gui(self) . . . 28
3.20.3.4 menu_401_403(self, event) . . . 28
3.20.3.5 on_about(self, e) . . . 28
3.20.3.6 on_check_manual(self, e) . . . 28
3.20.3.7 on_defaults(self, e) . . . 28
3.20.3.8 on_exit(self, e) . . . 28
3.20.3.9 on_flip_mode(self, e) . . . 28
3.20.3.10 on_flip_tabbed(self, e) . . . 28
3.20.3.11 on_flip_twave(self, e) . . . 28
3.20.3.12 on_mass_list(self, e) . . . 29
3.20.3.13 on_motion(self, xpos, ypos) . . . 29
3.20.3.14 on_save_figure_dialog(self, e) . . . 29
3.20.3.15 on_save_figure_eps(self, e) . . . 29
3.20.3.16 on_save_figure_pdf(self, e) . . . 29
3.20.3.17 on_save_figure_png(self, e, kwargs) . . . 29
3.20.3.18 on_save_figure_small(self, e) . . . 29
3.20.3.19 save_all_figures(self, extension, extension2='', e=0, header=None, kwargs) . . . 29
3.20.3.20 setup_main_panel(self) . . . 30
3.20.3.21 setup_menu(self) . . . 30
3.20.3.22 setup_shortcuts(self) . . . 30
3.20.3.23 setup_tool_tips(self) . . . 30
3.20.3.24 shrink_all_figures(self) . . . 30
3.20.3.25 shrink_figure(self, plot) . . . 30
3.21 masstools.ManualSelection Class Reference . . . 30
3.22 MassModelFitter.mass Class Reference . . . 31
3.23 MassDefects.MassDefectWindow Class Reference . . . 32
3.24 MassFitter.MassFitter Class Reference . . . 33
3.25 masstools.MassSelection Class Reference . . . 34
3.26 mzMLimporter.mzMLimporter Class Reference . . . 36
3.27 nativez.NativeZ Class Reference . . . 36

3.28 datacollector.NetworkFrame Class Reference . . . 38
3.29 peakstructure.Peak Class Reference . . . 38
3.29.1 Detailed Description . . . 39
3.29.2 Constructor & Destructor Documentation . . . 39
3.29.2.1 __init__(self) . . . 39
3.30 peakstructure.Peaks Class Reference . . . 39
3.30.1 Detailed Description . . . 40
3.30.2 Constructor & Destructor Documentation . . . 40
3.30.2.1 __init__(self) . . . 40
3.30.3 Member Function Documentation . . . 40
3.30.3.1 add_peaks(self, parray) . . . 40
3.30.3.2 default_params . . . 40
3.30.3.3 get_mass_defects . . . 40
3.30.3.4 score_peaks . . . 40
3.31 peakwidthtools.PeakTools1d Class Reference . . . 40
3.32 peakwidthtools.PeakTools2d Class Reference . . . 42
3.33 twitter_interface.PinWindow Class Reference . . . 43
3.34 plot1d.Plot1d Class Reference . . . 44
3.35 plot2d.Plot2d Class Reference . . . 44
3.36 plot2d.Plot2dMass Class Reference . . . 45
3.37 PlottingWindow.PlottingWindow Class Reference . . . 46
3.38 miscwindows.SaveFigureDialog Class Reference . . . 47
3.39 GUniDec.Shell Class Reference . . . 48
3.40 miscwindows.SingleInputDialog Class Reference . . . 48
3.41 peaklistsort.TestListCtrl Class Reference . . . 49
3.42 masstools.TestListCtrl Class Reference . . . 49
3.43 masstools.TestListCtrl2 Class Reference . . . 49
3.44 masstools.TestListCtrl3 Class Reference . . . 50
3.45 IM_windows.TestListCtrl4 Class Reference . . . 51
3.46 masstools.TestListCtrlMatch Class Reference . . . 51
3.47 masstools.TestListCtrlPanel Class Reference . . . 52
3.48 peaklistsort.TestListCtrlPanel Class Reference . . . 52
3.49 masstools.TestListCtrlPanel2 Class Reference . . . 53
3.50 masstools.TestListCtrlPanel3 Class Reference . . . 53
3.51 IM_windows.TestListCtrlPanel4 Class Reference . . . 54
3.52 masstools.TestListCtrlPanelMatch Class Reference . . . 55
3.53 import_wizard_treectrl.TreeCtrl Class Reference . . . 55
3.54 import_wizard_treectrl.TreeCtrlPanel Class Reference . . . 55
3.54.1 Member Function Documentation . . . 56
3.54.1.1 add_children . . . 56

3.54.1.2 add_root . . . 56
3.55 twitter_interface.TwitterWindow Class Reference . . . 56
3.56 unidec.UniDec Class Reference . . . 58
3.56.1 Constructor & Destructor Documentation . . . 59
3.56.1.1 __init__(self) . . . 59
3.56.2 Member Function Documentation . . . 59
3.56.2.1 autocorrelation . . . 59
3.56.2.2 autointegrate . . . 59
3.56.2.3 center_of_mass . . . 59
3.56.2.4 check_badness(self) . . . 59
3.56.2.5 convolve_peaks(self) . . . 60
3.56.2.6 cross_validate . . . 60
3.56.2.7 export_config . . . 60
3.56.2.8 export_params(self, e) . . . 60
3.56.2.9 fit_all_masses(self) . . . 60
3.56.2.10 get_charge_peaks(self) . . . 60
3.56.2.11 initialize(self) . . . 60
3.56.2.12 integrate . . . 60
3.56.2.13 kendrick_continuous . . . 61
3.56.2.14 kendrick_peaks . . . 61
3.56.2.15 load_config(self, f_name) . . . 61
3.56.2.16 load_default(self) . . . 61
3.56.2.17 load_state(self, load_path) . . . 61
3.56.2.18 mass_grid_to_f_grid(self) . . . 61
3.56.2.19 normalize_peaks(self) . . . 61
3.56.2.20 open_file(self, file_name, file_directory, kwargs) . . . 62
3.56.2.21 pick_peaks(self) . . . 62
3.56.2.22 process_data(self, kwargs) . . . 62
3.56.2.23 process_mass_data(self) . . . 62
3.56.2.24 raw_process . . . 62
3.56.2.25 reset_config(self) . . . 62
3.56.2.26 run_unidec . . . 63
3.56.2.27 save_default(self) . . . 63
3.56.2.28 unidec_imports . . . 63
3.57 GUniDec.UniDecApp Class Reference . . . 63
3.57.1 Detailed Description . . . 65
3.57.2 Member Function Documentation . . . 65
3.57.2.1 export_config . . . 65
3.57.2.2 import_config . . . 65
3.58 unidecstructure.UniDecConfig Class Reference . . . 65

3.58.1 Detailed Description . . . 67
3.58.2 Constructor & Destructor Documentation . . . 68
3.58.2.1 __init__(self) . . . 68
3.58.3 Member Function Documentation . . . 68
3.58.3.1 check_badness(self) . . . 68
3.58.3.2 config_export(self, name) . . . 68
3.58.3.3 config_import(self, name) . . . 68
3.58.3.4 default_colormaps(self) . . . 68
3.58.3.5 default_file_names(self) . . . 68
3.58.3.6 default_high_res(self) . . . 68
3.58.3.7 default_zero_charge(self) . . . 68
3.58.3.8 initialize(self) . . . 69
3.58.3.9 initialize_system_paths(self) . . . 69
3.58.3.10 print_config(self) . . . 69
3.59 unidec_tests.UniDecTest Class Reference . . . 69
3.60 import_wizard_grid.WizardGrid Class Reference . . . 70
3.60.1 Detailed Description . . . 70
3.60.2 Member Function Documentation . . . 70
3.60.2.1 fill_down(self, evt) . . . 70
3.60.2.2 set_labels(self, mode) . . . 70
3.60.2.3 showPopupMenu(self, evt) . . . 71
3.61 datacollector.XListCtrl Class Reference . . . 71
3.62 datacollector.YListCtrl Class Reference . . . 71
3.63 nativez.zoffset Class Reference . . . 72
3.64 ZoomBox.ZoomBox Class Reference . . . 72
3.64.1 Detailed Description . . . 73
3.64.2 Constructor & Destructor Documentation . . . 74
3.64.2.1 __init__ . . . 74
3.64.3 Member Function Documentation . . . 74
3.64.3.1 get_active(self) . . . 74
3.64.3.2 set_active(self, active) . . . 74
3.65 ZoomSpan.ZoomSpan Class Reference . . . 74
3.65.1 Detailed Description . . . 75
3.65.2 Constructor & Destructor Documentation . . . 76
3.65.2.1 __init__ . . . 76

Index **77**

Chapter 1

Hierarchical Index

1.1 Class Hierarchy

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

ColumnSorterMixin
- peaklistsort.TestListCtrlPanel . . . 52

unidec.DataContainer . . . 14

Dialog
- IM_windows.IMToolExtract . . . 19
- IM_windows.IMTools . . . 20
- masstools.AutocorrWindow . . . 7
- masstools.ManualSelection . . . 30
- masstools.MassSelection . . . 34
- miscwindows.AdditionalParameters . . . 5
- miscwindows.FileNameDialog . . . 16
- miscwindows.SaveFigureDialog . . . 47
- miscwindows.SingleInputDialog . . . 48
- nativez.NativeZ . . . 36
- peakwidthtools.PeakTools1d . . . 40
- peakwidthtools.PeakTools2d . . . 42
- twitter_interface.PinWindow . . . 43
- twitter_interface.TwitterWindow . . . 56

Frame
- datacollector.DataCollector . . . 12
- Extract2D.Extract2DPlot . . . 15
- import_wizard.ImportWizard . . . 18
- mainwindow.Mainwindow . . . 23
- MassDefects.MassDefectWindow . . . 32
- PlotAnimations.AnimationWindow . . . 6

Grid
- import_wizard_grid.WizardGrid . . . 70

UniFit.KDmodel . . . 21

UniFit.kdstruct . . . 22

ListCtrl
- datacollector.XListCtrl . . . 71
- datacollector.YListCtrl . . . 71
- IM_windows.TestListCtrl4 . . . 51
- masstools.CorrListCtrl . . . 10
- masstools.TestListCtrl . . . 49
- masstools.TestListCtrl2 . . . 49
- masstools.TestListCtrl3 . . . 50
- masstools.TestListCtrlMatch . . . 51

peaklistsort.TestListCtrl . . . 49
ListCtrlAutoWidthMixin
datacollector.XListCtrl . . . 71
datacollector.YListCtrl . . . 71
IM_windows.TestListCtrl4 . . . 51
masstools.CorrListCtrl . . . 10
masstools.TestListCtrl . . . 49
masstools.TestListCtrl2 . . . 49
masstools.TestListCtrl3 . . . 50
masstools.TestListCtrlMatch . . . 51
MassModelFitter.mass . . . 31
MassFitter.MassFitter . . . 33
mzMLimporter.mzMLimporter . . . 36
object
GUniDec.Shell . . . 48
GUniDec.UniDecApp . . . 63
Panel
datacollector.ListCtrlPanel . . . 23
IM_windows.TestListCtrlPanel4 . . . 54
import_wizard_treectrl.TreeCtrlPanel . . . 55
masstools.CorrListCtrlPanel . . . 10
masstools.TestListCtrlPanel . . . 52
masstools.TestListCtrlPanel2 . . . 53
masstools.TestListCtrlPanel3 . . . 53
masstools.TestListCtrlPanelMatch . . . 55
nativez.ColorList . . . 8
peaklistsort.TestListCtrlPanel . . . 52
peakstructure.Peak . . . 38
peakstructure.Peaks . . . 39
TextEditMixin
datacollector.XListCtrl . . . 71
datacollector.YListCtrl . . . 71
IM_windows.TestListCtrl4 . . . 51
masstools.CorrListCtrl . . . 10
masstools.TestListCtrl . . . 49
masstools.TestListCtrl2 . . . 49
masstools.TestListCtrl3 . . . 50
masstools.TestListCtrlMatch . . . 51
TreeCtrl
import_wizard_treectrl.TreeCtrl . . . 55
unidec.UniDec . . . 58
unidec_tests.UniDecTest . . . 69
unidecstructure.UniDecConfig . . . 65
Window
PlottingWindow.PlottingWindow . . . 46
ColorPlot.ColorPlot2D . . . 9
datacollector.NetworkFrame . . . 38
plot1d.BarChart . . . 7
plot1d.Plot1d . . . 44
plot2d.Plot2d . . . 44
plot2d.Plot2dMass . . . 45
plot3d.CubePlot . . . 10
nativez.zoffset . . . 72
ZoomBox.ZoomBox . . . 72
ZoomSpan.ZoomSpan . . . 74

