

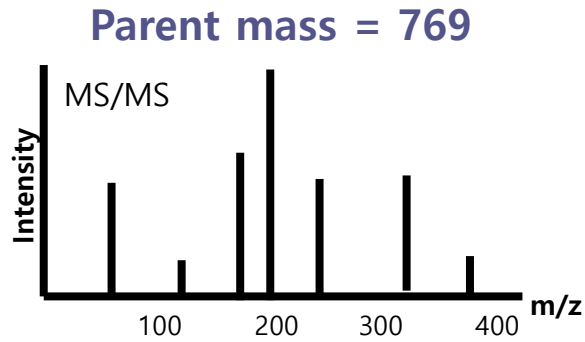
Blind PTM Search

2020.06

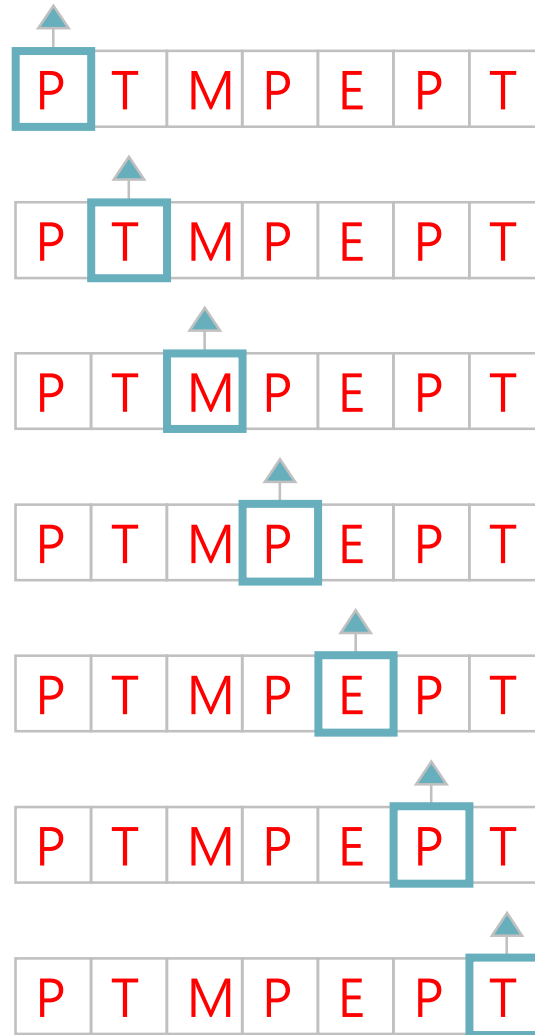
김현우

Complexity for analyzing modified peptides

Considering one modifications per peptide



PTMPEPT 753



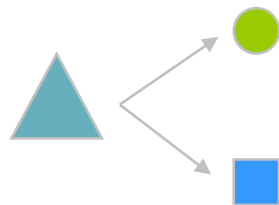
$O(N)$

Complexity for analyzing modified peptides

Considering two modifications per peptide



$$N(N-1)$$



$$\begin{aligned} 100 &= 1 + 99 \\ &= 2 + 98 \\ &= 3 + 97 \end{aligned}$$

...

...

$$= 101 + -1$$

$$= 102 + -2$$

...

...

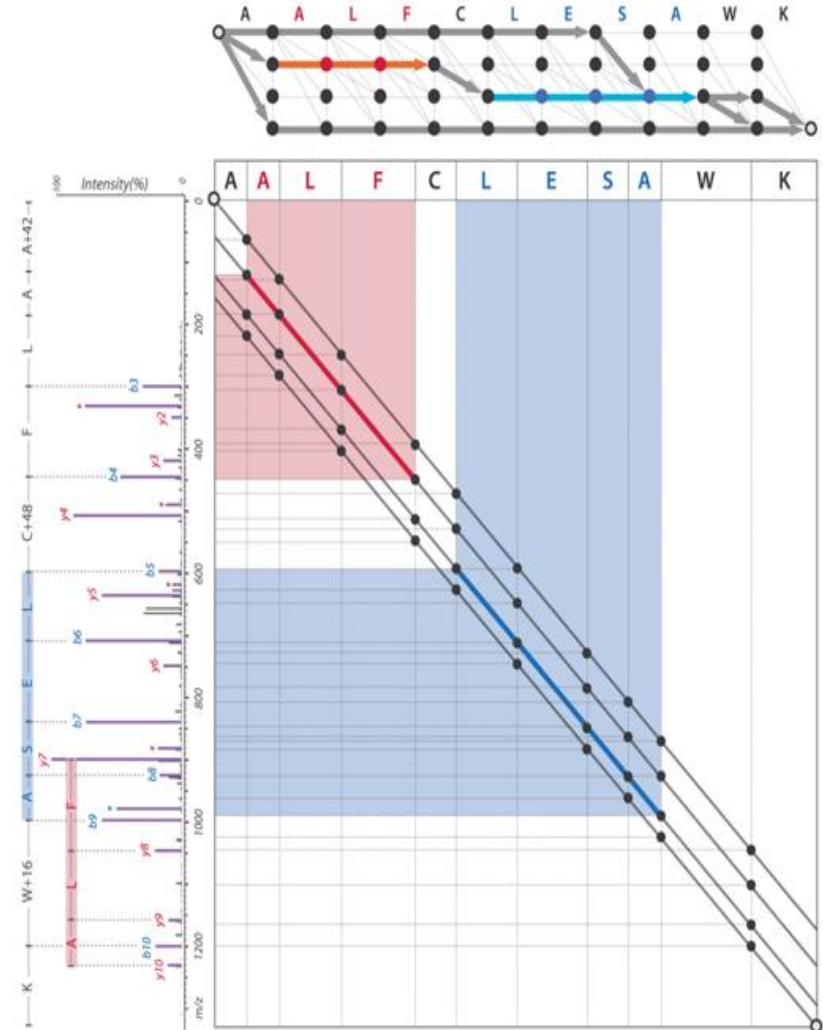
$$= 300 + -200$$

$$d \quad (-200 \sim +200)$$

$$O(dN^2)$$

Blind Modification Search

- **MODa**
 - Blind modification search tool
 - Novel modification search



Na, Seungjin, Nuno Bandeira, and Eunok Paek. "Fast multi-blind modification search through tandem mass spectrometry." *Molecular & Cellular Proteomics* 11.4 (2012): M111-010199.

Blind Modification Search

- **Mass-tolerant database search (OpenSearch)**
 - Using previous search tools
 - Sequest, Comet, ...
 - Use Ultra precursor mass tolerance
 - Precursor mass tolerance = 500 Da
- Drawback
 - A modification site can't be localized

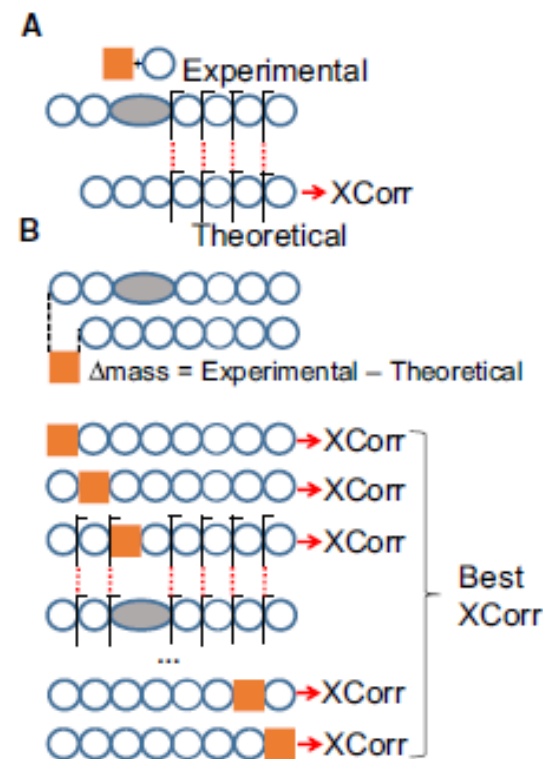
Blind Modification Search

- **Mass-tolerant database search (OpenSearch)**

- Using previous search tools
 - Sequest, Comet, ...
- Use Ultra precursor mass tolerance
 - Precursor mass tolerance = 500 Da

- Drawback
 - A modification site can't be localized

- Comet-PTM
 - OpenSearch + localization



Blind PTM Search 실습

MODa 실행을 위한 준비

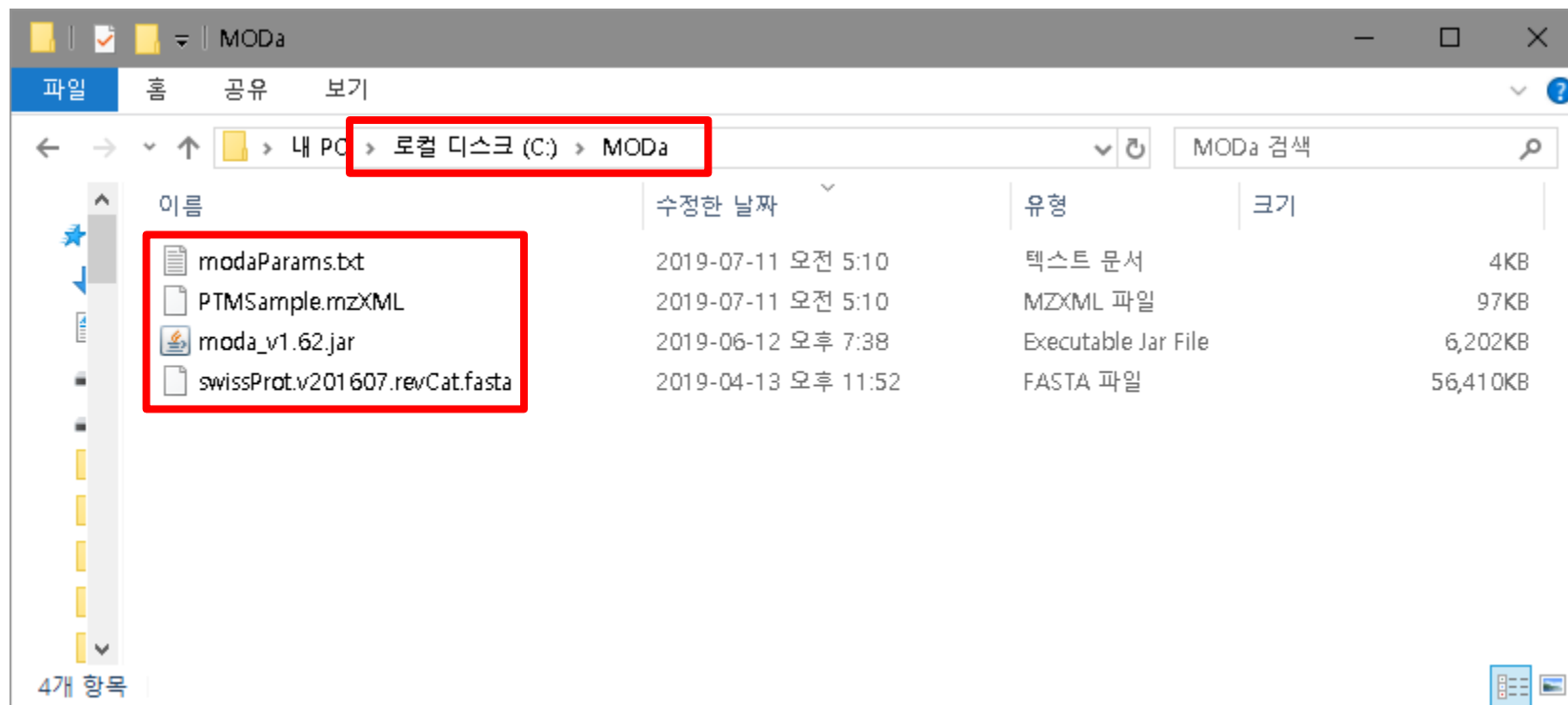
- **필요한 파일**

- MODa 실행 파일 (.jar)
 - moda_v1.62.jar
- Spectrum 파일 (.mzxml or .mzml)
 - PTMSample.mzXML
- Database 파일 (.fasta)
 - swissProt.v201607.revCat.fasta
- Parameter 파일 (.txt)
 - modaParams.txt

MODa 실행을 위한 준비

- 해당 파일을 복사

- C:\ 폴더에 MODa 폴더를 복사
- MODa 폴더 안에 있는 파일 확인



MODa Parameter

```
# Spectra=[FILENAME]
# Specifies a path to the spectra file to search
# Supported formats: *.mgf, *.pkl, *.dta, *mzXML
# In case of dta type, for multiple MS/MS scans, at least one blank line must be between each MS/MS scan
Spectra=PTMSample.mzXML

# Instrument=[TYPE(ESI-TRAP|ESI-QTOF)]
# Specifies the type of MS/MS instrument used (or best matched) for peptide fragmentation.
# According to an instrument type, a different fragmentation model is applied.
# Default value is ESI-TRAP
Instrument=ESI-QTOF

# Fasta=[FILENAME]
# Specifies a path to the database file (*.fasta) to search
Fasta=swissProt.v201607.revCat.fasta

# PeptTolerance=[MASS] / PPMTolerance=[VALUE]
# PeptTolerance sets parent mass tolerance in Dalton.
# PPMTolerance sets parent mass tolerance in ppm.
# Either PeptTolerance or PPMTolerance is applied as precursor mass tolerance. PeptTolerance has a default value of 3.
PeptTolerance=0.5
# PPMTolerance=10

# AutoPMCorrection=[0|1]
# If this parameter is set to 1 (this requires more search time),
# the program will automatically find the optimal parent mass for the input spectrum, regardless of specified PeptTolerance.
# The default value is 0 (interpreting the spectrum only within the range you specify).
AutoPMCorrection=0

# FragTolerance=[MASS]
# Sets a fragment ion mass tolerance in dalton, default value is 0.6
FragTolerance=

# BlindMode=[0|1|2]
# Sets the number of modifications per peptide, default value is 2
# 0 allows no modification per peptide (very fast),
# 1 allows one modification per peptide
# while 2 allows arbitrary modifications per peptide.
BlindMode=2
```

