VWA_generate_mz_diagrams

October 25, 2017

```
In [109]: import pandas as pd
          import numpy as np
          import math as mt
          import matplotlib.pyplot as plt

          from matplotlib import rcParams

In [110]: filetype = "png"        # "png" or "pdf"
          """str: Filetype of the outputfile

          Tested with "pdf" and "png"
          """

          figdpi = 200
          """int: DPI of the image output file
          """


          # correct DPI of figure if using pdf
          if filetype.lower() == "pdf":
              figdpi = 72

          params = {'backend': 'pdf',
                    'figure.dpi': figdpi,   # 72 for pdf
                    'axes.labelsize': 10,
                    'font.size': 10,
                    'legend.fontsize': 8,
                    'legend.frameon': True,
                    'xtick.labelsize': 8,
                    'ytick.labelsize': 8,
                    'font.family': 'serif',
                    'text.usetex': True,
                    'text.latex.unicode': True,
                    'axes.linewidth': 0.5,
                    'xtick.major.size': 4,   # major tick size in points
                    'xtick.minor.size': 2,   # minor tick size in points
                    'xtick.direction': 'out',
                    'ytick.major.size': 4,  # major tick size in points
                    'ytick.minor.size': 2,  # minor tick size in points
                    'ytick.direction': 'out',
                    }
          plt.rcParams.update(params)
```

```
In [111]: def __get_max_peak(x_value, raw_values):
              """Search for the local peak next to the x-value.

              The value searches in the near area of the given x-value for the maxi
              peak, which correspondends to the data.

              Args:
                  x_value (float): m/z value (x-coordinate) of the point, to be ann
                  raw_values (Pandas.DataFrame): Data values, which should be annot

              Returns:
                  y value of the peak, next to the given x value

              """
              #print(x_value)
              #print(raw_values[raw_values["m/z"] == x_value])
              raw_values_index = raw_values[raw_values["m/z"] == x_value].index[0]

              #print(raw_values_index)
              value, index = float(raw_values.loc[raw_values_index - 1, "intensity_

              #for z in range(-5, 15):
                  #if float(raw_values.loc[raw_values_index + z, "intensity_normali
                      #value, index = float(raw_values.loc[raw_values_index + z, "i
              return value
```

```
In [112]: def annotate_point(x1, y_pos=0, text='', raw_values=None):
              """Annotage a specific point.

              Annotate a point with a label. The label will be placed vertically
              with an additional line.

              The function uses the data values and searches for the peak of the
              value to be annotated. Therefore the ``raw_values`` parameter is usec

              Args:
                  x1 (float): m/z value (x-coordinate) of the point, to be annotate
                  y_pos (Optional[float]): Position of the label beginning (y-coorc
                      The value uses the scale of the datapoints.
                  text (str): Label text
                  raw_values (Pandas.DataFrame): Data values, which should be annot
```

```
    """

    delta_point_annotate_line_pixel = 1

    if raw_values is not None:

        if __get_max_peak(x1, raw_values) < (y_pos - delta_point_annotate
            xy_text = (x1, y_pos)
        else:
            xy_text = (x1, __get_max_peak(x1, raw_values) + delta_point_a

        plt.annotate(
            text, xy=(x1, __get_max_peak(x1, raw_values) + delta_point_an
            xytext=xy_text, textcoords='data',
            rotation=90, size=8, horizontalalignment='center', verticalal
            arrowprops=dict(arrowstyle='-', color="#808080", linewidth=0.

In [113]: def annotate_distance(x1=0, x2=0, y_pos=0, text='', raw_values=None, rota
    """Annotage the distance between two peaks

    Annotate the distance between two given peaks. The text can be placed
    given angle.


