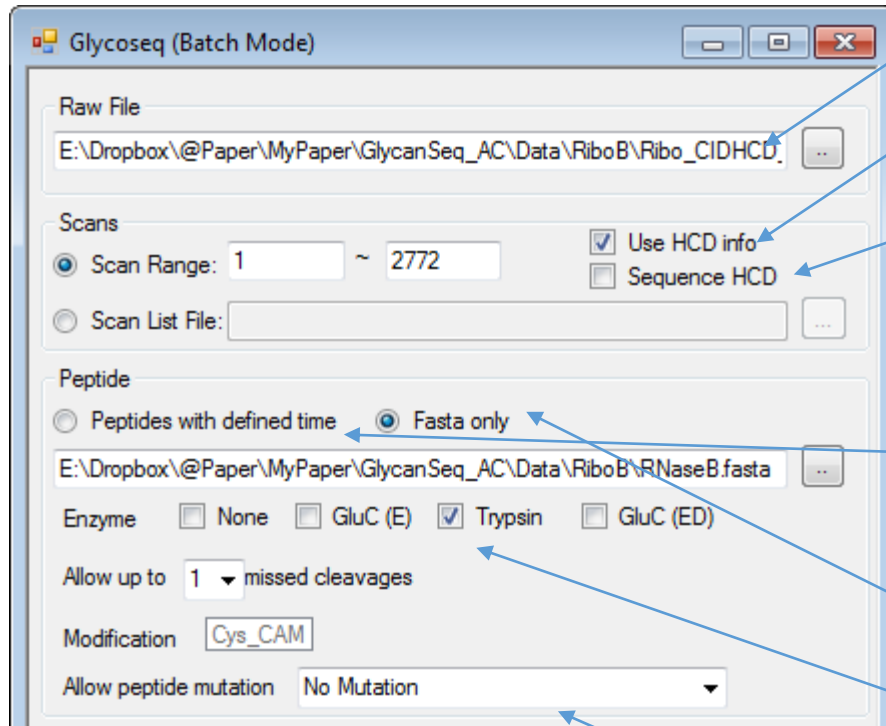


Suggestion setting are shown in the picture



- Raw File: Theomo Raw or mzXML
- Use HCD Info: if your raw file contain HCD scan, this can help guide CID sequencing
- Sequence HCD: sometimes HCD contains glycosidic bond fragments, and can be used for sequencing.
- Peptide with defined time: CSV format contain peptide search time information (Page 3)
- Fasta Only: input protein/peptide sequence in fasta format
 - Enzyme, missed cleavage: for protein sequence
 - For peptide fasta choose None and 0
 - Peptide mutation: generate and add mutated peptides

The screenshot shows a software window with the following settings:

- Composition upper bound:**
 - Hex: 99, HexNAc: 99, deHex: 0
 - Radio buttons: ☒ NeuAc, ☐ NeuGc
 - ☒ N-Linked
- Use glycan list:** ☐ (with an empty text field and a browse button)
- Tolerance:**
 - MS/MS (da): 0.8
 - Precursor (PPM): 10
 - ☒ Precursor in MS/MS
- Export:**
 - Get Top ? Rank: 3 (dropdown menu)
 - ☐ Only complete structure
 - Completed score reward: 1.0
 - ☐ Individual detail report
- Start:** A button at the bottom center.

- Composition upper bound: limit the number of glycan in the structure. eg. high mannose sample can be set as the picture shown
- Use glycan list: check if you have csv format glycan list
- Precursor in MS/MS: if CID contains precursor, it can help for sequencing
- Get top: export top n results
- Only complete structure: export completed structure
- Generate detail report: generate report for each scan (caution : lots of files, and long time)

Peptide with defined time

- CSV format
- Header name
 - Protein_Name
 - Peptide_Sequence
 - Start_Search_Time_(Mins)
 - End_Search_Time_(Mins)

```
Protein_Name,Peptide_Sequence,Start_Search_Time_(Mins),End_Search_Time_(Mins)  
CC112 HUMAN,AISSK,99.79108,101.01841
```

Protein/peptide fasta

```
>sp|P03455|HEMA_I76AI Hemagglutinin OS=Influenza A virus (strain  
MKAILLVLLCTFAATNADTLCIGYHANNSTDVDTVLEKNVTVTHSVNLLDRHNGKLCK  
LGGIAPLHLGKCNIAGRLLGNPECELLTVSSWSYIVETSKSDNGTCYPGDFINYEELRE  
QLSSVSSFERFEIFPKTSSWPNHETNRGVTAACPYAGANSFYRNLIWLVKKENSYPKLSK  
SYVNNKGKEVLVLWGIHHPPTSTDQQSLYQNADAYVFGSSKYNRKFKPEIAARPKVRGQ  
AGRMSYYWTLIEPGDTITFEATGNLVVPRYAFAMNRGSGSGIIWDAPVHDCNTKCQTPK  
GAINTSLPFQNIHPVTIGECPKYVKSTKLRLMATGLRNVPSIQSRGLFGAIAGFIEGGWTG  
MIDGWYGYHHQNEQGSGYAADQRSTQNAIDGITNKNVSVIEKMNTQFTAVGKEFNHLEKR  
IENLNKKVDDGFLDIWTYNAELLVLLNERTLDFHDSNVKNLYEKVRSQLRNNAKEIGNG  
CFEFYHKCDDTCMESVKNGTYDYPKYSEESKLNREEIDGVKLESTRIYQILAIYSTVASS  
|LVLLVSLGAISFWMCSSNGSLOCRI
```

```
>IIIB-C1  
VVLNVNTE  
>IIIB-V1/V2_1  
CTNLKNDTNTNSSSGR  
>IIIB-V1/V2_2  
NCSFNISTSIR  
>IIIB-V1/V2/C2  
LDIIPIDNDTTSYTLTSCNTSVITQACPK  
>IIIB-C2_1  
TFNGTGPCTNVSTVQCTHGIR  
>IIIB-C2_2  
PVVSTQLLLNGSLAEEEVVIR  
>IIIB-C2_3  
SANFTDNAK  
>IIIB-C2_4  
TIIVQLNQSV  
>IIIB-C2_5  
INCTRPNNNTRK  
>IIIB-C3_1  
QAHCNISR  
>IIIB-C3_2  
WNNTLK  
>IIIB-C3_3_1  
LREQFGNNK  
>IIIB-C3_3_2  
LREQFGNNKT  
>IIIB-V4_1  
FFYCNSTQLFNSTWFNSTWSTK  
>IIIB-V4_2  
GSNNTEGSDTITLPCR  
>IIIB-C4  
CSSNITGLLLTR  
>IIIB-V5  
DGGNSNNESEIFR
```