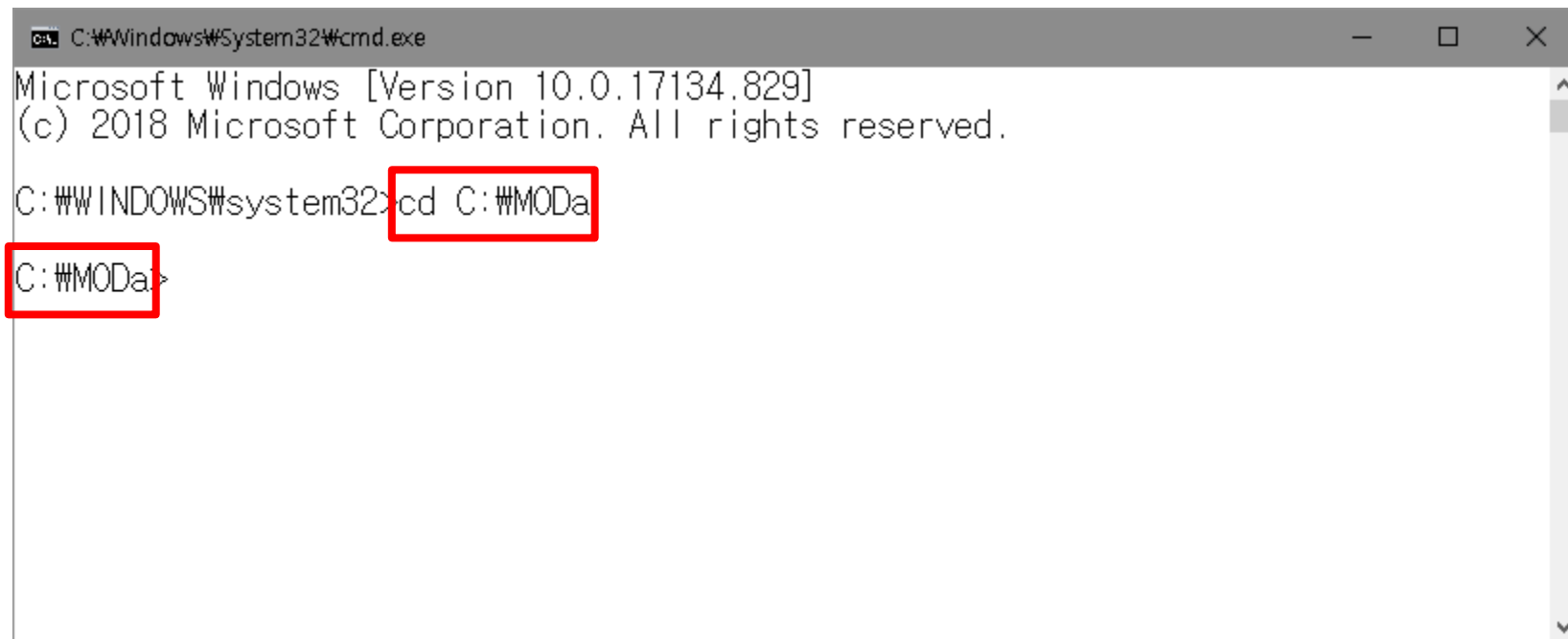
MODa 실행

- Cmd 창 실행
 - 시작메뉴
 - cmd 입력



MODa 실행

- **Cmd 창**
 - cd C:\MODa

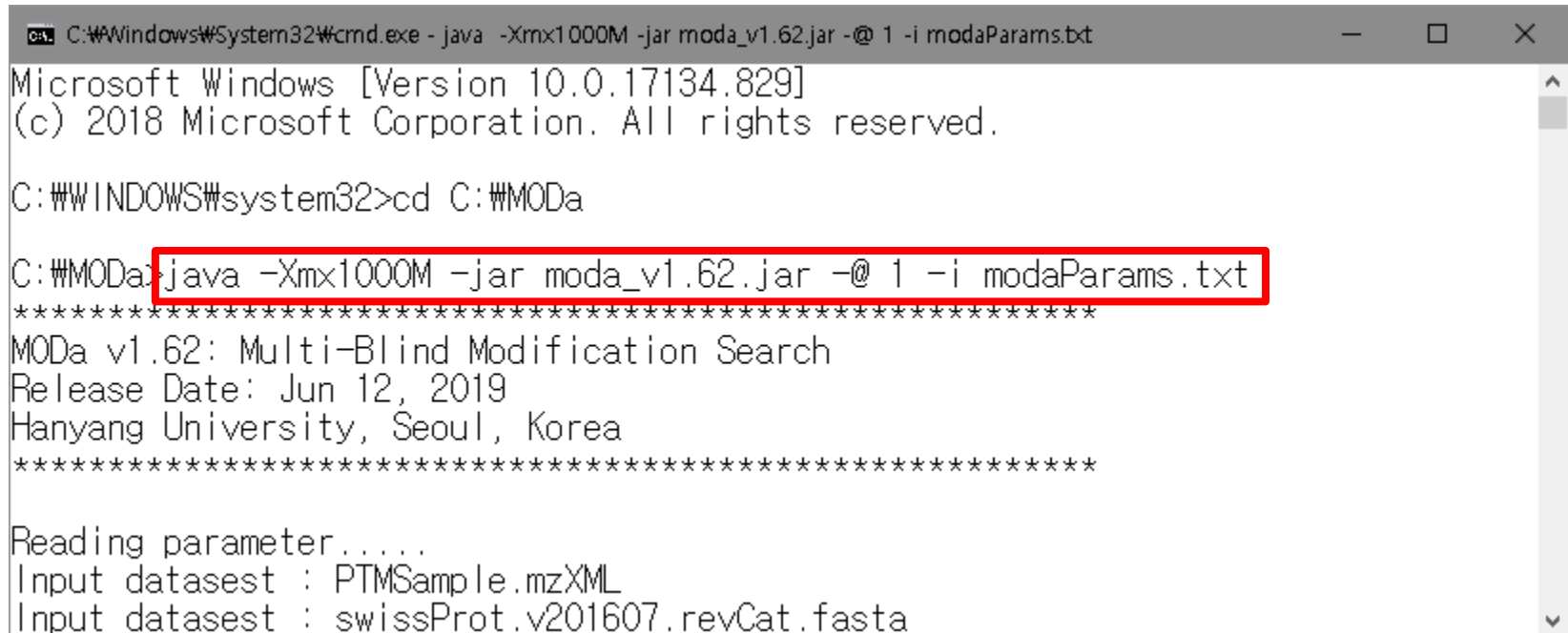


A screenshot of a Windows Command Prompt window. The title bar reads "C:\Windows\System32\cmd.exe". The window content shows the following text: "Microsoft Windows [Version 10.0.17134.829] (c) 2018 Microsoft Corporation. All rights reserved. C:\Windows\system32> cd C:\MODa". The command "cd C:\MODa" is highlighted with a red rectangular box. Below the command, the prompt "C:\MODa>" is also highlighted with a red rectangular box. The window has standard Windows window controls (minimize, maximize, close) in the top right corner.

MODa 실행

- Cmd 창

- `java -Xmx1000M -jar moda_v1.62.jar -@ 1 -i modaParams.txt`



```
C:\Windows\System32\cmd.exe - java -Xmx1000M -jar moda_v1.62.jar -@ 1 -i modaParams.txt
Microsoft Windows [Version 10.0.17134.829]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Windows\system32>cd C:\MODa

C:\MODa>java -Xmx1000M -jar moda_v1.62.jar -@ 1 -i modaParams.txt
*****
MODa v1.62: Multi-Blind Modification Search
Release Date: Jun 12, 2019
Hanyang University, Seoul, Korea
*****

Reading parameter.....
Input dataset : PTMSample.mzXML
Input dataset : swissProt.v201607.revCat.fasta
```

MODa 실행 결과

- Cmd 창

- `java -Xmx1000M -jar moda_v1.62.jar -@ 1 -i modaParams.txt`

```
C:\Windows\System32\cmd.exe
C:\#MODa>java -Xmx1000M -jar moda_v1.62.jar -@ 1 -i modaParams.txt
*****
MODa v1.62: Multi-Blind Modification Search
Release Date: Jun 12, 2019
Hanyang University, Seoul, Korea
*****

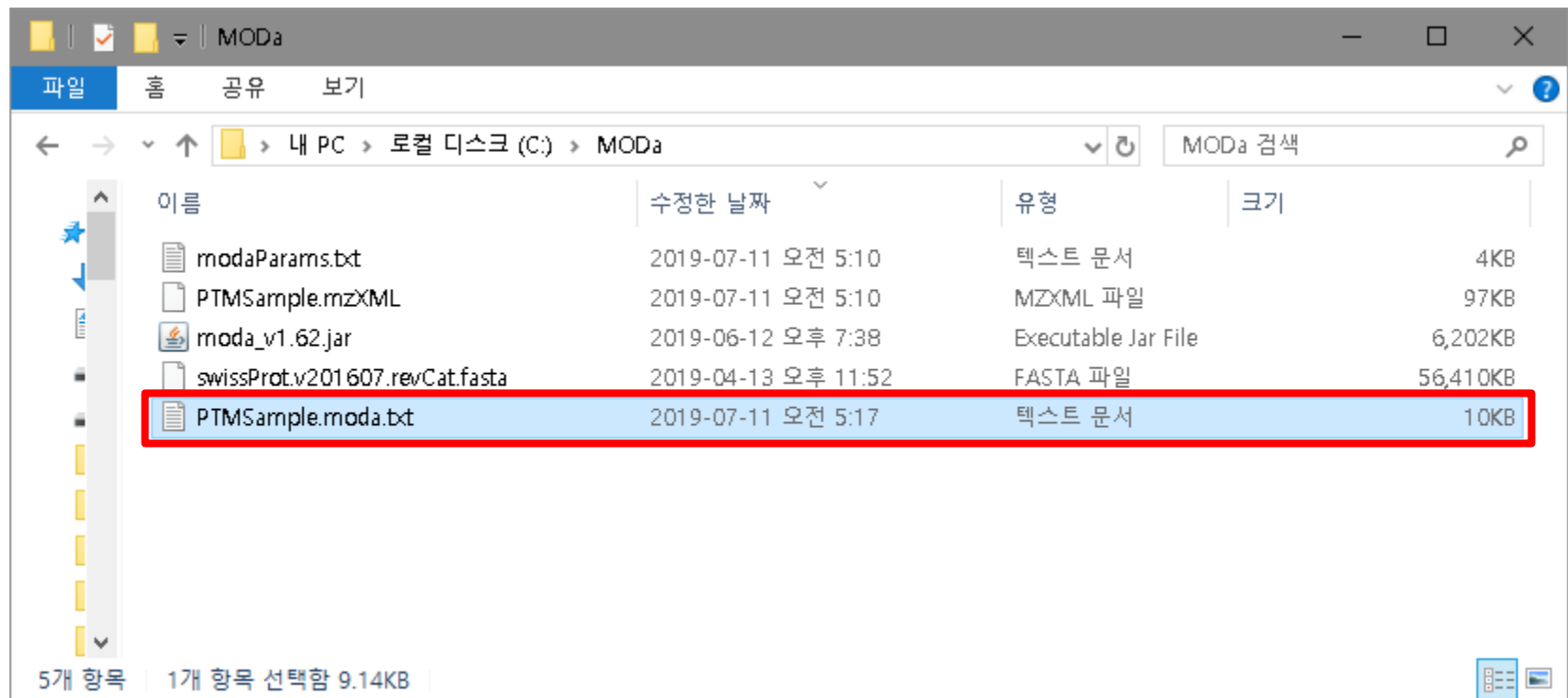
Reading parameter.....
Input dataset : PTMSample.mzXML
Input dataset : swissProt.v201607.revCat.fasta
Fixed Mod : 57.021464 is added to amino acid 'C'

Starting MOD-Alignment for multi-blind modification search!
Reading MS/MS spectra..... 20 scans
Reading protein database..... 84328 proteins / 48563476 residues (1)

0-thread was created!
moda | 1 at 0-thread
moda | 2 at 0-thread
moda | 3 at 0-thread
moda | 4 at 0-thread
moda | 5 at 0-thread
moda | 6 at 0-thread
moda | 7 at 0-thread
moda | 8 at 0-thread
moda | 9 at 0-thread
moda | 10 at 0-thread
moda | 11 at 0-thread
moda | 12 at 0-thread
moda | 13 at 0-thread
moda | 14 at 0-thread
moda | 15 at 0-thread
moda | 16 at 0-thread
moda | 17 at 0-thread
moda | 18 at 0-thread
moda | 19 at 0-thread
moda | 20 at 0-thread
[MOD-A] Elapsed Time : 295 Sec
```

MODa 실행 결과

- PTMSample.moda.txt 확인



MODa 실행 결과

- PTMSample.moda.txt 확인

```
PTMSample.moda.txt - 메모장
파일(F) 편집(E) 서식(O) 보기(V) 도움말(H)
MODa v1.62

>>C:\#MODa\#PTMSample.mzXML      1      2178.0520      3      20326
2177.9456      0.1064 96      1.0000 R.G+144NFGGSFAGSFGGAGGHAPGVAR.K sp|P52272      628~650
2178.0467      0.0053 90      1.0000 K.R+18AVGPAHGGAGGFSAGFSGGFNGR-30.E XXX_sp|P52272      81~104
2177.9456      0.1064 89      0.9999 R.A+174YGPAGHGGAGGFSAGFSGGFNGR-30.E XXX_sp|P52272      82~104
2177.8919      0.1601 62      0.8695 -.MAESGGSSGGAGGG+177GAFGAGPGER-76.P sp|Q53HC5      1~25
2177.8738      0.1782 61      0.3812 R.H+269RGSNKGA+76SGAEGGHGAAR.A XXX_sp|C9JTQ0      138~157

>>C:\#MODa\#PTMSample.mzXML      2      3085.3101      3      21713
3085.2065      0.1036 114      1.0000 R.R+144FSDTCFLDTDGQATCDACAPGYTGR.R sp|P98160      824~849
3085.1054      0.2047 114      1.0000 R.F+300SDTCFLDTDGQATCDACAPGYTGR.R sp|P98160      825~849
3085.3076      0.0025 108      1.0000 R.R+18GTYPACADCTAQQGDTDLFCTDSFR-30R.S XXX_sp|P98160      3543~3569
3085.2065      0.1036 108      1.0000 R.G+174TYGPACADCTAQQGDTDLFCTDSFR-30R.S XXX_sp|P98160      3544~3569
3085.2065      0.1036 107      1.0000 R.R+18GTYPACADCTAQQGDTDLFCTDSF+126R.R XXX_sp|P98160      3543~3569

>>C:\#MODa\#PTMSample.mzXML      3      3569.7368      4      21975
3569.6269      0.1098 87      0.9976 K.V+144LLESGASIEDHNENGHTPLMEAGSAGHVEVAR.L sp|Q75179      352~384
3569.6208      0.1160 79      0.9924 R.A+174VEVHGASGAEMLPHTGNENHDEISAGSELLVK-2.V XXX_sp|Q75179      2221~2253
3569.6644      0.0724 62      0.6444 K.VLLNEGANI ED+90HNENGHTPLMEAA-14SAGHVEVAR.V sp|Q81WZ3      323~355
3569.6582      0.0785 58      0.3082 R.A+174VEVHGASA-14AEMLPHTGNENHDEIN-56AGENLLVK.V XXX_sp|Q81WZ3      2189~2221
3569.8837      -0.1469 51      0.0507 R.AQACAFWNRLFP-28KLLSATGMQGPAGSAGRRGVGAR-61.Q sp|P22303-4      557~591

>>C:\#MODa\#PTMSample.mzXML      4      2740.3641      3      23213
2740.2517      0.1124 117      1.0000 R.S+144YPAPGAGHVQEEESNL SLQALESR.Q sp|Q13155      34~58
2740.2517      0.1124 113      1.0000 R.S+174ELAQSLNSEEQVHGAGPAPGYSR-30.G XXX_sp|Q13155      264~288
2740.3841      -0.0200 66      0.8671 K.LNPTTPPV+36RAGVQEESSPR-64YTGETQR.K XXX_sp|Q9BUF7      10~34
2740.3074      0.0567 66      0.8192 R.AFG+344RPKESEEK-20KKPKSEEK.D XXX_sp|P83916      72~92
2740.3932      -0.0291 63      0.8702 R.AALSFLNGKW-49VKK+1ERE+96ESTETNR.S sp|Q9P2N2-2      632~654

>>C:\#MODa\#PTMSample.mzXML      5      3686.6560      4      25501
3686.5500      0.1059 106      1.0000 R.RGY+144QLSDVDGYTCEDIDECALPTGGHICSYR.C sp|P23142      467~497
```

