

SPS Recommended Graphical User Interface

In this section a layout for a recommended graphical user interface is shown, as well as how it should be linked to the parameter file (*sps.params*). At the bottom half of the page the parameters are shown in brackets with their default values (e.g. TOLERANCE_PM=0-3Da).

1 Spectrum files:

2 Database:

Parent mass tolerance: **3**

Peak mass tolerance: **4**

☒ Discard low quality spectra **6**

Minimum quality:

Cysteine protecting group: **5**

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

☒ MS-Cluster **7**

☒ Advanced spectrum alignment parameters

Minimum spectrum overlap: **8**

Minimum # matched peaks: **9**

Minimum % matched score: **10**

☒ Require transitive spectrum alignments **11**

Maximum alignment p-value: **12**

Maximum modification mass: **13**

☒ Advanced homology mapping parameters

Minimum # matched peaks: **14**

CLUSTALW min score: **15**

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)