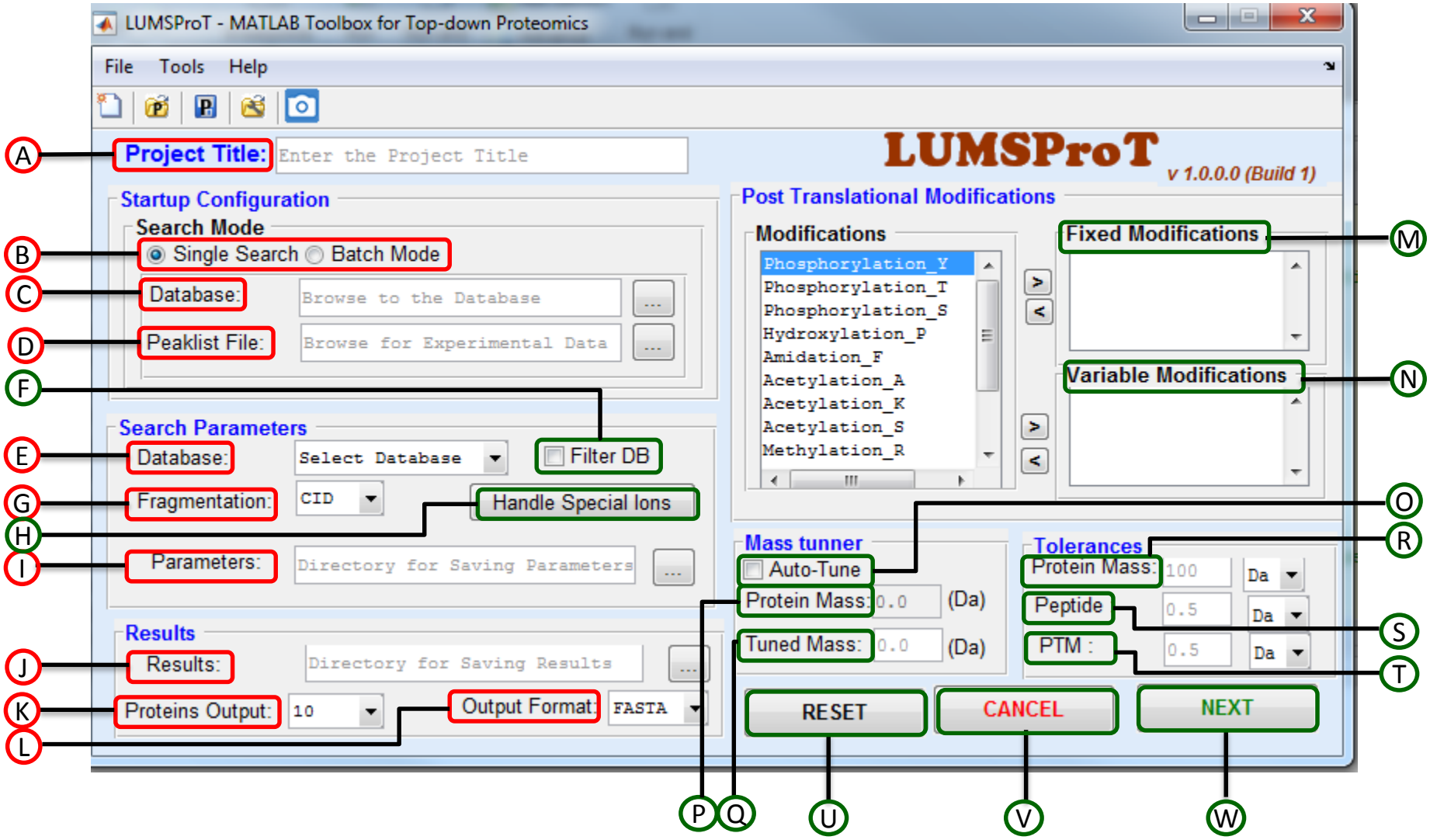
LUMSProT

MATLAB Toolbox
for
Top-down Proteomics

Manual

WINDOW 1: LUMSProT MATLAB Toolbox for Top-down Proteomics



WINDOW 1: LUMSProT MATLAB Toolbox for Top-down Proteomics

A. In order to start a project, user has to enter the 'Project title' first (for My project)

B. Select the search mode according to your requirement (i.e. single search or batch mode). Batch mode option will lead to drop down menu of 'file type'.

