Portable Proteomics Pipeline (P3)
MSGF Benchmark

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1. Files:

```
## [1] "TCGA_13-1489_42-2590_36-2529_117C_W_PNNL_B2S5_f11.mzML"


## [1] "ID_003632_9011437E.fasta"
```

2. Identification:

`MSGFPlus.jar` was downloaded from https://omics.pnl.gov/software/ms-gf. Identification was run multiple times (within or without Docker), and resulted the same results.

Identification with different switches resulted different results.

```
# Command Line (Without Switch)
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_no_switch.mzid \
-d ID_003632_9011437E.fasta

# 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


## [1] "TCGA_13-1489_42-2590_36-2529_117C_W_PNNL_B2S5_f11_no_switch.mzid"
## [2] "TCGA_13-1489_42-2590_36-2529_117C_W_PNNL_B2S5_f11.mzid"
```

3. Result from PNNL

```
## [1] 12695
```

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

```
##       Scan MSGFDB_SpecEValue Peptide
## 12947 3823        0.04856372  SPAGGG
## 12948 4099        0.05022644  PGGAGM
```

4. Result from MSGF+ without any switches (sorted by SpecE-Value)

```
##          scan number(s) ms-gf:denovoscore ms-gf:specevalue
## X9740.1           10815               277     4.434865e-30
## X8340.1            9275               234     2.157325e-27
## X10711.1          11883               157     1.386474e-25
##                                  pepseq
## X9740.1  SHSTEPGLVLTLGQGDVGQLGLGENVMER
## X8340.1          DLYANTVLSGGTTMYPGIADR
## X10711.1     ILGGVISAISEAAAQYNPEPPPPR
```

```
##          scan number(s) ms-gf:denovoscore ms-gf:specevalue
## X13036.1          14441               381     4.861374e-08
## X10464.1          11612               279     5.246882e-08
##                                  pepseq
## X13036.1     KETDLKQIQTLIQGTQTRLKYSQNELEMIKK
## X10464.1 AGISEAQLTDAETSKLIYDFIEDQGGLEAVRQEMR
```

Reading the MZID file manually

```
java -Xmx2000M -XX:+UseConcMarkSweepGC -cp \
../P3/MSGFPlus.jar edu.ucsd.msjava.ui.MzIDToTsv -i \
TCGA_13-1489_42-2590_36-2529_117C_W_PNNL_B2S5_f11_no_switch.mzid \
-showQValue 1 -showDecoy 1 -unroll 1
```

```
##   ScanNum                            Peptide             Protein SpecEValue
## 1   10815 R.SHSTEPGLVLTLGQGDVGQLGLGENVMER.K ref|NP_001041660.1   4.43e-30
## 2   10815 R.SHSTEPGLVLTLGQGDVGQLGLGENVMER.K ref|NP_001041659.1   4.43e-30
## 3   10815 R.SHSTEPGLVLTLGQGDVGQLGLGENVMER.K ref|NP_001041664.1   4.43e-30
```

5. Results with switches

```
##          scan number(s) ms-gf:denovoscore ms-gf:specevalue
## X11197.1          12418               321     6.104450e-34
## X9050.1           10056               258     4.553317e-33
```

```
## X9060.1              10067             288      9.340615e-33
##                                    pepseq
## X11197.1 VYLASLETLDNGKPFQESYALDLDEVIK
## X9050.1    CLCLPSYVGALCEQDTETCDYGWHK
## X9060.1    CLCLPSYVGALCEQDTETCDYGWHK


##           scan number(s) ms-gf:denovoscore ms-gf:specevalue      accession
## X13036.1          14441               345      2.196462e-06 ref|NP_060250.2
## X10464.1          11612               279      2.280634e-06 ref|NP_000487.1
##                                    pepseq
## X13036.1 FILPNVSTPVSDAFKTQMELLQAGLSRTPTR
## X10464.1  GDYKDSSDFGAPHPQVQSVRRIRDMQWHQR
```

Reading the MZID file manually

```
##    ScanNum
## 1    12418
## 2    10056
## 3    10056
##                                                                    Peptide
## 1                 R.+144.102VYLASLETLDNGK+144.102PFQESYALDLDEVIK+144.102.V
## 2 R.+144.102C+57.021LC+57.021LPSYVGALC+57.021EQDTETC+57.021DYGWHK+144.102.F
## 3 R.+144.102C+57.021LC+57.021LPSYVGALC+57.021EQDTETC+57.021DYGWHK+144.102.F
##    SpecEValue
## 1   6.10e-34
## 2   4.55e-33
## 3   4.55e-33
```

7. Filtering (PNNL -> Docker)

a. Spec-Evalue 10^{-10}

From PNNL

There are **4633** rows remained.

