VWA_Analyse_LC-ESI-MS

October 25, 2017

In [22]:
```
def cc(arg):
    return mcolors.to_rgba(arg, alpha=0.6)
```

In [23]:
```
def detect_peaks(x, mph=None, mpd=1, threshold=0, edge='rising',
                 kpsh=False, valley=False, show=False, ax=None):

    """Detect peaks in data based on their amplitude and other features.

    Parameters
    ----------
    x : 1D array_like
        data.
    mph : {None, number}, optional (default = None)
        detect peaks that are greater than minimum peak height.
    mpd : positive integer, optional (default = 1)
        detect peaks that are at least separated by minimum peak distance
        number of data).
    threshold : positive number, optional (default = 0)
        detect peaks (valleys) that are greater (smaller) than `threshold`
        in relation to their immediate neighbors.
    edge : {None, 'rising', 'falling', 'both'}, optional (default = 'risi
        for a flat peak, keep only the rising edge ('rising'), only the
        falling edge ('falling'), both edges ('both'), or don't detect a
        flat peak (None).
    kpsh : bool, optional (default = False)
        keep peaks with same height even if they are closer than `mpd`.
    valley : bool, optional (default = False)
        if True (1), detect valleys (local minima) instead of peaks.
    show : bool, optional (default = False)
        if True (1), plot data in matplotlib figure.
    ax : a matplotlib.axes.Axes instance, optional (default = None).

    Returns
    -------
    ind : 1D array_like
        indeces of the peaks in `x`.
```

```
    Notes
    -----
    The detection of valleys instead of peaks is performed internally by s
    negating the data: `ind_valleys = detect_peaks(-x)`

    The function can handle NaN's

    See this IPython Notebook [1]_.

    References
    ----------
    .. [1] http://nbviewer.ipython.org/github/demotu/BMC/blob/master/noteb

    Examples
    --------
    >>> from detect_peaks import detect_peaks
    >>> x = np.random.randn(100)
    >>> x[60:81] = np.nan
    >>> # detect all peaks and plot data
    >>> ind = detect_peaks(x, show=True)
    >>> print(ind)

    >>> x = np.sin(2*np.pi*5*np.linspace(0, 1, 200)) + np.random.randn(200
    >>> # set minimum peak height = 0 and minimum peak distance = 20
    >>> detect_peaks(x, mph=0, mpd=20, show=True)

    >>> x = [0, 1, 0, 2, 0, 3, 0, 2, 0, 1, 0]
    >>> # set minimum peak distance = 2
    >>> detect_peaks(x, mpd=2, show=True)

    >>> x = np.sin(2*np.pi*5*np.linspace(0, 1, 200)) + np.random.randn(200
    >>> # detection of valleys instead of peaks
    >>> detect_peaks(x, mph=0, mpd=20, valley=True, show=True)

    >>> x = [0, 1, 1, 0, 1, 1, 0]
    >>> # detect both edges
    >>> detect_peaks(x, edge='both', show=True)

    >>> x = [-2, 1, -2, 2, 1, 1, 3, 0]
    >>> # set threshold = 2
    >>> detect_peaks(x, threshold = 2, show=True)
    """

    x = np.atleast_1d(x).astype('float64')
    if x.size < 3:
        return np.array([], dtype=int)
    if valley:
        x = -x
```

```
    # find indices of all peaks
    dx = x[1:] - x[:-1]
    # handle NaN's
    indnan = np.where(np.isnan(x))[0]
    if indnan.size:
        x[indnan] = np.inf
        dx[np.where(np.isnan(dx))[0]] = np.inf
    ine, ire, ife = np.array([[], [], []], dtype=int)
    if not edge:
        ine = np.where((np.hstack((dx, 0)) < 0) & (np.hstack((0, dx)) > 0)
    else:
        if edge.lower() in ['rising', 'both']:
            ire = np.where((np.hstack((dx, 0)) <= 0) & (np.hstack((0, dx))
        if edge.lower() in ['falling', 'both']:
            ife = np.where((np.hstack((dx, 0)) < 0) & (np.hstack((0, dx))
    ind = np.unique(np.hstack((ine, ire, ife)))
    # handle NaN's
    if ind.size and indnan.size:
        # NaN's and values close to NaN's cannot be peaks
        ind = ind[np.in1d(ind, np.unique(np.hstack((indnan, indnan-1, indn
    # first and last values of x cannot be peaks
    if ind.size and ind[0] == 0:
        ind = ind[1:]
    if ind.size and ind[-1] == x.size-1:
        ind = ind[:-1]
    # remove peaks < minimum peak height
    if ind.size and mph is not None:
        ind = ind[x[ind] >= mph]
    # remove peaks - neighbors < threshold
    if ind.size and threshold > 0:
        dx = np.min(np.vstack([x[ind]-x[ind-1], x[ind]-x[ind+1]]), axis=0)
        ind = np.delete(ind, np.where(dx < threshold)[0])
    # detect small peaks closer than minimum peak distance
    if ind.size and mpd > 1:
        ind = ind[np.argsort(x[ind])][::-1]  # sort ind by peak height
        idel = np.zeros(ind.size, dtype=bool)
        for i in range(ind.size):
            if not idel[i]:
                # keep peaks with the same height if kpsh is True
                idel = idel | (ind >= ind[i] - mpd) & (ind <= ind[i] + mpd
                    & (x[ind[i]] > x[ind] if kpsh else True)
                idel[i] = 0  # Keep current peak
        # remove the small peaks and sort back the indices by their occurr
        ind = np.sort(ind[~idel])

    if show:
        if indnan.size:
            x[indnan] = np.nan
```

```
            if valley:
                x = -x
            _plot(x, mph, mpd, threshold, edge, valley, ax, ind)

        return ind


    def _plot(x, mph, mpd, threshold, edge, valley, ax, ind):
        """Plot results of the detect_peaks function, see its help."""
        try:
            import matplotlib.pyplot as plt
        except ImportError:
            print('matplotlib is not available.')
        else:
            if ax is None:
                _, ax = plt.subplots(1, 1, figsize=(8, 4))

            ax.plot(x, 'b', lw=1)
            if ind.size:
                label = 'valley' if valley else 'peak'
                label = label + 's' if ind.size > 1 else label
                ax.plot(ind, x[ind], '+', mfc=None, mec='r', mew=2, ms=8,
                        label='%d %s' % (ind.size, label))
                ax.legend(loc='best', framealpha=.5, numpoints=1)
            ax.set_xlim(-.02*x.size, x.size*1.02-1)
            ymin, ymax = x[np.isfinite(x)].min(), x[np.isfinite(x)].max()
            yrange = ymax - ymin if ymax > ymin else 1
            ax.set_ylim(ymin - 0.1*yrange, ymax + 0.1*yrange)
            ax.set_xlabel('Data #', fontsize=14)
            ax.set_ylabel('Amplitude', fontsize=14)
            mode = 'Valley detection' if valley else 'Peak detection'
            ax.set_title("%s (mph=%s, mpd=%d, threshold=%s, edge='%s')"
                         % (mode, str(mph), mpd, str(threshold), edge))
            # plt.grid()
            plt.show()
```