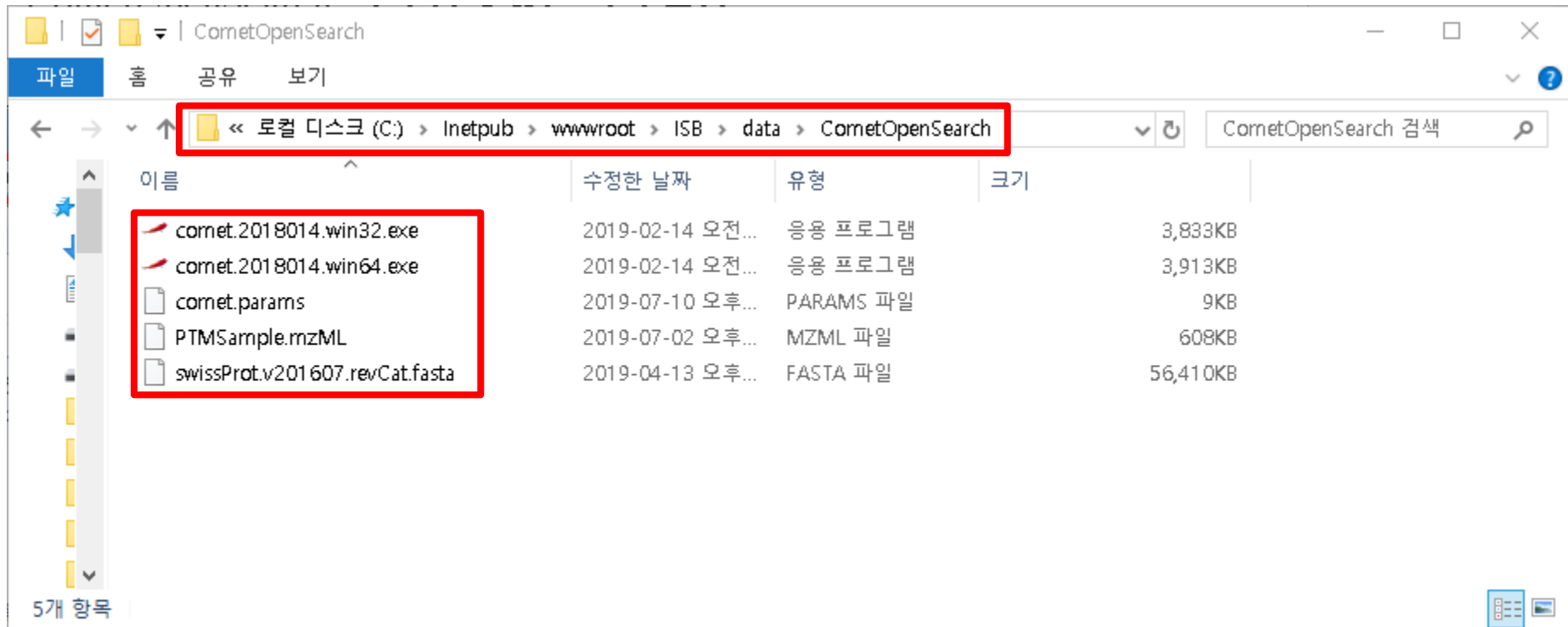

Comet OpenSearch 실행을 위한 준비

- **필요한 파일**
 - Comet-PTM 실행 파일 (.exe)
 - comet.2018014.win64.exe
 - comet.2018014.win32.exe
 - Spectrum 파일 (.mzxml or .mzml)
 - PTMSample.mzML
 - Database 파일 (.fasta)
 - swissProt.v201607.revCat.fasta
 - Parameter 파일 (.params)
 - comet.params

Comet OpenSearch 실행을 위한 준비

- **결과 파일을 TPP에서 사용할 수 있도록 복사**

- C:\Inetpub\wwwroot\ISB\data 폴더에 CometOpenSearch 폴더를 복사
- CometOpenSearch 폴더 안에 있는 파일 확인



Comet Parameter

```
# Comet MS/MS search engine parameters file.
# Everything following the '#' symbol is treated as a comment.

database_name = swissProt.v201607.revCat.fasta
decoy_search = 0                # 0=no (default), 1=concatenated search, 2=separate search

num_threads = 0                 # 0=poll CPU to set num threads; else specify num threads directly (max 64)

#
# masses
#
peptide_mass_tolerance = 500    # 0=amu, 1=mmu, 2=ppm
peptide_mass_units = 0          # 0=average masses, 1=monoisotopic masses
mass_type_parent = 1            # 0=average masses, 1=monoisotopic masses
mass_type_fragment = 1          # 0=MH+ (default), 1=precursor m/z; only valid for amu/mmu tolerances
precursor_tolerance_type = 0    # 0=off, 1=on -1/0/1/2/3 (standard C13 error), 2= -8/-4/0/4/8 (for +4/+8 labeling)
isotope_error = 0

#
# search enzyme
#
search_enzyme_number = 1        # choose from list at end of this params file
num_enzyme termini = 2          # 1 (semi-digested), 2 (fully digested, default), 8 C-term unspecific , 9 N-term unspecific
allowed_missed_cleavage = 0    # maximum value is 5; for enzyme search

#
# Up to 9 variable modifications are supported
# format: <mass> <residues> <0=variable/else binary> <max_mods_per_peptide> <term_distance> <n/c-term> <required>
# e.g. 79.966331 STY 0 3 -1 0 0
#
variable_mod01 = 0.0 M 0 3 -1 0 0
max_variable_mods_in_peptide = 2
require_variable_mod = 0

#
# fragment ions
```

Comet OpenSearch 실행

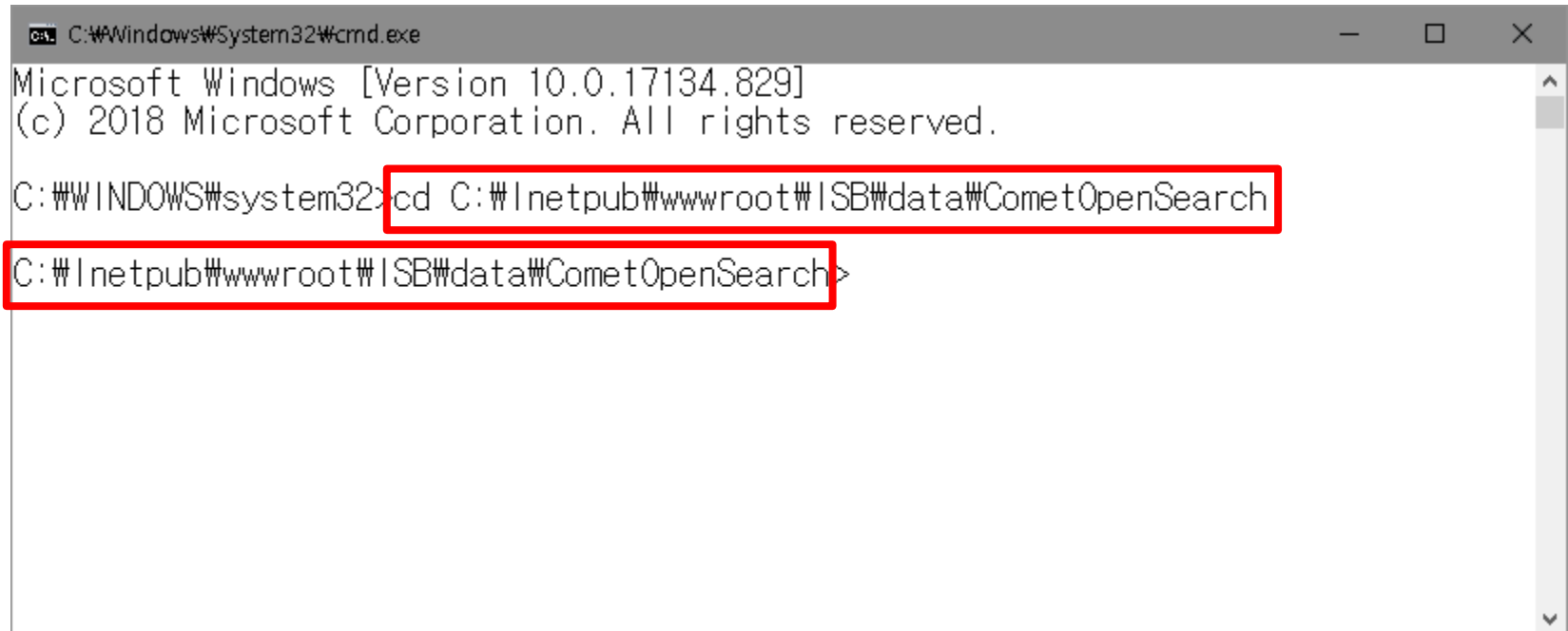
- Cmd 창 실행
 - 시작메뉴
 - cmd 입력



Comet OpenSearch 실행

- **Cmd 창**

- `cd C:\Inetpub\wwwroot\ISB\data\CometOpenSearch`



A screenshot of a Windows Command Prompt window. The title bar reads "C:\Windows\System32\cmd.exe". The window content shows the following text: "Microsoft Windows [Version 10.0.17134.829] (c) 2018 Microsoft Corporation. All rights reserved." followed by the command "C:\Windows\system32>cd C:\Inetpub\wwwroot\ISB\data\CometOpenSearch" and the resulting prompt "C:\Inetpub\wwwroot\ISB\data\CometOpenSearch>". The command and the new prompt are highlighted with red rectangular boxes.

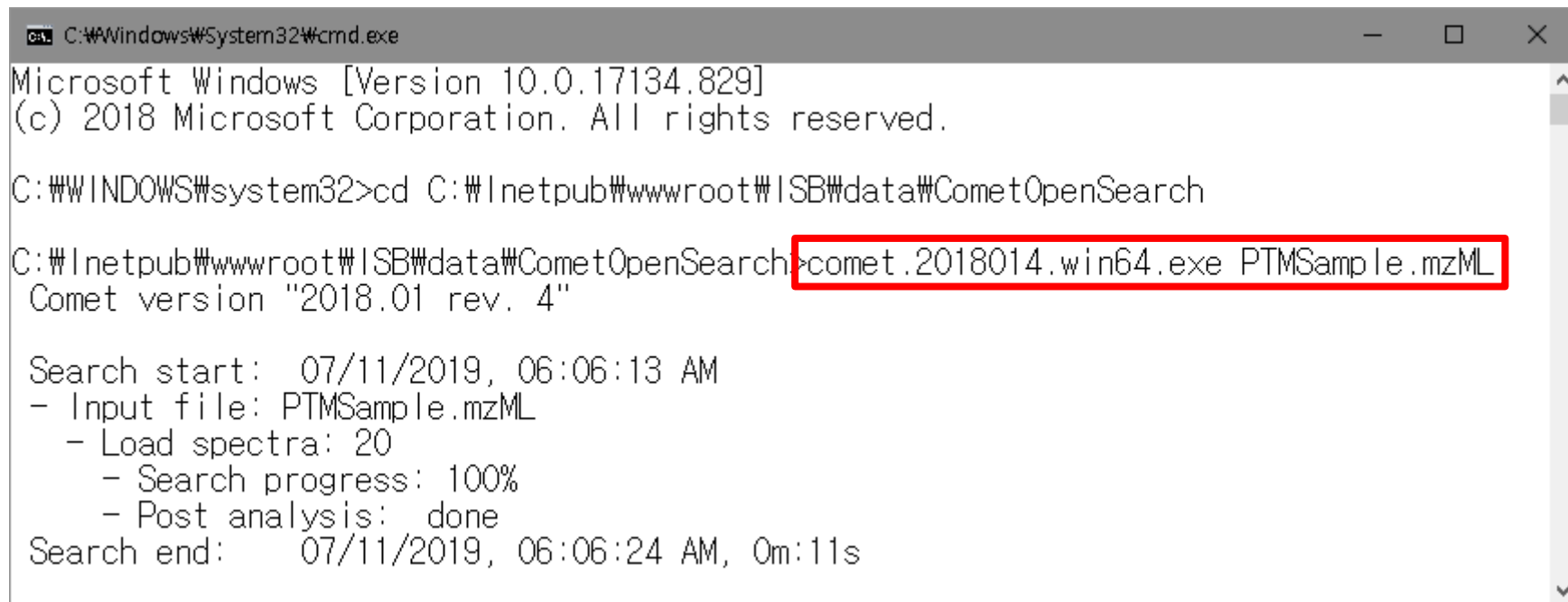
```
C:\Windows\System32\cmd.exe
Microsoft Windows [Version 10.0.17134.829]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Windows\system32>cd C:\Inetpub\wwwroot\ISB\data\CometOpenSearch
C:\Inetpub\wwwroot\ISB\data\CometOpenSearch>
```

Comet OpenSearch 실행

- Cmd 창

- comet.2018014.win64.exe PTMSample.mzML



```
C:\Windows\System32\cmd.exe
Microsoft Windows [Version 10.0.17134.829]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Windows\system32>cd C:\inetpub\wwwroot\ISB\data\CometOpenSearch

C:\inetpub\wwwroot\ISB\data\CometOpenSearch>comet.2018014.win64.exe PTMSample.mzML
Comet version "2018.01 rev. 4"

Search start: 07/11/2019, 06:06:13 AM
- Input file: PTMSample.mzML
  - Load spectra: 20
    - Search progress: 100%
    - Post analysis: done
Search end: 07/11/2019, 06:06:24 AM, 0m:11s
```

