

# MASCOT Distiller : 機能



- rawデータからピークを判定し抽出

- decharge

[多価フラグメントピークを認識し1価相当のm/zに変換]

- キメラスペクトル作成

[複数ペプチド由来のMS/MSデータを認識]

[1つのMS/MSデータに複数のprecursor値]

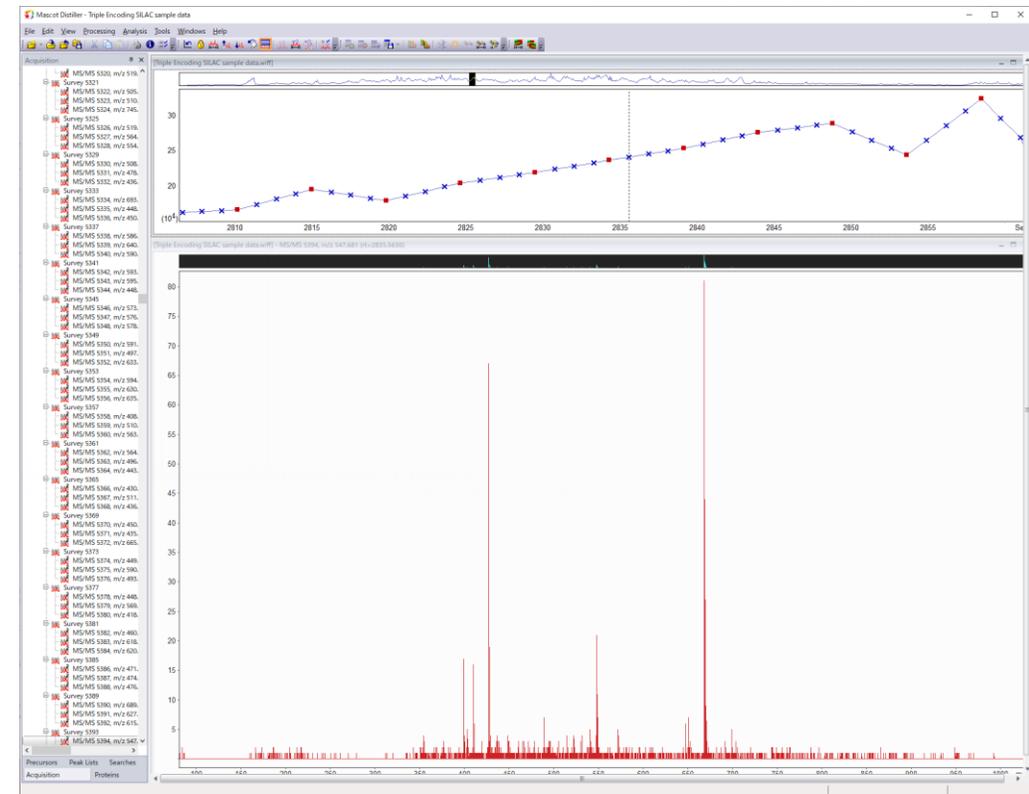
- Mascot Daemonと連動

[追加のモジュールでできるようになる事]