Chapter 2

Class Index

2.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

miscwindows.AdditionalParameters . . . 5
PlotAnimations.AnimationWindow . . . 6
masstools.AutocorrWindow . . . 7
plot1d.BarChart . . . 7
nativez.ColorList . . . 8
ColorPlot.ColorPlot2D . . . 9
masstools.CorrListCtrl . . . 10
masstools.CorrListCtrlPanel . . . 10
plot3d.CubePlot . . . 10
datacollector.DataCollector . . . 12
unidec.DataContainer . . . 14
Extract2D.Extract2DPlot . . . 15
miscwindows.FileNameDialog . . . 16
import_wizard.ImportWizard . . . 18
IM_windows.IMToolExtract . . . 19
IM_windows.IMTools . . . 20
UniFit.KDmodel . . . 21
UniFit.kdstruct . . . 22
datacollector.ListCtrlPanel . . . 23
mainwindow.Mainwindow . . . 23
masstools.ManualSelection . . . 30
MassModelFitter.mass . . . 31
MassDefects.MassDefectWindow . . . 32
MassFitter.MassFitter . . . 33
masstools.MassSelection . . . 34
mzMLimporter.mzMLimporter . . . 36
nativez.NativeZ . . . 36
datacollector.NetworkFrame . . . 38
peakstructure.Peak . . . 38
peakstructure.Peaks . . . 39
peakwidthtools.PeakTools1d . . . 40
peakwidthtools.PeakTools2d . . . 42
twitter_interface.PinWindow . . . 43
plot1d.Plot1d . . . 44
plot2d.Plot2d . . . 44
plot2d.Plot2dMass . . . 45
PlottingWindow.PlottingWindow . . . 46
miscwindows.SaveFigureDialog . . . 47

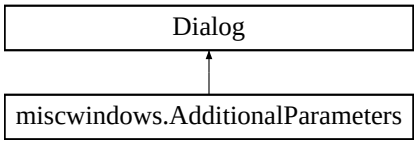
GUniDec.Shell . . . 48
miscwindows.SingleInputDialog . . . 48
peaklistsort.TestListCtrl . . . 49
masstools.TestListCtrl . . . 49
masstools.TestListCtrl2 . . . 49
masstools.TestListCtrl3 . . . 50
IM_windows.TestListCtrl4 . . . 51
masstools.TestListCtrlMatch . . . 51
masstools.TestListCtrlPanel . . . 52
peaklistsort.TestListCtrlPanel . . . 52
masstools.TestListCtrlPanel2 . . . 53
masstools.TestListCtrlPanel3 . . . 53
IM_windows.TestListCtrlPanel4 . . . 54
masstools.TestListCtrlPanelMatch . . . 55
import_wizard_treectrl.TreeCtrl . . . 55
import_wizard_treectrl.TreeCtrlPanel . . . 55
twitter_interface.TwitterWindow . . . 56
unidec.UniDec . . . 58
GUniDec.UniDecApp . . . 63
unidecstructure.UniDecConfig . . . 65
unidec_tests.UniDecTest . . . 69
import_wizard_grid.WizardGrid . . . 70
datacollector.XListCtrl . . . 71
datacollector.YListCtrl . . . 71
nativez.zoffset . . . 72
ZoomBox.ZoomBox . . . 72
ZoomSpan.ZoomSpan . . . 74

Chapter 3

Class Documentation

3.1 miscwindows.AdditionalParameters Class Reference

Inheritance diagram for miscwindows.AdditionalParameters:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, config)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)

Public Attributes

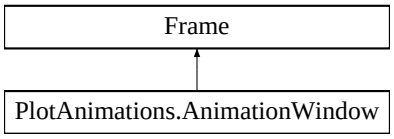
- **config**
- **pnl**
- **vbox**
- **sb**
- **sbs**
- **hbox5**
- **inputbox5**
- **hbox6**
- **inputbox6**
- **hbox6b**
- **inputbox6b**

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

- C:/Python/UniDec/miscwindows.py

3.2 PlotAnimations.AnimationWindow Class Reference

Inheritance diagram for PlotAnimations.AnimationWindow:



Public Member Functions

- def **__init__** (self, parent, datalist, config=None, yvals=None, mode="1D", args, kwargs)
- def **on_close** (self, e)
- def **update** (self, frame_number)
- def **newplot** (self)
- def **init** (self)
- def **on_play** (self, e)
- def **RefreshPlot** (self)
- def **on_next** (self, e)
- def **on_back** (self, e)
- def **update_framerate** (self, e)

Public Attributes

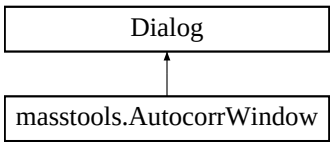
- **mode**
- **config**
- **datalist**
- **yvals**
- **dim**
- **pos**
- **play**
- **panel**
- **sizer**
- **plot**
- **controlsizer**
- **sb**
- **sbs**
- **frslider**
- **playbutton**
- **nextbutton**
- **backbutton**
- **ctlautoscale**
- **data**
- **xlim**
- **ylim**
- **animation**

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

- C:/Python/UniDec/PlotAnimations.py

3.3 masstools.AutocorrWindow Class Reference

Inheritance diagram for masstools.AutocorrWindow:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, config, massdat)
- def **Go** (self, e)
- def **PickPeaks** (self, e)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)

Public Attributes

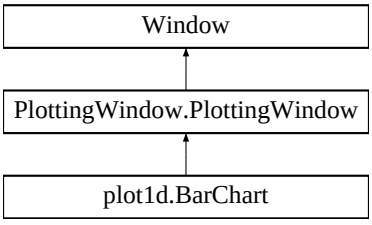
- **config**
- **massdat**
- **pnl**
- **vbox**
- **hbox**
- **sb**
- **sbs**
- **plot1**
- **listpanel**
- **corr**
- **corrx**
- **pks2**
- **peaks**

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

- C:/Python/UniDec/masstools.py

3.4 plot1d.BarChart Class Reference

Inheritance diagram for plot1d.BarChart:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **plotrefreshtop** (self, X, Y, titlestr, xstr, ystr, colortab, peakval)
- def **plotadd** (self, X, Y, colval, newlabel)
- def **plotaddlegend** (self)
- def **plotadddot** (self, X, Y, colval, markval)
- def **PaintAgain** (self, bins, kwargs)
- def **PlotClear** (self)
- def **on_save_fig_dialog** (self, evt)
- def **on_save_fig** (self, evt, path, kwargs)

Public Attributes

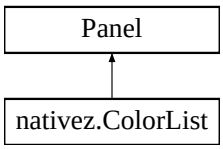
- **flag**
- **subplot1**
- **labels**

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

- C:/Python/UniDec/plot1d.py

3.5 nativez.ColorList Class Reference

Inheritance diagram for nativez.ColorList:



Public Member Functions

- def __init__ (self, parent)
- def **AddLineEmpty** (self)
- def **AddLine** (self, zoff)
- def **ReturnData** (self)
- def **SuperDelete** (self)

Public Attributes

- **ultimateList**
- **buttontot**
- **colorbox**
- **zoffouts**

3.5.1 Detailed Description

3.5.2 Constructor & Destructor Documentation

3.5.2.1 def nativez.ColorList.__init__ (*self, parent*)

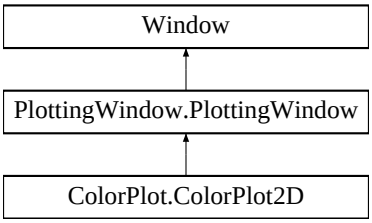
```
Constructor
```

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

- C:/Python/UniDec/nativez.py

3.6 ColorPlot.ColorPlot2D Class Reference

Inheritance diagram for ColorPlot.ColorPlot2D:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **ColorPlot** (self, mzgrid, mzax, dtax, ztab)
- def **PaintAgain** (self, bins, kwargs)
- def **on_save_fig** (self, evt, path, kwargs)
- def **PlotClear** (self)

Public Attributes

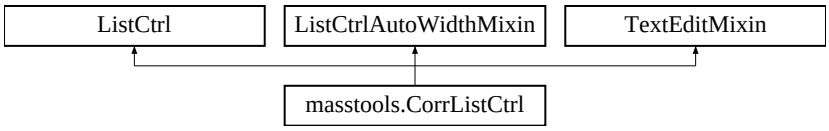
- **flag**
- **data_x_lim**
- **data_y_lim**
- **data_lims**
- **mzgrid**
- **mzlen**
- **dtlen**
- **zlen**
- **ztot**
- **zind**
- **ztab**
- **skew**
- **topcmap**
- **colors**
- **subplot1**
- **norm**
- **cax**
- **cbar**

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

- C:/Python/UniDec/ColorPlot.py

3.7 masstools.CorrListCtrl Class Reference

Inheritance diagram for masstools.CorrListCtrl:



Public Member Functions

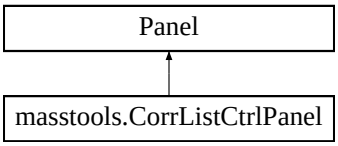
- def **__init__**
- def **Populate** (self, pks)
- def **Clear** (self)

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

- C:/Python/UniDec/masstools.py

3.8 masstools.CorrListCtrlPanel Class Reference

Inheritance diagram for masstools.CorrListCtrlPanel:



Public Member Functions

- def **__init__** (self, parent)
- def **OnUseNative** (self, event)

Public Attributes

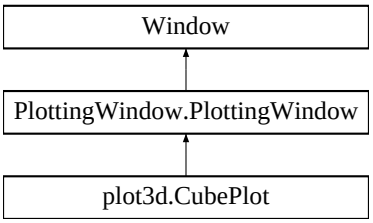
- **useNative**
- **list**

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

- C:/Python/UniDec/masstools.py

3.9 plot3d.CubePlot Class Reference

Inheritance diagram for plot3d.CubePlot:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **cubeplot** (self, xaxis, yaxis, zaxis, C, C2, C3, xlab, ylab, zlab, config)
- def **on_save_fig_dialog** (self, evt)
- def **on_save_fig** (self, evt, path, kwargs)
- def **PaintAgain** (self, bins)
- def **PlotClear** (self)
- def **MakeIsoMatrices** (self)
- def **IsometricProjection** (self, x, y, z)
- def **Isogrids** (self)
- def **IsoTicks** (self, ax, col)
- def **IsoLabs** (self, xticlab, yticlab, zticlab, ax, col)
- def **IsoLines** (self)