Comet OpenSearch 실행

- Comet OpneSearch 실행 완료

- Comet version
- Spectrum 개수
- 시작시간 및 종료시간

```
C:\Windows\System32\cmd.exe
Microsoft Windows [Version 10.0.17134.829]
(c) 2018 Microsoft Corporation. All rights reserved.

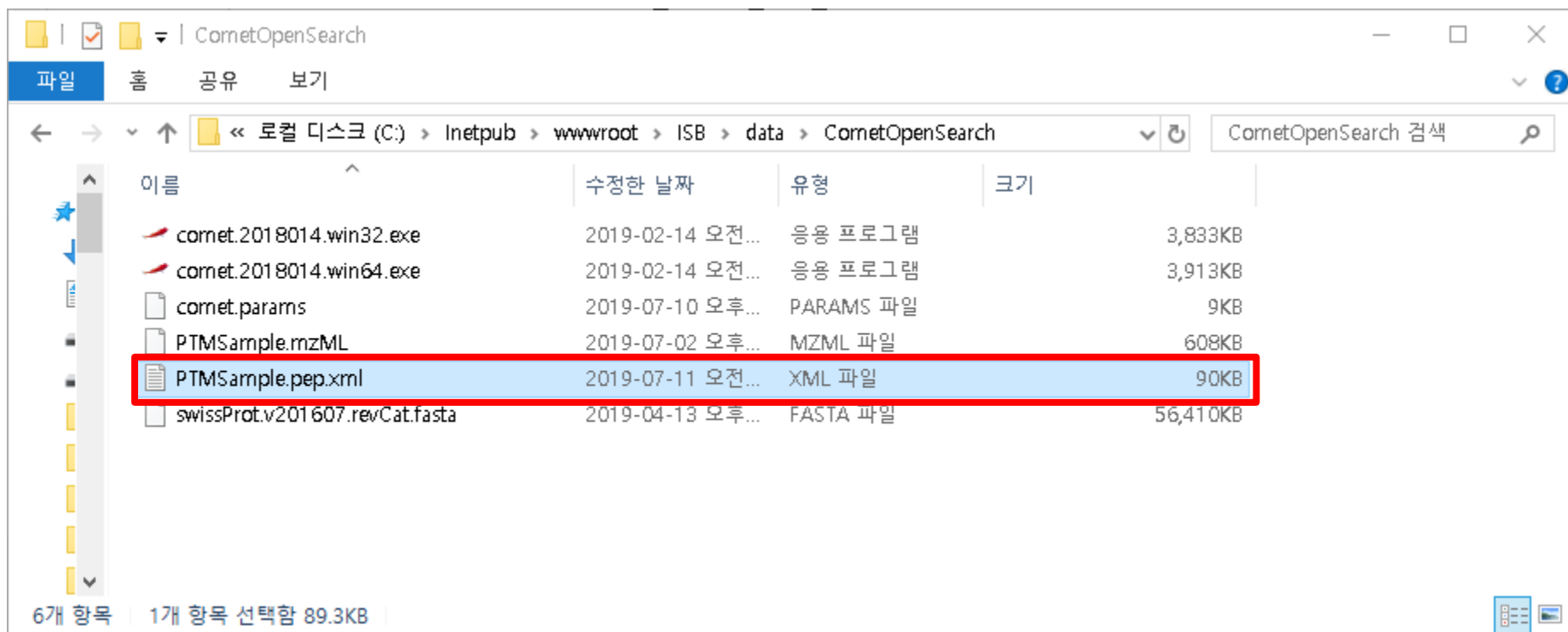
C:\WINDOWS\system32>cd C:\inetpub\wwwroot\ISB\data\CometOpenSearch

C:\inetpub\wwwroot\ISB\data\CometOpenSearch>comet.2018014.win64.exe PTMSample.mzML
Comet version "2018.01 rev. 4"

Search start: 07/11/2019, 06:06:13 AM
- Input file: PTMSample.mzML
  - Load spectra: 20
    - Search progress: 100%
    - Post analysis: done
Search end: 07/11/2019, 06:06:24 AM, 0m:11s
```

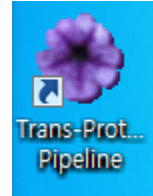
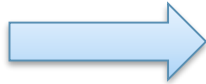
Comet OpenSearch 실행 결과

- PTMSample.pep.xml 확인 (TPP 사용)



TPP 실행 및 로그인

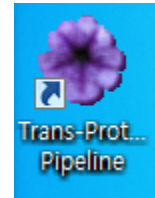
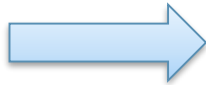
- **TPP 실행**
 - 바탕화면에 아이콘 실행



TPP 실행 및 로그인

- **TPP 실행**

- 바탕화면에 아이콘 실행



- **TPP 웹페이지에서 로그인**

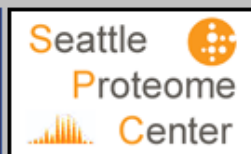
- User Name: guest
 - Password: guest

ISB/SPC Trans Proteomic Pipeline - login

User Name:

Password:

Login

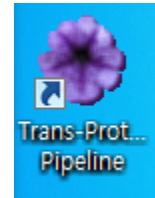
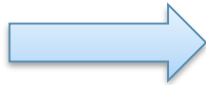


TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

TPP 실행 및 로그인

- **TPP 실행**

- 바탕화면에 아이콘 실행



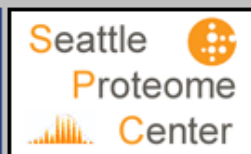
- **TPP 웹페이지에서 로그인**

- User Name: guest
 - Password: guest
 - Login 클릭

ISB/SPC Trans Proteomic Pipeline - login

User Name:

Password:



TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

Comet OpenSearch 실행 결과

- Comet OpenSearch 결과 확인

- Files
- Browse Files 클릭

ISB/SPC Trans Proteomic Pipeline - home

Home | Files | Account | Pre-Process | mzXML Utils | Analysis Pipeline (Comet) | Decoy | Utilities | SpectraST Tools | Jobs

You are logged in as guest. Log Out

Home | Files | ACCOUNT | PRE-PROCESS | mzXML UTILS | ANALYSIS PIPELINE | DECOY | UTILITIES | SPECTRAST TOOLS | JOBS

Messages [Show / Hide]

• Welcome, guest.

ISB/SPC Trans Proteomic Pipeline - home

Home | Files | Account | Pre-Process | mzXML Utils | Analysis Pipeline (Comet) |

Browse Files

Update Paths

mzIdent

Messages [Show / Hide]

SPC Tools

SPC Tools Wiki

Sashimi

SPCTools-Discuss at Google Groups

INSTITUTE FOR Systems Biology Revolutionizing science. Enhancing life.

Seattle Proteome Center

TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

Comet OpenSearch 실행 결과

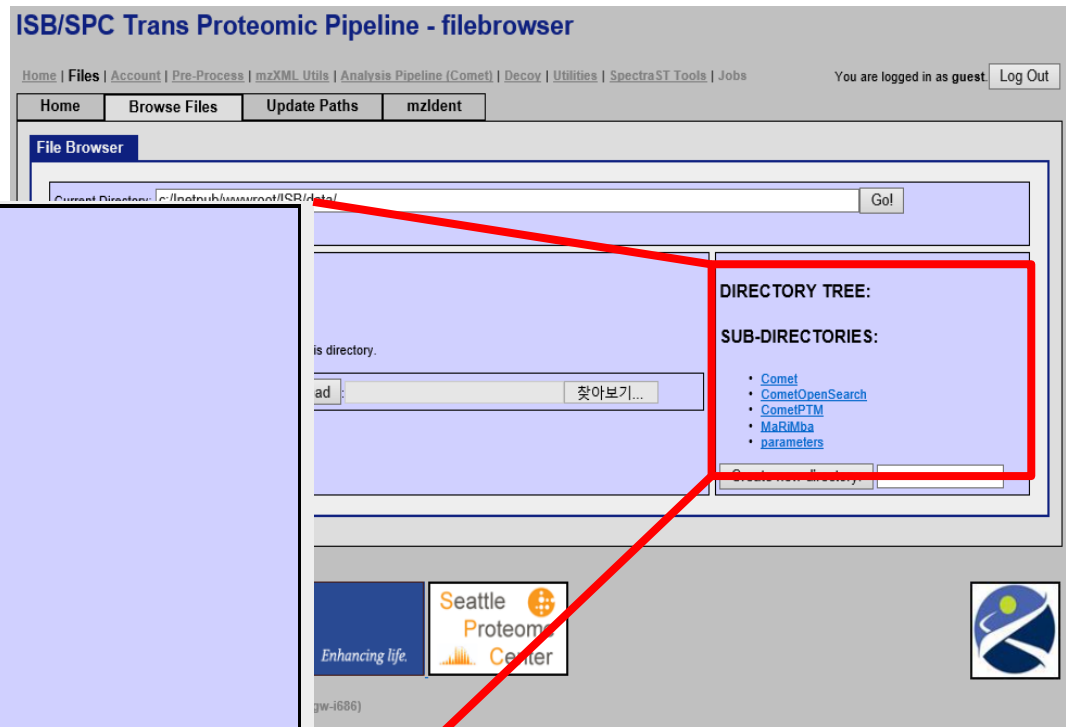
- Comet OpenSearch 결과 확인
 - CometOpenSearch 클릭

DIRECTORY TREE:

SUB-DIRECTORIES:

- [Comet](#)
- [CometOpenSearch](#)
- [CometPTM](#)
- [MaRiMba](#)
- [parameters](#)

Create new directory:



Comet OpenSearch 실행 결과

- Comet OpenSearch 결과 확인
 - [PepXML](#) 클릭

ISB/SPC Trans Proteomic Pipeline - filebrowser

Home | Files | Account | Pre-Process | mzXML Utils | Analysis Pipeline (Comet) | Decoy | Utilities | SpectraST Tools | Jobs

You are logged in as guest. Log Out

Home Browse Files Update Paths mzIdent

File Browser

Current Directory: c:/inetpub/wwwroot/ISB/data/CometOpenSearch/ Go

Set as Working Directory

FILES: (*.*)

☐ Select/Unselect All

File Name	View?	Size	Date Modified
<input type="checkbox"/> PTMSample.mzML	[Pep3D Edit]	607.6 KB	Tue Jul 2 17:43:19 2019
<input type="checkbox"/> PTMSample.pep.xml	[PepXML Edit]	89.4 KB	Thu Jul 11 06:06:24 2019
<input type="checkbox"/> comet.2018014.win32.exe	---	3.7 MB	Thu Feb 14 07:50:40 2019
<input type="checkbox"/> comet.2018014.win64.exe	---	3.8 MB	Thu Feb 14 07:48:00 2019
<input type="checkbox"/> comet.params	[View Edit]	8.3 KB	Wed Jul 10 23:03:43 2019
<input type="checkbox"/> swissProt.v201607.revCat.fasta	[View]	55.1 MB	Sat Apr 13 23:52:09 2019

6 files found

Delete Copy Paste S3 Sync Download Upload

찾아보기...

DIRECTORY TREE:

- Go up to: [data](#)
- Current: |--CometOpenSearch

SUB-DIRECTORIES:

- No subdirectories found in this folder.

Create new directory:

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Seattle
Proteome
Center

TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

Comet OpenSearch 실행 결과

- Comet OpenSearch 결과 확인

Summary	Display Options	Pick Columns	Filtering Options	Other Actions	[Hide options]
---------	-----------------	--------------	-------------------	---------------	------------------

Sorting: spectrum

desc

asc

Update Page

pepXML file: c:/inetpub/wwwroot/ISB/data/CometOpenSearch/PTMSample.pep.xml

Trypsin digest, COMET search engine, quantitation: [none]

displaying 20 of 20 total spectra, page 1 of 1

19 unique peptides, 19 unique stripped peptides, 19 unique proteins, 18 single hits

Peptide Viewer: 2000 SPECIES

Page 1 of 1

1

FIRST 1 LAST

SPECTRUM	SCAN	KCORR	DELTA	EXPECT	IONS	PEPTIDE	PROTEIN	CALC MASS
PTMSample.20326.20326.3	20326	4.241	0.519	2.55E-08	23/88	R.GNFGGSFAGSFGGAGGHAPGVAR.K	spIP52272IHNRPM_HUMAN +1	2033.945620
PTMSample.21713.21713.3	21713	3.137	0.522	5.13E-06	16/96	R.FSDTC160.03FLDTDGQATC160.03DAC160.03APGYTGR.R	spIP98160IPGBM_HUMAN	2785.105430
PTMSample.21975.21975.4	21975	4.598	0.531	4.15E-08	26/192	K.VLLESGASIEDHNEGHPTPLMEAGSAGHVEVAR.L	spIO75179IANR17_HUMAN +6	3425.626995
PTMSample.23213.23213.3	23213	4.019	0.565	5.75E-08	19/96	R.SYGPAAGAGHVQEEENSLSLQALESR.Q	spIQ13155IAMP2_HUMAN	2596.251758
PTMSample.25501.25501.4	25501	3.867	0.434	4.18E-06	21/174	R.GYQLSDVDGVGTC160.03EDIDEC160.03ALPTGGHIC160.03SYR.C	spIP23142IFBLN1_HUMAN +3	3386.448957
PTMSample.25540.25540.3	25540	3.662	0.538	7.90E-09	23/116	R.GYQLSDVDGVGTC160.03EDIDEC160.03ALPTGGHIC160.03SYR.C	spIP23142IFBLN1_HUMAN +3	3386.448957
PTMSample.26739.26739.4	26739	4.025	0.486	8.02E-06	23/186	K.TEVQEEVVATPVPHPTDLAAGTLFGPGQATR.F	spIQ6NUN9IZN746_HUMAN +2	3414.669178
PTMSample.28714.28714.4	28714	4.354	0.466	4.99E-07	26/162	R.DLPASLSAPMSAAHLQAMHAQSAELQR.L	spIP54259IATN1_HUMAN	2958.444009
PTMSample.30428.30428.4	30428	2.998	0.246	6.94E-03	14/144	R.APDEPQQAQVPHVWGVEVAGAPALR.L	spIQ8IVT2IMISP_HUMAN	2708.345933
PTMSample.30518.30518.4	30518	4.691	0.500	7.18E-07	27/192	R.QGAPPAAGQGALVELTPTPGGLALVSPFYHTR.A	spIQ9BV19ICA050_HUMAN	3219.678895
PTMSample.30806.30806.3	30806	4.001	0.066	1.21E-06	23/88	K.ISMFC160.03HVEPEQVIC160.03VHDVSSIYR.V	spIP17812IPYRG1_HUMAN	2804.308428
PTMSample.33097.33097.4	33097	3.365	0.285	6.58E-03	13/156	K.DHPWHIQSC160.03C160.03ALTGEGLC160.03QGLEWMTSR.I	spIQ96KC2IARL5B_HUMAN	3228.399779
PTMSample.33276.33276.3	33276	3.840	0.503	6.95E-08	22/84	R.YQSTGEFLQGVGHVYVDLSP.K	spIP21589ISNTD_HUMAN	2424.207374
PTMSample.33353.33353.4	33353	4.890	0.559	3.65E-07	22/222	R.AVYTSVQAQYSTAGVFQQSNLLSHSVQAADHLSISPR.G	spIQ6ZSR9IYJ005_HUMAN	4075.003536
PTMSample.33512.33512.3	33512	3.649	0.537	5.20E-08	22/96	R.GAGYTFQDQISETFNHANGTLTVSR.A	spIP62714IP2AB_HUMAN +1	2654.272494
PTMSample.34405.34405.3	34405	4.234	0.591	9.57E-14	25/100	R.VSFSYAGLSGDDPDLGPAHVTVIAR.Q	spIQ98TV4ITMM43_HUMAN	2642.334031
PTMSample.34889.34889.4	34889	3.627	0.284	3.28E-03	16/216	R.TMIGPEMNFVHLTHIGSGEMGAGDGLAMTGAVQEQMR.S	spIQ9NRR8IC42S1_HUMAN	3872.777641
PTMSample.38041.38041.3	38041	3.280	0.363	9.36E-04	14/88	R.NDFQLIGIQDGYLSLLQDSGEVR.E	spIP63241IIFSA1_HUMAN +1	2579.286747
PTMSample.38125.38125.4	38125	4.113	0.515	9.01E-07	25/198	R.IASAC160.03DELSC160.03EFLLAGAGGAGAGAAPGPHLPPR.G	spIQ7Z7E8IUB2Q1_HUMAN	3302.617617
PTMSample.39654.39654.4	39654	5.086	0.582	2.06E-09	29/198	R.EGSGIGALDSNLDWSHNFNMLGYDHTQSTELTR.L	spIO75390ICISY_HUMAN	3825.732917

jump to FIRST 1 LAST

PepXML Viewer: c:/inetpub/wwwroot/ISB/data/CometOpenSearch/PTMSample.pep.xml
 This program displays peptide data stored in PepXML files.
 Developed at [Institute for Systems Biology / Seattle Proteome Center](#)
 version: TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

