pXtract User Guide

Introduction

pXtract2.0 is a portable application which means you can use it without installation. After downloading the software, you need to unzip the file. There are two executable files, pXtract.exe and xtract.exe. pXtract.exe provides an user interface, while xtract.exe actually do the job of data extraction. You can either choose to use the user interface or directly use the kernel program (xtract.exe). To use the kernel program well, this user guide can give you some instructions.

xtract2.0.0.5 is a command line program used to extract text-plain spectra from binary Thermo Scientific RAW files. The supporting output formats are MS1, MS2, MGF, and PFD. Xcalibur must be installed first due to the invocation of Thermo's Xcalibur APIs in this program. In order to obtain data generated on an LTQ-Orbitrap or LTQ-FTMS, Xcalibur v2.0.5 or a later version is required, and Xcalibur v2.2 is a must for data from a QE equipment.

Usage

This program runs in two ways. One way (see Use Configuration File) is

xtract.exe *configuration_file_path*

The other way (see Use Console Switches) is

xtract.exe [OPTION]… [FILE]…

In terms of the first way, parameter *configuration_file_path* is the path of the configuration file, which you need to set some values, including basic options that you must assign values to as well as advanced options if you would like to use them. For the second way, all files to be converted follow up the command name directly, and switches are designed to control the options as in the first way. The Next two sections will contain a detailed instruction for the use of options in the first manner and switches in the second manner.

Use Configuration File

Basic Options

The basic options part starts with a header named **`[required]`** followed by two options. One of them is **`extension`**, and the other is **`input_file_path`**. Each option should go in a newline, and any line begins with **#** will be regarded as annotations. Go to the Configuration File Sample part for an institutive understanding of these rules.

`extension`=MS1|MS2

This option specifies which export format to get and the legitimate value can be one of the following four values, which are MS1, MS2, MGF, and PFD, or their combinations, which are

separated by a vertical line. Since these values are case insensitive, mgf, or Mgf would be fine.

input_file_path=F:\data\directory\|F:\data\raw\data.raw

This option guides you to set the RAW files you want to convert. You can set directory paths or the whole file paths. When directory is set, all files of .raw in that directory will be in account. Several locations are separated by a single vertical line. The conflict of file name should be avoided.

Advanced Options

The following six options go under a header named **[optional]**, which means these options can be omitted. When they are not showed up, the default value will be taken.

output_file_path=F:\data\output\

This option instructs the program to export all of the outputs in the directory you set. If the directory does not exist, the program will create one. When this option is omitted, all of the outputs will be in the same directory with its own RAW file.

activation=NONE

This option orders the program to export a particular type of activation spectra of MS/MS. The allowed values are NONE and ALL. The default is NONE, which means to put different activation types in different files. ALL means put different activation types in one file. It should be noticed that this option only take effect when you want to export MS/MS spectra.

centroided=ON

This option specifies whether the exported spectra should be centroided or not. If the RAW itself is centroided, what value of this option is taken matters nothing. However, when the RAW file is profile, setting on this option will do take effect. The legitimate value could be ON and OFF. Default is ON.

mz=7

This option specifies the decimal place of m/z ratio. Its value goes from 1 to 9, and the default value is 7.

intensity=6

This option specifies the decimal place of intensity. Its value goes from 1 to 9, and the default value is 6.

charge=2-3

This option specifies the charge range of the spectra whose charge would not be decided by the Xcalibur APIs, and then it will be exported several same spectra peaks lists with different charge which goes in this range. The range could be any interval between 1 and 9. Default is 2-3.

Configuraiton File Sample

```
# xtract.ini
# The following setting order program to extract MS1 spectra
# from RAWs in the directory of F:\data\directory\ and also
# the RAW F:\data\raw\data.raw. The results will be holding in
# the directory F:\data\output\. Since it is going to export
# MS1, activation setting will be negelected. All spectra will
# export as centroided. The decial place of m/z ratio and
# intensity will be 7 and 6. The charge range will be 2 to 3.
[required]
extension=MS1
input_file_path=F:\data\directory\|F:\data\raw\data.raw
[optional]
output_file_path=F:\data\output\
activation=ALL
centroided=ON
mz=7
intensity=6
charge=2-3
```

Use Console Switches

xtract.exe support 13 switches, which have the same functions as the options in previous section.

-a

Take effect for MS/MS. Turn on this switch to hold different activation types spectra in one file. Turn off to split in different files. Same duty as **activation.**

-c

Make results centroided. In deault case, this switch is on. Same as **centroided**.

--help

Get help information.

-i

The decimal place of intensity. The value goes from 1 to 9. Default is –i 6.

-m

The decimal place of m/z ratio. The value goes from 1 to 9. Default is –m 7.

-mgf

Export MGF extension file(s).

-ms

Export MS1 and MS2 files.

-ms1

Export MS1 files.

-ms2

Export MS2 files.

-o

Outputs directory. E.g. –o F:\data\output\.

-p

Make results profile. In default case, this switch is off.

-pfd

Export PFD files.

-z

Charge range of the spectra. The range could be any interval between 1 and 9. Default is –z 2-3.

