pParse+ User Guide

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Introduction

pParse+ is a software tool for extracting MS\MS spectra from *.RAW format. It inspects the isolation windows corresponding to each MS\MS spectra and exports the most possible precursors. Besides pParse+ recalibrates the mass of monoisotopic peak and could detect co-eluted precursors. Currently, users can set co-eluted as '0' to export only one recalibrated precursor monoisotopic peak for each MS\MS scan.
pParse+ do not need install. You can use it after decompressed it into a folder.

Recommended Minimum System Requirements

- CPU: Pentium III or higher
- Main Memory: 1GB
- Operating System: Windows XP/Vista/7/8
- **Xcalibur 2.1 or higher**

Usage 1

a. Set the parameters. A template of parameter configure file named pParse.para can be found in the folder where pParse+ is decompressed.
b. Save the parameter configure file and open command line prompt in current folder, run pParse+ as follow.

```
pParse.exe   pParse.para
```

Usage 2

Now pParse has 21 options and each option has a default value. Users need configure a few of them to run pParse. For example, both

```
pParse.exe –D D:\mydata\First.raw
```

and

```
pParse.exe –D D:\mydata\
```

are legal.

The command line

pParse.exe

will print a detailed user guide about usage of more options.

How to Set the Parameters?

To correctly run pParse+, users need to set a few parameters. Some of the parameters are very important. For example, if **co-eluted** is set as 1, pParse will export all co-eluted precursors.
Usually, users only need to set datapath to run pParse.exe.

```
[Basic Options]
datapath=E:\MannData\
# both folder or file is legal.
[Advanced Option]
co-elute=0
# 0, do not export co-eluted precursors.
# 1, export co-eluted precursors.
input_format=raw
# raw/ms1
isolation_width=2
# default=2.
mars_threshold=-0.68
trainingset=.\TrainingSet.txt
ipv_file=.\IPV.txt.
[0/1 Switches]
output_mgf=1
output_mars_y=0
delete_msn=0
rewrite_files=0
export_unchecked_mono=0
cut_similiar_mono=1
output_trainingdata=0
check_activationcenter=1
output_all_mars_y=0
debug_mode=0
```

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pParse+用户手册

软件简介

pParse+是一个支持从 RAW 格式导出 MGF 格式串联质谱图的软件。下载好压缩包后，解压即可使用。

pParse+目前具有导出共洗脱母离子和不导出共洗脱母离子两种模式，可以在参数文件中的 co-eluted 项目下修改。

最小系统配置要求

- 处理器：Pentium III 以上
- 内存：1GB
- 操作系统：Windows XP/Vista/7/8
- Xcalibur 2.1 或者更高版本

使用方法 1

首先配置好参数文件，解压后的文件夹中包含了一个参数文件模板：

pParse.para

配置好参数后，在当前目录下打开命令行，执行：

pParse.exe pParse.para

使用方法 2

pParse+现在有 21 个命令行开关可以控制，每一个开关都有默认参数。用户可以仅仅配置其中一小部分，就可以正常运行 pParse+。比如说:

pParse.exe -D D:\mydata\First.raw

或者

pParse.exe -D D:\mydata\First.raw -O E:\mydata

分别处理单个 RAW 和批处理文件夹内的所有 RAW。

单独键入命令：

pParse.exe

会输出一个比较详细使用说明，此外，如果用户不小心删除了 pParse.para，这一命令还会生成一份参数文件模板。

参数文件配置说明

pParse+正常执行依赖于参数文件的正确配置，大部分参数不需要用户修改，常规使用，仅需配置 datapath 参数即可。

```
# This is standard pParse configure file
# Time: 2014.1.6
# '#'后面可以添加注释，文件中可以任意空行。

[基本参数]
datapath=E:\MannData\
# 文件夹和文件均可.
[高级选项]
co-elute=0
# 0, 不导出共洗脱母离子.
# 1, 导出共洗脱母离子.
input_format=raw
# raw/ms1
isolation_width=2
# 默认值 2.
mars_threshold=-0.68
trainingset=.\TrainingSet.txt
ipv_file=.\IPV.txt.
[其他开关]
output_mgf=1
output_mars_y=0
delete_msn=0
rewrite_files=0
export_unchecked_mono=0
cut_similiar_mono=1
output_trainingdata=0
check_activationcenter=1
output_all_mars_y=0
debug_mode=0
```