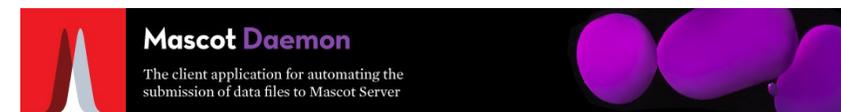
- denovo sequencing

- Distiller上で検索結果を受け取り、rawデータと検索結果を結び付ける

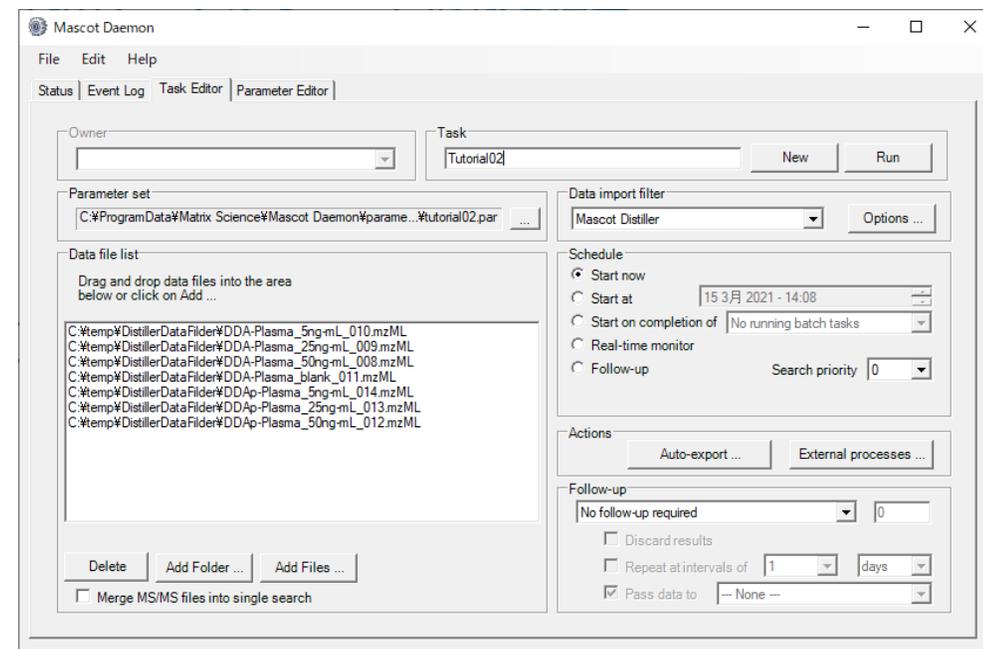
- 定量解析



# MASCOT Daemon: 機能



- 複数のデータを同一検索条件で検索実施
- rawデータ変換プログラム (Distiller, ProteoWizard MSconvert)の適用
- データの結合
- CSVファイル出力
- 装置付属のソフトウェアを使わず MASCOT検索が可能