    Args:
        x1 (float): m/z value (x-coordinate) of the left point
        x2 (float): m/z value (x-coordinate) of the right point
        y_pos (Optional[float]): Position of the label beginning (y-coord
            The value uses the scale of the datapoints.
        text (str): Label text
        raw_values (Pandas.DataFrame): Data values, which should be annot
        rotate_text (Optional[int]): Rotation of the label, should be 0 o

    """

    delta_point_annotate_line_pixel = 1

    if raw_values is not None:
        if __get_max_peak(x1, raw_values) < (y_pos - delta_point_annotate
            plt.annotate(
                '', xy=(x1, __get_max_peak(x1, raw_values) + delta_point_
                xytext=(x1, y_pos), textcoords='data',
                arrowprops=dict(arrowstyle='-', color="#808080", linewidt

        if __get_max_peak(x2, raw_values) < (y_pos - delta_point_annotate
            plt.annotate(
                '', xy=(x2, __get_max_peak(x2, raw_values) + delta_point_
                xytext=(x2, y_pos), textcoords='data',
                          arrowprops=dict(arrowstyle='-', color="#808080", linewidt

              plt.annotate(
                  '', xy=(x1, y_pos), xycoords='data',
                  xytext=(x2, y_pos), textcoords='data',
                  arrowprops=dict(arrowstyle='<|-,head_length=0.4,head_width=0.1',
                                  color="black", linewidth=0.6, shrinkA=0.05, shrin
              plt.annotate(
                  text, xy=((x1 if x1 <= x2 else x2) + mt.fabs((x1 - x2)) / 2, y_po
                  rotation=rotate_text, size=8,
                  horizontalalignment='center', verticalalignment='bottom',
                  xytext=(0, 2), textcoords='offset points')

          # Helper functions

In [114]: def __figsize_and_margins(plotsize, subplots=(1, 1), **absolute_margins):
              """Determine figure size and margins from plot size and absolute marg

              Args:
                  plotsize: (width, height) of plot area in inch
                  subplots: (nrows, ncols) of subplots
                  left, right, top, bottom: absolute margins around plot area
                  wspace, hspace: width and height spacing between subplots

              Returns:
                   size: figure size for figsize argument of figure()
                   margins: relative margins dict suitable for subplots_adjust()

              Example: making 2x2 grid of 3" square plots with specific spacings:

                 sz, rm = figsize_and_margins((3,3), (2,2), left=1, right=.5,
                                                            top=.5, bottom=1,
                                                            wspace=.5, hspace=.5)
                 figure(figsize=sz)
                 subplots_adjust(**rm)
                 subplot(221); subplot(222)
                 subplot(223); subplot(224)

              Source: http://scipy-central.org/item/65/1/absolute-plot-size-and-mar
              """

              pw, ph = plotsize
              nr, nc = subplots
              amarg = absolute_margins
              # dictionary for relative margins
              # initialize from rcParams with margins not in amarg
              rmarg = dict((m, rcParams['figure.subplot.' + m])
                           for m in ('left', 'right', 'top', 'bottom', 'wspace', 'h
                           if m not in amarg
                           )
