

User Manual of EpiProfileLite

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A. Requirements:

1. Windows system (Windows 7 or later version, any Intel or AMD x86-64 processor, RAM with 2 GB or more).
2. Xcalibur and Matlab should be installed firstly.

B. Instructions:

1. modify the input parameters (open the folder 'EpiProfileLite', open the file 'paras.txt', put your data path after 'raw_path', set other parameters following the instructions).
2. start Matlab (in the folder 'EpiProfileLite', doubly click the file 'EpiProfileLite.m').
3. run EpiProfileLite (in the Matlab Command Window input “EpiProfileLite” and press “Enter”).

The results are under the data path (histone_layouts and histone_ratios.xls).

C. Steps:

Step 1 (modify the input parameters)

```
[EpiProfileLite]
```

```
% the datapath of raw files
```

```
raw_path= C:\F\Exp28_EpiProfile\RAW
```

```
% 1: Human, 2: Mouse
```

```
norganism=1
```

```
% 1: histone_normal, 2: histone_SILAC, 3: histone_C13, 4: histone_N15, 5: histone_13CD3
```

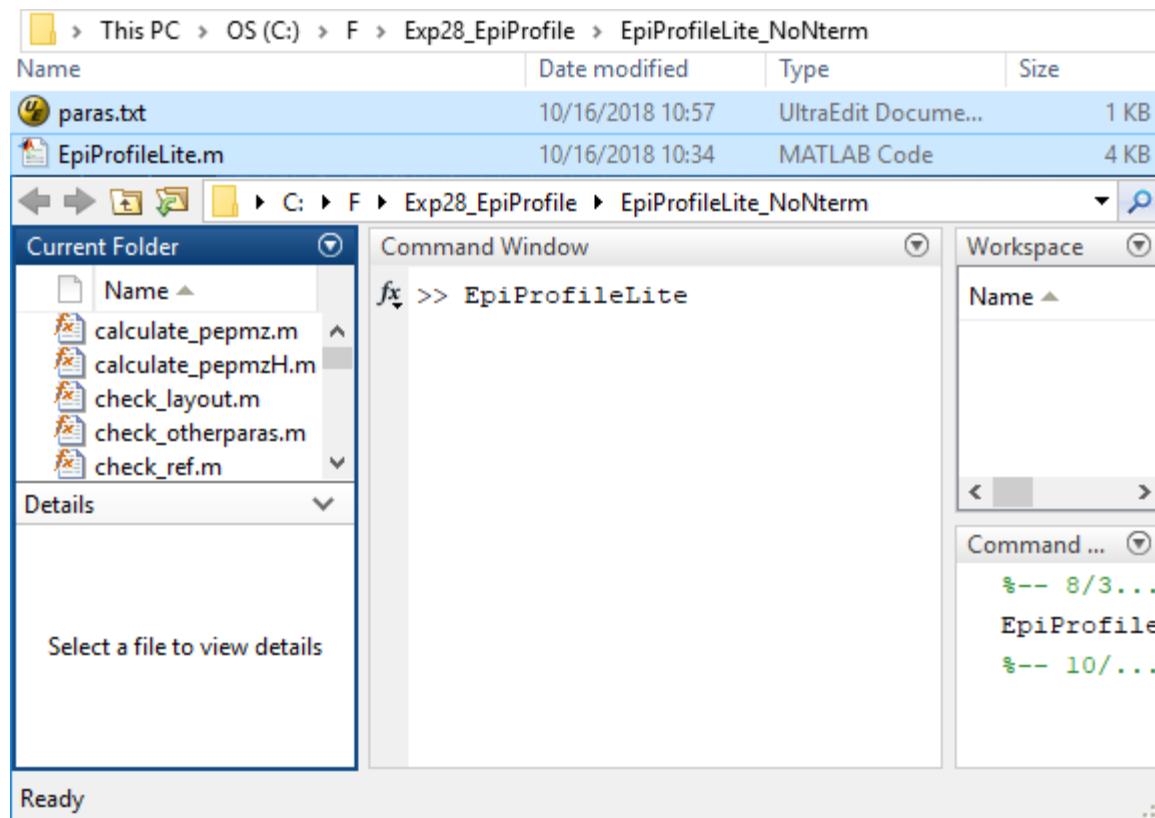
```
nsources=1
```

```
% if histone_N15, 0: N14 light Mods, 1: N15 light Mods, 2: N14 heavy Mods, 3: N15 heavy Mods, 4: 0+1, 5: 0+3
```