C. Browse and select the protein database

D. Browse and upload experimental data (Peaklist file for Single mode; .mzxml/ .mgf/.txt file for Batch mode)

E. Select Database from the drop down menu

F. User can filter database by checking the option -'Filter DB'

G. Select the 'Fragmentation technique' from drop down menu.

H. 'Handle Special Ions' option will lead to a new window where user can select the fragmentation ions option (i.e. a', b', y', z", a*, b*,y*, z' ions)

I. User can select a file to store the selected parameters

J. User can select a file to store the results

K. Set the protein output (for example 10, 20, 30 etc.)

L. Select the 'Output Format' from the drop down menu

M. User can opt for required fixed 'Post translation Modifications' from the list of modifications

N. Similarly, various 'Variable Modifications' are also selected from the list

O. Check the option 'Auto-tune' for tuning protein mass and proceed to the next step

P. After uploading the MS input file, user can see the 'Protein mass' in the box

Q. Tuned mass can be seen when user proceed to the next step

R. Set the tolerance value for protein mass (Unit can be changed by clicking on the drop down arrow)

S. Set the tolerance value for Peptide

T. Set the tolerance value for Post Translational Modification (PTM)

U. User can clear the already uploaded data by clicking on 'Reset' option

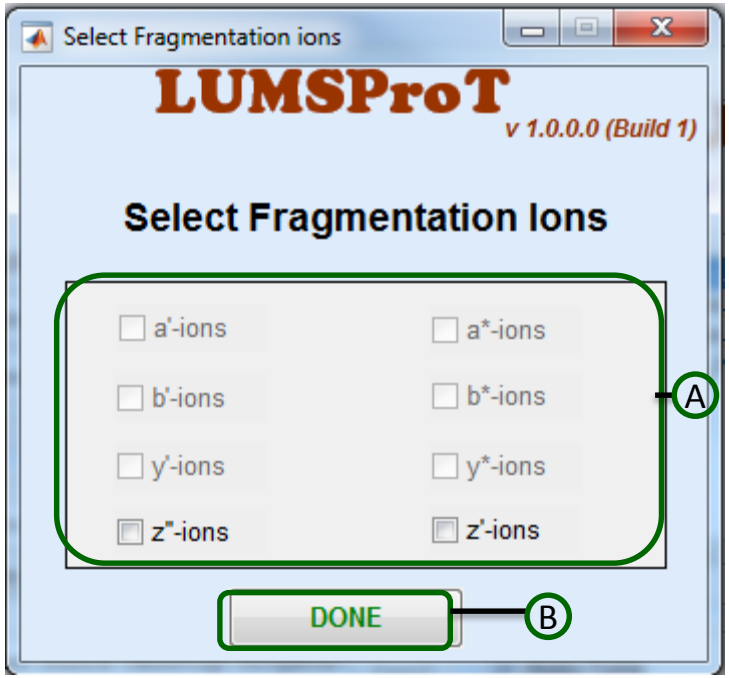
V. Click on ' Cancel' option to close the window