              # subplots_adjust wants wspace and hspace relative to plotsize:
              if 'wspace' in amarg:
                  rmarg['wspace'] = float(amarg['wspace']) / pw
              if 'hspace' in amarg:
                  rmarg['hspace'] = float(amarg['hspace']) / ph
              # in terms of the relative margins:
              # width  * (right - left)
              #    = ncols * plot_width  + (ncols - 1) * wspace * plot_width
              # height * (top - bottom)
              #    = nrows * plot_height + (nrows - 1) * hspace * plot_height
              # solve for width and height, using absolute margins as necessary:
              width = float((nc + (nc - 1) * rmarg['wspace']) * pw + amarg.get('lef
                  rmarg.get('right', 1) - rmarg.get('left', 0))
              height = float((nr + (nr - 1) * rmarg['hspace']) * ph + amarg.get('to
                  rmarg.get('top', 1) - rmarg.get('bottom', 0))

              # now we can get any remaining relative margins
              if 'left' in amarg:
                  rmarg['left'] = float(amarg['left']) / width
              if 'right' in amarg:
                  rmarg['right'] = 1 - float(amarg['right']) / width
              if 'top' in amarg:
                  rmarg['top'] = 1 - float(amarg['top']) / height
              if 'bottom' in amarg:
                  rmarg['bottom'] = float(amarg['bottom']) / height
              # return figure size and relative margins
              return (width, height), rmarg

In [115]: def __get_ax_size(ax, fig):
              """
              Source: http://scipy-central.org/item/65/1/absolute-plot-size-and-ma
              """
              bbox = ax.get_window_extent().transformed(fig.dpi_scale_trans.inverte
              width, height = bbox.width, bbox.height
              width *= fig.dpi
              height *= fig.dpi
              return width, height

In [116]: def __conv_inch(length_mm):
              """Converts a length from millimeters to inch

              Args:
                  length_mm (int,float): length in millimeters to be converted

              Returns:
                  float: The converted length in inch
```

```
    """
    return length_mm / 25.4
```

In [117]:

```
def generate_massspectra_plot_automatic_labels(input_filename, output_fil
    print("Generate {0} mass spectra plot ({1}.{2}) from {3}.[xy/txt]".fo


    # min and max value of the x axis
    min_xaxis = 50
    max_xaxis = 425

    # dimensions of the single plot
    figwidth_mm = 141
    left_margin_mm = 14
    right_margin_mm = 2
    top_margin_mm = 26
    bottom_margin_mm = 13

    plotwidth_mm = figwidth_mm - left_margin_mm - right_margin_mm
    plotheight_mm = plotwidth_mm * 0.8

    hspace_mm = 0.1  # horizontal space between two plots

    # read xy input data
    raw_values = pd.read_csv(input_filename + ".xy", sep=" ", names=["m/z
                             dtype={"m/z": np.float64, "intensity": np.fl
    # normalize input data
    max_val = np.max(raw_values['intensity'])
    raw_values["intensity_normalized"] = raw_values['intensity'] / max_va

    # read txt captions
    caption_values = pd.read_csv(input_filename + ".txt", sep=";", names=

    # find maximum value for each annotate peak - necessary for later cal
    for i in caption_values.index:
        raw_values_index = raw_values[raw_values["m/z"] == caption_values
        value, index = float(raw_values.loc[raw_values_index - 5, "intens

