CJunction User Guide

2021/06/24

Step1: Setting parameters

Step2: Importing the results of de novo sequencing of MS data

Step3: Setting the path to the output file

Step4: Selecting the "Get Junction Peptide" option

Step5: Clicking "Start" to run the program

In the second step above, the input file needs to satisfy the following format, with the contents of each line separated by commas: name of the MS raw file, scan number of the MS2 spectrum, peptide identified by de novo sequencing, monoisotopic mass of the precursor ion, and charge, respectively.

```
39_20,0.02&0.05.csv  x

 1 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLALVPR,483.33044,2
 2 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLAVLPR,483.33044,2
 3 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLAVLPR,483.33044,2
 4 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLGLLPR,483.33044,2
 5 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLGLLPR,483.33044,2
 6 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLLAVPR,483.33044,2
 7 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLLGLPR,483.33044,2
 8 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLVALPR,483.33044,2
 9 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLVALPR,483.33044,2
10 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003,VVVLVLAPR,483.33044,2
11 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,FPLFGVAR,453.76578,2
12 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,FPLFGVAR,453.76578,2
13 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,FPLFRAR,453.76578,2
14 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,FPLFVGAR,453.76578,2
15 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,FPLFVGAR,453.76578,2
16 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,FPLGVFAR,453.76578,2
17 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,LMLFGVAR,453.76578,2
18 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,LMLFGVAR,453.76578,2
19 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,MLLFGVAR,453.76578,2
20 "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026,MLLFGVAR,453.76578,2
```

1. When the program is finished running, two files are available: Result.txt and JunctionPeptide.fasta.
2. In the Result.txt, all of the possible junction peptides corresponding to the MS2 spectrum are shown after the colon in each row.
3. JunctionPeptide.fasta provides all possible non-redundant junction peptides enumerated from the MS dataset.

Result

JunctionPeptide

Result.txt ✕

```
 1  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10003:VVVLALVPR;
 2  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10026:;
 3  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10036:;
 4  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10039:;
 5  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10040:;
 6  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10043:;
 7  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10044:;
 8  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10047:;
 9  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10052:;
10  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10057:;
11  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10065:;
12  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10076:;
13  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10083:;
14  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10087:;
15  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10093:;
16  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10096:;
17  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10102:;
18  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10120:LLPALZAFR;
19  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10136:;
20  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10145:;
21  "20150708_QE3_UPLC8_DBJ_QC_HELA_39frac_Trypsin_1.raw",10148:;
```

JunctionPeptide.fasta ✕

```
 1  >JunctionPeptide_1
 2  VVVLALVPR
 3  >JunctionPeptide_2
 4  LLPALMAFR
 5  >JunctionPeptide_3
 6  FLLLLSGPK
 7  >JunctionPeptide_4
 8  LFLLLSGPK
 9  >JunctionPeptide_5
10  FGNLLLFLK
11  >JunctionPeptide_6
12  APTMLLFLK
13  >JunctionPeptide_7
14  KKMLLPGR
15  >JunctionPeptide_8
16  LLPALMAFR
17  >JunctionPeptide_9
18  LLMALLPR
19  >JunctionPeptide_10
20  DHTVRSTGPAK
```