In [24]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from matplotlib import colors as mcolors
from scipy.signal import argrelextrema
from scipy.signal import find_peaks_cwt

from numpy import trapz
```

In [25]:
```
data = pd.io.parsers.read_csv("Kuerbis_Analyse_7min_LC-ESI-MS_12min.csv")

helpvalue = ['617', '619', '629', '631', '633.23', '633.29', '645', '647.2
```

```
        #helpvalue = ['619', '633.23', '645', '647', '675', '821']

        xs = data[['Zeit']].values
        xs = np.hstack(xs)

        list_x_values = []
        list_y_values = []
        list_catabolite = []
        list_isomer = []
```

In [26]:
```
        ys = 0
        i = 0
        highest_peak = []

        fig = plt.figure(figsize=(20,10))
        ax = plt.axes()

        area_617 = 0
        area_619 = 0
        area_631 = 0
        area_63329 = 0
        area_645 = 0
        area_647 = 0
        area_659 = 0
        area_661 = 0
        area_675 = 0
        area_793 = 0
        area_795 = 0
        area_807 = 0
        area_809 = 0
        area_821 = 0

        height_617 = 0
        height_619 = 0
        height_631 = 0
        height_63329 = 0
        height_645 = 0
        height_647 = 0
        height_659 = 0
        height_661 = 0
        height_675 = 0
        height_793 = 0
        height_795 = 0
        height_807 = 0
        height_809 = 0
        height_821 = 0

        distance_for_integration = 0.1
```

```
for h in helpvalue:
    ys = data[[helpvalue[i]]].values
    ys = np.hstack(ys)

    highest_peak.append(ys.max())