        for z in range(-5, 15):
            if float(raw_values.loc[raw_values_index + z, "intensity_norm
                value, index = float(raw_values.loc[raw_values_index + z,

        caption_values.loc[i, "m/z"] = float(raw_values.loc[index, "m/z"]
        caption_values.loc[i, "intensity_normalized"] = value  # add inte

    # dimension for the annotations in pixel
    delta_x_text_labels_mm = 3.8
    delta_point_annotate_line_mm = 1
```

```
label_annotate_arm_high_mm = 5.3
delta_y_diagonal_annotate_arm_mm = 3.5
delta_y_baseline_axistop_mm = 6.3
delta_label_mznumber_pixel_mm = 7

fsize, margins = __figsize_and_margins(plotsize=(__conv_inch(plotwidt
                                       subplots=(1, 1),
                                       left=__conv_inch(left_margin_m
                                       top=__conv_inch(top_margin_mm)
                                       wspace=0.01, hspace=__conv_inc
fig = plt.figure(figsize=fsize, )
plt.subplots_adjust(**margins)
ax = fig.add_subplot(111)

# delta_dimension in pixel calculate from mm
delta_x_text_labels_pixel = __conv_inch(delta_x_text_labels_mm) * fig
delta_point_annotate_line_pixel = __conv_inch(delta_point_annotate_li
label_annotate_arm_high_pixel = __conv_inch(label_annotate_arm_high_m
delta_y_diagonal_annotate_arm = __conv_inch(delta_y_diagonal_annotate
delta_y_baseline_axistop = __conv_inch(delta_y_baseline_axistop_mm) *
delta_label_mznumber_pixel = __conv_inch(delta_label_mznumber_pixel_m

# plot spectra line
ax.plot(raw_values["m/z"], raw_values["intensity_normalized"], color=

# set x axes range
if min_xaxis is not None and max_xaxis is not None:
    ax.set_xlim([int(min_xaxis), int(max_xaxis)])

length_x_axis_pixel, length_y_axis_pixel = __get_ax_size(ax, fig)
x_axis_min, x_axis_max = ax.get_xlim()
y_axis_min, y_axis_max = ax.get_ylim()

list_text_pos = list()
if len(caption_values.index) > 0:

    # annotate from basepeak
    basepeak_index = caption_values[caption_values["intensity_normali
    if len(basepeak_index) == 0:
        basepeak_index = [len(caption_values) / 2]

    # annotate peaks left frome basepeak
    for z in caption_values.loc[:basepeak_index[0], "m/z"].sort_index
        x_value_pixel = (z - x_axis_min) / (x_axis_max - x_axis_min)

        if len(list_text_pos) == 0:
            list_text_pos.append(x_value_pixel)
        else:
```

```
        if x_value_pixel > list_text_pos[-1] + delta_x_text_label
            list_text_pos.append(x_value_pixel)
        else:
            list_text_pos.append(list_text_pos[-1] + delta_x_text

# annotate peaks right from basepeak
if basepeak_index[0] + 1 in caption_values.index:
    for z in caption_values.loc[basepeak_index[0] + 1:, "m/z"]:
        x_value_pixel = (z - x_axis_min) / (x_axis_max - x_axis_m

        if x_value_pixel < list_text_pos[0] - delta_x_text_labels
            list_text_pos.insert(0, x_value_pixel)
        else:
            list_text_pos.insert(0, list_text_pos[0] - delta_x_te

# move annotation to left, if the label is out of the axes range
if len(list_text_pos) > 0 and max(list_text_pos) >= length_x_axis
    print("move labels to left")
    calc_delta = max(list_text_pos) - length_x_axis_pixel
    for index in range(len(list_text_pos) - 1, 0, -1):
        print("change", list_text_pos[index], calc_delta)
        if index > 1 and list_text_pos[index] - calc_delta > list
