

Sipros

Proteomics data analysis software

PTM_instructions

Create configure file

Please refer to <http://code.google.com/p/sipros/wiki/ConfigureFileSetting> for technical details. An example is available at <http://code.google.com/p/sipros/source/browse/trunk/Sipros3.0/Sipros-src/SiprosConfigPTM.cfg>

FT1 and FT2 files

Please refer to <http://code.google.com/p/raxport/> for generating FT1 and FT2 files

Pre-processing

The current version of scripts has been tested using Python 2.7.2, so if you are using different versions of Python (2.6.X or 3.X), you are encouraged to try with Python 2.7.2. If you want to use reverseseq.py, Biopython is required.

```
cd Sipros-ProRata_V3.0_Linux/scripts
```

Generate reverse sequence

```
python reverseseq.py -i original_database_file -o output_database_file
```

The step will generate a new database file with reverse sequences

Run Sipros

The easiest way for running Sipros is

```
./Sipros -c configurefilename -w workingdirectory
```

Sipros will use all .FT2 files in the working directory. Results (.sip files) will be saved on working directory by default. You can specify output directory by specifying -o. If you just want to specify one FT2 file, you can use -f like,

```
./Sipros -c configurefilename -f FT2filename
```

If you want to slice screen output, please add -s. In Sipros_openmp_mpi, you are allowing to specify -g like

```
./Sipros -g configurefiledirectory -w workingdirectory
```

if you have many configure files.

Please note that you can get help information by flag -h.

Post-processing

The current version of scripts has been tested using Python 2.7.2, so if you are using different versions of Python (2.6.X or 3.X), you are encouraged to try with Python 2.7.2. If you want to use pro2ptm.py, Biopython is required.

```
cd Sipros-ProRata_V3.0_Linux/scripts
```

Peptide filtering

```
python sipros_peptides_filtering.py -c configurefile -w workingdirectory
```

All sip files, output files of Sipros, should be in the working directory. The step will generate related psm.txt and pep.txt

Peptide assembling

```
python sipros_peptides_assembling.py -c configurefile -w workingdirectory
```

The psm.txt and pep.txt files generated by the filtering step will be used in this step. And the step will generate pro.txt, pro2pep.txt, and pro2psm.txt files.

Pro2ptm (Biopython needs to be installed)

```
python pro2ptm.py -c configurefile -w workingdirectory
```

Script pro2ptm.py will generate pro2ptm.txt file

If you also need pro2ptm.prorata.txt file, please run pro2ptm.py first and add ProRata_LabelFree_Peptide.txt, a output file of ProRata, to the working directory. Then run

```
python prorata_pro2ptm.py -w workingdirectory
```

This step will generate pro2ptm.prorata.txt file.