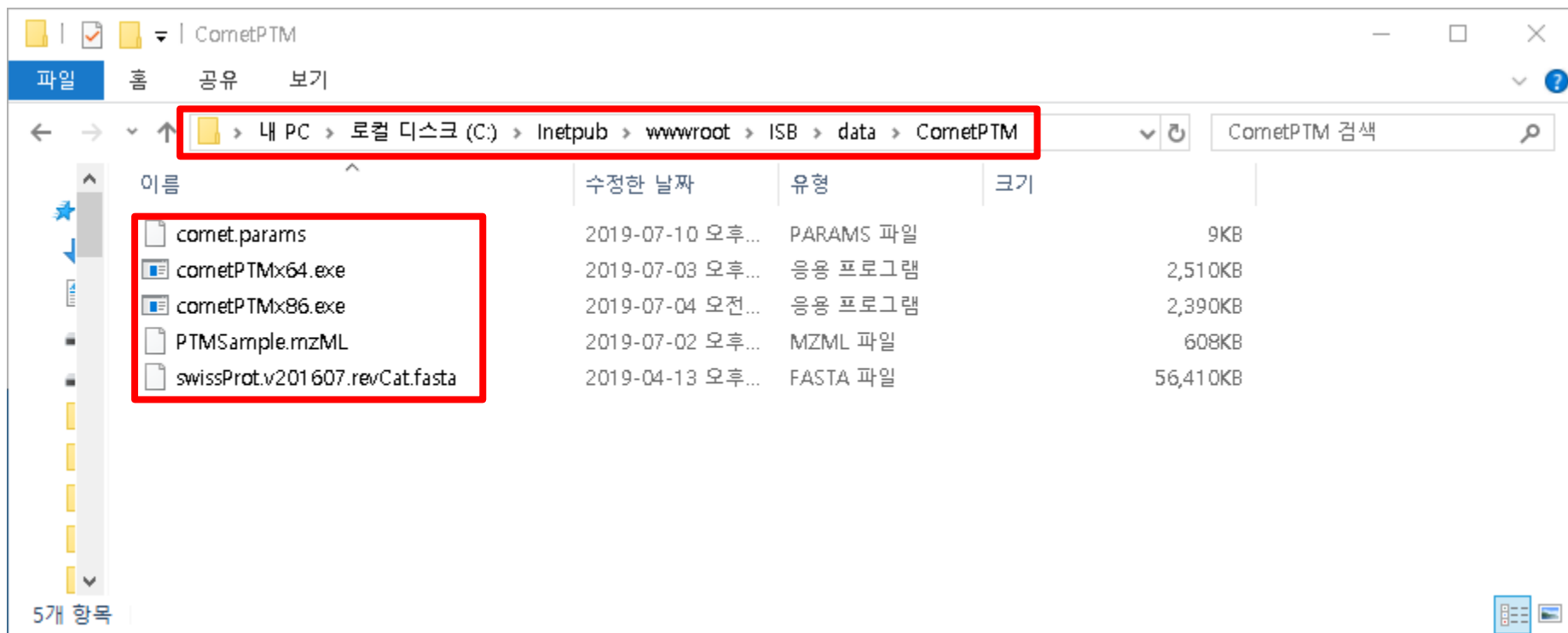
XHTML 1.0

Comet-PTM 실행을 위한 준비

- **필요한 파일**
 - Comet-PTM 실행 파일 (.exe)
 - cometPTMx64.exe
 - cometPTMx86.exe
 - Spectrum 파일 (.mzxml or .mzml)
 - PTMSample.mzML
 - Database 파일 (.fasta)
 - swissProt.v201607.revCat.fasta
 - Parameter 파일 (.params)
 - comet.params

Comet-PTM 실행을 위한 준비

- **결과 파일을 TPP에서 사용할 수 있도록 복사**
 - C:\Inetpub\wwwroot\ISB\data 폴더에 CometPTM 폴더를 복사
 - CometPTM 폴더 안에 있는 파일 확인



Comet-PTM Parameter

```
# Comet MS/MS search engine parameters file.
# Everything following the '#' symbol is treated as a comment.

database_name = swissProt.v201607.revCat.fasta
decoy_search = 0                # 0=no (default), 1=concatenated search, 2=separate search

num_threads = 0                 # 0=poll CPU to set num threads; else specify num threads directly (max 64)

#
# CNIC / comet-iq / comet-PTM specific
#
# do deltaX search for: (-delta_tolerance_outer < deltaMass < -delta_tolerance_inner) OR
#                      (+delta_tolerance_inner < deltaMass < +delta_tolerance_outer)
#
use_delta_xcorr      = 1        # 0=no (default), 1=yes
delta_outer_tolerance = 500     # ignored if use_delta_xcorr 0, default 320
delta_inner_tolerance = 0       # ignored if use_delta_xcorr 0, default 0.8
use_delta_back_jumps  = 0       # 0=no (default), 1=yes
use_delta_forward_jumps = 0     # 0=no (default), 1=yes
dont_calc_pseudo_non_mod = 1    # 0=yes, calculate pseudo nonmod (default), 1=avoid calculating pseudo non_mod

#
# masses
#
peptide_mass_tolerance = 500
peptide_mass_units = 0          # 0=amu, 1=mmu, 2=ppm
mass_type_parent = 1            # 0=average masses, 1=monoisotopic masses
mass_type_fragment = 1          # 0=average masses, 1=monoisotopic masses
precursor_tolerance_type = 0     # 0=MH+ (default), 1=precursor m/z; only valid for amu/mmu tolerances
isotope_error = 0               # 0=off, 1=on -1/0/1/2/3 (standard C13 error), 2= -8/-4/0/4/8 (for +4/+8 labeling)

#
# search enzyme
#
search enzyme number = 1        # choose from list at end of this params file
```

Comet-PTM 실행

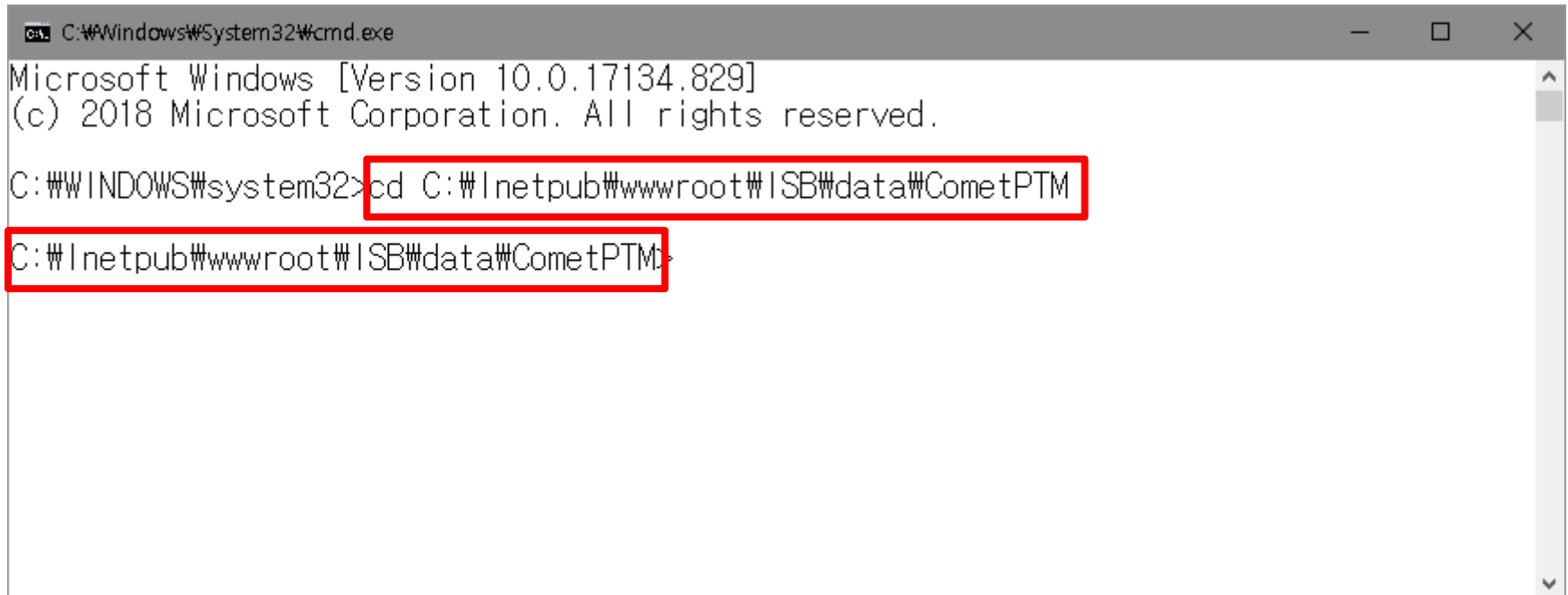
- Cmd 창 실행
 - 시작메뉴
 - cmd 입력



Comet-PTM 실행

- Cmd 창

- cd C:\Inetpub\wwwroot\ISB\data\CometPTM

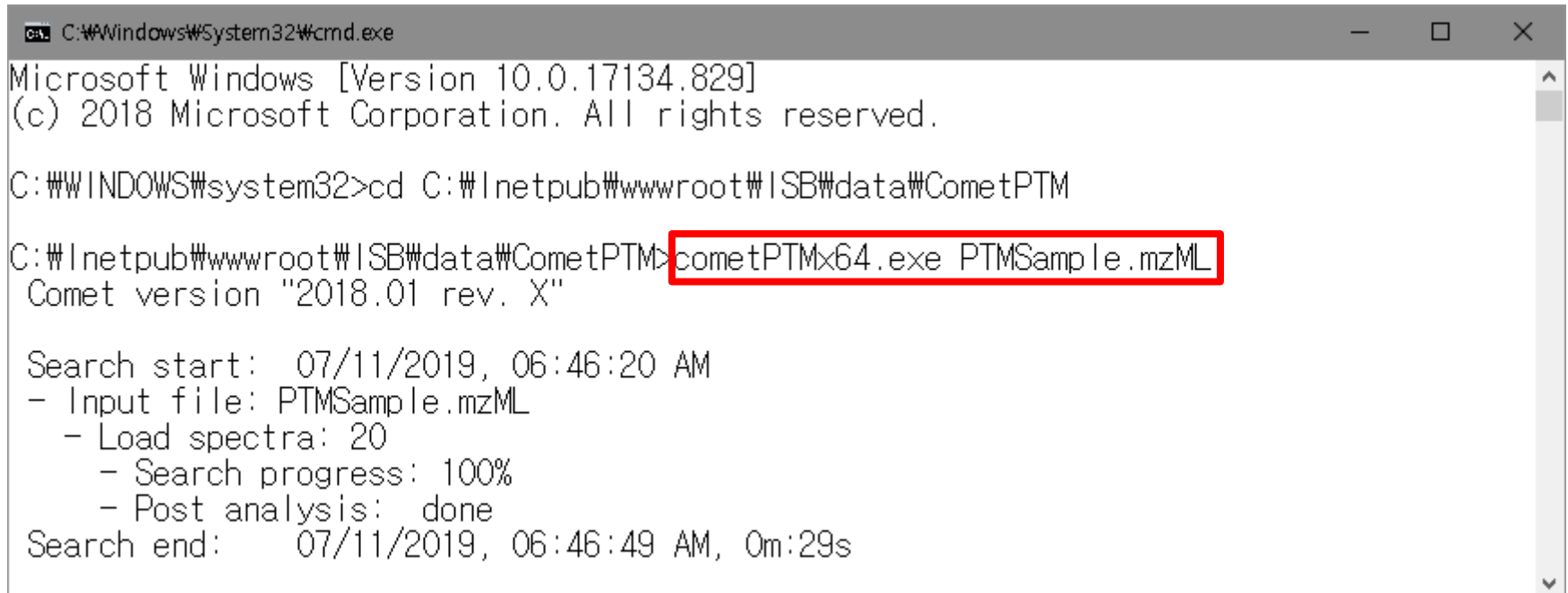


```
C:\Windows\System32\cmd.exe
Microsoft Windows [Version 10.0.17134.829]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Windows\system32>cd C:\Inetpub\wwwroot\ISB\data\CometPTM
C:\Inetpub\wwwroot\ISB\data\CometPTM>
```