Public Attributes

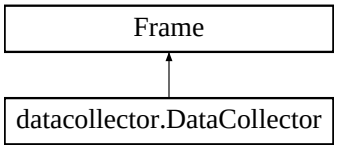
- **flag**
- **subplot1**
- **alpha**
- **beta**
- **bins**
- **N**
- **cmap**
- **col**
- **xaxis**
- **yaxis**
- **zaxis**
- **xlen**
- **ylen**
- **zlen**
- **xticlab**
- **yticlab**
- **zticlab**
- **xticloc**
- **yticloc**
- **zticloc**
- **cbar**
- **datalims**
- **A**
- **B**
- **P**
- **C**
- **PC**

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

- C:/Python/UniDec/plot3d.py

3.10 datacollector.DataCollector Class Reference

Inheritance diagram for datacollector.DataCollector:



Public Member Functions

- def **__init__** (self, parent, title, config=None, pks=None, args, kwargs)
- def **LoadXfromPeaks** (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 **OnMotion** (self, xpos, ypos)
- def **update_get** (self, e)
- def **update_set** (self, e)
- def **data_extract**
- def **on_run**
- 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)

Public Attributes

- **directory**
- **config**
- **pks**
- **gridparams**
- **filemenu**
- **menuSave**
- **menuLoad**
- **menuSaveFigPNG**
- **menuSaveFigPDF**
- **toolsmenu**
- **experimentalmenu**
- **menuAnimation**

- menuAnimation2
- menu2dGrid
- menudefect
- menulocalpath
- menuabsolutepath
- menumsmsnorm
- menuautocorr
- 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**
- **data**
- **var1**
- **grid**
- **xlabel**
- **xcolors**
- **aniwindow**
- **compress**

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

- C:/Python/UniDec/datacollector.py

3.11 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**

3.11.1 Constructor & Destructor Documentation

3.11.1.1 def unidec.DataContainer.__init__ (*self*)

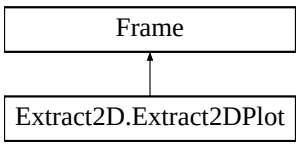
```
Initialize DataContainer with empty arrays.
:return: None
```

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

- C:/Python/UniDec/unidec.py

3.12 Extract2D.Extract2DPlot Class Reference

Inheritance diagram for Extract2D.Extract2DPlot:



Public Member Functions

- def **__init__** (self, parent, datalist, config=None, yvals=None, directory=None, header=None, params=None, args, kwargs)
- def **modparams** (self)
- def **getfromgui** (self)
- def **makegrid** (self)
- def **extractall** (self)
- def **makeplot** (self)
- def **makeplottotal** (self)
- def **makeplotwap** (self)
- def **on_close** (self, e)
- def **on_back** (self, e)
- def **on_next** (self, e)
- def **on_total** (self, e)
- 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**

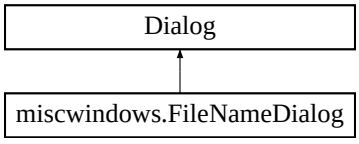
- **pos**
- **yvals**
- **storediscrete**
- **panel**
- **sizer**
- **plot1**
- **plot2**
- **controlsizer**
- **controlsizer1**
- **ctlm0**
- **ctlm1**
- **ctlm2**
- **ctlm1min**
- **ctlm1max**
- **ctlm2min**
- **ctlm2max**
- **ctlwindow**
- **ctlnorm**
- **controlsizer2**
- **backbutton**
- **nextbutton**
- **totalbutton**
- **wapbutton**
- **m0**
- **m1**
- **m2**
- **m1minmax**
- **m2minmax**
- **window**
- **normflag**
- **grids**
- **m1range**
- **m2range**
- **m2grid**
- **massgrid**
- **igrid**

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

- C:/Python/UniDec/Extract2D.py

3.13 miscwindows.FileNameDialog Class Reference

Inheritance diagram for miscwindows.FileNameDialog:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, config)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)

Public Attributes

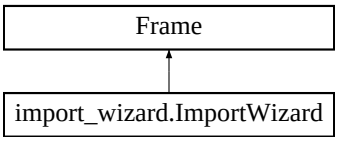
- **config**
- **defaultin**
- **defaultout**
- **defaultconf**
- **defaultmassfile**
- **defaulttruncfile**
- **defaultofile**
- **defaultmatchfile**
- **defaultpeaksfile**
- **pnl**
- **vbox**
- **sb**
- **sbs**
- **hbox1**
- **inputbox**
- **hbox2**
- **confbox**
- **hbox3**
- **outputbox**
- **hbox4**
- **massbox**
- **hbox5**
- **truncbox**
- **hbox6**
- **obox**
- **hbox7**
- **matchbox**
- **hbox8**
- **peakbox**
- **inboxval**
- **outboxval**
- **confboxval**
- **truncval**
- **massfileval**
- **ofileval**
- **matchfileval**
- **peaksfileval**

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

- C:/Python/UniDec/miscwindows.py

3.14 import_wizard.ImportWizard Class Reference

Inheritance diagram for 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**

3.14.1 Member Function Documentation

3.14.1.1 def import_wizard.ImportWizard.export_file (*self, evt*)

```
Export import file for later import
```

3.14.1.2 def import_wizard.ImportWizard.export_then_load (*self, evt*)

```
save file then load it
```

3.14.1.3 def import_wizard.ImportWizard.get_folder_path (*self, evt*)

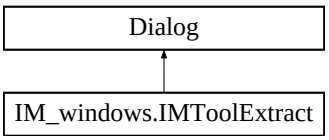
```
Get path to folder and place in txtctrl
```

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

- C:/Python/UniDec/import_wizard.py

3.15 IM_windows.IMToolExtract Class Reference

Inheritance diagram for IM_windows.IMToolExtract:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, massdat, ccsdat, mccsgrid, config, pks)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)
- def **loadpeaks** (self, e)
- def **getfromgui** (self, e)
- def **OnAdd** (self, e)
- def **OnPlot** (self, e)

Public Attributes

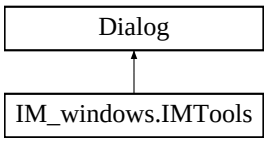
- **config**
- **massdat**
- **ccsdat**
- **totalgrid**
- **pks**
- **ztab**
- **zstrings**
- **pnl**
- **vbox**
- **sb**
- **sbs**
- **plot1**
- **plot2**
- **plotsizer**
- **sb2**
- **sbs2**
- **gbox1c**
- **ctlzout**
- **masspanel**
- **addbutton**
- **plotbutton**
- **hboxend**
- **okButton**
- **closeButton**
- **zout**
- **zoutgrid**
- **ccsproj**

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

- C:/Python/UniDec/IM_windows.py

3.16 IM_windows.IMTools Class Reference

Inheritance diagram for IM_windows.IMTools:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, data3, config)
- def **SetupPanel** (self)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)
- def **loadtogui** (self, e)
- def **getfromgui** (self, e)
- def **OnAdd** (self, e)
- def **OnPlot** (self, e)
- def **OnFlipTWave** (self, e)

Public Attributes

- **defaultconfig**
- **config**
- **data3**
- **pnl**
- **pnl2**
- **flag**
- **vbox**
- **sb**
- **sbs**
- **plot**
- **ctlsizer**
- **sb2**
- **sbs2**
- **gbox1c**
- **ctltwave**
- **ctlvolt**
- **ctlpressure**
- **ctltemp**
- **ctlgasmass**
- **ctlto**
- **ctldriftlength**
- **twave**
- **ctltcal1**
- **ctltcal2**
- **ctledc**
- **vbox2**
- **masspanel**
- **addbutton**

- **plotbutton**
- **hboxend**
- **okButton**
- **closeButton**

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

- C:/Python/UniDec/IM_windows.py

3.17 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, numpts)
- 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**

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

- C:/Python/UniDec/UniFit.py

3.18 UniFit.kdstruct Class Reference

Public Member Functions

- def **__init__** (self)

Public Attributes

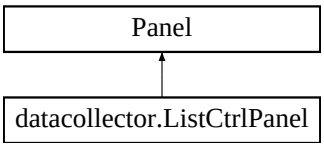
- **pconc**
- **lconc**
- **ureact**
- **nprottab**
- **nligtab**
- **paths**
- **pfrees**
- **lfrees**
- **weights**
- **nodelist**
- **kds**
- **degen**
- **maxsites**
- **nfactors**

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

- C:/Python/UniDec/UniFit.py

3.19 datacollector.ListCtrlPanel Class Reference

Inheritance diagram for datacollector.ListCtrlPanel:



Public Member Functions

- def **__init__** (self, parent, type="X", size=(200, 400)
- def **OnUseNative** (self, event)
- def **OnRightClick** (self, event)
- def **OnPopupOne** (self, event)
- def **OnPopupTwo** (self, event)
- def **OnPopupThree** (self, event)
- def **OnPopupFour** (self, event)

Public Attributes

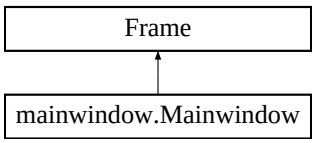
- **useNative**
- **list**
- **popupID1**
- **popupID2**
- **popupID3**
- **popupID4**
- **selection**

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

- C:/Python/UniDec/datacollector.py

3.20 mainwindow.Mainwindow Class Reference

Inheritance diagram for mainwindow.Mainwindow:



Public Member Functions

- def __init__ (self, parent, title, config)
- 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_flip_mode (self, e)
- def on_flip_tabbed (self, e)
- def on_flip_twave (self, e)
- 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**
- **open_bmp**
- **next_bmp**
- **report_bmp**
- **A_bmp**
- **ud_bmp**
- **system**
- **displaysize**
- **tabbed**
- **imflag**
- **twave**
- **filemenu**
- **toolsmenu**
- **analysismenu**
- **advancedmenu**
- **experimentalmenu**
- **menuOpen**
- **menuOpenRaw**
- **menuLoadState**
- **menuSaveState**
- **menuLoad**
- **menuLoadDefault**
- **menuSaveDefault**
- **defaultmenu**
- **menuDefault1**
- **menuDefault2**
- **menufigdialog**
- **figmenu**
- **menuSaveFigure0**

- menuSaveFigure1s
- menuSaveFigure1
- menuSaveFigure2
- menuSaveFigure4
- menuAbout
- menuExit
- menuBatch
- menuBatch2
- menuBatchRaw
- menuImportWizard
- menuWidth
- menuManualFile
- menuMassFile
- menuPlotZ
- menucollect
- menuExport
- menuFitNorm
- menukendrick
- menu2Dgrid
- menuintegrate
- menumatch
- menucom
- menucolor1d
- menuoffset
- menuimtools
- menuimtools2
- menunativeccs
- menuReset
- menuUnidecPath
- menuFileName
- menuflipmode
- menufliptabbed
- Tweet
- menuAdditionalParameters
- menuDeisotope
- menuCrossValidate
- menusuperbatch
- menumassprocess
- menupastespectrum
- menuerrors
- menuBar
- plot1
- plot2
- plot3
- plot4
- plot5
- plot6
- plot1im
- plot1fit
- plot2ccs
- plot5mccs
- plot5ccsz
- plot3color
- plot9
- plot10