W. After filing all the requirements, user can proceed further by clicking on 'Next' option below.

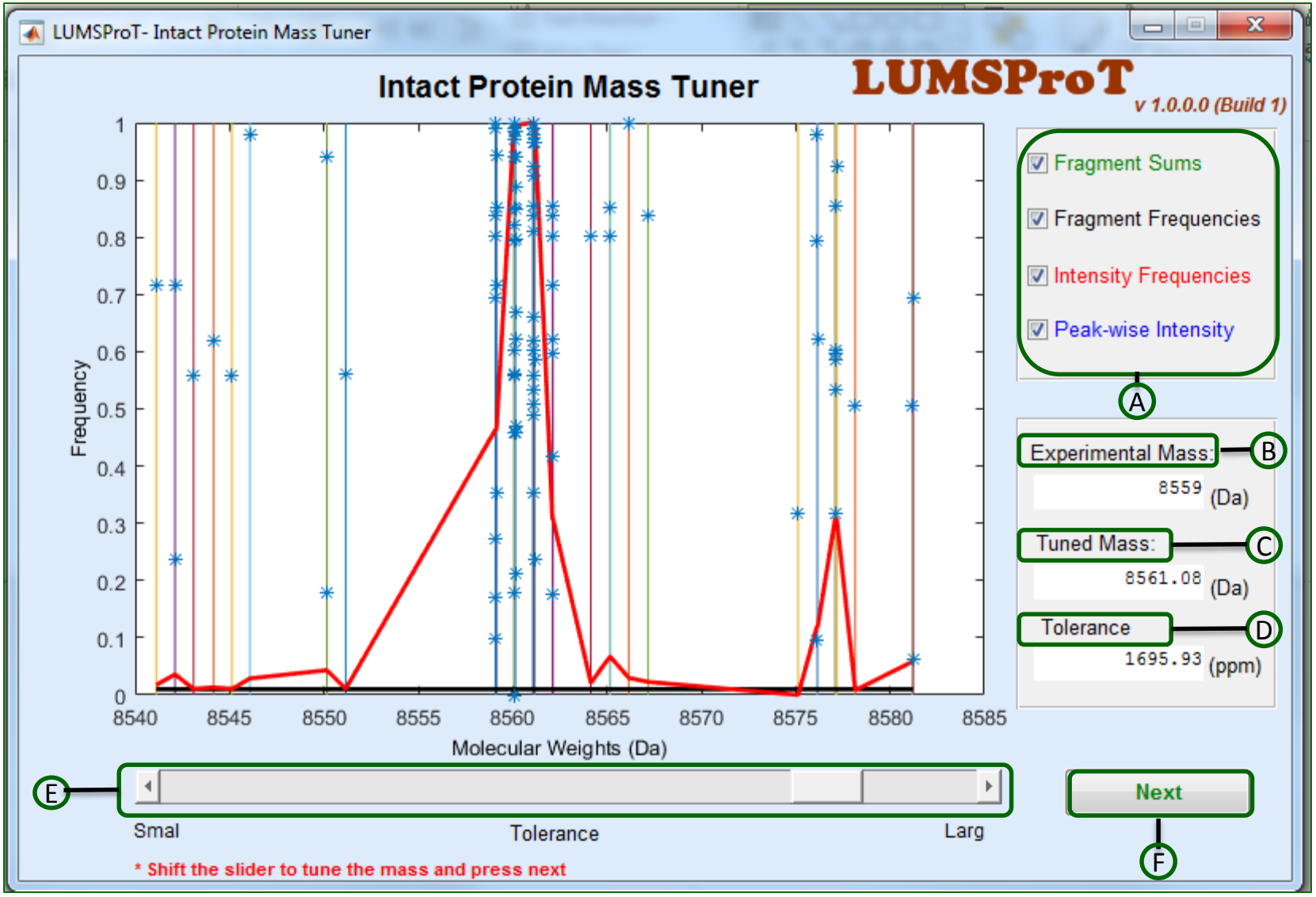
Window 2: Select Fragmentation Ions

A. ‘Handle Special Ions’ in the previous window, option leads to a new window where user can select the fragmentation ions option (i.e. a’, b’, y’, z”, a*, b*,y*, z’ ions)

B. Click on ‘Done’ to record the selection



Window 3: Intact Protein Mass Tuner



Window 3: Intact Protein Mass Tuner

A. Graph between ‘Frequency’ on Y-axis and ‘Molecular weight’ on X-axis is shown when a used selected ‘Auto-tune’ option from the previous window. Graph represents Fragment Sums, Fragment Frequencies, Intensity Frequencies and Peak-wise Intensity displayed by green, black, red and blue colors respectively. User can select from the list of Attributes to be represented in the graph.

