

Program to generate k-permuted decoy database

The source code to generate k-permuted decoy databases is implemented in the Python programming language. To run the code, do the following steps.

Install Python

- 1 Download Python version 2.7 or later from <https://www.python.org/downloads>. The Python can be installed on user machines running any operating system such as Windows, Linux or Unix, Mac OS X, and Other.
- 2 The program command can be executed in the shell/terminal of the Linux/Unix and Mac OS X operating systems. For the Windows OS, command prompt can be used to execute the program after setting the path and environmental variables for the Python.
- 3 Guideline to set path and environmental variables in Windows:
 - From the Desktop, right-click My Computer and click Properties.
 - In the System Properties window, click on the Advanced tab.
 - In the Advanced section, click the Environment Variables button.
 - Finally, in the Environment Variables window, highlight the Path variable in the Systems Variable section and click the Edit button. Add or modify the path lines with the path of installed python. Each different path is separated with a semicolon for example:

```
C:\Program Files;C:\Winnt;C:\Python
```

Command to run program

To execute the source code, run the following command:

```
python permuted_peptides.py -in <path to fasta sequence file> [optional parameter]
```

Required parameter:

-in <input_file>

The full path to the file containing FASTA sequences. This parameter is required.

Optional parameters:

-h or -help

This shows help message.

-perm <Integer>

The number of random permutations (i.e., k) you want to generate for each sequence in the Fasta file (default=100)

-seed <Integer>

Initialize the random number generator (default=3343)

-max-length <Integer>

The maximum peptide length when all possible permutations can be used (default=7)

-out <output_file>

The full path and the name of the output file (default=decoys.fasta)

-iupac <True or False>

Generate permuted peptides with Any(X), Asparagine (B), and Glutamine (Z) amino acids in addition to standard 20 amino acids (default=False)