- **peakpanel**
- **openbutton**
- **procbutton**
- **udbutton**
- **ppbutton**
- **autobutton**
- **ctlminmz**
- **ctlmaxmz**
- **ctlmindt**
- **ctlmaxdt**
- **ctlsmoothdt**
- **ctlsubbuffdt**
- **subtypectl**
- **dataprepbutton**
- **ctlbuff**
- **ctlsmooth**
- **ctlbinsize**
- **ctlpusher**
- **ctlintthresh**
- **ctladductmass**
- **ctlaccelvolt**
- **ctlbintype**
- **ctlconvertflag**
- **ctltwave**
- **ctlvolt**
- **ctlpressure**
- **ctltemp**
- **ctlgasmass**
- **ctlto**
- **ctldriftlength**
- **ctltcal1**
- **ctltcal2**
- **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**
- **ctlnativeccslb**
- **ctlnativeccsub**
- **ctlwindow**
- **ctlthresh**
- **ctlnorm**
- **plotbutton**
- **plotbutton2**
- **ctl2dcm**
- **ctlpeakcm**
- **ctldiscrete**
- **ctlpublicationmode**
- **ctlrawflag**
- **ctlthresh2**
- **ctlsep**
- **ctlintlb**
- **ctlintub**
- **replotbutton**
- **compositebutton**
- **cubeplotbutton**
- **pngs**
- **figsize**
- **rect**

3.20.1 Detailed Description

```
Main UniDec GUI Window.
```

3.20.2 Constructor & Destructor Documentation

3.20.2.1 def mainwindow.Mainwindow.__init__ (*self, parent, title, config*)

```
initialize window and feed in links to presenter and config.

:param parent: GUniDec Presenter -> self.pres
:param title: Window title (string)
:param config: UniDecConfig object ->self.config
:return: None
```

3.20.3 Member Function Documentation

3.20.3.1 def mainwindow.Mainwindow.clear_all_plots (*self, flag =* 0)

```
Clear All Plots
:return: None
```

3.20.3.2 def mainwindow.Mainwindow.export_gui_to_config (*self*)

```
Exports parameters from the GUI to the config object.
:return: None
```

3.20.3.3 def mainwindow.Mainwindow.import_config_to_gui (*self*)

```
Imports parameters from the config object to the GUI.
:return: None
```

3.20.3.4 def mainwindow.Mainwindow.menu_401_403 (*self, event*)

```
Menu function to adjust the UniDec core function (agreesiveflag).
:param event: wx Event
:return: None
```

3.20.3.5 def mainwindow.Mainwindow.on_about (*self, e*)

```
Displays message about program
:param e:
:return:
```

3.20.3.6 def 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
```

3.20.3.7 def mainwindow.Mainwindow.on_defaults (*self, e*)

```
Resets the configuration to a default predefined in the unidecstructure file.
:param e: Menu event
:return: None
```

3.20.3.8 def mainwindow.Mainwindow.on_exit (*self, e*)

```
Exit the Program
:param e: Dummy wx event
:return: None
```

3.20.3.9 def mainwindow.Mainwindow.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
```

3.20.3.10 def mainwindow.Mainwindow.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
```

3.20.3.11 def mainwindow.Mainwindow.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
```

3.20.3.12 def 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
```

3.20.3.13 def 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
```

3.20.3.14 def 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
```

3.20.3.15 def mainwindow.Mainwindow.on_save_figure_eps (*self, e*)

```
Save all figures as EPS
:param e: Dummy wx event
:return: None
```

3.20.3.16 def mainwindow.Mainwindow.on_save_figure_pdf (*self, e*)

```
Saves all figures as PDF
:param e: Dummy wx event
:return: None
```

3.20.3.17 def mainwindow.Mainwindow.on_save_figure_png (*self, e, kwargs*)

```
Save all figures as PNG
:param e: Dummy wx event
:param kwargs: keywards to pass to matplotlib savefig
:return: None
```

3.20.3.18 def 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
```

3.20.3.19 def 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 keywards 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)
```

3.20.3.20 def mainwindow.Mainwindow.setup_main_panel (*self*)

```
Lays Out Main Panel. Binds some functions to presenter.
:return: None
```

3.20.3.21 def mainwindow.Mainwindow.setup_menu (*self*)

```
Sets menu and binds menu objects to functions in presenter and window
:return: None
```

3.20.3.22 def mainwindow.Mainwindow.setup_shortcuts (*self*)

```
Setup shortcuts in GUI. Binds key combinations to functions in presenter (self.pres)
:return: None
```

3.20.3.23 def mainwindow.Mainwindow.setup_tool_tips (*self*)

```
Sets Tool Tips for items on the Main Panel
:return: None
```

3.20.3.24 def 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
```

3.20.3.25 def mainwindow.Mainwindow.shrink_figure (*self, plot*)

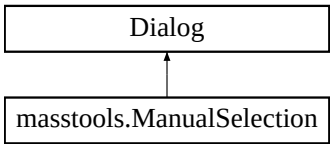
```
Automatically shrinks the plot to a figure size in inches set in self.figsize.
:param plot: Plot object to shrink
:return: None
```

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

- C:/Python/UniDec/mainwindow.py

3.21 masstools.ManualSelection Class Reference

Inheritance diagram for masstools.ManualSelection:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, config, data)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)
- def **OnClear** (self, e)
- def **OnAdd** (self, e)
- def **OnAddFromPlot** (self, e)
- def **OnPlot** (self, e)
- def **OnImport** (self, e)

Public Attributes

- **data**
- **config**
- **defaulttrunclist**
- **newtrunclist**
- **pnl**
- **vbox**
- **vbox2**
- **plot1**
- **hbox**
- **sb**
- **sbs**
- **importbutton**
- **clearbutt**
- **addbutton**
- **addbutton2**
- **plotbutton**
- **sb2**
- **sbs2**
- **masslistbox**
- **truncfilename**
- **importtrunc**

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

- C:/Python/UniDec/masstools.py

3.22 MassModelFitter.mass Class Reference

Public Member Functions

- def **__init__** (self, args)
- def **LoadGuesses** (self, mass0)
- def **MakePeakList** (self)
- def **f0** (self, array, peaks, run)
- def **f0s** (self, array, peaks, run)
- def **ComparePeaks** (self, peaks)

Public Attributes

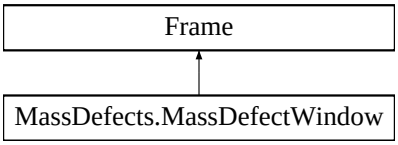
- **mass0**
- **mass1**
- **mass2**
- **dist1**
- **dist1limits**
- **dist2**
- **dist2limits**
- **adduction**
- **psfun**
- **resolution**
- **thresh**
- **intensity**
- **num1**
- **num2**
- **int1**
- **int2**
- **num2grid**
- **massgrid**
- **int2grid**
- **intgrid**
- **masspeaks**

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

- C:/Python/UniDec/MassModelFitter.py

3.23 MassDefects.MassDefectWindow Class Reference

Inheritance diagram for MassDefects.MassDefectWindow:



Public Member Functions

- def **__init__** (self, parent, datalist, config=None, yvals=None, pks=None, value=None, dir=None, show=True, args, kwargs)
- def **OnClose** (self, e)
- def **getfromgui** (self)
- def **makegrid** (self)
- def **extractall** (self)
- def **makeplot** (self)
- def **makeplottotal** (self)
- def **on_back** (self, e)
- def **on_next** (self, e)
- def **on_total** (self, e)
- def **on_peaks** (self, e)
- def **on_save_fig** (self, e)
- def **on_save_figPDF** (self, e)
- def **on_add_line** (self, e)

Public Attributes

- **directory**
- **parent**
- **filemenu**
- **menuSaveFigPNG**
- **menuSaveFigPDF**
- **plotmenu**
- **menuaddline**
- **menuBar**
- **config**
- **datalist**
- **pos**
- **yvals**
- **panel**
- **sizer**
- **plot1**
- **plot2**
- **controlsizer**
- **ctlm0**
- **ctlwindow**
- **controlsizer2**
- **backbutton**
- **nextbutton**
- **totalbutton**
- **pks**
- **peaksbutton**
- **radiobox**
- **radiobox2**
- **radiobox3**
- **ylab**
- **m0**
- **window**
- **ktype**
- **factor**
- **xlab**
- **xaxis**
- **kmass**
- **nominalkmass**
- **kmdefectexact**
- **defects**
- **nominal**
- **m2grid**
- **igrid**

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

- C:/Python/UniDec/MassDefects.py

3.24 MassFitter.MassFitter Class Reference

Public Member Functions

- def **__init__** (self, massdat, finarray, psfun, args)
- def **Fit** (self, args)

Public Attributes

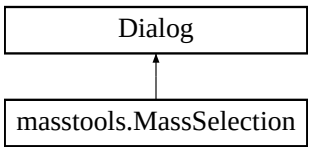
- **massdat**
- **finarray**
- **psfun**
- **initguess**
- **fit**
- **fitdat**

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

- C:/Python/UniDec/MassFitter.py

3.25 masstools.MassSelection Class Reference

Inheritance diagram for masstools.MassSelection:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI**
- def **OnSim** (self, e)
- def **OnPlot** (self, e)
- def **OnRightClick** (self, event)
- def **OnPopupOne** (self, event)
- def **OnRightClick2** (self, event)
- def **OnPopup2** (self, event)
- def **OnMatchI** (self, e)
- def **OnMatchAll** (self, e)
- def **Match** (self)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)
- def **OnPopulateButton** (self, e)
- def **OnPopulateButton2** (self, e)
- def **OnPopulateButton3** (self, e)
- def **OnClear** (self, e)
- def **OnAdd** (self, e)
- def **OnAdd2** (self, e)
- def **OnClear2** (self, e)
- def **OnImport** (self, e)
- def **OnImport2** (self, e)

Public Attributes

- massdat
- config
- defaultmasslist
- defaultoligolist
- defaultmatchlist
- newmasslist
- oligos
- matchlist
- newmatchlist
- pks
- pnl
- vbox
- hbox
- sb
- sbs
- peakpop
- importbutton
- oligopop
- oligopop2
- clearbutt
- addbutton
- simbutton
- masslistbox
- sb2
- sbs2
- clearbutt2
- addbutton2
- importbutton2
- plotbutton
- buttonbox
- hbox3
- oligomerlistbox
- sb4
- sbs4
- matchlbutt
- matchAllbutt
- matchlistbox
- hbox2
- newpeaks
- popupID1
- selection
- popupID2
- oligomasslist
- oligonames
- matches
- error
- peaks
- names
- oligoshort
- mfilename
- importmass
- ofilename
- importolig

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

- C:/Python/UniDec/masstools.py

3.26 mzMLimporter.mzMLimporter Class Reference

Public Member Functions

- def **__init__** (self, path, args, kwargs)
- def **GetData** (self)