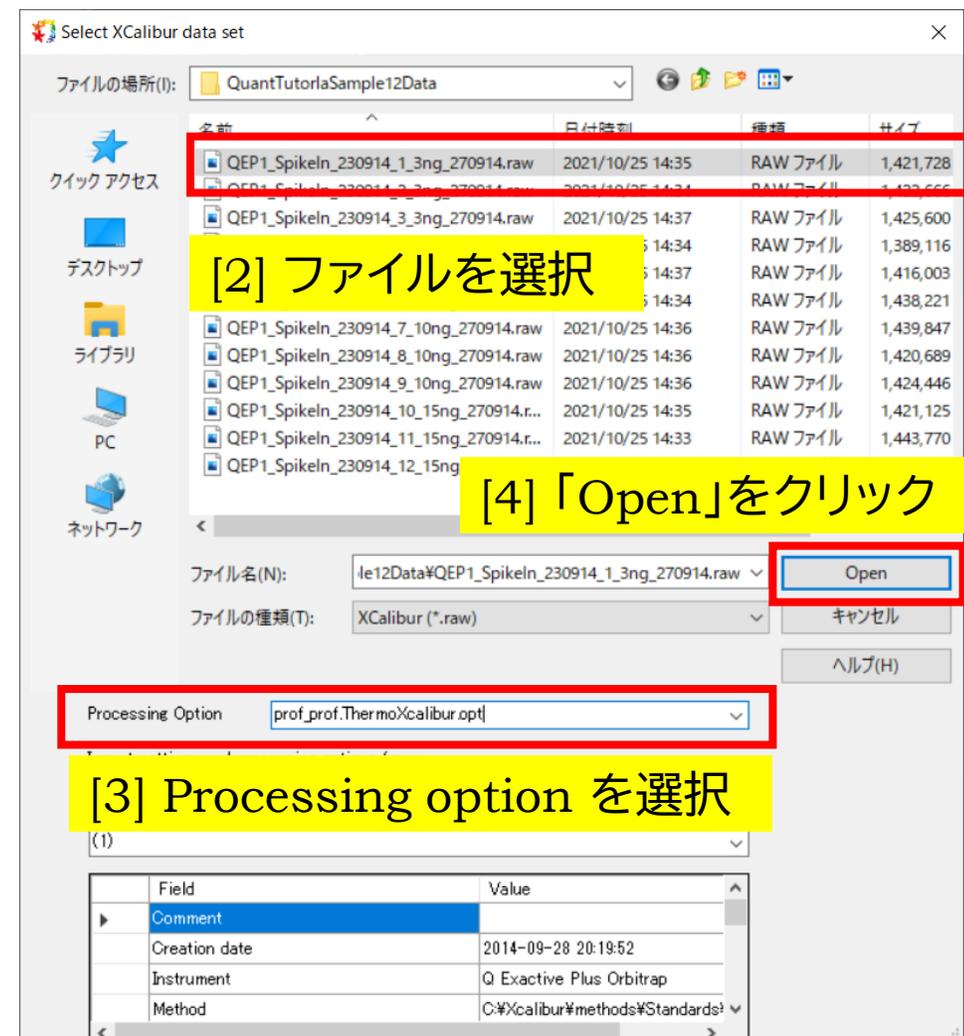
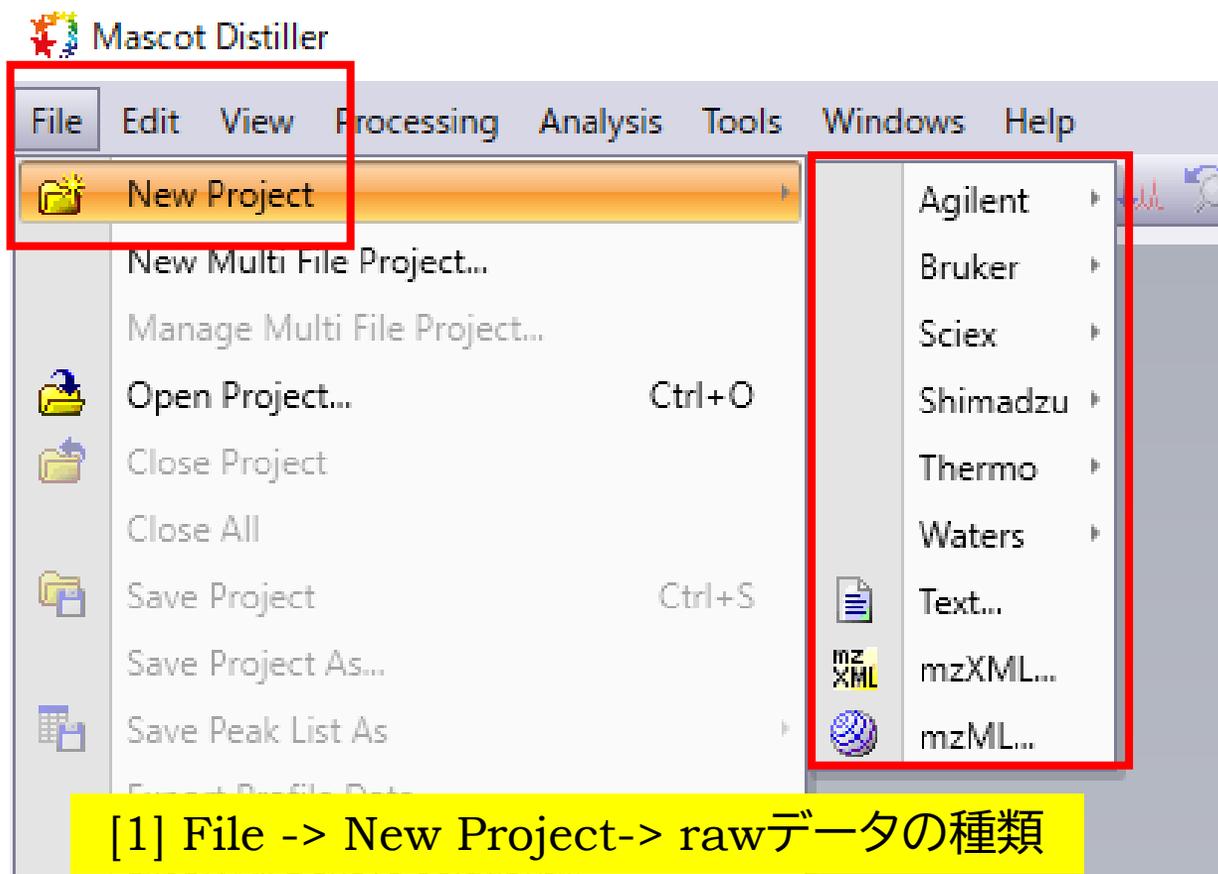