    if (i == 0):
        print(helpvalue[i])
        area_617 = trapz(ys, dx=distance_for_integration)
        height_617 = ys.max()
    elif (i == 1):
        print(helpvalue[i])
        area_619 = trapz(ys, dx=distance_for_integration)
        height_619 = ys.max()
    elif (i == 3):
        print(helpvalue[i])
        area_631 = trapz(ys, dx=distance_for_integration)
        height_631 = ys.max()
    elif (i == 5):
        print(helpvalue[i])
        area_63329 = trapz(ys, dx=distance_for_integration)
        height_63329 = ys.max()
    elif (i == 6):
        print(helpvalue[i])
        area_645 = trapz(ys, dx=distance_for_integration)
        height_645 = ys.max()
    elif (i == 7):
        print(helpvalue[i])
        area_647 = trapz(ys, dx=distance_for_integration)
        height_647 = ys.max()
    elif (i == 10):
        print(helpvalue[i])
        area_659 = trapz(ys, dx=distance_for_integration)
        height_659 = ys.max()
    elif (i == 11):
        print(helpvalue[i])
        area_661 = trapz(ys, dx=distance_for_integration)
        height_661 = ys.max()
    elif (i == 12):
        print(helpvalue[i])
        area_675 = trapz(ys, dx=distance_for_integration)
        height_675 = ys.max()
    elif (i == 13):
        print(helpvalue[i])
        area_793 = trapz(ys, dx=distance_for_integration)
        height_793 = ys.max()
    elif (i == 14):
```

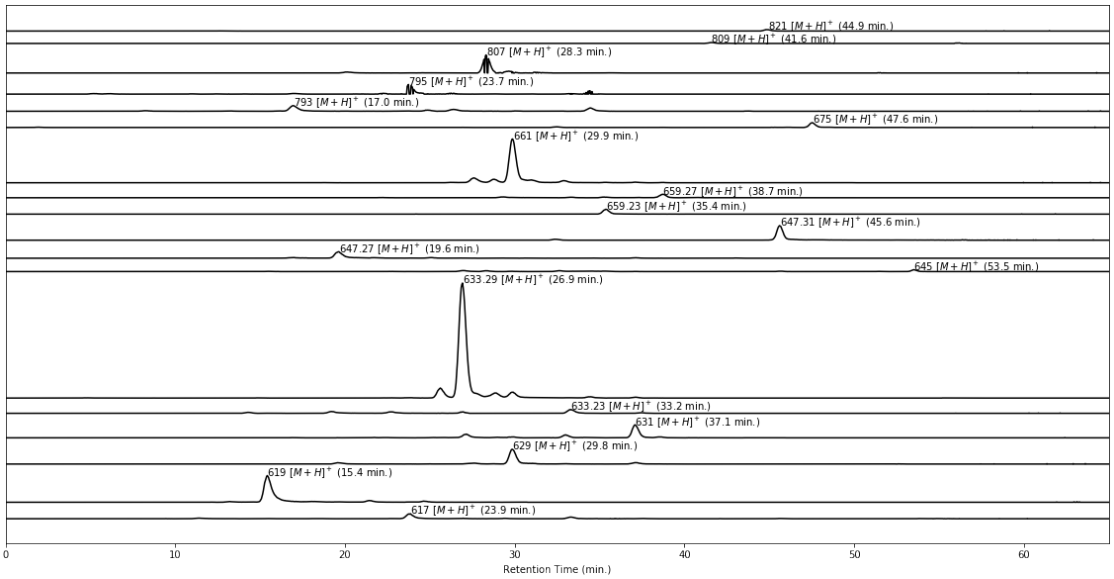
```
            print(helpvalue[i])
            area_795 = trapz(ys, dx=distance_for_integration)
            height_795 = ys.max()
        elif (i == 15):
            print(helpvalue[i])
            area_807 = trapz(ys, dx=distance_for_integration)
            height_807 = ys.max()
        elif (i == 16):
            print(helpvalue[i])
            area_809 = trapz(ys, dx=distance_for_integration)
            height_809 = ys.max()
        elif (i == 17):
            print(helpvalue[i])
            area_821 = trapz(ys, dx=distance_for_integration)
            height_821 = ys.max()

        i = i+1

Ka_617 = area_631/area_617
Kh_617 = height_631/height_617
Ka_619 = area_63329/area_619
Kh_619 = height_63329/height_619
Ka_645 = area_659/area_645
Kh_645 = height_659/height_645
Ka_647 = area_661/area_647
Kh_647 = height_661/height_647
Ka2_647 = area_675/area_647
Kh2_647 = height_675/height_647
Ka_793 = area_807/area_793
Kh_793 = height_807/height_793
Ka2_793 = area_821/area_793
Kh2_793 = height_821/height_793
Ka_795 = area_809/area_795
Kh_795 = height_809/height_795

print('Ka_617')
print(Ka_617)
print(Kh_617)
print('Ka_619')
print(Ka_619)
print(Kh_619)
print('Ka_645')
print(Ka_645)
print(Kh_645)
print('Ka_647')
print(Ka_647)
print(Kh_647)
print('Ka2_647')
```