用户手册

软件简介

pXtract2.0 是一个支持导出 RAW 格式文件的绿色软件，无需安装可以直接运行。下载好压缩包后先将包内文件解压到一个目录中，可以看到有两个可执行文件 pXtract.exe 与 xtract.exe，pXtract.exe 提供界面配置参数，xtract.exe 是用于导出数据的核心程序。您可以选择使用界面程序，或者直接用核心程序。如果使用核心程序，您需要按照本手册中的叙述设置参数。

xtract2.0.0.5 是用来将 Thermo Scientific RAW 格式文件导出为普通文本格式的工具，它所支持的导出格式包括 MS1、MS2、MGF 与 PFD。在运行该工具前请先安装 Xcalibur，其提供的一些应用程序接口（API）会被 xtract2.0.0.5 调用。值得注意，在导出 LTQ-Orbitrap 或者 LTQ-FTMS 生成的数据时，Xcalibur 的版本至少是 v2.0.5，而在导出 Q Exactive 仪器生成的数据时，版本至少是 v2.2。

基本用法

该程序可通过两种方式设置参数，一种是通过配置文本文件（参见配置文件的用法），命令形式为

xtract.exe *configuration_file_path*

另一种是直接使用控制台开关（参见命令行函数的用法），命令形式为

xtract.exe [OPTION]… [FILE]…

在第一种方式中，*configuration_file_path* 表示配置文件的路径。在配置文件中，通过设置其中的基本参数与高级参数可以得到不同形式的结果文件。在第二种方式中，通过设置控制台开关进行配置参数，与第一种方法中的效果等同。下面两部分会详细介绍另种方式中的参数设置。

配置文件的用法

基本参数

配置文件中基本参数以**[required]**标识，意思是必须有这部分参数。基本参数共两个，一个设置导出格式 **extension**，另一个设置输入路径 **input_file_path**。配置文件中每个参数项都应独占一行，注释行以**#**打头，具体可参考配置文件样本一节。

extension=MS1|MS2

该参数指定导出格式，合法取值为 MS1、MS2、MGF 与 PFD。该选项为多值选项，值之间以竖线间隔。对于取值，大小写不敏感，所以 mgf 或者 Mgf 等等都是合法值，后面的参数亦同。

input_file_path=F:\data\directory\|F:\data\raw\data.raw

该参数指定输入文件路径，合法取值为 RAW 文件名或者包含 RAW 文件的目录名，要求绝对路径。该选项为多值选项，值之间以竖线间隔。文件名相同的路径应避免同时出现否则会出现文件覆盖可能得不到预期结果。

高级参数

接下来的六个参数以**[optional]**作为标识，意在有无均可。如果没有设置，会取用缺省值。

output_file_path=F:\data\output\

该参数指定输出文件目录，如果指定目录不存在，程序会默认创建。该选项为单值选项，额外的设置可能引起错误。缺省值为各自的 RAW 导出后的文件在与原 RAW 相同的目录下。

activation=NONE

该参数指定导出二级谱的碎裂类型是分文件存储还是用单个文件存储，当值为 NONE 时，分文件导出不同的碎裂类型，而当值为 ALL 时，所有类型会放置在一个文本文件中。该参数只针对二级谱，对一级谱无效。缺省值为 NONE。

centroided=ON

该参数指定导出的谱图是否进行中心化，取值为 ON 或 OFF，ON 表示中心化，OFF 表示不中心化。缺省值为 ON。

mz=7

该参数指定导出谱图质荷比的小数点位数，取值为 1 至 9。缺省值为 7.

intensity=6

该参数指定导出谱图强度的小数点位数，取值为 1 至 9。缺省值为 6.

charge=2-3

该参数指定二级谱中仪器无法确定电荷的谱图应该导出的电荷范围，取值为 1 至 9 间的任何一个区间。缺省值为 2-3.

配置文件样本

```
# xtract.ini
# The following setting order program to extract MS1 spectra
```

```
# from RAWs in the directory of F:\data\directory\ and also
# the RAW F:\data\raw\data.raw. The results will be holding in
# the directory F:\data\output\. Since it is going to export
# MS1, activation setting will be negelected. All spectra will
# export as centroided. The decial place of m/z ratio and
# intensity will be 7 and 6. The charge range will be 2 to 3.
[required]
extension=MS1
input_file_path=F:\data\directory\|F:\data\raw\data.raw
[optional]
output_file_path=F:\data\output\
activation=ALL
centroided=ON
mz=7
intensity=6
charge=2-3
```

命令行参数的用法

xtract.exe 支持 13 个控制开关，功能与配置文件中的参数一致。除去开关外，命令行中的其余参数均被识别为待转换的 RAW 文件或者待转换 RAW 文件所在目录。

-a

仅对二级谱有效。打开这个开关，不同的碎裂类型会被导出在一个文件中，默认此开关被关闭。功能同 **activation**。

-c

对导出谱图进行中心化。默认此开关被打开。功能同 **centroided**。

--help

获取帮助信息。

-i

设置导出谱图强度的小数点位数。默认值为-i 6。

-m

设置导出谱图质荷比的小数点位数。 默认值为 –m 7。

-mgf

设置导出 MGF 格式。默认开启。

-ms

设置导出 MS1 与 MS2 格式。默认关闭。

-ms1

设置导出 MS1 格式。默认关闭。

-ms2

设置导出 MS2 格式。默认关闭。

-o

设置输出文件路径。例如–o F:\data\output\。

-p

对导出谱图不进行中心化。默认此开关关闭。功能同 **centroided**。

-pfd

设置导出 PFD 格式。默认关闭。

-z

设置仪器无法确定电荷谱图应导出的电荷范围，取值区间为 1 至 9 的任意区间，缺省值为-z 2-3。