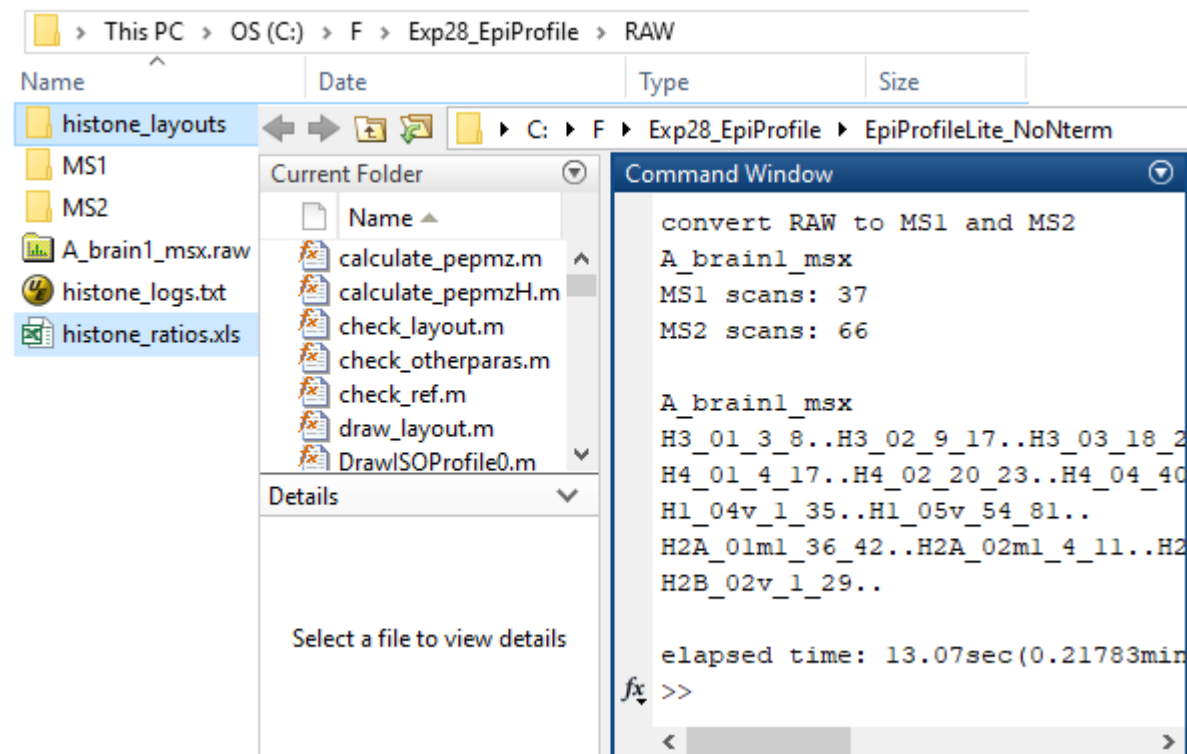
```
nsubtype=0
```

Step 2&3 (start Matlab and run EpiProfileLite)

Start and Run



Results



D. Advanced options

Note: these are advanced options which might need the author's help (zuoyuan@pennmedicine.upenn.edu).

1. Some options in 'paras.txt'. If "nsource=2", set "nsubtype=0" for SILAC of light and heavy R, and set "nsubtype=1" for SILAC of light and heavy K and R. "nsource=3" means two (2) ¹³C on acetylation. "nsource=4" and if "nsubtype" contains 15N means all N in each amino acid is labeled by 15N. "nsource=5" means ¹³CD₃ on methylation and Methionine. Currently, only "nsource=1" works.
2. How to set the peptide mass tolerance? In 'check_otherparas.m', the default setting is "def_ptol = 15", which means 15 ppm. If the mass tolerance is shifted to 20 or 30 ppm, then the value of "def_ptol" should be changed.
3. How to add a new PTM? In 'GetMods.m', the form and mass of a PTM can be added (e.g., cr is on K with the mass of 68.026215). In the corresponding *.m file (e.g. H3_02_9_17.m), the new PTM (e.g. K9cr) can be added into the function of 'init_histone', 'calculate_layout'. Again, it is better to ask the author to add a new PTM!!!

E. Trouble shooting

1. If Xcalibur is installed but EpiProfile cannot use Xcalibur to convert RAW to MS1 and MS2, then MSFileReader need be installed, which can be downloaded from <https://thermo.flexnetoperations.com>.
2. In addition to MATLAB, EpiProfile2.0 uses the following 3 toolboxes: Statistics and Machine Learning Toolbox, Curve Fitting Toolbox, and Bioinformatics Toolbox.
3. The application file 'xtract.exe' in the folder of 'EpiProfile' will expire on the end day of each year. Therefore, it needs be updated in the beginning of each year.