From Docker

There are **1665** rows remained.

```
## [1] "==Head=="
```

```
##       Scan MSGFDB_SpecEValue                 Peptide ms-gf:specevalue
## 3641 12418      6.104450e-34 VYLASLETLDNGKPFQESYALDLDEVIK     6.104450e-34
```

```
## 2717 10056      4.553317e-33    CLCLPSYVGALCEQDTETCDYGWHK      4.553317e-33
##                                 pepseq
## 3641 VYLASLETLDNGKPFQESYALDLDEVIK
## 2717    CLCLPSYVGALCEQDTETCDYGWHK


## [1] "==Tail=="


##       Scan MSGFDB_SpecEValue          Peptide ms-gf:specevalue
## 2508 9513      2.871564e-13    NIIGSSPVADFSAIK      8.381110e-05
## 223  1927      5.243567e-25 CCYDGACVNNDETCEQR      9.379988e-05
##                     pepseq
## 2508 LVDETEGQCGETDPNSEMPR
## 223        HECCFRYHCTGCCFR
```

Differences

Data from Docker is matched with from PNNL using scan number as ID. MSGFDB_SpecEValue, Peptide are values from PNNL. ms-gf:specevalue, pepseq are the corresponding values from Docker Container. There are 4621 of rows in total with 1227 exact match.

325 with the same peptide identification and different spec-evalue, 3069 of different peptide identification as well different spec-evalues (12 of them are unmatched values).

```
## [1] "==Unmatched=="


##       Scan MSGFDB_SpecEValue       Peptide ms-gf:specevalue pepseq
## 2291 8856      1.119096e-15 CSEGVFLLTTTPR             NA   <NA>
## 1416 6555      6.590530e-15  CQSLQEELDFRK             NA   <NA>


## [1] "==Different Spec eValues=="


##        Scan MSGFDB_SpecEValue                          Peptide
## 3127 11078      5.495878e-31       MGLDPACQVDIICGDHLLEQYQTLR
## 2548  9602      2.682754e-30 WSGPLSLQEVDEQPQHPLHVTYAGAAVDELGK
##      ms-gf:specevalue                          pepseq
## 3127    7.059070e-31       MGLDPACQVDIICGDHLLEQYQTLR
## 2548    1.788561e-30 WSGPLSLQEVDEQPQHPLHVTYAGAAVDELGK


## [1] "==Different Peptides identification and different Spec Evalues=="


##       Scan MSGFDB_SpecEValue                      Peptide ms-gf:specevalue
## 2595  9730      6.005831e-22     FFDHSGTLVMDAYEPEISR      2.231272e-20
## 4204 13789      4.811341e-14 NAQMAQSPILLLGGAASTLLQNR      6.118720e-19
##                     pepseq
## 2595 DLYANTVLSGGTTMYPGIADR
## 4204   IQTQLNLIHPDIFPLLTSFR
```

b. Spec-Evalue 10^{-15}

From PNNL

There are 2511 rows remained.

From Docker

There are 767 rows remained.

```
## [1] "==Head=="
```

```
##        Scan MSGFDB_SpecEValue                        Peptide ms-gf:specevalue
## 1763 12418     6.104450e-34 VYLASLETLDNGKPFQESYALDLDEVIK    6.104450e-34
## 1170 10056     4.553317e-33    CLCLPSYVGALCEQDTETCDYGWHK    4.553317e-33
##                                 pepseq
## 1763 VYLASLETLDNGKPFQESYALDLDEVIK
## 1170    CLCLPSYVGALCEQDTETCDYGWHK
```

```
## [1] "==Tail=="
```

```
##     Scan MSGFDB_SpecEValue           Peptide ms-gf:specevalue
## 49 1876     1.449447e-17    QNEAAVGNCAEHMR     3.858078e-05
## 50 1927     5.243567e-25 CCYDGACVNNDETCEQR     9.379988e-05
##           pepseq
## 49    DSFMRHRGHCER
## 50 HECCFRYHCTGCCFR
```

Differences

Data from Docker is matched with from PNNL using scan number as ID. MSGFDB_SpecEValue, Peptide are values from PNNL. ms-gf:specevalue, pepseq are the corresponding values from Docker Container. There are 2511 of rows in total with 572 exact match.