# MASCOT Daemon + Distiller どんな時にお勧めか

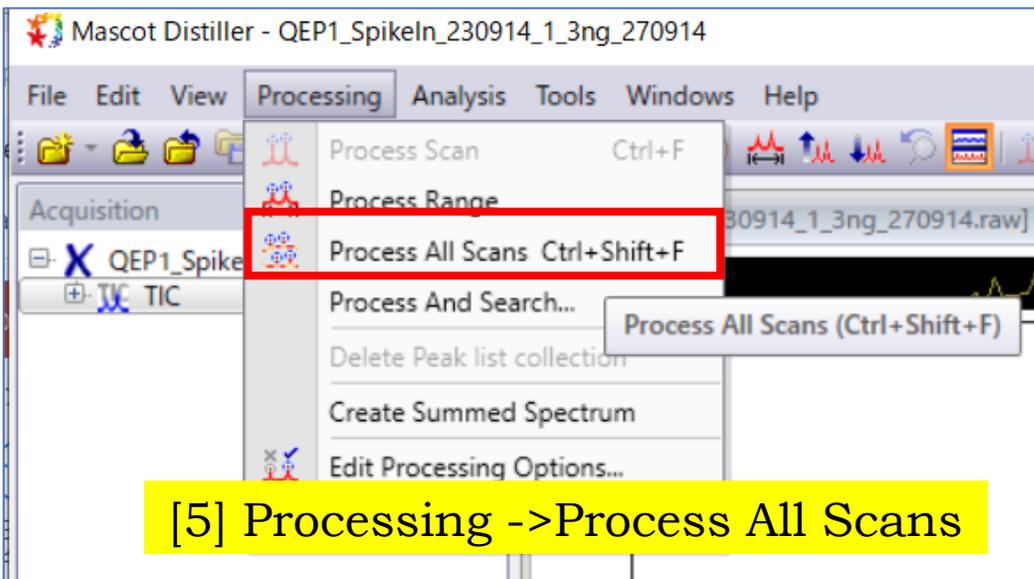


- 複数の装置のデータ解析において、ピーク抽出プログラムを揃えたい
- 他社ソフトウェア以外の解析方法でMASCOT検索したい
- decharge機能 [多価フラグメントピークを認識し1価相当のm/zに変換] を使いたい
- キメラスペクトル作成 [複数ペプチド由来のMS/MSデータを認識] 機能を使いたい

