Supplmental Figure 1: Sequest parameters file used for peptide and PTM identification

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[SEQUEST]
database_name = C:\Xcalibur\database\swissprot_human.fasta
first_database_name = C:\Xcalibur\database\swissprot_human.fasta
second_database_name =
peptide_mass_tolerance = 2.5000
create_output_files = 1                 ; 0=no, 1=yes
ion_series = 0 1 1 0.0 1.0 0.0 0.0 0.0 0.0 0.0 1.0 0.0
fragment_ion_tolerance = 0.0            ; leave at 0.0 unless you have real poor data
num_output_lines = 12                   ; # peptide results to show
num_description_lines = 12              ; # full protein descriptions to show for top N peptides
num_results = 500             ; # of results to process
show_fragment_ions = 0                  ; 0=no, 1=yes
print_duplicate_references = 1          ; 0=no, 1=yes
enzyme_number = 1
diff_search_options = 1 NQ 16.0 MW 0.000 X 0.000 X 0.000 X 0.000 X 0.000 X
term_diff_search_options = 0.000 42.000 ; c term, n term diff mods
max_num_differential_AA_per_mod = 4     ; max # of modified AA per diff. mod in a peptide
nucleotide_reading_frame = 0            ; 0=proteinDB, 1-6, 7=forward three, 8=reverse three, 9=all six
mass_type_parent = 1                    ; 0=average masses, 1=monoisotopic masses
mass_type_fragment = 1                  ; 0=average masses, 1=monoisotopic masses
normalize_xcorr = 0                     ; use normalized xcorr in ouput file
remove_precursor_peak = 0               ; 0=no, 1=yes
ion_cutoff_percentage = 0.0             ; prelim. score cutoff % as a decimal number i.e. 0.30 for 30%
protein_mass_filter = 0 0               ; enter protein mass min & max value ( 0 for both = unused)\n
max_num_internal_cleavage_sites = 2     ; maximum value is 5; for enzyme search
match_peak_count = 0                    ; number of auto-detected peaks to try matching (max 5)
match_peak_allowed_error = 1            ; number of allowed errors in matching auto-detected peaks
match_peak_tolerance = 1.0              ; mass tolerance for matching auto-detected peaks
partial_sequence =
sequence_header_filter =


residues_in_upper_case = 0              ; 0=no, 1=yes

add_Cterm_protein = 0.0000              ; added to protein C-terminus (only C-term peptide affected)
add_Nterm_protein = 0.0000              ; added to protein N-terminus (only N-term peptide affected)
add_Cterm_peptide = 0.0000              ; added to each peptide C-terminus
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add_Nterm_peptide = 0.0000             ; added to each peptide N-terminus
add_G_Glycine = 0.0000                 ; added to G - avg.  57.0519, mono.  57.02146
add_A_Alanine = 0.0000                 ; added to A - avg.  71.0788, mono.  71.03711
add_S_Serine =  0.0000                 ; added to S - avg.  87.0782, mono.  87.03203
add_P_Proline = 0.0000                 ; added to P - avg.  97.1167, mono.  97.05276
add_V_Valine = 0.0000                  ; added to V - avg.  99.1326, mono.  99.06841
add_T_Threonine = 0.0000               ; added to T - avg. 101.1051, mono. 101.04768
add_C_Cysteine = 57.02                 ; added to C - avg. 103.1388, mono. 103.00919
add_L_Leucine = 0.0000                 ; added to L - avg. 113.1594, mono. 113.08406
add_I_Isoleucine = 0.0000              ; added to I - avg. 113.1594, mono. 113.08406
add_X_LorI = 0.0000                    ; added to X - avg. 113.1594, mono. 113.08406
add_N_Asparagine = 0.0000              ; added to N - avg. 114.1038, mono. 114.04293
add_O_Ornithine = 0.0000               ; added to O - avg. 114.1472, mono  114.07931
add_B_avg_NandD = 0.0000               ; added to B - avg. 114.5962, mono. 114.53494
add_D_Aspartic_Acid = 0.0000           ; added to D - avg. 115.0886, mono. 115.02694
add_Q_Glutamine = 0.0000               ; added to Q - avg. 128.1307, mono. 128.05858
add_K_Lysine = 0.0000                  ; added to K - avg. 128.1741, mono. 128.09496
add_Z_avg_QandE = 0.0000               ; added to Z - avg. 128.6231, mono. 128.55059
add_E_Glutamic_Acid = 0.0000           ; added to E - avg. 129.1155, mono. 129.04259
add_M_Methionine = 0.0000              ; added to M - avg. 131.1926, mono. 131.04049
add_H_Histidine = 0.0000               ; added to H - avg. 137.1411, mono. 137.05891
add_F_Phenylalanine = 0.0000           ; added to F - avg. 147.1766, mono. 147.06841
add_R_Arginine = 0.0000                ; added to R - avg. 156.1875, mono. 156.10111
add_Y_Tyrosine = 0.0000                ; added to Y - avg. 163.1760, mono. 163.06333
add_W_Tryptophan = 0.0000              ; added to W - avg. 186.2132, mono. 186.07931

[SEQUEST_ENZYME_INFO]
0.  No_Enzyme              0      -           -
1.  Trypsin_Strict         1      KR          -
2.  Trypsin                1      KRLNH       -
3.  Chymotrypsin           1      FWYL        -
4.  Chymotrypsin_WYF       1      FWY         -
5.  Clostripain            1      R           -
6.  Cyanogen_Bromide       1      M           -
7.  IodosoBenzoate         1      W           -
8.  Proline_Endopept       1      P           -
9.  Staph_Protease         1      E           -
10. Trypsin_K              1      K           P
11. Trypsin_R              1      R           P
12. GluC                   1      ED          -
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13. LysC	1	K	-
14. AspN	0	D	-
15. Elastase	1	ALIV	P
16. Elastase/Tryp/Chymo	1	ALIVKRWFY	P
17. Trypsin/Chymo	1	KRLFWYN	-