            list_text_pos[index] = list_text_pos[index] - calc_de
            break
        else:
            list_text_pos[index] = list_text_pos[index] - calc_de

for i in caption_values.index:

    label_x_pos = list_text_pos.pop()
    x_value = float(caption_values.loc[i, "m/z"])
    y_value = float(caption_values.loc[i, "intensity_normalized"]
    label_text = str(caption_values.loc[i, "caption"])

    x_value_pixel = (x_value - x_axis_min) / (x_axis_max - x_axis
    y_value_pixel = (y_value - y_axis_min) / (y_axis_max - y_axis
    label_y_pos_pixel = length_y_axis_pixel + delta_y_baseline_ax
    length_y_annotation_line = label_y_pos_pixel - y_value_pixel
    label_annotate_arm_low_pixel = length_y_annotation_line - lab

    if label_annotate_arm_low_pixel < 0:
        label_annotate_arm_low_pixel = 0

    ax.annotate("{:.0f}".format(x_value),
                xy=(x_value_pixel, y_value_pixel + delta_point_ar
                xycoords='axes pixels', rotation=90,
                xytext=(label_x_pos, label_y_pos_pixel),
                textcoords='axes pixels', size=8,
                    arrowprops=dict(arrowstyle="-",
                                    connectionstyle="arc,angleA=-90,a
                                                    ",angleB= 90,armB
                                                    ",rad=0", linewid
                    horizontalalignment='center', verticalalignment='
        ax.annotate(label_text,
                    xy=(x_value_pixel, y_value_pixel + delta_point_an
                    xycoords='axes pixels', rotation=90,
                    xytext=(label_x_pos, label_y_pos_pixel + delta_la
                    textcoords='axes pixels', size=8,
                    horizontalalignment='center', verticalalignment='
                    )

# remove top and right axis
ax.spines['top'].set_visible(False)
ax.spines['right'].set_visible(False)
ax.get_xaxis().tick_bottom()
ax.get_yaxis().tick_left()

# label axes
ax.set_xlabel(r"$m/z$")
ax.set_ylabel(r"$Intensity\,[\%]$")

# set x labels
plt.xticks(rotation='vertical')
start, end = ax.get_xlim()
ax.xaxis.set_ticks(np.arange(start, end + 1, 25))

# set y labels
ax.set_ylim(0, 100)
start, end = ax.get_ylim()
ax.yaxis.set_ticks(np.arange(start, end + 1, 10))

# set grid
plt.grid(True, axis="y", color='black', linestyle=':', linewidth=0.1)
plt.show()

plt.savefig(output_filename + "." + filetype, dpi=fig.dpi, format=fil
plt.close()
```

```
In [118]: def generate_massspectra_two_plot_manual_annotation(input_filename1, inpu
              print("Generate {0} mass spectra plot ({1}.{2}) from {3}.xy and {4}.x



              # min and max value of the x axis
              min_xaxis = 50
              max_xaxis = 475
```

```
# labels
label1 = "Substance 1"
label2 = "Substance 2"

# dimensions of the single plot
figwidth_mm = 141
left_margin_mm = 14
right_margin_mm = 2
top_margin_mm = 5
bottom_margin_mm = 13

plotwidth_mm = figwidth_mm - left_margin_mm - right_margin_mm
plotheight_mm = plotwidth_mm * 0.8

hspace_mm = 25  # horizontal space between two plots

# read xy input data
raw_values1 = pd.read_csv(input_filename1 + ".xy", sep=" ", names=["m
                          dtype={"m/z": np.float64, "intensity": np.f
# normalize input data
max_val = np.max(raw_values1['intensity'])
raw_values1["intensity_normalized"] = raw_values1['intensity'] / max_

# read xy input data
raw_values2 = pd.read_csv(input_filename2 + ".xy", sep=" ", names=["m