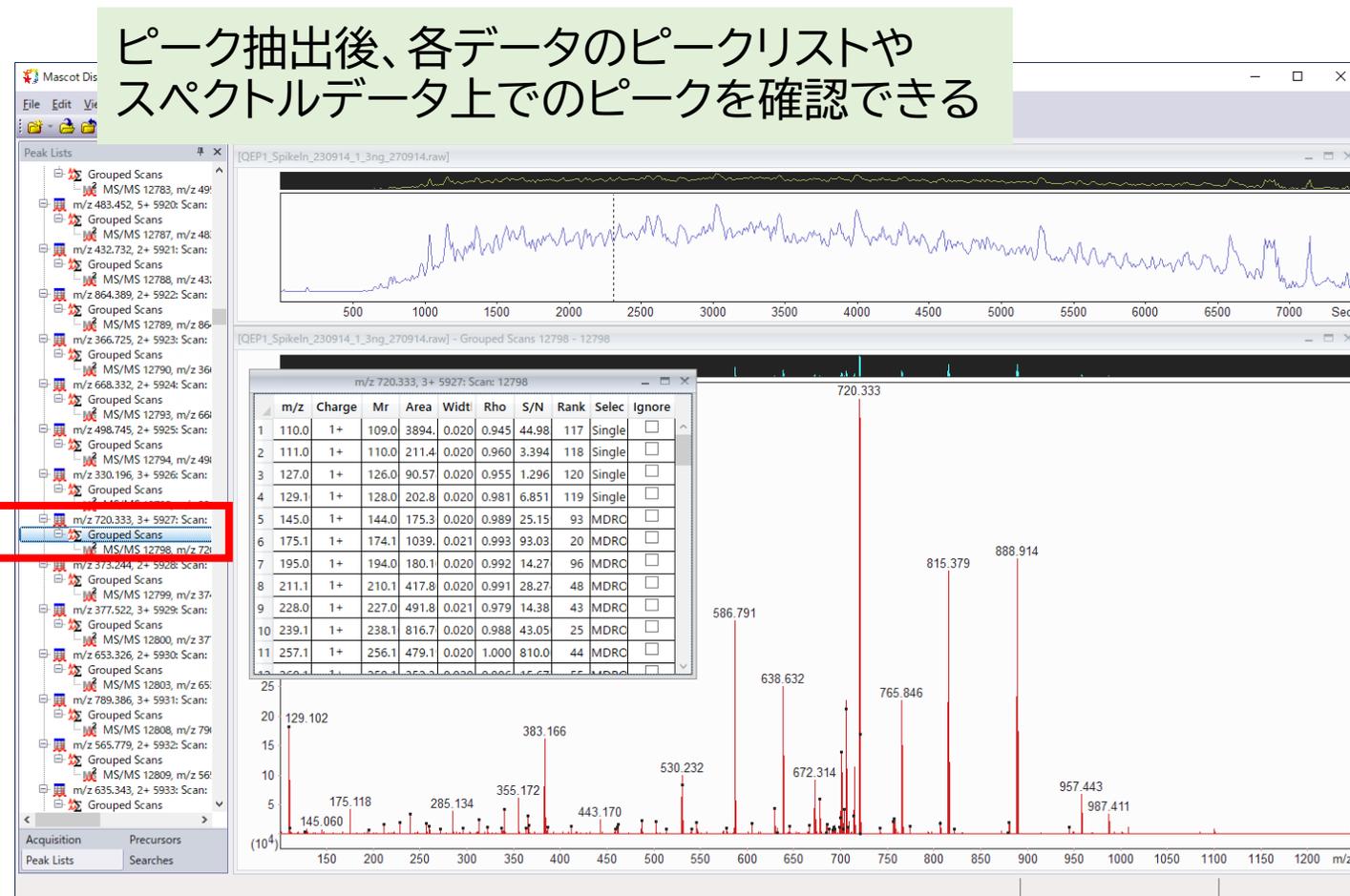
# Distiller上での操作手順：raw ファイルの読み込み



# Distiller上での操作手順：ピーク抽出



[5] Processing ->Process All Scans



# Distiller上での操作手順：MASCOT 検索



Mascot Distiller - QEP1\_SpikeIn\_230914\_1\_3ng\_1data\*

File Edit View Processing **Analysis** Tools Windows Help

Mascot Search All Peaklists...

Denovo Search Current peaklist...  
Digest Protein... Mascot Search (All Tags)...  
Fragment Peptide... Current Tag...  
Analysis Info All Tags in Current Peaklist...  
Calculate XIC...

Peak Lists

Grouped Scans  
MS/MS 12783, m/z 483.452, 5+ 5920:  
Grouped Scans  
MS/MS 12787, m/z 432.732, 2+ 5921:  
Grouped Scans  
MS/MS 12788, m/z 864.389, 2+ 5922:  
Grouped Scans  
MS/MS 12789, m/z 366.725, 2+ 5923:  
Grouped Scans  
MS/MS 12790, m/z 366.725, 2+ 5923:

[6] Analysis  
-> Mascot Search  
-> All Peaklists

Mascot Search (localhost)

### MASCOT MS/MS Ions Search

Your name: takaesu Email: [ ]

Search title: C:\temp\replicatesDataset\QEP1\_SpikeIn\_230914\_1\_3ng\_270914.raw

