

# pParse User Guide

Version 2.0.0

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pFind Group

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# Before software installation

- ❖ **pParse is written by C++.**
- ❖ **Please install 64-bit MSFileReader first.**
- ❖ **Windows 7 and above**
  - **64 bit version**
  - **.NET Framework 4.5 environment**

# Software registration and installation

- ❖ Send the registration information to [pparse@ict.ac.cn](mailto:pparse@ict.ac.cn), and you'll get a software download link.
- ❖ pParse doesn't need to install. You can use it directly after decompressing “pParseStandAlone\_X64.zip” into a folder.
- ❖ The contents of the folder pParseStandAlone\_X64 are as follows:

 pParse.cfg	2017/5/26 17:06	1 KB
 pParse+ User Guide.pdf	2017/3/30 12:35	629 KB
 IPV.txt	2017/3/30 12:35	566 KB
 TrainingSet.txt	2017/3/30 12:35	144 KB
 pParse.exe	2017/3/30 12:35	389 KB
 xtract_raw.exe	2017/3/30 12:35	2,823 KB
 xtract_wiff.exe	2017/4/23 15:54	24 KB
 Clearcore.Licensing.dll	2015/11/11 13:47	122 KB
 Clearcore2.Data.AnalystDataProvider...	2015/11/11 13:47	96 KB
 Clearcore2.Data.CommonInterfaces.dll	2015/11/11 13:47	20 KB

## ❖ Two usable methods

- Usage 1:

Run pParse with parameter file

*pParse.exe pParse.para*

- Usage 2:

Run pParse with command line parameters

*pParse.exe -D D:\data\1.raw*

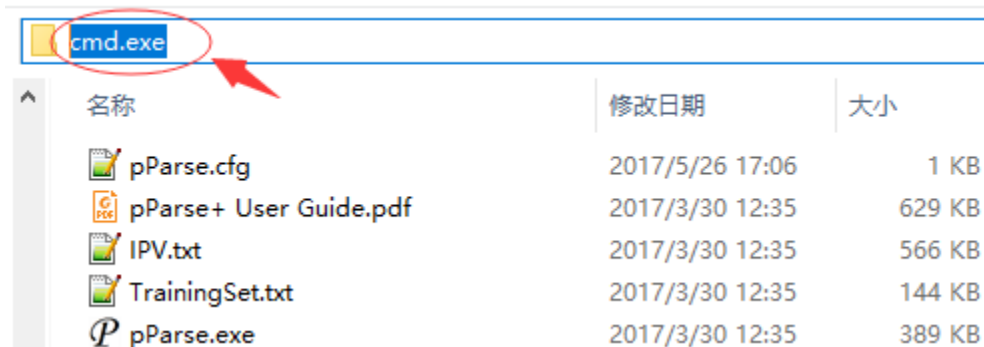
# Software usage 1

## ❖ Step 1

- Double click “pParse.exe” to generate a parameter file.

## ❖ Step 2

- Run “cmd.exe” in the folder where pParse was installed.



# Software usage 1

## ❖ Step 3

- Configure parameter file.
  - Set the parameter “datapath”, “co-elute” and “input\_format”.
  - Keep other parameters default.

```
5 [Basic Options]
6 datapath = E:\dataSet\std8\1.RAW
7
8 [Advanced Options]
9 co-elute = 1
10 # 0, output single precursor for single scan;
11 # 1, output all co-eluted precursors.
12 input_format = raw
13 # raw / msl
14 isolation_width = 2
15 # 2 / 2.5 / 3 / 4
16 mars_threshold = -0.5
17 ipv_file = .\IPV.txt
18 trainingset = EmptyPath
```

# Software usage 1

## ❖ Step 4

- Run command “*pParse.exe pParse.para*”.

```
C:\Windows\System32\cmd.exe
Microsoft Windows [版本 10.0.15063]
(c) 2017 Microsoft Corporation. 保留所有权利。

E:\pParseStandAlone_X64>pParse.exe pParse.para

*****
      pParse2.0 (x64) from pFind Studio
      Email  : pfind@ict.ac.cn
      Website: http://pfind.ict.ac.cn
*****

[pParse] Rawlist completes
[pParse] Calling pXtract to export MS1 and MS2 files...
[pXtract] The software will expire in 01/01/2018
[pXtract] Begin to extract E:\dataSet\std8\std8_trypsin_denovo_20090729.RAW
[pXtract] pXtract tries to use MSFilerReader
[pXtract] <Output files>: 100.00%
[pXtract] Output Files Completed!
[pXtract] == == == Time elapsed: 28.715s. == == ==
[pParse] MS1list completes.
[pParse] Processing std8_trypsin_denovo_20090729.ms1
[pParse] Loading MS1 and MS2 files...
[pParse] Loading MS1 Spectra Number: 2132
[pParse] Loading MS2 Spectra Number: 4752
[pParse] Writing MS1 to PF...
```



# Software usage 2

## ❖ Step 1

- Run “pParse.exe” to get usable command line parameters.

```
E:\pParseStandAlone_X64>pParse.exe

*****
<      pParse2.0 (x64) from pFind Studio      >
<      Email  : pfind@ict.ac.cn              >
<      Website: http://pfind.ict.ac.cn       >
*****

pParse Version-Release-2.0.8(x64)

What's New:
[2014.11.26] Bug      : RTINSECONDS is exported correctly.
[2014.11.25] Upgrade: SVM training set can be exported.
[2014.10.22] Upgrade: Crash report is available in pParse 2.0.
[2014.09.29] Bug      : The RAWs from Fusion instruments are supported.

Usage via config files:
pParse.exe pParse.para

Attention:
Carefully configured parameter file is required!
A standard parameter file named 'pParse.para' is generated.
```

# Software usage 2

## ❖ Step 1

- Run “pParse.exe” to get usable command line parameters.

```
More Options:
-D datapath          default (D:\data\)
-L logfilepath      default (the same with datapath)
-O outputpath       default (the same with datapath)
-W isolation_width  default (2)
-F input_format     default (raw) optional (wiff)
-C co-elute         default (1)
-S cut_similiar_mono default (1)
-I ipv_file         default (. \IPV. txt)
-M mars_model       default (4)
-T trainingset      default (. \TrainingSet. txt)
-m output_mgf       default (1)
-p output_pf        default (1)
-d delete_msn       default (0)
-a check_activationcenter default (1)
-g debug_mode       default (0)
-r rewrite_files    default (0)
-t mars_threshold   default (-0.5)
-u export_unchecked_mono default (0)
-y output_all_mars_y default (0)
-Y output_mars_y    default (0)
-s output_trainingdata default (0)
-R recalibrate_window default (7)
-v outputsvmlight   default (0)
```

# Software usage 2

## ❖ Step 2

- Use following command to run pParse

*pParse.exe -D D:\data\1.raw*

- Or (Keep other parameters default)

*pParse.exe -D D:\data\1.raw -O E:\data*

# Result files

## ❖ csv files

- Precursors information, same with .mgf file.

## ❖ pf files

- Binary files , including \*.pf1, \*.pf2, \*.pf1idx, \*.pf2idx.
- Used for pFind search engine.

## ❖ pParsePlusLog.txt

- pParse log file.

## ❖ xtract files

- Intermediate result file.



❖ **Thank you for using pParse!**

❖ **If you have any questions, please contact**  
**[pparse@ict.ac.cn](mailto:pparse@ict.ac.cn)**.