Public Attributes

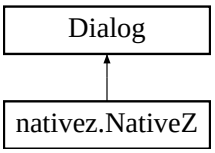
- **msrun**
- **data**

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

- C:/Python/UniDec/mzMLimporter.py

3.27 nativez.NativeZ Class Reference

Inheritance diagram for nativez.NativeZ:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, xvals, yvals, zdat, config, pks)
- def **OnReplot** (self, e)
- def **PlotZoffs** (self)
- def **MakePlot7** (self, e)
- def **on_edit** (self, event)
- def **on_delete** (self, event)
- def **fit** (self, e)
- def **update** (self, e)
- def **OnReset** (self, e)
- def **UpdateList** (self)
- def **PopulateList** (self, e)
- def **onadd** (self, e)
- def **MakeFArray** (self, min, max)
- def **fastextract** (self, f, width)
- def **Extract** (self, e)
- def **GetMaxima** (self)
- def **PeakExtract** (self)
- def **SaveFig** (self, e)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)

Public Attributes

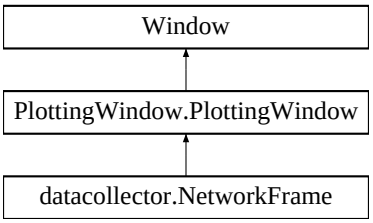
- **config**
- **pks**
- **xlen**
- **ylen**
- **xvals**
- **yvals**
- **newgrid**
- **pnl**
- **vbox**
- **sb**
- **sbs**
- **hbox0**
- **plot1**
- **plot2**
- **plot3**
- **plot4**
- **plot5**
- **plot6**
- **plot7**
- **hbox1**
- **addbutton**
- **fitbutton**
- **resetbutton**
- **extractbutton**
- **massoffset**
- **ctlfilt**
- **savefigbutt**
- **replotbutton**
- **hbox2**
- **list**
- **hbox3**
- **zoffs**
- **eshape**
- **offsetgrid**
- **ftot**
- **f**
- **offsetvalue**
- **extracts**
- **maxes**
- **peakextracts**
- **peakextractsarea**
- **zoffouts**

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

- C:/Python/UniDec/nativez.py

3.28 datacollector.NetworkFrame Class Reference

Inheritance diagram for datacollector.NetworkFrame:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **on_save_fig** (self, evt, path, kwargs)
- def **Clear** (self)

Public Attributes

- **axes**
- **flag**

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

- C:/Python/UniDec/datacollector.py

3.29 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**

3.29.1 Detailed Description

```
Class for a single peak. Contains all key parameters for describing and plotting the peak.
```

3.29.2 Constructor & Destructor Documentation

3.29.2.1 def peakstructure.Peak.__init__ (*self*)

```
Initialize all parameters for the peak to defaults
```

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

- C:/Python/UniDec/peakstructure.py

3.30 peakstructure.Peaks Class Reference

Public Member Functions

- def __init__ (self)
- def add_peaks (self, parray)
- def default_params
- def get_mass_defects
- def score_peaks

Public Attributes

- **peaks**
- **plen**
- **changed**
- **masses**
- **convolved**
- **composite**
- **peakcolors**
- **markers**
- **colormap**
- **textmarkers**
- **marklen**

3.30.1 Detailed Description

```
Class containing all useful data about peaks.

The peaks themselves are of the Peak class and contained within the self.peaks list.
```

3.30.2 Constructor & Destructor Documentation

3.30.2.1 def peakstructure.Peaks.__init__ (*self*)

```
Initialize Peaks class and set empty values
:return: None
```

3.30.3 Member Function Documentation

3.30.3.1 def peakstructure.Peaks.add_peaks (*self, parray*)

```
Create peak objects from an array
:param parray: N x 2 array containing (mass, height) of each peak.
:return: None
```

3.30.3.2 def 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
```

3.30.3.3 def 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 0=(0,1), 1=(-0.5,0.5)
:return: None
```

3.30.3.4 def peakstructure.Peaks.score_peaks (*self, thresh =* 0, *ci =* 0.99)

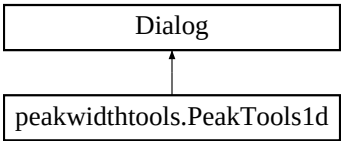
```
For each peak, assign a score of the fractional number of charge states observed.
:param thresh: Optional threshold to define a noise floor.
:return: None
```

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

- C:/Python/UniDec/peakstructure.py

3.31 peakwidthtools.PeakTools1d Class Reference

Inheritance diagram for peakwidthtools.PeakTools1d:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, config, data)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)
- def **OnReset** (self, e)
- def **OnCenter** (self, e)
- def **OnPlot** (self, e)
- def **OnFit** (self, e)

Public Attributes

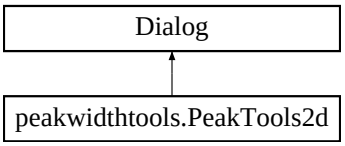
- **config**
- **data**
- **topmax**
- **topmin**
- **mzsig**
- **length**
- **psfun**
- **pnl**
- **vbox**
- **sb**
- **sbs**
- **plot1**
- **hbox11**
- **hbox10**
- **centerbutton**
- **hbox9**
- **ctlpsfun**
- **fitbutton**
- **plotbutton**
- **hbox8**
- **ctlmzsig**
- **hbox6**
- **errorbox**
- **hbox7**
- **resbox**
- **centdat**
- **mzsig2**
- **mid**
- **scale**
- **psguess**
- **res**
- **cent**
- **cent2**

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

- C:/Python/UniDec/peakwidthtools.py

3.32 peakwidthtools.PeakTools2d Class Reference

Inheritance diagram for peakwidthtools.PeakTools2d:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, data3, data2, config)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)
- def **OnFlip** (self, e)
- def **OnReset** (self, e)
- def **OnCenter** (self, e)
- def **OnPlot** (self, e)
- def **OnFit** (self, e)

Public Attributes

- **mz**
- **dt**
- **int**
- **C**
- **data**
- **topdata**
- **topmax**
- **topmin**
- **config**
- **mzsig**
- **dtsig**
- **length**
- **psfun**
- **fitmid**
- **fitsig**
- **pnl**
- **vbox**
- **sb**
- **sbs**
- **plot1**
- **hbox11**
- **hbox10**
- **centerbutton**
- **flipbutton**
- **hboxsigs**
- **outmzsig**
- **hboxsigs2**
- **outdtsig**
- **hbox9**

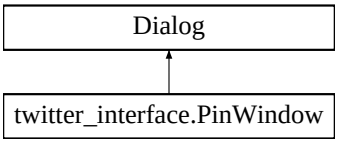
- **ctlpsfun**
- **fitbutton**
- **plotbutton**
- **hbox8**
- **ctlmzsig**
- **hbox6**
- **errorbox**
- **flag**
- **pos**
- **intdt**
- **data2**
- **centdat**
- **mzsig2**
- **mid**
- **scale**
- **psguess**
- **cent**
- **cent2**

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

- C:/Python/UniDec/peakwidthtools.py

3.33 twitter_interface.PinWindow Class Reference

Inheritance diagram for twitter_interface.PinWindow:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)

Public Attributes

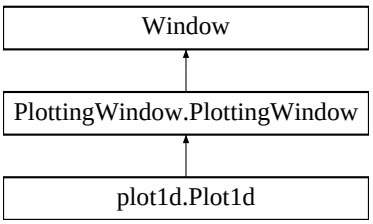
- **pnl**
- **vbox**
- **sbs**
- **inputbox**
- **pin**

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

- C:/Python/UniDec/twitter_interface.py

3.34 plot1d.Plot1d Class Reference

Inheritance diagram for plot1d.Plot1d:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **plotrefreshtop** (self, X, Y, titlestr, xstr, ystr, lab, config, args, kwargs)
- def **plotrefreshtopspan** (self, X, Y, titlestr, xstr, ystr, kwargs)
- def **plotrefreshtopbox** (self, X, Y, titlestr, xstr, ystr, args, kwargs)
- def **plotadd** (self, X, Y, colval, newlabel)
- def **plotaddspan** (self, X, Y, colval, newlabel)
- def **plotadddot** (self, X, Y, colval, markval)
- def **plotaddlegend**
- def **addtext** (self, txt, x, y, kwargs)
- def **filledplot** (self, x, y, color)
- def **textremove** (self)
- def **PaintAgain** (self, bins, kwargs)
- def **on_save_fig_dialog** (self, evt)
- def **on_save_fig** (self, evt, path, kwargs)
- def **Histogram**
- def **PlotClear** (self, args)

Public Attributes

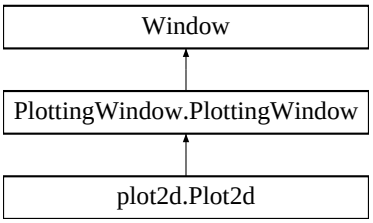
- **flag**
- **text**
- **lines**
- **kda**
- **subplot1**
- **X**
- **labels**

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

- C:/Python/UniDec/plot1d.py

3.35 plot2d.Plot2d Class Reference

Inheritance diagram for plot2d.Plot2d:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **contourplot**
- def **on_save_fig_dialog** (self, evt)
- def **on_save_fig** (self, evt, path, kwargs)
- def **PaintAgain** (self, bins, kwargs)
- def **PlotClear** (self)

Public Attributes

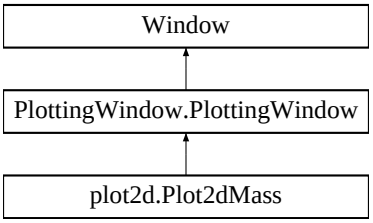
- **flag**
- **subplot1**
- **ticcol**
- **norm**
- **cbar**

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

- C:/Python/UniDec/plot2d.py

3.36 plot2d.Plot2dMass Class Reference

Inheritance diagram for plot2d.Plot2dMass:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **contourplot**
- def **on_save_fig_dialog** (self, evt)
- def **on_save_fig** (self, evt, path, kwargs)
- def **PaintAgain** (self, bins, kwargs)
- def **PlotClear** (self)
- def **PlotNativeZ**

Public Attributes

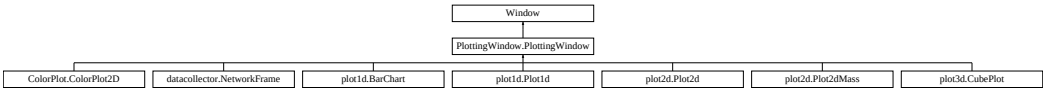
- **flag**
- **nativez**
- **kda**
- **xvals**
- **yvals**
- **subplot1**
- **ticcol**
- **norm**
- **cbar**

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

- C:/Python/UniDec/plot2d.py

3.37 PlottingWindow.PlottingWindow Class Reference

Inheritance diagram for PlottingWindow.PlottingWindow:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **set_link** (self, link)
- def **contour** (self)
- def **save_contour** (self, path, kwargs)
- def **repaint** (self)
- def **set_color**
- def **size_handler** (self, args, kwargs)
- def **setup_zoom**

Public Attributes

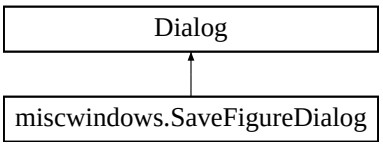
- **figure**
- **int**
- **smash**
- **link**
- **canvas**
- **resize**
- **cbar**
- **colors**
- **index2color**
- **cm_dict**
- **zoom**

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

- C:/Python/UniDec/PlottingWindow.py

3.38 miscwindows.SaveFigureDialog Class Reference

Inheritance diagram for miscwindows.SaveFigureDialog:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI** (self, config)
- def **OnClose** (self, e)
- def **OnCloseCancel** (self, e)
- def **on_choose_dir** (self, e)