Database(s): SwissProt (AA)

Amino acid (AA): AmbystomaMexicanum, Caudata, contaminants, cRAP, IPI\_human, M\_smeigmatis\_2, M\_smeigmatis\_ATCC700084, Mouse, NCBIprot

Taxonomy: All entries

Enzyme: Trypsin Allow up to: 1 missed cleavages

Quantitation: None

Crosslinking: None

Fixed modifications: Carbamidomethyl (C)

Variable modifications: Oxidation (M)

Display all modifications:

Peptide tol. ±: 0.1 Da # <sup>13</sup>C: 0 MS/MS tol. ±: 0.1 Da

Peptide charge: 2+ Monoisotopic:  Average

Data file: [ ]

Data format: Mascot generic Precursor: [ ] m/z

Instrument: ESI-TRAP Error tolerant:

Decoy:

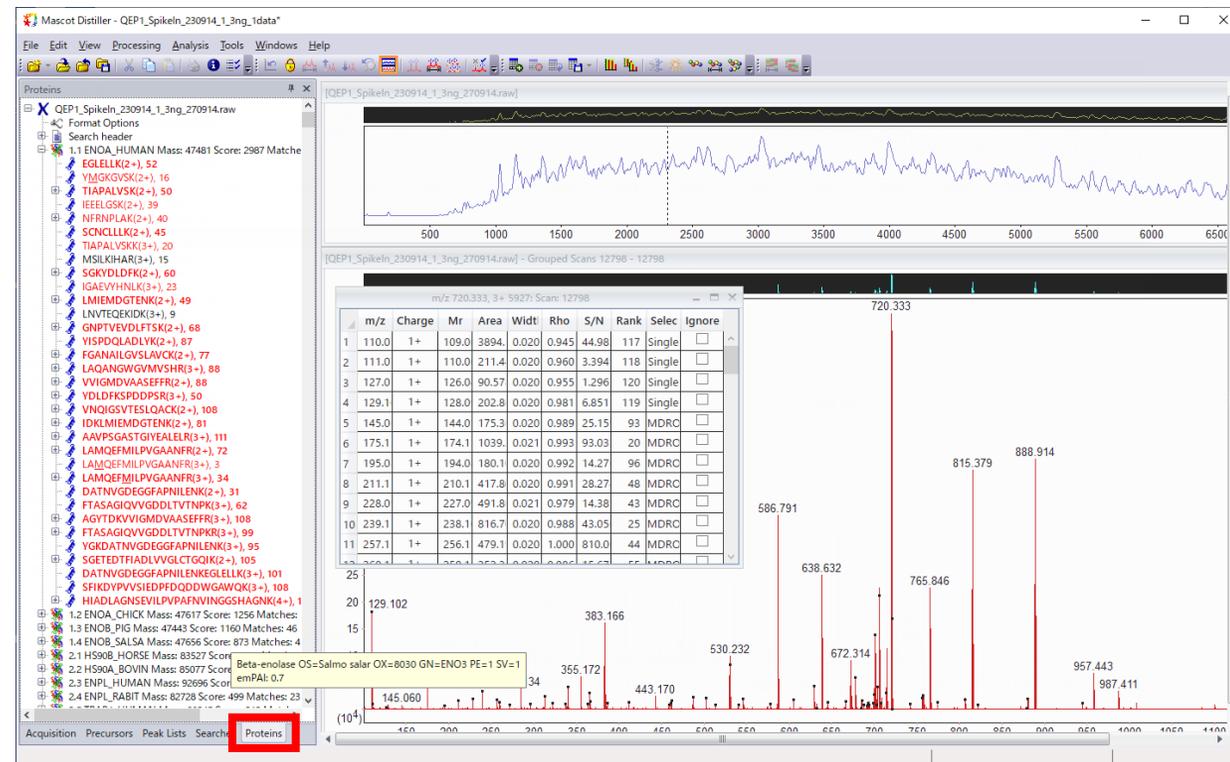
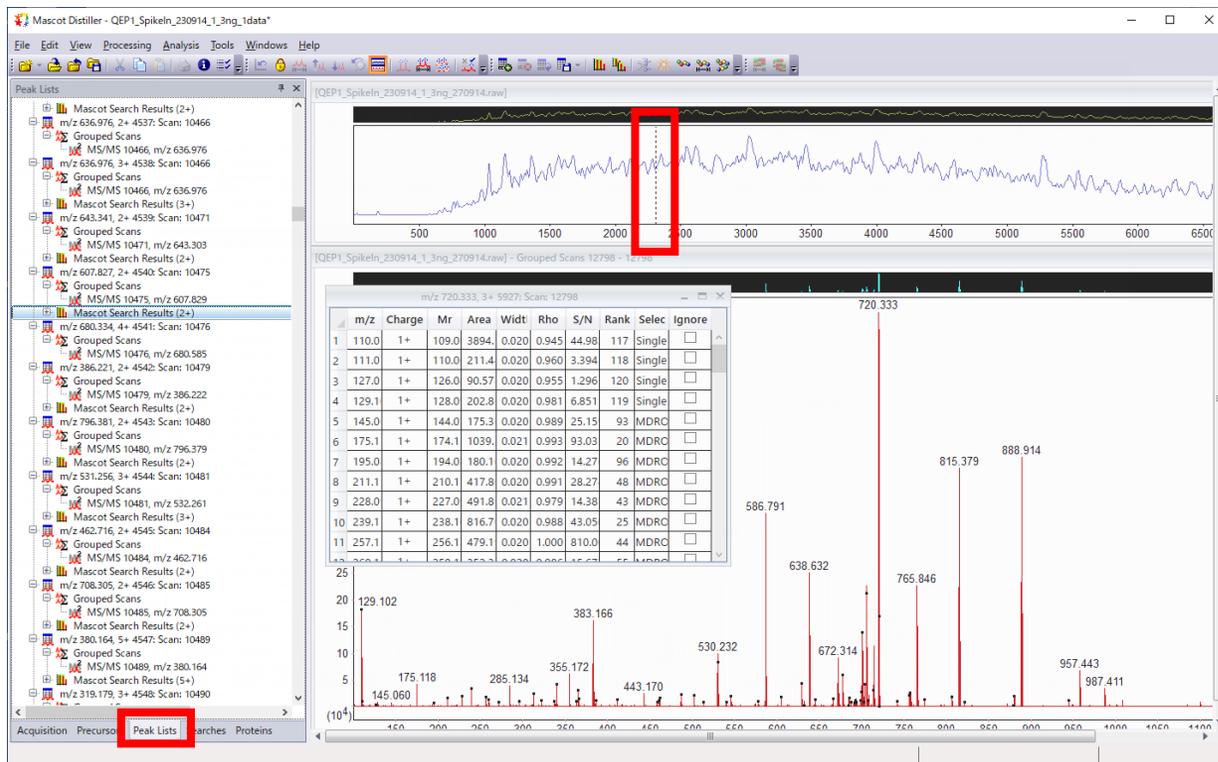
Start Search ... Reset Form