```
print(Ka2_647)
print(Kh2_647)
print('Ka_793')
print(Ka_793)
print(Kh_793)
print('Ka2_793')
print(Ka2_793)
print(Kh2_793)
print('Ka_795')
print(Ka_795)
print(Kh_795)


highest_peak = np.array(highest_peak).max()

ys = 0
i=0
previous_mass = 0

for h in helpvalue:
    ys = data[[helpvalue[i]]].values
    ys = np.hstack(ys)

    y = []
    for x in ys:
        y.append(((x/highest_peak)*100)+previous_mass+10)

    y = np.array(y)

    previous_mass = y.max()
    x_max_arg = y.argmax()

    #local_maxima = argrelextrema(y, np.greater, order=200)
    #local_maxima = find_peaks_cwt(y, np.arange(1, 350))
    local_maxima = detect_peaks(y, mph=0.04, mpd=350)
    #first_isomer = np.partition(np.array(y).flatten(), -1)[-1]
    #first_isomer = np.round(np.array(np.hstack(y)[local_maxima])).argsort
    #print(first_isomer)
    #y_help = np.sort(y[local_maxima])

    line = plt.plot(xs, y, color = 'black', label = h + '[M+H]^+^')
    ax.annotate(xy=(xs[x_max_arg], previous_mass), s = h + r' $[M+H]^+$ ('

    list_x_values.append(xs[x_max_arg])
    list_y_values.append(previous_mass)
    list_catabolite.append(h)

    #u=1
```

```
                #for x in xs[local_maxima]:
                    #ax.annotate(xy=(x, y[np.where(x)]), s = h + r' $[M+H]^+$-Isomer

                    #list_x_values.append(x)
                    #list_y_values.append(y[np.where(x)])
                    #list_catabolite.append(h)
                    #list_isomer.append(u)

                    #u = u+1

                i = i+1

            plt.yticks([])
            plt.xlabel('Retention Time (min.)')
            plt.xlim(0,65)
            plt.savefig('Kuerbis_Analyse_Reaktion3h_LC-ESI-MS.png')
            plt.show()
```

```
617
619
631
633.29
645
647.27
659.27
661
675
793
795
807
809
821
Ka_617
2.04496546098
2.61835424334
Ka_619
3.72894401481
4.30577315565
Ka_645
0.952718937384
1.90972196983
Ka_647
4.46006879328
6.6850336666
Ka2_647
0.50313171312
0.722832075087
Ka_793
```

```
0.998319279587
3.20375262079
Ka2_793
0.112793086295
0.266083083593
Ka_795
0.118012120986
0.093094387365
```




```
In [27]: data = pd.io.parsers.read_csv("Kuerbis_Analyse_7min_LC-ESI-MS_12min_Spektr

         xs = data[['Time']].values
         xs = np.hstack(xs)

         ys = data[['Intensity']].values
         ys = np.hstack(ys)

In [28]: fig = plt.figure(figsize=(20,10))
         ax = plt.axes()


         #ax.annotate(xy=(xs[x_max_arg], previous_mass), s = h + r' $[M+H]^+$ ('+st

         highest_peak = np.array(ys).max()
         y = []
         for z in ys:
             y.append(((z/highest_peak)*100))
```

```
ys = y

line = plt.plot(xs, ys, color = 'black', label = '')

highest_peak = np.array(list_y_values).max()
helper = []
for t in list_y_values:
    helper.append(((t/highest_peak)*100))
list_y_values = helper

i = 0
for index in list_x_values:
    h = list_catabolite[i]
    #u = list_isomer[i]
    text = h + r' $[M+H]^+$ ('+str(np.round(index, 1))+' min.)'
    plt.annotate(
            text, xy=(index, 0), xycoords='data',
            xytext=(index, list_y_values[i]), textcoords='data',
            rotation=0, size=12, horizontalalignment='center', verticalali
            arrowprops=dict(arrowstyle='-', color="#808080", linewidth=0.4
    i = i+1

#ax.annotate(xy=(x, y[np.where(x)]), s = h + r' $[M+H]^+$-Isomer '+str(u)+

plt.xlabel('Retention Time (min.)')
plt.ylabel('Relative abundance')
plt.xlim(0,65)
plt.savefig('Kuerbis_Analyse_Ganzes_Spektrum.png')
plt.show()
```