Public Attributes

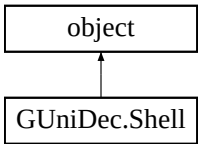
- **config**
- **directory**
- **header**
- **extension**
- **transparent**
- **rect**
- **figsize**
- **pnl**
- **vbox**
- **sb**
- **sbs**
- **hbox**
- **dirinput**
- **dirbutton**
- **hbox5**
- **headerbox**
- **hbox6**
- **extbox**
- **tbox**
- **hbox7**
- **widebox**
- **tallbox**
- **hbox8**
- **b1**
- **b2**
- **b3**
- **b4**

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

- C:/Python/UniDec/miscwindows.py

3.39 GUniDec.Shell Class Reference

Inheritance diagram for GUniDec.Shell:



Public Member Functions

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

Public Attributes

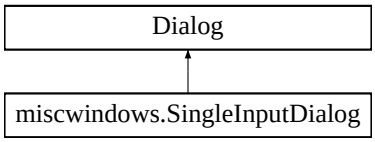
- **shell**
- **shellwindow**

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

- C:/Python/UniDec/GUniDec.py

3.40 miscwindows.SingleInputDialog Class Reference

Inheritance diagram for miscwindows.SingleInputDialog:



Public Member Functions

- def **__init__** (self, args, kwargs)
- def **InitUI**
- def **OnClose** (self, e)

Public Attributes

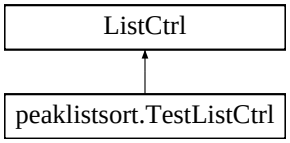
- **pnl**
- **vbox**
- **hbox**
- **inputbox**
- **value**

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

- C:/Python/UniDec/miscwindows.py

3.41 peaklistsort.TestListCtrl Class Reference

Inheritance diagram for peaklistsort.TestListCtrl:



Public Member Functions

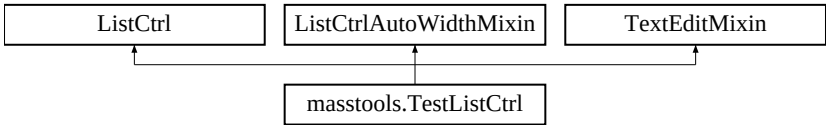
- def **__init__**

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

- C:/Python/UniDec/peaklistsort.py

3.42 masstools.TestListCtrl Class Reference

Inheritance diagram for masstools.TestListCtrl:



Public Member Functions

- def **__init__**
- def **Populate** (self, listctrldata)
- def **Clear** (self)
- def **AddLine** (self)
- def **GetList** (self)

Public Attributes

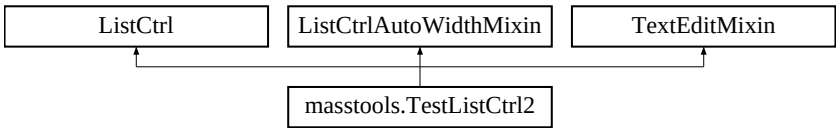
- **currentItem**

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

- C:/Python/UniDec/masstools.py

3.43 masstools.TestListCtrl2 Class Reference

Inheritance diagram for masstools.TestListCtrl2:



Public Member Functions

- def **__init__**
- def **Clear** (self)
- def **AddLine** (self)
- def **Populate** (self, data)
- def **GetList** (self)

Public Attributes

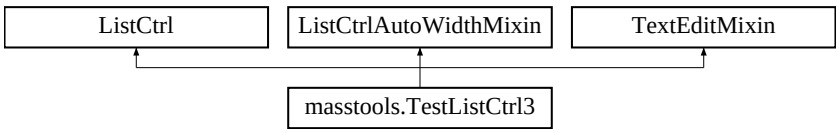
- **index**

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

- C:/Python/UniDec/masstools.py

3.44 masstools.TestListCtrl3 Class Reference

Inheritance diagram for masstools.TestListCtrl3:



Public Member Functions

- def **__init__**
- def **Clear** (self)
- def **AddLine** (self, line=[0)
- def **Populate**
- def **GetList** (self)

Public Attributes

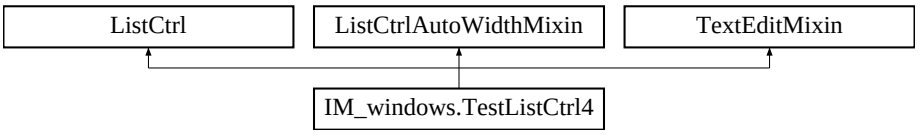
- **imflag**

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

- C:/Python/UniDec/masstools.py

3.45 IM_windows.TestListCtrl4 Class Reference

Inheritance diagram for IM_windows.TestListCtrl4:



Public Member Functions

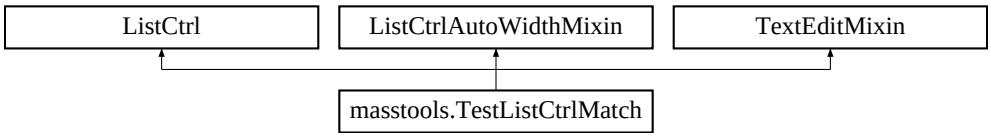
- def **__init__**
- def **Clear** (self)
- def **AddLine**
- def **Populate**
- def **GetList** (self)

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

- C:/Python/UniDec/IM_windows.py

3.46 masstools.TestListCtrlMatch Class Reference

Inheritance diagram for masstools.TestListCtrlMatch:



Public Member Functions

- def **__init__**
- def **Clear** (self)
- def **Populate** (self, data1, data2, data3, data4)
- def **GetList** (self)

Public Attributes

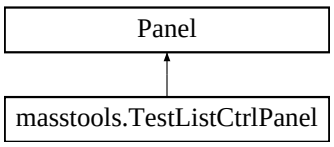
- **index**

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

- C:/Python/UniDec/masstools.py

3.47 masstools.TestListCtrlPanel Class Reference

Inheritance diagram for masstools.TestListCtrlPanel:



Public Member Functions

- def **__init__** (self, parent)
- def **OnUseNative** (self, event)

Public Attributes

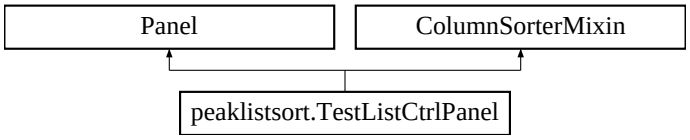
- **useNative**
- **list**

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

- C:/Python/UniDec/masstools.py

3.48 peaklistsort.TestListCtrlPanel Class Reference

Inheritance diagram for peaklistsort.TestListCtrlPanel:



Public Member Functions

- def **__init__** (self, parent)
- def **Clear** (self)
- def **AddData**
- def **GetListCtrl** (self)
- def **OnColClick** (self, event)
- def **OnRightClick** (self, event)
- def **OnItemSelected** (self, event)
- def **OnPopupOne** (self, event)
- def **OnPopupTwo** (self, event)
- def **OnPopupThree** (self, event)
- def **OnPopupFour** (self, event)
- def **OnPopupFive** (self, event)

Public Attributes

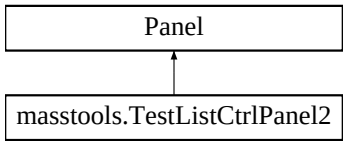
- **index**
- **list_ctrl**
- **EVT_DELETE_SELECTION_2**
- **EVT_CHARGE_STATE**
- **remove**
- **pks**
- **popupID1**
- **popupID2**
- **popupID3**
- **popupID4**
- **popupID5**
- **currentItem**
- **selection**
- **selection2**

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

- C:/Python/UniDec/peaklistsort.py

3.49 masstools.TestListCtrlPanel2 Class Reference

Inheritance diagram for masstools.TestListCtrlPanel2:



Public Member Functions

- def **__init__** (self, parent)
- def **OnUseNative** (self, event)

Public Attributes

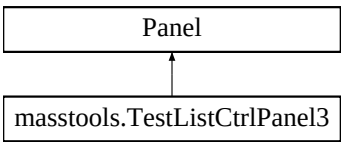
- **useNative**
- **list**

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

- C:/Python/UniDec/masstools.py

3.50 masstools.TestListCtrlPanel3 Class Reference

Inheritance diagram for masstools.TestListCtrlPanel3:



Public Member Functions

- def **__init__**
- def **OnRightClick** (self, e)
- def **OnPopupOne** (self, e)
- def **OnUseNative** (self, event)

Public Attributes

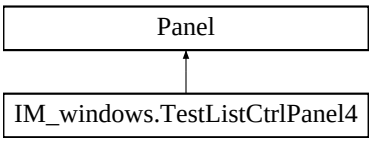
- **useNative**
- **list**
- **popupID1**
- **selection**

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

- C:/Python/UniDec/masstools.py

3.51 IM_windows.TestListCtrlPanel4 Class Reference

Inheritance diagram for IM_windows.TestListCtrlPanel4:



Public Member Functions

- def **__init__** (self, parent, size=(200, 200)
- def **OnUseNative** (self, event)

Public Attributes

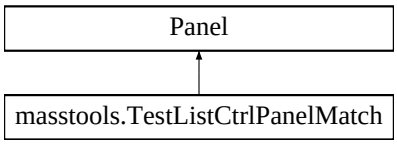
- **useNative**
- **list**

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

- C:/Python/UniDec/IM_windows.py

3.52 masstools.TestListCtrlPanelMatch Class Reference

Inheritance diagram for masstools.TestListCtrlPanelMatch:



Public Member Functions

- def **__init__** (self, parent)
- def **OnUseNative** (self, event)

Public Attributes

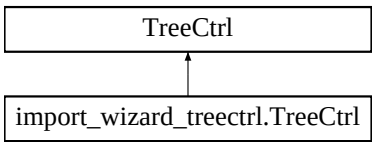
- **useNative**
- **list**

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

- C:/Python/UniDec/masstools.py

3.53 import_wizard_treectrl.TreeCtrl Class Reference

Inheritance diagram for import_wizard_treectrl.TreeCtrl:



Public Member Functions

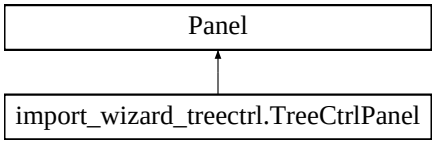
- def **__init__** (self, parent, id, pos, size, style)

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

- C:/Python/UniDec/import_wizard_treectrl.py

3.54 import_wizard_treectrl.TreeCtrlPanel Class Reference

Inheritance diagram for 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**

3.54.1 Member Function Documentation

3.54.1.1 def import_wizard_treectrl.TreeCtrlPanel.add_children (*self, parent, path, depth_limit* = `1`)

```
Recursively adds children up to the depth specified
```

3.54.1.2 def import_wizard_treectrl.TreeCtrlPanel.add_root (*self, name, data* = `None`)

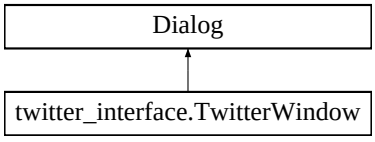
```
Add root folder to tree
    returns root object
```