                          dtype={"m/z": np.float64, "intensity": np.f
# normalize input data
max_val = np.max(raw_values2['intensity'])
raw_values2["intensity_normalized"] = raw_values2['intensity'] / max_

fsize, margins = __figsize_and_margins(plotsize=(__conv_inch(plotwidt
                                       subplots=(1, 1),
                                       left=__conv_inch(left_margin_m
                                       top=__conv_inch(top_margin_mm)
                                       wspace=0.01, hspace=__conv_inc
fig = plt.figure(figsize=fsize, )
plt.subplots_adjust(**margins)

ax = fig.add_subplot(211)

# plot spectra line
plt1, = ax.plot(raw_values1["m/z"], raw_values1["intensity_normalized
legend = plt.legend(handles=[plt1], loc=2)
legend.get_frame().set_linewidth(0)

# set x axes range
if min_xaxis is not None and max_xaxis is not None:
    ax.set_xlim([int(min_xaxis), int(max_xaxis)])

# annotate plot1
annotate_point(253, 60, r'Peak 1', raw_values1)
annotate_distance(385, 403, 45, r'$-18$', raw_values1, rotate_text=90
annotate_distance(367, 385, 45, r'$-18$', raw_values1, rotate_text=90
annotate_distance(321, 349, 75, r'$xy$', raw_values1, rotate_text=0)
annotate_point(403, 60, r'Peak 2', raw_values1)

# remove top and right axis
ax.spines['top'].set_visible(False)
ax.spines['right'].set_visible(False)
ax.get_xaxis().tick_bottom()
ax.get_yaxis().tick_left()

# label axes
ax.set_ylabel(r"$Intensity\,[\%]$")

# set x labels
plt.xticks(rotation='vertical')
start, end = ax.get_xlim()
ax.xaxis.set_ticks(np.arange(start, end + 1, 25))

# set y labels
ax.set_ylim(0, 100)
start, end = ax.get_ylim()
ax.yaxis.set_ticks(np.arange(start, end + 1, 10))

# set grid
plt.grid(True, axis="y", color='black', linestyle=':', linewidth=0.1)

# set x labels
plt.xticks(rotation='vertical')
start, end = ax.get_xlim()
ax.xaxis.set_ticks(np.arange(start, end + 1, 25))
# set y labels
ax.set_ylim(0, 100)
start, end = ax.get_ylim()
ax.yaxis.set_ticks(np.arange(start, end + 1, 10))
# set grid
plt.grid(True, axis="y", color='black', linestyle=':', linewidth=0.1)

# generate plot2
ax = fig.add_subplot(212)

plt2, = ax.plot(raw_values2["m/z"], raw_values2["intensity_normalized
                label=label2)
legend = plt.legend(handles=[plt2], loc=2)
```

```
              legend.get_frame().set_linewidth(0)

              # set x axes range
              if min_xaxis is not None and max_xaxis is not None:
                  ax.set_xlim([int(min_xaxis), int(max_xaxis)])

              # annotate
              annotate_point(253, 60, r'Peak I', raw_values2)
              annotate_point(189, 60, r'189', raw_values2)
              annotate_point(215, 60, r'215', raw_values2)
              annotate_distance(385, 445, 30, r'Multiple'"\n"r'line'"\n"'annotation
              annotate_distance(367, 385, 45, r' -18', raw_values2, rotate_text=90)
              annotate_distance(349, 367, 45, r' -18', raw_values2, rotate_text=90)
              annotate_distance(321, 349, 75, r'xy', raw_values2, rotate_text=0)
              annotate_point(445, 60, r'Peak 2', raw_values2)

              # remove top and right axis
              ax.spines['top'].set_visible(False)
              ax.spines['right'].set_visible(False)
              ax.get_xaxis().tick_bottom()
              ax.get_yaxis().tick_left()

              # label axes
              ax.set_xlabel(r"$m/z$")
              ax.set_ylabel(r"$Intensity\,[\%]$")

