

1 Spectrum files:

2 Database:

Parent mass tolerance: **3**

Peak mass tolerance: **4**

Cysteine protecting group: **5**

☒ Discard low quality spectra **6** ☒ MS-Cluster **7**

Minimum quality:

☒ Advanced spectrum alignment parameters

Minimum spectrum overlap: **8** ☒ Require transitive spectrum alignments **11**

Minimum # matched peaks: **9** Maximum alignment p-value: **12**

Minimum % matched score: **10** Maximum modification mass: **13**

☒ Advanced homology mapping parameters

Minimum # matched peaks: **14** CLUSTALW min score: **15**

None
IAA (+57 Da)
NIPAA (+99 Da)

- 1** Input spectrum files (INPUT_SPECS_MS)
- 2** Input protein sequence files (FASTA_DATABASE)
- 3** Parent mass tolerance, in Da (TOLERANCE_PM=0-3Da)
- 4** Peak mass tolerance, in Da (TOLERANCE_PEAK=0.0.4Da)
- 5** Cysteine protecting group (AMINO_ACID_MASSES)
- 6** Minimum spectrum quality (MIN_SPECTRUM_QUALITY=0-1.0)
- 7** Cluster repeated spectra (CLUSTER_MIN_SIZE=0/1)
- 8** Minimum percentage of spectrum mass overlap (MIN_OVERLAP_AREA=0-1.0)
- 9** Minimum number of matched peaks (MIN_MATCHED_PEAKE=0-8)
- 10** Minimum percentage of matched peaks score (MIN_RATIO=0-1.0)
- 11** Require transitive spectrum alignments (FILTER_TRIGS=1/0)
- 12** Maximum alignment p-value (MAX_PVALUE=0-1.0)
- 13** Maximum modification mass (MAX_MOD_MASS=0-200)
- 14** Minimum number of matched peaks (MIN_MATCHED_PEAKE_DB=0-12)
- 15** Minimum score for clustalw protein/protein sequence alignments (CLUSTALW_MINSORE)