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

- C:/Python/UniDec/import_wizard_treectrl.py

3.55 twitter_interface.TwitterWindow Class Reference

Inheritance diagram for 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

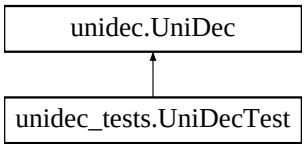
- **pngs**
- **codes**
- **imflag**
- **previewsize**
- **APP_KEY**
- **APP_SECRET**
- **pnl**
- **vbox**
- **sb**
- **sbs**
- **hbox1**
- **loginbutton**
- **userbox**
- **hbox2**
- **inputbox2**
- **countbox**
- **hbox3**
- **imagechoice**
- **previewbutton**
- **hbox4**
- **emptyimg**
- **imageCtrl**
- **hbox5**
- **tweetbutton**
- **OAUTH_TOKEN**
- **OAUTH_TOKEN_SECRET**
- **screen_name**
- **imageFile**
- **url**
- **pinwindow**
- **pin**

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

- C:/Python/UniDec/twitter_interface.py

3.56 unidec.UniDec Class Reference

Inheritance diagram for 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 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 export_params (self, e)
- def process_mass_data (self)
- def center_of_mass
- def fit_all_masses (self)
- def get_charge_peaks (self)
- 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

- **config**
- **data**
- **pks**
- **autopeaks**
- **peakparams**
- **massfit**
- **massfitdat**
- **errorgrid**

3.56.1 Constructor & Destructor Documentation

3.56.1.1 def unidec.UniDec.__init__ (*self*)

```
UniDec Engine

Consists of three main subclasses: Config, DataContiner, Peaks

:return: None
```

3.56.2 Member Function Documentation

3.56.2.1 def 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
:return: float. First peak in autocorrelation.
```

3.56.2.2 def 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.
```

3.56.2.3 def 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)
```

3.56.2.4 def unidec.UniDec.check_badness (*self*)

```
Check for problematic variables, such as upper bounds less than lower bounds and raise warning if found.
:return:
```

3.56.2.5 def unidec.UniDec.convolve_peaks (*self*)

```
Convolve Peaks with Peak Shape
:return: None
```

3.56.2.6 def unidec.UniDec.cross_validate (*self, numcrosstot* = 5)

```
Experimental function to perform cross validation
:param numcrosstot: Number of cross validation routines to perform
:return: mean, stddtev (mean and standard deviaition of mass distribution following cross validation)
```

3.56.2.7 def 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
```

3.56.2.8 def 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
```

3.56.2.9 def 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)
```

3.56.2.10 def 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))
```

3.56.2.11 def unidec.UniDec.initialize (*self*)

```
Initialize Config, DataContainer, and Peaks
:return: None
```

3.56.2.12 def unidec.UniDec.integrate (*self, limits, data* = None)

```
Trapezoid ntegrate 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.
:return: None
```

3.56.2.13 def 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)
```

3.56.2.14 def 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.
```

3.56.2.15 def unidec.UniDec.load_config (*self, f_name*)

```
Import UniDec Configuration File
:param f_name: File name
:return: None
```

3.56.2.16 def unidec.UniDec.load_default (*self*)

```
Loads config from default location set at self.config.defaultconfig
:return: None
```

3.56.2.17 def 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
```

3.56.2.18 def 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)
```

3.56.2.19 def 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
```

3.56.2.20 def 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
:return: None
```

3.56.2.21 def unidec.UniDec.pick_peaks (*self*)

```
Detect, Normalize, and Output Peaks
:return: None
```

3.56.2.22 def 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
```

3.56.2.23 def 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
```

3.56.2.24 def 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)
```

3.56.2.25 def unidec.UniDec.reset_config (*self*)

```
Resets UniDec config to default. Should not reset paths or filenames.
:return: None
```

3.56.2.26 def 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)
```

3.56.2.27 def unidec.UniDec.save_default (*self*)

```
Saves existing config in default location set at self.config.defaultconfig
:return: None
```

3.56.2.28 def unidec.UniDec.unidec_imports (*self*, *efficiency* = `False`)

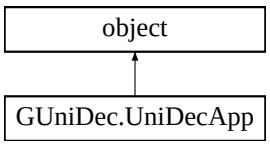
```
Imports files output from the UniDec core executable into self.data.
:param efficiency: If True, it will ignore the larger files to speed up the run.
:return: None
```

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

- C:/Python/UniDec/unidec.py

3.57 GUniDec.UniDecApp Class Reference

Inheritance diagram for 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** (self, e)
- def **on_open_file**
- def **on_save_state**
- def **on_load_state** (self, e)
- def **on_raw_open** (self, e)
- def **on_load_conf_file** (self, e)

- def **on_save_default** (self, e)
- def **on_load_default** (self, e)
- def **on_paste_spectrum** (self, e)
- def **on_reset** (self, e)
- def **on_dataprep_button** (self, e)
- def **on_unidec_button** (self, e)
- def **after_unidec_run** (self)
- def **on_pick_peaks** (self, e)
- def **on_plot_peaks** (self, e)
- def **on_peak_errors** (self, e)
- def **check_badness** (self)
- def **warn**
- def **on_auto** (self, e)
- def **makeplot1** (self, e)
- def **makeplot2** (self, e)
- def **makeplot3** (self, e)
- def **makeplot4** (self, a)
- def **makeplot5** (self, a)
- def **makeplot6**
- def **on_plot_composite** (self, e)
- def **make_im_plots** (self)
- def **on_plot_nativeccs** (self, e)
- def **on_replot** (self, e)
- def **make_cube_plot** (self, e)
- def **on_delete** (self, e)
- def **on_charge_states** (self, e)
- def **on_plot_offsets** (self, e)
- def **plot_integral**
- def **on_integrate**
- def **on_smash** (self)
- def **on_charge_plot** (self, e)
- def **on_batch_raw** (self, e)
- def **on_manual** (self, e)
- def **on_match** (self, e)
- def **on_mass_tools**
- def **on_peak_width_tool** (self, e)
- def **on_additional_parameters** (self, e)
- def **on_unidec_path** (self, e)
- def **on_file_name** (self, e)
- def **on_data_collector** (self, e)
- def **on_import_wizard** (self, e)
- def **on_im_tools** (self, e)
- def **on_im_extract** (self, e)
- def **on_tweet** (self, e)
- def **on_kendrick** (self, e)
- def **on_2d_grid** (self, e)
- def **on_nativez_tools** (self, e)
- def **on_export_params** (self, e)
- def **on_mass_process** (self, e)
- def **on_center_of_mass** (self, e)
- def **on_zerocharge_mass** (self, e)
- def **on_fit_masses** (self, e)
- def **on_batch**
- def **on_batch2** (self, e)
- def **on_super_batch** (self, e)
- def **on_cross_validate** (self, e)
- def **on_pdf_report** (self, e)

Public Attributes

- **eng**
- **view**
- **twittercodes**

3.57.1 Detailed Description

```
Main UniDec GUI Application.

Presenter contains UniDec engine at self.eng and main GUI window at self.view
```

3.57.2 Member Function Documentation

3.57.2.1 def 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
:return: None
```

3.57.2.2 def 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
```

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

- C:/Python/UniDec/GUniDec.py

3.58 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_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**
- **intthresh**
- **minmz**
- **maxmz**
- **numit**
- **zzsig**
- **startz**
- **endz**
- **numz**
- **mzsig**
- **psfun**
- **massub**
- **masslb**
- **msig**
- **molig**
- **massbins**
- **adductmass**
- **damp**
- **aggressiveflag**
- **suppression**
- **isotopemode**
- **peakwindow**
- **peakthresh**
- **peakplotthresh**
- **separation**
- **peaknorm**
- **error**
- **mtabsig**
- **poolflag**
- **nativezub**
- **nativezlb**
- **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**
- **gridparams**
- **cmaps**
- **badtest**
- **warning**
- **system**
- **defaultUnidecDir**
- **defaultUnidecName**
- **defaultIMName**
- **UniDecPath**
- **UniDecName**
- **UniDecIMName**
- **UniDecDir**
- **UniDecIMPath**
- **rawreaderpath**
- **cdcreaderpath**
- **defaultconfig**

3.58.1 Detailed Description

```
Class containing all options and configurations for UniDec GUI and Program. Contains methods to export and imp
config to text file for running UniDec core binaries and for storing parameters for GUI.
```

3.58.2 Constructor & Destructor Documentation

3.58.2.1 def unidecstructure.UniDecConfig.__init__ (*self*)

```
Initialize Everything. Set default paths and run self.initialize
:return: UniDecConfig object
```

3.58.3 Member Function Documentation

3.58.3.1 def 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
```

3.58.3.2 def 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
```

3.58.3.3 def 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
```

3.58.3.4 def unidecstructure.UniDecConfig.default_colormaps (*self*)

```
Get default matplotlib colormaps and set names to self.cmaps. Ignores CMRmap and CMRmap_r because the caused
problems.
:return: None
```

3.58.3.5 def 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
```

3.58.3.6 def unidecstructure.UniDecConfig.default_high_res (*self*)

```
Sets some defaults for high resolution spectra. Leaves other values unchanged.
:return: None
```

3.58.3.7 def 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
```

3.58.3.8 def unidecstructure.UniDecConfig.initialize (*self*)

```
Initialize configuration parameters but not paths. Runs self.default_colormaps
:return: None
```

3.58.3.9 def unidecstructure.UniDecConfig.initialize_system_paths (*self*)

```
Initialize initial paths for UniDec directories
:return: None
```

3.58.3.10 def unidecstructure.UniDecConfig.print_config (*self*)

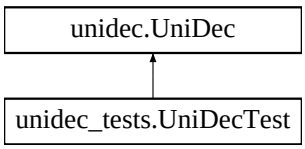
```
Simple debugging command to read in the config file and print out its contents.
:return: None
```

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

- C:/Python/UniDec/unidecstructure.py

3.59 unidec_tests.UniDecTest Class Reference

Inheritance diagram for 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)

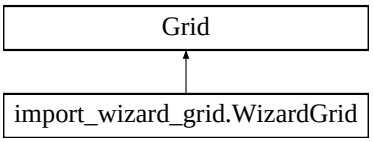
Additional Inherited Members

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

- C:/Python/UniDec/unidec_tests.py

3.60 import_wizard_grid.WizardGrid Class Reference

Inheritance diagram for 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**

3.60.1 Detailed Description

```
Grid for data import wizard
```

3.60.2 Member Function Documentation

3.60.2.1 def import_wizard_grid.WizardGrid.fill_down (*self, evt*)

```
Try to fill down the columnn
```

3.60.2.2 def import_wizard_grid.WizardGrid.set_labels (*self, mode*)

```
Set initial column headers based on mode
    0 - Linear
    1 - T-wave
```

3.60.2.3 def import_wizard_grid.WizardGrid.showPopupMenu (*self, evt*)

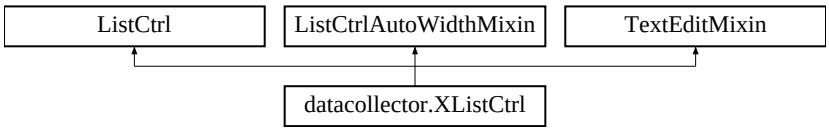
```
Create and display a popup menu on right-click event
```

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

- C:/Python/UniDec/import_wizard_grid.py

3.61 datacollector.XListCtrl Class Reference

Inheritance diagram for datacollector.XListCtrl:



Public Member Functions

- def **__init__**
- def **Populate**
- def **Clear** (self)
- def **AddLine**
- def **GetList** (self)
- def **GetMaxes** (self)