              # set x labels
              plt.xticks(rotation='vertical')
              start, end = ax.get_xlim()
              ax.xaxis.set_ticks(np.arange(start, end + 1, 25))

              # set y labels
              ax.set_ylim(0, 100)
              start, end = ax.get_ylim()
              ax.yaxis.set_ticks(np.arange(start, end + 1, 10))

              # set grid
              plt.grid(True, axis="y", color='black', linestyle=':', linewidth=0.1)
              plt.show()

              plt.savefig(output_filename + "." + filetype, dpi=fig.dpi, format=fil
              plt.close()

In [119]: def generate_massspectra_plot_distance_peak_manual_annotation(input_filen
              print("Generate {0} mass spectra plot ({1}.{2}) from {3}.[xy/txt]".fo


              # min and max value of the x axis
```

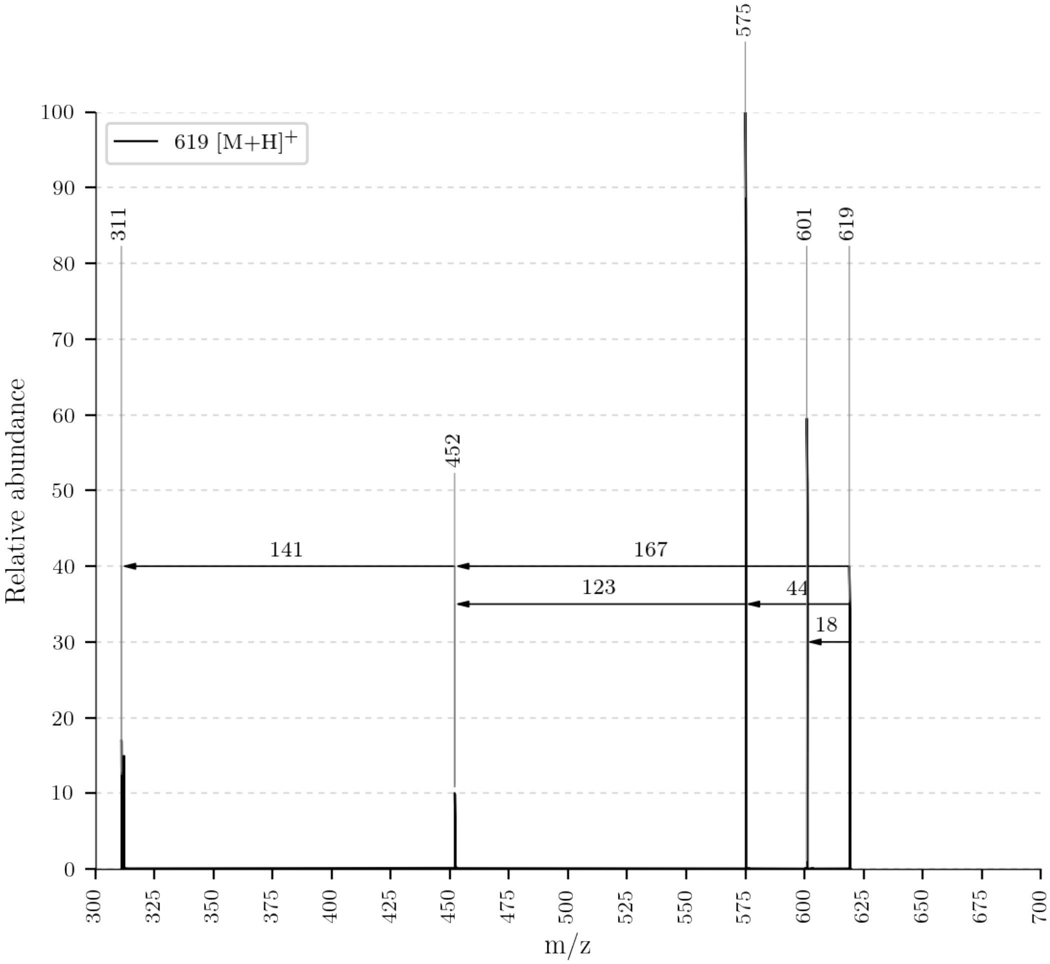
```
min_xaxis = 300
max_xaxis = 700

plotSubstance = '619 [M+H]^+^'

# dimensions of the single plot
figwidth_mm = 141
left_margin_mm = 14
right_margin_mm = 2
top_margin_mm = 5
bottom_margin_mm = 13

plotwidth_mm = figwidth_mm - left_margin_mm - right_margin_mm
plotheight_mm = plotwidth_mm * 0.8

hspace_mm = 0.1  # horizontal space between two plots

# read xy input data
raw_values = pd.read_csv(input_filename + ".xy", sep=" ", names=["m/z
                         dtype={"m/z": np.float32, "intensity": np.fl
# normalize input data
max_val = np.max(raw_values['intensity'])
raw_values["intensity_normalized"] = (raw_values['intensity'] / max_v

fsize, margins = __figsize_and_margins(plotsize=(__conv_inch(plotwidt
                                       subplots=(1, 1),
                                       left=__conv_inch(left_margin_m
                                       top=__conv_inch(top_margin_mm)
                                       wspace=0.01, hspace=__conv_inc
fig = plt.figure(figsize=fsize, )
plt.subplots_adjust(**margins)
ax = fig.add_subplot(111)

# plot spectra line
line1 = ax.plot(raw_values["m/z"], raw_values["intensity_normalized"]
plt.legend([plotSubstance],loc=2)

# set x axes range
if min_xaxis is not None and max_xaxis is not None:
    ax.set_xlim([int(min_xaxis), int(max_xaxis)])

# annotations
# length in data value (in %)
annotate_distance(619, 601, 30, '$18$', raw_values, rotate_text=0)
annotate_distance(619, 575, 35, '$44$', raw_values, rotate_text=0)
annotate_distance(619, 452, 40, '$167$', raw_values, rotate_text=0)
annotate_distance(575, 452, 35, '$123$', raw_values, rotate_text=0)
annotate_distance(452, 311, 40, '$141$', raw_values, rotate_text=0)
```

```
annotate_point(619, 83, r'619', raw_values)
annotate_point(601, 83, r'601', raw_values)
annotate_point(575, 110, r'575', raw_values)
annotate_point(452, 53, r'452', raw_values)
annotate_point(311, 83, r'311', raw_values)

#633
#annotate_distance(633, 601, 5, '$32$', raw_values, rotate_text=0)
#annotate_distance(633, 583, 10, '$50$', raw_values, rotate_text=0)
#annotate_distance(633, 557, 15, '$76$', raw_values, rotate_text=0)
#annotate_distance(633, 510, 20, '$123$', raw_values, rotate_text=0)
#annotate_distance(633, 496, 25, '$137$', raw_values, rotate_text=0)
#annotate_distance(633, 478, 30, '$155$', raw_values, rotate_text=0)
#annotate_distance(633, 460, 35, '$173$', raw_values, rotate_text=0)
#annotate_distance(633, 367, 40, '$266$', raw_values, rotate_text=0)
#annotate_distance(633, 337, 45, '$296$', raw_values, rotate_text=0)