170 with the same peptide identification and different spec-evalue, 1769 of different peptide identification as well different spec-evalues (0 of them are unmatched values).

```
## [1] "==Unmatched=="
```

```
## [1] Scan                MSGFDB_SpecEValue Peptide           ms-gf:specevalue
## [5] pepseq
## <0 rows> (or 0-length row.names)
```

```
## [1] "==Different Spec eValues=="
```

```
##         Scan MSGFDB_SpecEValue                          Peptide
## 1437 11078     5.495878e-31        MGLDPACQVDIICGDHLLEQYQTLR
## 1057  9602     2.682754e-30 WSGPLSLQEVDEQPQHPLHVTYAGAAVDELGK
##        ms-gf:specevalue                          pepseq
## 1437    7.059070e-31        MGLDPACQVDIICGDHLLEQYQTLR
## 1057    1.788561e-30 WSGPLSLQEVDEQPQHPLHVTYAGAAVDELGK


## [1] "==Different Peptides identification and different Spec Evalues=="


##         Scan MSGFDB_SpecEValue            Peptide ms-gf:specevalue
## 1091 9730     6.005831e-22 FFDHSGTLVMDAYEPEISR     2.231272e-20
## 123  3378     2.191136e-20    ASGNYATVISHNPETKK     2.189761e-14
##                    pepseq
## 1091 DLYANTVLSGGTTMYPGIADR
## 123      NKPGPYSSVPPPSAPPPK
```

c. Spec-Evalue 10^{-20}

From PNNL

There are **936** rows remained.

From Docker

There are **223** rows remained.

```
## [1] "==Head=="


##         Scan MSGFDB_SpecEValue                          Peptide ms-gf:specevalue
## 571 12418     6.104450e-34 VYLASLETLDNGKPFQESYALDLDEVIK     6.104450e-34
## 327 10056     4.553317e-33    CLCLPSYVGALCEQDTETCDYGWHK     4.553317e-33
##                          pepseq
## 571 VYLASLETLDNGKPFQESYALDLDEVIK
## 327    CLCLPSYVGALCEQDTETCDYGWHK


## [1] "==Tail=="


##    Scan MSGFDB_SpecEValue            Peptide ms-gf:specevalue
## 19 3273     1.342643e-21 ESCNPQDCVPEVDENCKDK     2.671039e-05
## 12 1927     5.243567e-25    CCYDGACVNNDETCEQR     9.379988e-05
##                    pepseq
## 19 AEGAYYDNHSVVYLDHGENGEK
## 12        HECCFRYHCTGCCFR
```

Differences

Data from Docker is matched with from PNNL using scan number as ID. MSGFDB_SpecEValue, Peptide are values from PNNL. ms-gf:specevalue, pepseq are the corresponding values from Docker Container. There are 936 of rows in total with 165 exact match.

54 with the same peptide identification and different spec-evalue, 717 of different peptide identification as well different spec-evalues (0 of them are unmatched values).

```
## [1] "==Unmatched=="


## [1] Scan              MSGFDB_SpecEValue Peptide            ms-gf:specevalue
## [5] pepseq
## <0 rows> (or 0-length row.names)


## [1] "==Different Spec eValues=="


##      Scan MSGFDB_SpecEValue                            Peptide
## 450 11078     5.495878e-31        MGLDPACQVDIICGDHLLEQYQTLR
## 284  9602     2.682754e-30 WSGPLSLQEVDEQPQHPLHVTYAGAAVDELGK
##      ms-gf:specevalue                          pepseq
## 450     7.059070e-31        MGLDPACQVDIICGDHLLEQYQTLR
## 284     1.788561e-30 WSGPLSLQEVDEQPQHPLHVTYAGAAVDELGK


## [1] "==Different Peptides identification and different Spec Evalues=="


##      Scan MSGFDB_SpecEValue              Peptide ms-gf:specevalue
## 299  9730     6.005831e-22  FFDHSGTLVMDAYEPEISR     2.231272e-20
## 401 10627     4.148874e-23 GMSLNLEPDNVGVVVFGNDK     7.877905e-10
##                     pepseq
## 299 DLYANTVLSGGTTMYPGIADR
## 401    GNAEPDPPVRLFQIHGNDK
```