Comet-PTM 실행

- **Cmd 창**
 - cometPTMx64.exe PTMSample.mzML



```
C:\Windows\System32\cmd.exe
Microsoft Windows [Version 10.0.17134.829]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Windows\system32>cd C:\inetpub\wwwroot\ISB\data\CometPTM

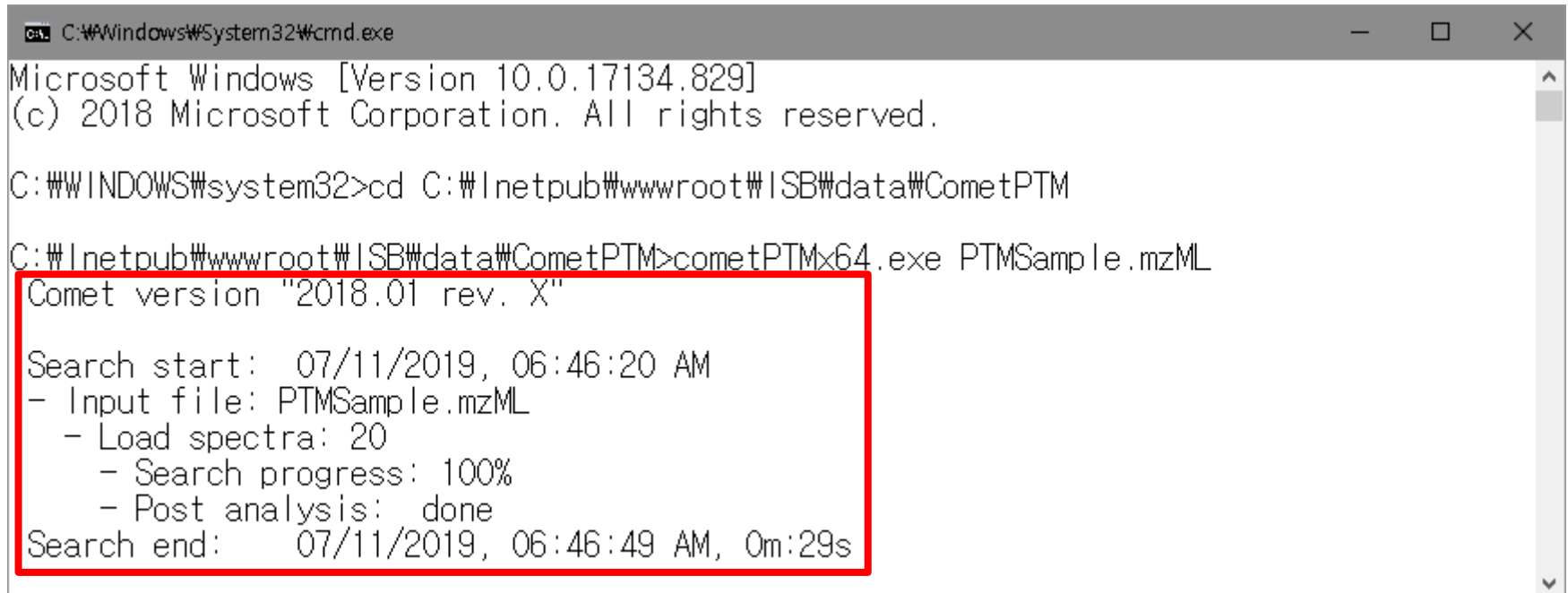
C:\inetpub\wwwroot\ISB\data\CometPTM>cometPTMx64.exe PTMSample.mzML
Comet version "2018.01 rev. X"

Search start: 07/11/2019, 06:46:20 AM
- Input file: PTMSample.mzML
  - Load spectra: 20
    - Search progress: 100%
    - Post analysis: done
Search end: 07/11/2019, 06:46:49 AM, 0m:29s
```

Comet-PTM 실행

- **Comet OpneSearch 실행 완료**

- Comet version
- Spectrum 개수
- 시작시간 및 종료시간



```
C:\Windows\System32\cmd.exe
Microsoft Windows [Version 10.0.17134.829]
(c) 2018 Microsoft Corporation. All rights reserved.

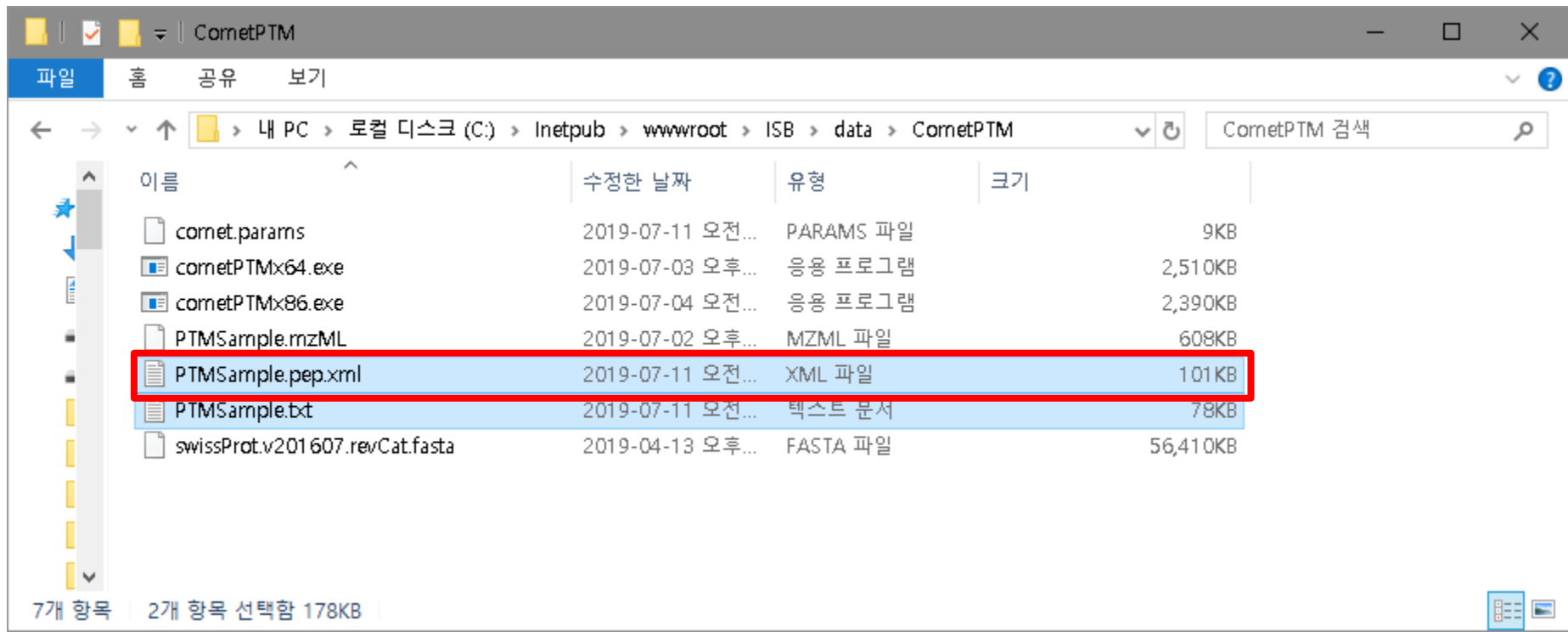
C:\WINDOWS\system32>cd C:\inetpub\wwwroot\ISB\data\CometPTM

C:\inetpub\wwwroot\ISB\data\CometPTM>cometPTMx64.exe PTMSample.mzML
Comet version "2018.01 rev. X"

Search start:  07/11/2019, 06:46:20 AM
- Input file: PTMSample.mzML
  - Load spectra: 20
    - Search progress: 100%
    - Post analysis:  done
Search end:    07/11/2019, 06:46:49 AM, 0m:29s
```

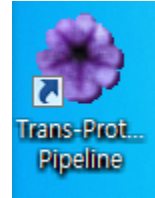
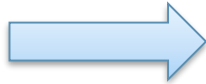
Comet-PTM 실행 결과

- PTMSample.pep.xml 확인 (TPP 사용)



TPP 실행 및 로그인

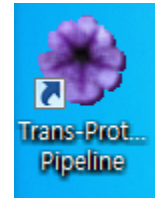
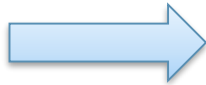
- **TPP 실행**
 - 바탕화면에 아이콘 실행



TPP 실행 및 로그인

- **TPP 실행**

- 바탕화면에 아이콘 실행



- **TPP 웹페이지에서 로그인**

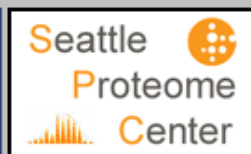
- User Name: guest
 - Password: guest

ISB/SPC Trans Proteomic Pipeline - login

User Name:

Password:

Login

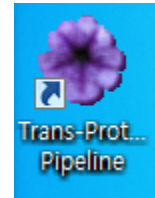
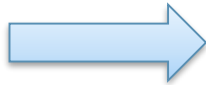


TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

TPP 실행 및 로그인

- **TPP 실행**

- 바탕화면에 아이콘 실행



- **TPP 웹페이지에서 로그인**

- User Name: guest
 - Password: guest
 - Login 클릭

ISB/SPC Trans Proteomic Pipeline - login

User Name:

Password:

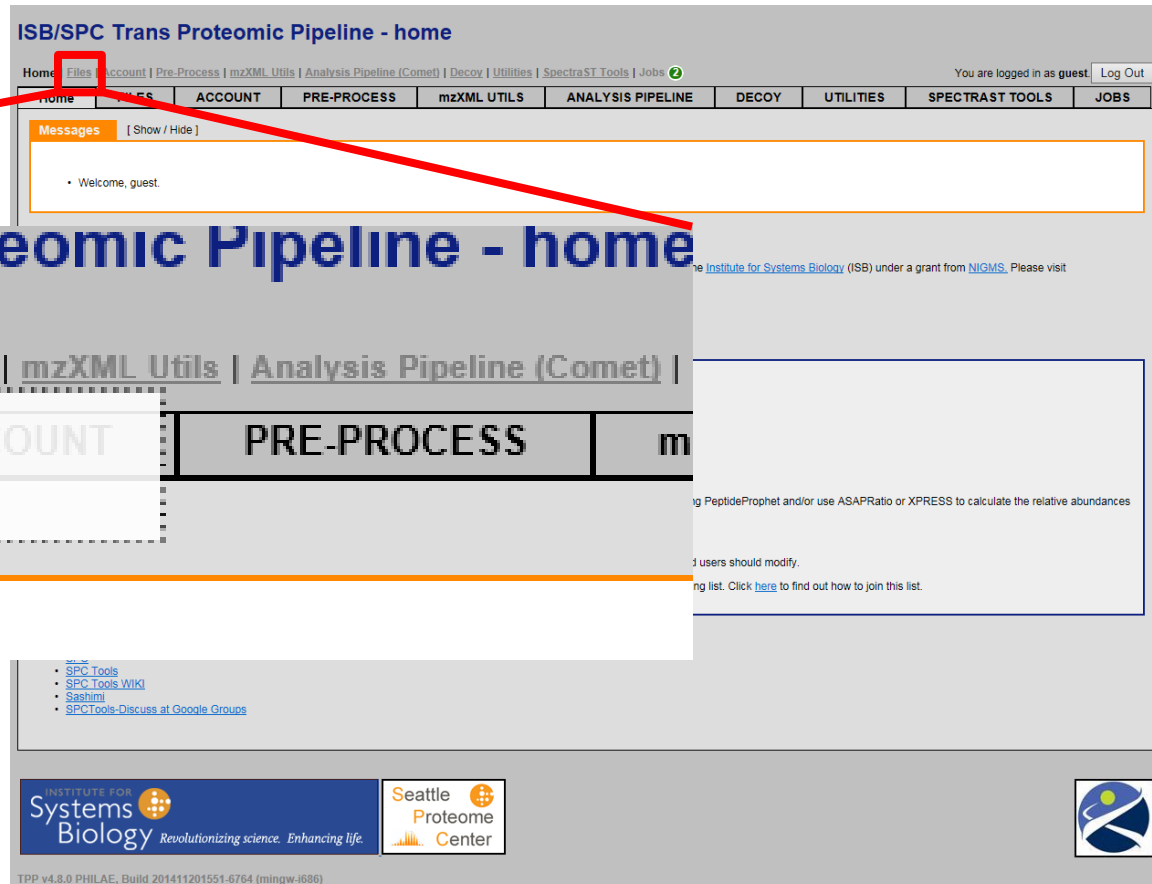


TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

Comet-PTM 실행 결과

- Comet-PTM 결과 확인

- Files
- Browse Files 클릭



ISB/SPC Trans Proteomic Pipeline - home

Home | Files | Account | Pre-Process | mzXML Utils | Analysis Pipeline (Comet) | Decoy | Utilities | SpectraST Tools | Jobs

You are logged in as guest. Log Out

Home | Files | ACCOUNT | PRE-PROCESS | mzXML UTILS | ANALYSIS PIPELINE | DECOY | UTILITIES | SPECTRAST TOOLS | JOBS

Messages [Show / Hide]

• Welcome, guest.

ISB/SPC Trans Proteomic Pipeline - home

Home | Files | Account | Pre-Process | mzXML Utils | Analysis Pipeline (Comet) | Decoy | Utilities | SpectraST Tools | Jobs

Home | Files | ACCOUNT | PRE-PROCESS | mzXML UTILS | ANALYSIS PIPELINE | DECOY | UTILITIES | SPECTRAST TOOLS | JOBS

Browse Files

Update Paths

mzIdent

Messages [Show / Hide]

SPC Tools

SPC Tools Wiki

Sashimi

SPCTools-Discuss at Google Groups

Institute for Systems Biology

Seattle Proteome Center

TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

Comet-PTM 실행 결과

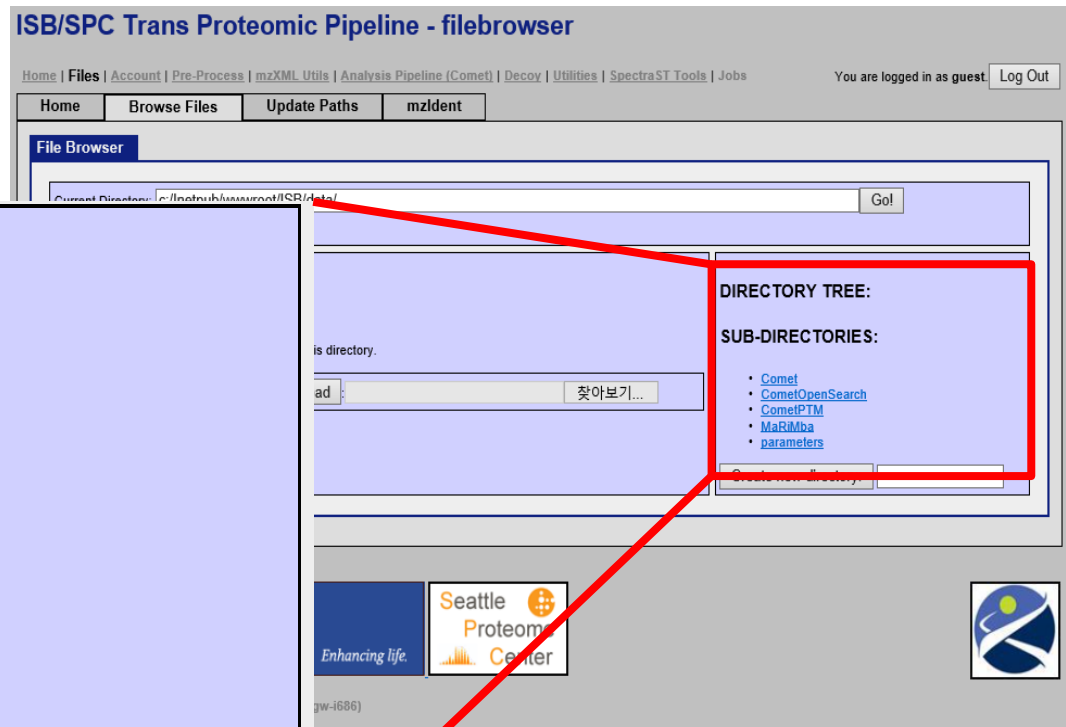
- Comet-PTM 결과 확인
 - CometPTM 클릭

DIRECTORY TREE:

SUB-DIRECTORIES:

- [Comet](#)
- [CometOpenSearch](#)
- [CometPTM](#)
- [MaRiMba](#)
- [parameters](#)

Create new directory:



Comet-PTM 실행 결과

- Comet-PTM 결과 확인
 - [PepXML](#) 클릭

ISB/SPC Trans Proteomic Pipeline - filebrowser

Home | Files | Account | Pre-Process | mzXML Utils | Analysis Pipeline (Comet) | Decoy | Utilities | SpectraST Tools | Jobs

You are logged in as guest. [Log Out](#)

Home Browse Files Update Paths mzIdent

File Browser

Current Directory: [Go!](#) [Set as Working Directory](#)

FILES: (*.*)

☐ Select/Unselect All

File Name	View?	Size	Date Modified
<input type="checkbox"/> PTMSample.mzML	[Pep3D] [Edit]	607.6 KB	Tue Jul 2 17:43:19 2019
<input type="checkbox"/> PTMSample.pep.xml	[PepXML] [Edit]	100.5 KB	Thu Jul 11 06:46:49 2019
<input type="checkbox"/> comet.params	[View] [Edit]	8.9 KB	Thu Jul 11 06:44:09 2019
<input type="checkbox"/> cometPTMx64.exe	---	2.5 MB	Wed Jul 3 18:28:53 2019
<input type="checkbox"/> cometPTMx86.exe	---	2.3 MB	Thu Jul 4 01:04:06 2019
<input type="checkbox"/> swissProt.v201607.revCat.fasta	[View]	55.1 MB	Sat Apr 13 23:52:09 2019

6 files found

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DIRECTORY TREE:

- Go up to: [data](#)
- Current: |--CometPTM

SUB-DIRECTORIES:

- No subdirectories found in this folder.

Create new directory:

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Seattle Proteome Center

TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

Comet-PTM 실행 결과

• Comet-PTM 결과 확인

Summary
Display Options
Pick Columns
Filtering Options
Other Actions
[Hide options]

pepXML file: c:/inetpub/wwwroot/ISB/data/CometPTM/PTMSample.pep.xml
Trypsin digest, COMET search engine, quantitation: [none]
displaying 20 of 20 total spectra, page 1 of 1
19 unique peptides, 19 unique stripped peptides, 19 unique proteins, 18 single hits
PepXML Viewer: 2008-07-03

Sorting: spectrum desc asc
Update Page

Page 1 of 1
1 FIRST 1 LAST

SPECTRUM	SCAN	XCORR	DELTA	EXPECT	IONS	PEPTIDE	PROTEIN	CALC. MASS
PTMSample.20326.20326.3	20326	6.850	0.584	1.29E-10	23/88	R.GNFGGSFAGSFGGAGGHAPGVAR.R	spIP52272IHNRPM_HUMAN +1	2033.945620
PTMSample.21713.21713.3	21713	6.580	0.703	1.04E-15	16/96	R.FSDTC160.03FLDTGQATC160.03DAC160.03APGYTGR.R	spIP98160IPGEM_HUMAN	2785.105430
PTMSample.21975.21975.4	21975	7.073	0.678	8.33E-14	26/192	K.VLLESGASTEDHNENGHTPLMEAGSAGHVEVAR.L	spIQ75179ANR17_HUMAN +6	3425.626995
PTMSample.23213.23213.3	23213	6.758	0.661	2.97E-12	19/96	R.SYGPAPGAGHVQEEENSLQLALESR.Q	spIQ13155IAMP2_HUMAN	2596.251758
PTMSample.25501.25501.4	25501	7.290	0.676	2.99E-15	21/174	R.GYQLSDVDGVTC160.03EDIDEC160.03ALPTGGHIC160.03SYR.C	spIP23142IFBLN1_HUMAN +3	3386.448957
PTMSample.25540.25540.3	25540	6.611	0.690	1.61E-11	23/116	R.GYQLSDVDGVTC160.03EDIDEC160.03ALPTGGHIC160.03SYR.C	spIP23142IFBLN1_HUMAN +3	3386.448957
PTMSample.26739.26739.4	26739	7.184	0.656	3.19E-13	23/186	K.TEVQEEVVATPVHPTDLEAHGTLFGPGQATR.F	spIQ6NUN9IZN746_HUMAN +2	3414.669178
PTMSample.28714.28714.4	28714	6.536	0.584	7.52E-09	26/162	R.DLPASLSAPMSAAHQLOAMHAQSAELQR.L	spIP54259IATN1_HUMAN	2958.444009
PTMSample.30428.30428.4	30428	6.636	0.605	1.75E-10	14/144	R.APDEPQQAQVPHVWGVEVAGAPALR.L	spIQ8IVT2IMISP_HUMAN	2708.345933
PTMSample.30518.30518.4	30518	7.482	0.587	2.64E-08	27/192	R.QGAPPAAGQGALVELITPGGLALVSPYHTR.A	spIQ9BV19CA050_HUMAN	3219.678895
PTMSample.30806.30806.3	30806	7.027	0.031	4.95E-09	23/88	K.ISMFC160.03HVEPEQVIC160.03VHDVSSIYR.V	spIP17812PYRG1_HUMAN	2804.308428
PTMSample.33097.33097.4	33097	6.873	0.563	1.17E-11	13/156	K.DHPWHIQSC160.03C160.03ALTGEGLC160.03QGLEWHTSR.I	spIQ96KC2IARL5B_HUMAN	3228.399779
PTMSample.33276.33276.3	33276	6.856	0.601	1.81E-10	22/84	R.YQSGTGEFLQVGGIHHVYDLR.K	spIP21589ISNTD_HUMAN	2424.207374
PTMSample.33353.33353.4	33353	7.179	0.638	1.79E-13	22/222	R.AVYTSVQAQYSTAGTVQSSNLLSHSVQAADHLDSISPR.G	spIQ6ZSR9IYJ005_HUMAN	4075.003536
PTMSample.33512.33512.3	33512	6.802	0.673	2.97E-15	22/96	R.GAGYTFQGDISETFNHANGLILVSR.A	spIP62714IPP2AB_HUMAN +1	2654.272494
PTMSample.34405.34405.3	34405	6.610	0.647	5.34E-16	25/100	R.VSFYAGLSGDDPDGLGPAHVTVIAR.Q	spIQ9BTV4ITMM43_HUMAN	2642.334031
PTMSample.34889.34889.4	34889	7.314	0.599	1.84E-11	16/216	R.TMIGEPMNFVHLTHIGSGEMGAGDLAMTGAVGQMR.S	spIQ9NRR8IC42S1_HUMAN	3872.777641
PTMSample.38041.38041.3	38041	6.558	0.525	2.48E-09	14/88	R.NDFQLIGIQDGLSLLQDSGEVR.F	spIP63241IFSA1_HUMAN +1	2579.286747
PTMSample.38125.38125.4	38125	6.722	0.681	2.77E-13	25/198	R.IASAC160.03LDELSC160.03EFLLAGAGGAGAGAAGPHLPFR.G	spIQ7Z7E8UB2Q1_HUMAN	3302.617617
PTMSample.39654.39654.4	39654	8.738	0.711	2.09E-15	29/198	R.EGSGIGATDSNLWSHNFNTMLGYTDHQSTELTR.L	spIQ75390ICISY_HUMAN	3825.732917

jump to FIRST 1 LAST

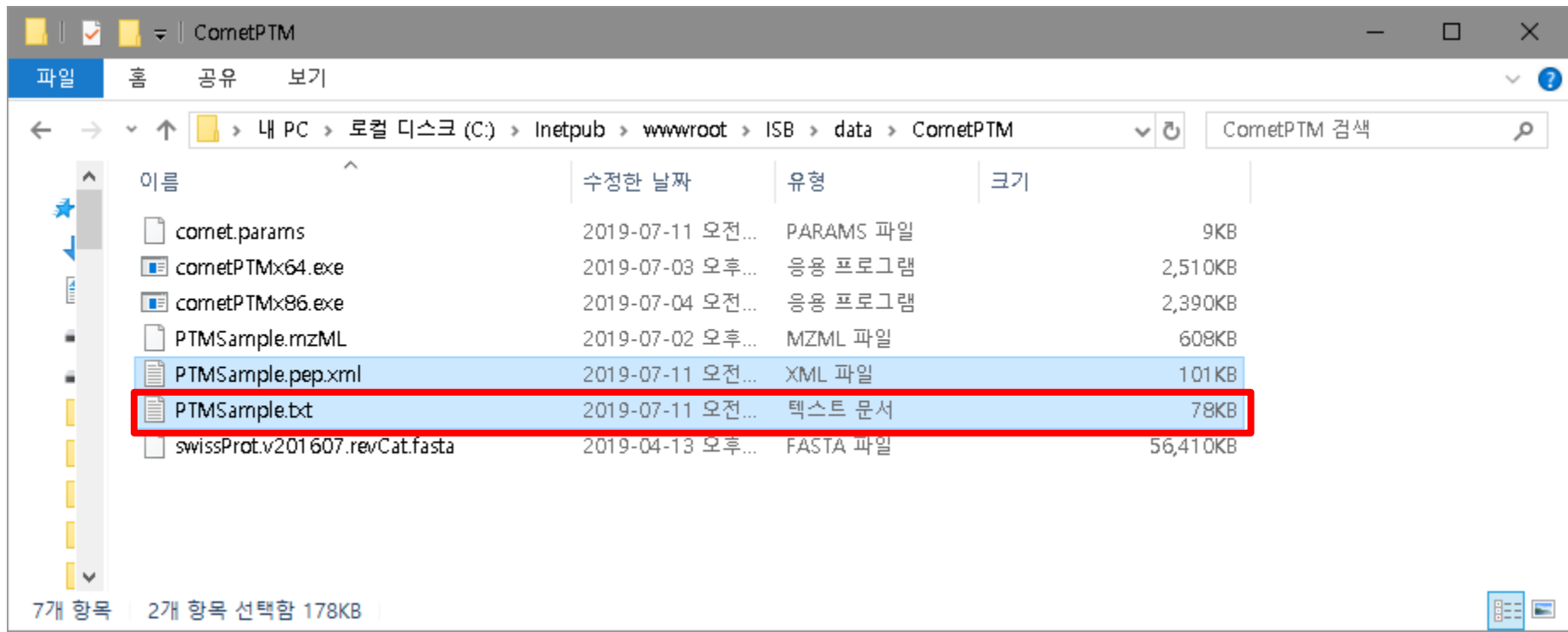
PepXML Viewer: c:/inetpub/wwwroot/ISB/data/CometPTM/PTMSample.pep.xml
This program displays peptide data stored in PepXML files.
Developed at [Institute for Systems Biology / Seattle Proteome Center](#)
version: TPP v4.8.0 PHILAE, Build 201411201551-6764 (mingw-i686)

W3C XHTML 1.0

Comet-PTM 실행 결과

- Comet-PTM 결과 확인 [2]

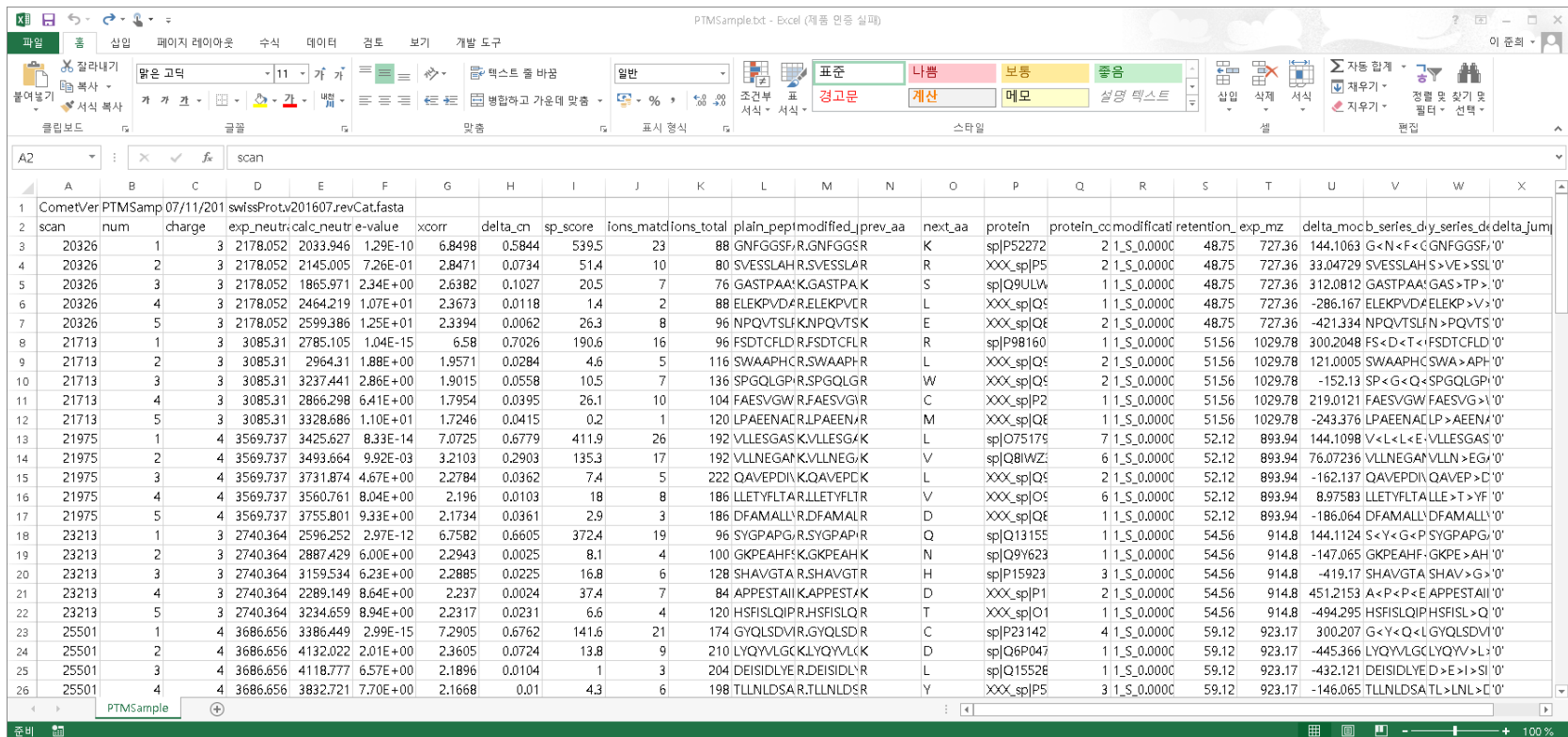
- C:\Inetpub\wwwroot\ISB\data\CometPTM 폴더 이동