#annotate_distance(633, 313, 50, '$320$', raw_values, rotate_text=0)
#annotate_distance(633, 287, 55, '$346$', raw_values, rotate_text=0)
#annotate_distance(510, 496, 5, '$14$', raw_values, rotate_text=0)
#annotate_distance(510, 478, 10, '$32$', raw_values, rotate_text=0)
#annotate_distance(510, 369, 65, '$141$', raw_values, rotate_text=0)
#annotate_distance(510, 337, 60, '$173$', raw_values, rotate_text=0)
#annotate_distance(460, 442, 5, '$18$', raw_values, rotate_text=0)
#annotate_distance(460, 432, 10, '$28$', raw_values, rotate_text=0)
#annotate_distance(460, 400, 15, '$60$', raw_values, rotate_text=0)
#annotate_distance(460, 337, 20, '$123$', raw_values, rotate_text=0)
#annotate_distance(460, 325, 25, '$135$', raw_values, rotate_text=0)
#annotate_distance(460, 297, 30, '$163$', raw_values, rotate_text=0)
#annotate_distance(337, 319, 65, '$18$', raw_values, rotate_text=0)
#annotate_distance(337, 309, 60, '$28$', raw_values, rotate_text=0)

#annotate_point(633, 83, r'633', raw_values)
#annotate_point(601, 110, r'601', raw_values)
#annotate_point(583, 83, r'583', raw_values)
#annotate_point(557, 83, r'557', raw_values)
#annotate_point(510, 83, r'510', raw_values)
#annotate_point(496, 83, r'496', raw_values)
#annotate_point(478, 83, r'478', raw_values)
#annotate_point(460, 83, r'460', raw_values)
#annotate_point(442, 83, r'442', raw_values)
#annotate_point(432, 83, r'432', raw_values)
#annotate_point(400, 83, r'400', raw_values)
#annotate_point(369, 93, r'369', raw_values)
#annotate_point(367, 83, r'367', raw_values)
#annotate_point(337, 83, r'337', raw_values)
#annotate_point(325, 73, r'325', raw_values)
#annotate_point(319, 83, r'319', raw_values)
```

```
              #annotate_point(313, 73, r'313', raw_values)
              #annotate_point(309, 83, r'309', raw_values)
              #annotate_point(297, 73, r'297', raw_values)
              #annotate_point(287, 83, r'287', raw_values)

              # remove top and right axis
              ax.spines['top'].set_visible(False)
              ax.spines['right'].set_visible(False)
              ax.get_xaxis().tick_bottom()
              ax.get_yaxis().tick_left()

              # label axes
              ax.set_xlabel("m/z")
              ax.set_ylabel("Relative abundance") #$Relative abundance\,[\%]$

              # set x labels
              plt.xticks(rotation='vertical')
              start, end = ax.get_xlim()
              ax.xaxis.set_ticks(np.arange(start, end + 1, 25))

              # set y labels
              ax.set_ylim(0, 100)
              start, end = ax.get_ylim()
              ax.yaxis.set_ticks(np.arange(start, end + 1, 10))

              # set grid
              plt.grid(True, axis="y", color='black', linestyle=':', linewidth=0.1)
              plt.savefig(output_filename + ".png")

              plt.show()
              plt.close()
```

```
In [120]: if __name__ == "__main__":
              # generate_massspectra_plot_automatic_labels("examples/inputs/substan

              generate_massspectra_plot_distance_peak_manual_annotation("data/raw/K

              # generate_massspectra_two_plot_manual_annotation("examples/inputs/su
```

```
Generate PNG mass spectra plot (data/ex2.png) from data/raw/Kuerbis_Analyse_Bindung
```


619 [M+H]+
575
311
601
619
452
141
167
123
44
18
Relative abundance
0
10
20
30
40
50
60
70
80
90
100
300
325
350
375
400
425
450
475
500
525
550
575
600
625
650
675
700
m/z

```
In [ ]:
```