Public Attributes

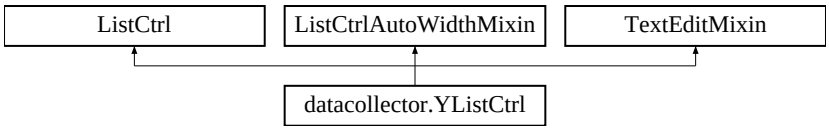
- **currentItem**

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

- C:/Python/UniDec/datacollector.py

3.62 datacollector.YListCtrl Class Reference

Inheritance diagram for datacollector.YListCtrl:



Public Member Functions

- def **__init__**
- def **Populate**
- def **Clear** (self)

- def **AddLine**
- def **GetList** (self)

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

- C:/Python/UniDec/datacollector.py

3.63 nativez.zoffset Class Reference

Public Member Functions

- def **__init__** (self, args)
- def **Make** (self, offset, intensity, index, color, marker)

Public Attributes

- **offset**
- **intensity**
- **index**
- **color**
- **marker**
- **id**
- **width**
- **nstate**
- **extractwidth**

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

- C:/Python/UniDec/nativez.py

3.64 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**

3.64.1 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()
```

3.64.2 Constructor & Destructor Documentation

3.64.2.1 def 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
```

3.64.3 Member Function Documentation

3.64.3.1 def ZoomBox.ZoomBox.get_active (*self*)

```
to get status of active mode (boolean variable)
```

3.64.3.2 def ZoomBox.ZoomBox.set_active (*self, active*)

```
Use this to activate / deactivate the RectangleSelector

    from your program with an boolean variable 'active'.
```

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

- C:/Python/UniDec/ZoomBox.py

3.65 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**

3.65.1 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
```

3.65.2 Constructor & Destructor Documentation

3.65.2.1 def 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
```

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

- C:/Python/UniDec/ZoomSpan.py

Index

__init__
    mainwindow::Mainwindow, 27
    nativez::ColorList, 9
    peakstructure::Peak, 39
    peakstructure::Peaks, 40
    unidec::DataContainer, 15
    unidec::UniDec, 59
    unidecstructure::UniDecConfig, 68
    ZoomBox::ZoomBox, 74
    ZoomSpan::ZoomSpan, 76

add_children
    import_wizard_treectrl::TreeCtrlPanel, 56
add_peaks
    peakstructure::Peaks, 40
add_root
    import_wizard_treectrl::TreeCtrlPanel, 56
autocorrelation
    unidec::UniDec, 59
autointegrate
    unidec::UniDec, 59

center_of_mass
    unidec::UniDec, 59
check_badness
    unidec::UniDec, 59
    unidecstructure::UniDecConfig, 68
clear_all_plots
    mainwindow::Mainwindow, 27
ColorPlot.ColorPlot2D, 9
config_export
    unidecstructure::UniDecConfig, 68
config_import
    unidecstructure::UniDecConfig, 68
convolve_peaks
    unidec::UniDec, 59
cross_validate
    unidec::UniDec, 60

datacollector.DataCollector, 12
datacollector.ListCtrlPanel, 23
datacollector.NetworkFrame, 38
datacollector.XListCtrl, 71
datacollector.YListCtrl, 71
default_colormaps
    unidecstructure::UniDecConfig, 68
default_file_names
    unidecstructure::UniDecConfig, 68
default_high_res
    unidecstructure::UniDecConfig, 68
default_params
    peakstructure::Peaks, 40
default_zero_charge
    unidecstructure::UniDecConfig, 68

export_config
    GUniDec::UniDecApp, 65
    unidec::UniDec, 60
export_file
    import_wizard::ImportWizard, 18
export_gui_to_config
    mainwindow::Mainwindow, 27
export_params
    unidec::UniDec, 60
export_then_load
    import_wizard::ImportWizard, 18
Extract2D.Extract2DPlot, 15

fill_down
    import_wizard_grid::WizardGrid, 70
fit_all_masses
    unidec::UniDec, 60

GUniDec.Shell, 48
GUniDec.UniDecApp, 63
GUniDec::UniDecApp
    export_config, 65
    import_config, 65
get_active
    ZoomBox::ZoomBox, 74
get_charge_peaks
    unidec::UniDec, 60
get_folder_path
    import_wizard::ImportWizard, 18
get_mass_defects
    peakstructure::Peaks, 40

IM_windows.IMToolExtract, 19
IM_windows.IMTools, 20
IM_windows.TestListCtrl4, 51
IM_windows.TestListCtrlPanel4, 54
import_config
    GUniDec::UniDecApp, 65
import_config_to_gui
    mainwindow::Mainwindow, 27
import_wizard.ImportWizard, 18
import_wizard::ImportWizard
    export_file, 18
    export_then_load, 18
    get_folder_path, 18

import_wizard_grid.WizardGrid, 70
import_wizard_grid::WizardGrid
    fill_down, 70
    set_labels, 70
    showPopupMenu, 70
import_wizard_treectrl.TreeCtrl, 55
import_wizard_treectrl.TreeCtrlPanel, 55
import_wizard_treectrl::TreeCtrlPanel
    add_children, 56
    add_root, 56
initialize
    unidec::UniDec, 60
    unidecstructure::UniDecConfig, 68
initialize_system_paths
    unidecstructure::UniDecConfig, 69
integrate
    unidec::UniDec, 60

kendrick_continuous
    unidec::UniDec, 60
kendrick_peaks
    unidec::UniDec, 61

load_config
    unidec::UniDec, 61
load_default
    unidec::UniDec, 61
load_state
    unidec::UniDec, 61

mainwindow.Mainwindow, 23
mainwindow::Mainwindow
    __init__, 27
    clear_all_plots, 27
    export_gui_to_config, 27
    import_config_to_gui, 27
    menu_401_403, 28
    on_about, 28
    on_check_manual, 28
    on_defaults, 28
    on_exit, 28
    on_flip_mode, 28
    on_flip_tabbed, 28
    on_flip_twave, 28
    on_mass_list, 28
    on_motion, 29
    on_save_figure_dialog, 29
    on_save_figure_eps, 29
    on_save_figure_pdf, 29
    on_save_figure_png, 29
    on_save_figure_small, 29
    save_all_figures, 29
    setup_main_panel, 29
    setup_menu, 30
    setup_shortcuts, 30
    setup_tool_tips, 30
    shrink_all_figures, 30
    shrink_figure, 30
mass_grid_to_f_grid
    unidec::UniDec, 61
MassDefects.MassDefectWindow, 32
MassFitter.MassFitter, 33
MassModelFitter.mass, 31
masstools.AutocorrWindow, 7
masstools.CorrListCtrl, 10
masstools.CorrListCtrlPanel, 10
masstools.ManualSelection, 30
masstools.MassSelection, 34
masstools.TestListCtrl, 49
masstools.TestListCtrl2, 49
masstools.TestListCtrl3, 50
masstools.TestListCtrlMatch, 51
masstools.TestListCtrlPanel, 52
masstools.TestListCtrlPanel2, 53
masstools.TestListCtrlPanel3, 53
masstools.TestListCtrlPanelMatch, 55
menu_401_403
    mainwindow::Mainwindow, 28
miscwindows.AdditionalParameters, 5
miscwindows.FileNameDialog, 16
miscwindows.SaveFigureDialog, 47
miscwindows.SingleInputDialog, 48
mzMLimporter.mzMLimporter, 36

nativez.ColorList, 8
nativez.NativeZ, 36
nativez.zoffset, 72
nativez::ColorList
    __init__, 9
normalize_peaks
    unidec::UniDec, 61

on_about
    mainwindow::Mainwindow, 28
on_check_manual
    mainwindow::Mainwindow, 28
on_defaults
    mainwindow::Mainwindow, 28
on_exit
    mainwindow::Mainwindow, 28
on_flip_mode
    mainwindow::Mainwindow, 28
on_flip_tabbed
    mainwindow::Mainwindow, 28
on_flip_twave
    mainwindow::Mainwindow, 28
on_mass_list
    mainwindow::Mainwindow, 28
on_motion
    mainwindow::Mainwindow, 29
on_save_figure_dialog
    mainwindow::Mainwindow, 29
on_save_figure_eps
    mainwindow::Mainwindow, 29
on_save_figure_pdf
    mainwindow::Mainwindow, 29
on_save_figure_png
    mainwindow::Mainwindow, 29

on_save_figure_small
mainwindow::Mainwindow, 29
open_file
unidec::UniDec, 61

peaklistsort.TestListCtrl, 49
peaklistsort.TestListCtrlPanel, 52
peakstructure.Peak, 38
peakstructure.Peaks, 39
peakstructure::Peak
__init__, 39
peakstructure::Peaks
__init__, 40
add_peaks, 40
default_params, 40
get_mass_defects, 40
score_peaks, 40
peakwidthtools.PeakTools1d, 40
peakwidthtools.PeakTools2d, 42
pick_peaks
unidec::UniDec, 62
plot1d.BarChart, 7
plot1d.Plot1d, 44
plot2d.Plot2d, 44
plot2d.Plot2dMass, 45
plot3d.CubePlot, 10
PlotAnimations.AnimationWindow, 6
PlottingWindow.PlottingWindow, 46
print_config
unidecstructure::UniDecConfig, 69
process_data
unidec::UniDec, 62
process_mass_data
unidec::UniDec, 62

raw_process
unidec::UniDec, 62
reset_config
unidec::UniDec, 62
run_unidec
unidec::UniDec, 62

save_all_figures
mainwindow::Mainwindow, 29
save_default
unidec::UniDec, 63
score_peaks
peakstructure::Peaks, 40
set_active
ZoomBox::ZoomBox, 74
set_labels
import_wizard_grid::WizardGrid, 70
setup_main_panel
mainwindow::Mainwindow, 29
setup_menu
mainwindow::Mainwindow, 30
setup_shortcuts
mainwindow::Mainwindow, 30
setup_tool_tips
mainwindow::Mainwindow, 30
showPopupMenu
import_wizard_grid::WizardGrid, 70
shrink_all_figures
mainwindow::Mainwindow, 30
shrink_figure
mainwindow::Mainwindow, 30

twitter_interface.PinWindow, 43
twitter_interface.TwitterWindow, 56

UniFit.KDmodel, 21
UniFit.kdstruct, 22
unidec.DataContainer, 14
unidec.UniDec, 58
unidec::DataContainer
__init__, 15
unidec::UniDec
__init__, 59
autocorrelation, 59
autointegrate, 59
center_of_mass, 59
check_badness, 59
convolve_peaks, 59
cross_validate, 60
export_config, 60
export_params, 60
fit_all_masses, 60
get_charge_peaks, 60
initialize, 60
integrate, 60
kendrick_continuous, 60
kendrick_peaks, 61
load_config, 61
load_default, 61
load_state, 61
mass_grid_to_f_grid, 61
normalize_peaks, 61
open_file, 61
pick_peaks, 62
process_data, 62
process_mass_data, 62
raw_process, 62
reset_config, 62
run_unidec, 62
save_default, 63
unidec_imports, 63
unidec_imports
unidec::UniDec, 63
unidec_tests.UniDecTest, 69
unidecstructure.UniDecConfig, 65
unidecstructure::UniDecConfig
__init__, 68
check_badness, 68
config_export, 68
config_import, 68
default_colormaps, 68
default_file_names, 68
default_high_res, 68

default_zero_charge, 68
initialize, 68
initialize_system_paths, 69
print_config, 69

ZoomBox.ZoomBox, 72
ZoomBox::ZoomBox
__init__, 74
get_active, 74
set_active, 74
ZoomSpan.ZoomSpan, 74
ZoomSpan::ZoomSpan
__init__, 76