Comet-PTM 실행 결과

• Comet-PTM 결과 확인 [2]

- C:\Inetpub\wwwroot\ISB\data\CometPTM 폴더 이동
- PTMSample.txt 파일 excel에서 열기



scan	num	charge	exp_neutral	calc_neutral	value	xcorr	delta_cn	sp_score	ions_matched	ions_total	plain_peptide	modified	prev_aa	next_aa	protein	protein_cm	modification	retention	exp_mz	delta_mob	b_series	d_y_series	delta_jum
20326	1	3	2178.052	2033.946	1.29E-10	6.8498	0.5844	539.5	23	88	GNFGGSF	R	GNFGGSF	K	sp P52272	2	1_S_0.0000	48.75	727.36	144.1063	G<N<F<G	GNFGGSF	'0'
20326	2	3	2178.052	2145.005	7.26E-01	2.8471	0.0734	51.4	10	80	SVESLAH	R	SVESLAH	R	XXX_sp P5	2	1_S_0.0000	48.75	727.36	33.04729	SVESLAH	S>VE>SSL	'0'
20326	3	3	2178.052	1865.971	2.34E+00	2.6382	0.1027	20.5	7	76	GASTPAA	K	GASTPAK	S	sp Q9ULW	1	1_S_0.0000	48.75	727.36	312.0812	GASTPAA	GAS>TP>	'0'
20326	4	3	2178.052	2464.219	1.07E+01	2.3673	0.0118	1.4	2	88	ELEKPV	D	ELEKPV	L	XXX_sp Q5	1	1_S_0.0000	48.75	727.36	-286.167	ELEKPV	D>ELEKPV	'0'
20326	5	3	2178.052	2599.386	1.25E+01	2.3394	0.0062	26.3	8	96	NPQVTS	L	NPQVTS	E	XXX_sp Q6	2	1_S_0.0000	48.75	727.36	-421.334	NPQVTS	L>NPQVTS	'0'
21713	1	3	3085.31	2785.105	1.04E-15	6.58	0.7026	190.6	16	96	FSDTCLD	R	FSDTCLD	R	sp P98160	1	1_S_0.0000	51.56	1029.78	300.2048	FS<D<T<	FSDTCLD	'0'
21713	2	3	3085.31	2964.31	1.88E+00	1.9571	0.0284	4.6	5	116	SWAAPHC	R	SWAAPHR	L	XXX_sp Q5	2	1_S_0.0000	51.56	1029.78	121.0005	SWAAPHC	SWA>APH	'0'
21713	3	3	3085.31	3237.441	2.86E+00	1.9015	0.0558	10.5	7	136	SPGQLGP	R	SPGQLGR	W	XXX_sp Q5	2	1_S_0.0000	51.56	1029.78	-152.13	SP<G<Q	SPGQLGP	'0'
21713	4	3	3085.31	2866.298	6.41E+00	1.7954	0.0395	26.1	10	104	FAESVGW	R	FAESVGR	C	XXX_sp P2	1	1_S_0.0000	51.56	1029.78	219.0121	FAESVGW	FAESVG>	'0'
21713	5	3	3085.31	3328.686	1.10E+01	1.7246	0.0415	0.2	1	120	LPAEENAC	R	LPAEENAR	M	XXX_sp Q6	1	1_S_0.0000	51.56	1029.78	-243.376	LPAEENAC	LP>AEENAC	'0'
21975	1	4	3569.737	3425.627	8.33E-14	7.0725	0.6779	411.9	26	192	VLLSESGA	K	VLLSEGA	L	sp O75179	7	1_S_0.0000	52.12	893.94	144.1098	V<L<L<E	VLLSEGA	'0'
21975	2	4	3569.737	3493.664	9.92E-03	3.2103	0.2903	135.3	17	192	VLLNEGAP	K	VLLNEGAK	V	sp Q8IWI	6	1_S_0.0000	52.12	893.94	76.07236	VLLNEGAP	VLLN>EG	'0'
21975	3	4	3569.737	3731.874	4.67E+00	2.2784	0.0362	7.4	5	222	QAVEPDI	K	QAVEPCK	L	XXX_sp Q5	2	1_S_0.0000	52.12	893.94	-162.137	QAVEPDI	QAVEP>D	'0'
21975	4	4	3569.737	3560.761	8.04E+00	2.196	0.0103	18	8	186	LLETYFL	T	LLETYFL	V	XXX_sp Q5	6	1_S_0.0000	52.12	893.94	8.97583	LLETYFL	TALLE>T	'0'
21975	5	4	3569.737	3755.801	9.33E+00	2.1734	0.0361	2.9	3	186	DFAMALL	R	DFAMALLR	D	XXX_sp Q6	1	1_S_0.0000	52.12	893.94	-186.064	DFAMALL	DFAMALL	'0'
23213	1	3	2740.364	2596.252	2.97E-12	6.7582	0.6605	372.4	19	96	SYGPAPG	R	SYGPAPIR	Q	sp Q13155	1	1_S_0.0000	54.56	914.8	144.1124	S<Y<G<P	SYGPAPG	'0'
23213	2	3	2740.364	2887.429	6.00E+00	2.2943	0.0025	8.1	4	100	GKPEAHF	K	GKPEAHK	N	sp Q9Y623	1	1_S_0.0000	54.56	914.8	-147.065	GKPEAHF	GKPE>AH	'0'
23213	3	3	2740.364	3159.534	6.23E+00	2.2885	0.0225	16.8	6	128	SHAVGTA	R	SHAVGTR	H	sp P15923	3	1_S_0.0000	54.56	914.8	-419.17	SHAVGTA	SHAV>G	'0'
23213	4	3	2740.364	2289.149	8.64E+00	2.237	0.0024	37.4	7	84	APPESTAI	K	APPESTAK	D	XXX_sp P1	2	1_S_0.0000	54.56	914.8	451.2153	A<P<P<E	APPESTAI	'0'
23213	5	3	2740.364	3234.659	8.94E+00	2.2317	0.0231	6.6	4	120	HSFISLQ	P	HSFISLQ	T	XXX_sp O1	1	1_S_0.0000	54.56	914.8	-494.295	HSFISLQ	P>HSFISL	'0'
25501	1	4	3686.656	3886.449	2.99E-15	7.2905	0.6762	141.6	21	174	GYQLSDV	R	GYQLSDR	C	sp P23142	4	1_S_0.0000	59.12	923.17	300.207	G<Y<Q<L	GYQLSDV	'0'
25501	2	4	3686.656	4132.022	2.01E+00	2.3605	0.0724	13.8	9	210	LQYVYLG	K	LQYVYLK	D	sp Q6P047	1	1_S_0.0000	59.12	923.17	-445.366	LQYVYLG	LQYVY>L	'0'
25501	3	4	3686.656	4118.777	6.57E+00	2.1896	0.0104	1	3	204	DEISIDLY	R	DEISIDLR	L	sp Q15528	1	1_S_0.0000	59.12	923.17	-432.121	DEISIDLY	D>E>I>S	'0'
25501	4	4	3686.656	3832.721	7.70E+00	2.1668	0.01	4.3	6	198	TLLNLSA	R	TLLNLSR	Y	XXX_sp P5	3	1_S_0.0000	59.12	923.17	-146.065	TLLNLSA	TL>LNL>C	'0'

Comet-PTM 실행 결과

- Comet-PTM 결과 확인 [2]
 - excel의 Y열에서 PTM의 질량과 위치 확인

	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z
1																			
2	delta_cn	sp_score	ions_matd	ions_total	plain_pept	modified_prev_aa	next_aa	protein	protein_cm	modification	retention_exp	mz	delta_mob	series_diy	series_de	delta_jum	delta_peptide		
3	0.5844	539.5	23	88	GNFGGSF	R.GNFGGS	K	sp P52272	2	1_S_0.0000	48.75	727.36	144.1063	G<N<F<GNFGGSF/0'			G[144.10]NFGGSFAGSFGGAGGHAPGVAR		
4	0.0734	51.4	10	80	SVESSLAH	R.SVESSLA	R	XXX_sp P5	2	1_S_0.0000	48.75	727.36	33.04729	SVESSLAH>S>VE>SSL/0'			SVESSLAHQSAQ[33.04]QQSSASAR		
5	0.1027	20.5	7	76	GASTPAA	K.GASTPA	K	sp Q9ULW	1	1_S_0.0000	48.75	727.36	312.0812	GASTPAA>GAS>TP>/0'			GASTPAASTLPTANGARP[312.08]AR		
6	0.0118	1.4	2	88	ELEKPVDA	R.ELEKPV	C	XXX_sp Q5	1	1_S_0.0000	48.75	727.36	-286.167	ELEKPVDA>ELEKPV>V>/0'			ELEKPVDAQ[-286.16]ASGNVVSADATHLER		
7	0.0062	26.3	8	96	NPOQVTS	L.KNPOQV	T	XXX_sp Q6	2	1_S_0.0000	48.75	727.36	-421.334	NPOQVTS>L>NPQVTS/0'			NPOQVTSLSI[-421.33]PLSTILEGSSGYAR		
8	0.7026	190.6	16	96	FSDTCLD	R.FSDTCL	R	sp P98160	1	1_S_0.0000	51.56	1029.78	300.2048	FS<D<T<FSDTCLD/0'			FS[300.20]DTCLDLDGQATCDACAPGYTGR		
9	0.0284	4.6	5	116	SWAAPHC	R.SWAAPH	R	XXX_sp Q5	2	1_S_0.0000	51.56	1029.78	121.0005	SWAAPHC>SWA>APH/0'			SWAAPHCALAEADPPPSAA[121.00]AGGEPGSDYGR		
10	0.0558	10.5	7	136	SPGQLGP	R.SPGQLG	R	XXX_sp Q5	2	1_S_0.0000	51.56	1029.78	-152.13	SP<G<Q<SPGQLGP/0'			S[-152.13]PGQLGPNDGEGAAATAQAEQEGGAAAEAEAR		
11	0.0395	26.1	10	104	FAESVGW	R.FAESVG	R	XXX_sp P2	1	1_S_0.0000	51.56	1029.78	219.0121	FAESVGW>FAESVG>L/0'			FAESVGWGPCLEGEQAGV[219.01]THEADGAPR		
12	0.0415	0.2	1	120	LPAEENAE	R.LPAEEN	A	XXX_sp Q6	1	1_S_0.0000	51.56	1029.78	-243.376	LPAEENAE>LP>AEEN/0'			LPAEENADETEEAQGSFLLS[-243.37]ALLCGLLVLAR		
13	0.6779	411.9	26	192	VLLSGAS	K.VLLESGA	K	sp O75179	7	1_S_0.0000	52.12	893.94	144.1098	V<L<L<E>VLLSGAS/0'			V[144.10]LLESGASIEDHNENHGTPLMEAGSAGHVEVAR		
14	0.2903	135.3	17	192	VLLNEGAN	K.VLLNEG	K	sp Q8IWZ	6	1_S_0.0000	52.12	893.94	76.07236	VLLNEGAN>VLLN>EG/0'			VLLNEGANIED[76.07]HNENHGTPLMEAGSAGHVEVAR		
15	0.0362	7.4	5	222	QAVEPDI	N.QAVEPD	C	XXX_sp Q5	2	1_S_0.0000	52.12	893.94	-162.137	QAVEPDI>QAVEP>D/0'			QAVEPDIIVSLGEGVGETI[-162.13]VSLSSGGNNPPGSPSTPESTPK		
16	0.0103	18	8	186	LLETYFLT	R.LLETYFL	T	XXX_sp O5	6	1_S_0.0000	52.12	893.94	8.97583	LLETYFLT>ALLE>T>YF/0'			LLETYFLTAECVDQGLQTLGLGQA[8.97]QAPDPWALR		
17	0.0361	2.9	3	186	DFAMALL	R.DFAMAL	L	XXX_sp Q6	1	1_S_0.0000	52.12	893.94	-186.064	DFAMALL>DFAMALL/0'			DFAMALLVASEMISFSLHFMQALCAFFNI[-186.06]ER		
18	0.6605	372.4	19	96	SYGPAPG	R.SYGPAP	R	sp Q13155	1	1_S_0.0000	54.56	914.8	144.1124	S<Y<G<P>SYGPAPG/0'			S[144.11]YGPAPGAGHVQVESNLSLALESR		
19	0.0025	8.1	4	100	GKPEAHF	K.GKPEAH	K	sp Q9Y623	1	1_S_0.0000	54.56	914.8	-147.065	GKPEAHF>GKPE>AH/0'			GKPEAHF[-147.06]SLVHYAGTVGDYNIAGWLDK		
20	0.0225	16.8	6	128	SHAVGTA	R.SHAVGT	R	sp P15923	3	1_S_0.0000	54.56	914.8	-419.17	SHAVGTA>SHAV>G>/0'			SHAVGTAG[-419.17]DMHTLPGHGALASGFTGPMMLGGR		
21	0.0024	37.4	7	84	APPESTAI	K.APPESTA	K	XXX_sp P1	2	1_S_0.0000	54.56	914.8	451.2153	A<P<P<E>APPESTAI/0'			A[451.21]PPESTAIIGNTTVVADISDR		
22	0.0231	6.6	4	120	HSFISLIQ	P.R.HSFISL	Q	XXX_sp O1	1	1_S_0.0000	54.56	914.8	-494.295	HSFISLIQ>HSFISL>Q/0'			HSFISLIQIDLPQPG[-494.29]VTGPEAGVSCIDGTGK		
23	0.6762	141.6	21	174	GYQLSDV	R.GYQLSD	R	sp P23142	4	1_S_0.0000	59.12	923.17	300.207	G<Y<Q<L>GYQLSDV/0'			G[300.20]YQLSDVDVGTCEIDICALPTGGHICSYR		
24	0.0724	13.8	9	210	LYQYVLG	C.KLYQYV	L	sp Q6P047	1	1_S_0.0000	59.12	923.17	-445.366	LYQYVLG>LQYQV>L>/0'			LYQYVLGQDQVLDL[-445.36]TVAHLEVCMPHPLPLAEGMDR		
25	0.0104	1	3	204	DEISIDLY	R.DEISIDL	R	sp Q15526	1	1_S_0.0000	59.12	923.17	-432.121	DEISIDLY>DE>SI/0'			DEISIDLYELEEEYSSSSSCEAN[-432.12]DLPLCEAYGR		
26	0.01	4.3	6	198	TLNLDSA	R.TLNLDS	R	XXX_sp P5	3	1_S_0.0000	59.12	923.17	-146.065	TLNLDSA>TL>LNL>C/0'			TLNLDSAHIF[-146.06]DMGLSAQSYVDHCGFCMISFSEK		