

A) Open searching

Workflows

FragPipe and its collection of tools support multiple proteomic workflows. Select and load an option from the dropdown menu below to configure all the tools. Workflows. Also [see the tutorial](#).

Select an option to load config for: or save current settings as workflow

Open search workflow for PTM analysis. MSFragger localization-aware open search (LOS) algorithm, with deisotoping, mass calibration, parameter optimization, and monoisotope correction enabled. Mass range -150 to 500 Da, with Met oxidation and protein N-term Acetyl included as variable modifications. PeptideProphet with extended mass model. Crystal-C for artifact removal. PTM-Shepherd for mass shift summarization.

☒ Run MSFragger

:

Common Options (Advanced Options are at the end of the page)

Peak Matching

Precursor mass tolerance - Fragment mass tolerance

Calibration and Optimization Isotope error Data type

Enable Open searching
Select the Open searching workflow

Ensure a wide mass tolerance
Define the maximum mass tolerance to 2,000.

B) Glycan-focused search

Modifications

Variable modifications

Max variable mods on a peptide Max combinations

Enabled	Site (editable)	Mass Delta (edita...	Max occurrences ...
<input checked="" type="checkbox"/>	M	15.9949	3
<input checked="" type="checkbox"/>	[^	42.0106	1
<input type="checkbox"/>	STY	79.96633	2
<input checked="" type="checkbox"/>	S	648.25	3
<input type="checkbox"/>	nE	-18.0106	1
<input checked="" type="checkbox"/>	S	692.28	3
<input type="checkbox"/>	site_07	0	1
<input type="checkbox"/>	site_08	0	1

Expected mass of glycans and residues
Define the expected mass (neutral mass).
Define the expected residues targeted for glycosylation.

Advanced Options

Mass Offsets

Restrict delta mass to

Expected mass of glycans and residues
Define the expected mass (neutral mass).
Define the expected residues targeted for glycosylation.

Glyco/Labile mods

Labile Modifications Search mode Diagnostic Ion Minimum Intensity

Y Ion Masses

Diagnostic Fragment Masses

Glycan-associated fragment mass
Define the expected Y ions (neutral mass).
Provide known Fragment / Oxonium ions (ensure MH⁺ provided).

Spectral Processing

Precursor mass mode

Min peaks Use top N peaks Min ratio

Clear m/z range -

Remove precursor peak removal m/z range -

Intensity transform

Open Search Options

Report mass shift as a variable mod

Track zero top N Add top N complementary

Zero bin accept expect Zero bin multiply expect

Delta mass exclude ranges

☒ Localize mass shift (LOS)