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Cancel

[7] 検索パラメーターを入力し、  
"Start Search"

# Distiller上での操作手順：MASCOT 検索結果受取



「Peak List」タブではScan numberとMASCOT検索結果を連動させた表示が可能

「Proteins」タブでは同定タンパク質並びにアサインペプチドの情報を確認

# Daemon+Distiller の操作手順 : Parameter Editor



Mascot Daemon

File Edit Help

Status | Event Log | Task Editor | **Parameter Editor**

Parameter set

Filename: C:\ProgramData\Matrix Science\Mas...default.par [New] [Open ...] [Save] [Save As ...]

All Searches

User name <mascot\_user\_full\_name> User email <mascot\_user\_email>

Search title <taskname> (<parameters>), submitted from Daemon on <localhost>

Taxonomy ..... Homo sapiens (human) Report top AUTO hits

Databases SwissProt [Select Databases] Protein mass kDa

Decoy  Enzyme Trypsin

Fixed modifications Carbamidomethyl (C) [Select Modifications] Max. missed cleavages 1

Variable modifications Oxidation (M) Monoisotopic  Average  Peptide charge 2+ and 3+

Peptide tol. ± 0.1 Da # 13C 0

MS/MS

MS/MS Ions search  Data format Mascot generic Instrument Default

Error tolerant search  MS/MS tol. ± 0.1 Da Quantitation None

Target PSM FDR 1% Crosslinking None

[1] 「Parameter Editor」タブをクリック

[3] 「Save」または「Save As」ボタンで設定ファイルを保存

[2] 検索条件を指定

# Daemon + Distiller の操作手順 : Task Editor



The screenshot displays the Mascot Daemon Task Editor window. The interface includes a menu bar (File, Edit, Help), a status bar (Status, Event Log, Task Editor, Parameter Editor), and several main sections: Owner, Task (with a text input field containing 'search test 01' and 'Run' and 'New' buttons), Parameter set (with a file path and a selection button), Data file list (with a list of files and an 'Add Files ...' button), Data import filter (with a dropdown menu set to 'Mascot Distiller' and an 'Options ...' button), Schedule (with radio buttons for 'Start now', 'Start at', 'Start on completion of', 'Real-time monitor', and 'Follow-up'), Actions (with 'Auto-export ...' and 'External processes ...' buttons), and Follow-up (with a dropdown menu set to 'No follow-up required' and a '0' input field).

[4] 「Task Editor」タブをクリック

[5] Task名を指定

[6] Parameter ファイルを選択

[7] 検索対象となるファイルを選択

[8] \*検索ファイルがrawデータの場合 rawデータを変換するプログラムとそのオプションを指定  
Optionについては次スライドで補足説明

[9] Runボタンを押して検索開始

## 補足説明 : Data import filterのOptionsダイアログ[MASCOT Distiller]



[a] RAWデータの種類を選択

[b] ピーク抽出に対する  
Distillerのパラメータセット  
ファイルを選択

The screenshot shows the 'Mascot Distiller data import options' dialog box. The 'Data File Format' dropdown is set to 'Thermo Xcalibur'. The 'Mascot Distiller Processing Options' field contains the path 'C:\ProgramData\Matrix S...%prof\_prof.ThermoXcalibur.opt'. The 'Output MS/MS Fragments as' section has 'MH+' selected. The 'Distiller Project' section has 'Save' checked. The 'Scan level parameters' section has 'Output INSTRUMENT=' checked and set to 'Default' for 'Unknown' scans.

[c] dechargeするときには「MH+」を選択



# Daemon + Distiller の操作手順：検索結果の確認



[11] rawデータのファイル名が記されたフォルダをクリックすると、結果のまとめが表示される

[10] 検索が完了すると、task名の前のマークがとなる。

**MASCOT Search Results**

User :  
E-mail :  
Search title : search test 01 (C:\ProgramData\Matrix Science\Mascot Daemon\parameters\daemondistiller.par), submitted from Daemon on T5820  
MS data file : C:\temp\replicatesDataset\QEP1\_SpikeIn\_230914\_1\_3ng\_270914.raw  
Database : SwissProt 2022\_02 (567,483 sequences; 204,940,973 residues)  
Taxonomy : Homo sapiens (human) (20,387 sequences)  
Timestamp : 22 Feb 2023 at 03:51:35 GMT

Re-search  All  Non-significant  Unassigned [\[help\]](#) Export As

Not what you expected? Try [the select summary](#).

- Search parameters
- Score distribution
- Modification statistics for all protein families
- Legend

**Protein Family Summary**

Format Significance threshold p< 0.05 Max. number of families AUTO [\[help\]](#)

[12] result file URL の項目をクリックすると、結果画面が表示される

**Protein families 1-10 (out of 1550)**

10 per page 1 2 3 4 5 6 ... 155 Next Expand all Collapse all

Accession contains Find Clear

1  1 ENOA\_HUMAN 4385 Alpha-enolase OS=Homo sapiens OX=9606 GN=ENO1 PE=1 SV...  
2 ENOB\_HUMAN 1652 Beta-enolase OS=Homo sapiens OX=9606 GN=ENO3 PE=1 SV...