

# Portable Proteomics Pipeline (P3)

## MSGF Benchmark

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### 1. Files:

```
## [1] "From PNNL: TCGA_13-1489_42-2590_36-2529_117C_W_PNNL_B2S5_f11_msgfdb_fht.txt"
```

```
## [1] "From Docker: TCGA_13-1489_42-2590_36-2529_117C_W_PNNL_B2S5_f11.txt"
```

### 2. Identification:

Identification used the following switches:

```
# Command Line (2)
java -Xmx8000M -jar P3/MSGFPlus.jar -s \
TCGA_13-1489_42-2590_36-2529_117C_W_PNNL_B2S5_f11.mzML -o \
TCGA_13-1489_42-2590_36-2529_117C_W_PNNL_B2S5_f11.mzid \
-d ID_003632_9011437E.fasta \
-t 10ppm -m 0 -inst 1 -e 1 -ti -1,2 -ntt 2 -tda 1 -minLength 6 \
-maxLength 50 -minCharge 2 -maxCharge 5 -n 1 -thread 7 \
-mod MSGFDB_Mods.txt -minNumPeaks 5 -addFeatures 1
```

### 3. Differences. Spec eValue = $10^{-10}$

#### a. From PNNL

```
## [1] "Remaining peptides: 4633"
```

```
## [1] "==== head ====="
```

##	Scan	MSGFDB_SpecEValue	Peptide
## 1	11612	1.481722e-36	IQDLTGLDVSTAEELQVANYGVGGQYEPHFDFAR
## 2	14441	8.834771e-36	LTPFIIQENLNLALNSASAIGCHVVNIGAEDLR

```
## [1] "==== tail ====="
```

##	Scan	MSGFDB_SpecEValue	Peptide
## 4634	7324	9.821299e-11	VTGTQPITCTWMK
## 4635	12688	9.998422e-11	SFLFQLLK

a. From Docker

```
## [1] "Remaining peptides: 882"
```

```
## [1] "==== head ====="
```

```
##      Scan  Spec_Evalue      PepSeq
## 4 14307 6.077710e-14      LWISNGGLADIFTVFAK
## 8 12726 2.039783e-14  LREQLG PVTQEFWDNLEKETEGLR
```

```
## [1] "==== tail ====="
```

```
##      Scan  Spec_Evalue      PepSeq
## 5904 3729 6.356413e-11      IFVHVSVLK
## 6218 4079 1.875725e-11  VHQLHTSRTFAK
```