

## **ToFIND version 1.0 (Oct 2011)**

### **INSTRUCTION**

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The **Time-of-Flight INterpretation moDule (ToFIND)** is a toolbox written in MATLAB language. It is used to process data obtained from Proton-Transfer-Reaction Time-of-Flight Mass Spectrometry (PTR-ToF-MS), the toolbox consists of two major files: ToFIND\_masscorr.m and ToFIND\_main.m.

### **INSTALLATION:**

Save those two files into any folder that is on the MATLAB search path. If the current folder containing those two files is not on MATLAB search path, set it in MATLAB by going to File>Set Path.

ToFIND has been tested successfully on MATLAB R2010a and latter versions, it depends on MATLAB Optimization Toolbox, make sure it is installed on your system. You can check the Dependency Report of the functions in the Editor window by going to Tools>Show Dependency Report.

The HDF5 file I/O depends on HDF5TOOLS, download it from:  
<http://www.mathworks.com/matlabcentral/fileexchange/17172-hdf5tools>

### **SYSTEM REQUIREMENT:**

At least 4 GB of memory, 6 GB memory preferred.

### **ToFIND\_masscorr.m**

This routine contains the main function (ToFIND\_masscorr) and subfunctions required to perform the mass correction on mass drift due to temperature variation. For detailed information on data processing algorithms refer to Müller, M., *et al.*, 2010 and DeCarlo, P., *et al.*, 2006.

#### **Syntax**

```
ToFIND_masscorr( )
```

#### **Description**

There is no argument input for this function. ToFIND\_masscorr will load the mass calibration parameters stored within each HDF5 file and use them as the initial value to perform mass correction, the output will be saved in a separate file.

**ALWAYS PERFORM MASS CORRECTION ON YOUR DATA FIRST!**

## ToFIND\_main.m

This routine contains the main function (ToFIND\_main) and subfunctions required to perform the data processing. For detailed information on data processing algorithms refer to Müller, M., *et al.*, 2010 and DeCarlo, P., *et al.*, 2006.

### Syntax

```
ToFIND_main(masstbl,peakList)
```

```
ToFIND_main(masstbl)
```

### Description

ToFIND\_main() performs curve fitting on peaks listed in `masstbl` by using the nonlinear least-squares method. It integrate the signal within the range for each peak and save the data in `.mat` file as the output.

ToFIND\_main(masstbl,peakList) does the calculation in manual mode.

ToFIND\_main(masstbl) does the calculation in automatic mode.

### Input Arguments

`masstbl` mass table that contains the exact  $m/z$  of the target peak

`peakList` peak list which contains the exact  $m/z$  for all the peaks within a nominal peak, including the target peak in `masstbl`. Refer to example below for syntax rules.

### Example

```
m=[33.03349,45.03349,59.04914,73.06479];  
p={[32.9979,33.03349],[44.9983,45.03349],59.04914,[72.9382,73.0270,73.06479]};  
ToFIND_main(m,p); % run in manual mode  
ToFIND_main(m); % run in automatic mode
```

`m` contains the exact  $m/z$  of the target peaks, while `p` contains the peak list for all peaks within each nominal peak. `m` can be a row or column vector, the exact  $m/z$  of the target peaks do not need to be in ascending or descending orders, it will be sorted latter by the program; `p` is a cell array, each element corresponds to the target peak in `m`, and it contains all the exact  $m/z$  within a nominal peak including the target peak. If there are more than one peak in a nominal peak, the element is a row vector in ascending order, otherwise, it is just the exact  $m/z$  of the target peak. ToFIND\_main has two calculation modes: when both `m` and `p` are supplied as inputs, it will do the calculation in manual mode, it uses the peak masses in `p` as parameters for curve fitting; if only `m` is supplied as input, it will do the calculation in automatic mode, all the peaks within a nominal peak will be found by a peak detection function and then they are used for curve fitting.

ALWAYS DO YOUR CALCULATIONS IN MANUAL MODE UNLESS YOU ARE VERY CONFIDENT OF YOUR DATA!

## REFERENCES

Müller, M., *et al.*, First eddy covariance flux measurements by PTR-TOF, *Atmos. Meas. Tech.*, 2010, 3, 387–395

DeCarlo, P., *et al.*, Field-Deployable, High-Resolution, Time-of-Flight Aerosol Mass Spectrometer, *Anal. Chem.*, 2006, 78, 8281–8289