B. ‘Experimental mass’ shows the mass of respective protein

C. ‘Tuned mass’ represents more accurate and precise protein mass

D. ‘Tolerance’ shows the value you set by shifting the slider

E. User can tune the mass by shifting the slider below, to left or right and press next

F. To proceed further, press ‘Next’

Window 4: Peptide Sequence Tags (PSTs)-LUMSProT

A. Tags will be filtered below the minimum length of PST selected from the drop down menu by the user

B. Tags will be filtered below the maximum length of PST selected from the drop down menu by the user

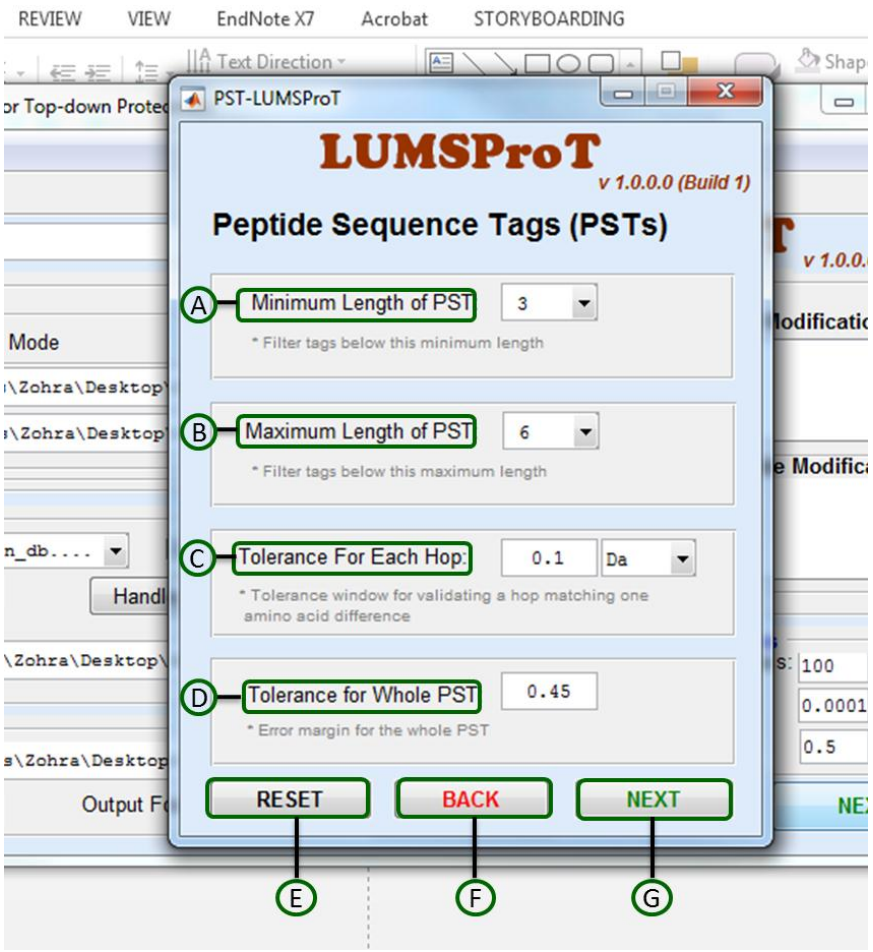
C. Set the 'Tolerance for each Hop'

D. 'Tolerance for Whole PST' shows error margin for the whole PST

E. Click 'Reset' to clear the already selected data

F. Click on 'Cancel' option to close the window

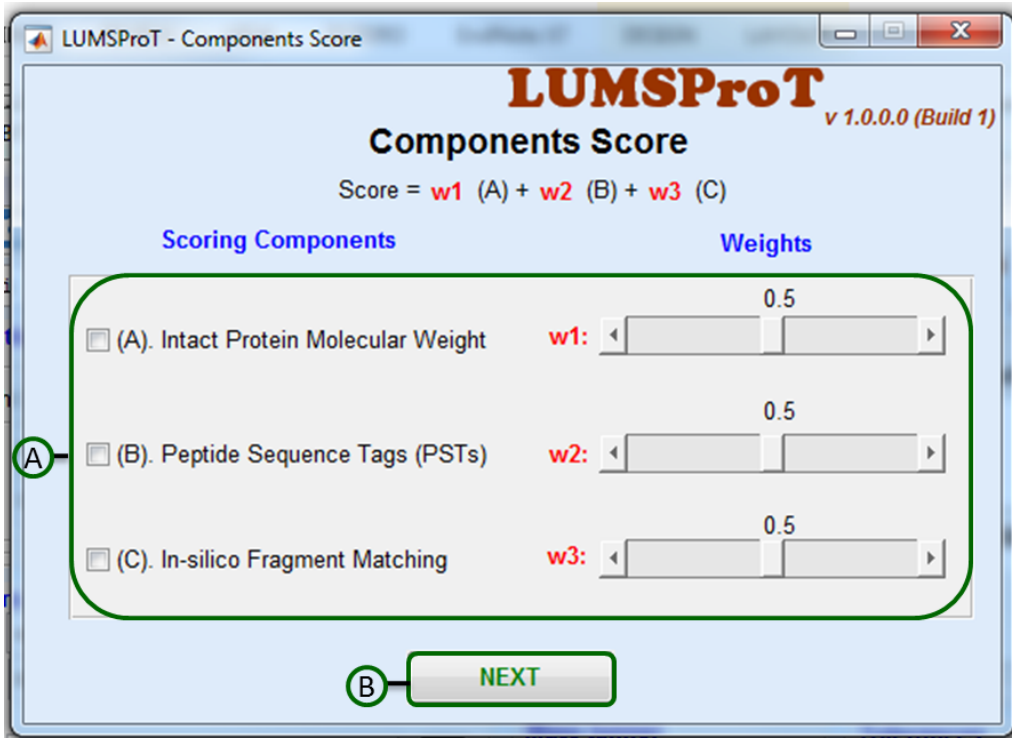
G. Click 'Next' to proceed to the next window



Window 5: LUMSProT-Components Score

A. Check the Scoring Components from the list and set their respective weights by shifting the slider left or right accordingly

B. Click ‘Next’ to proceed

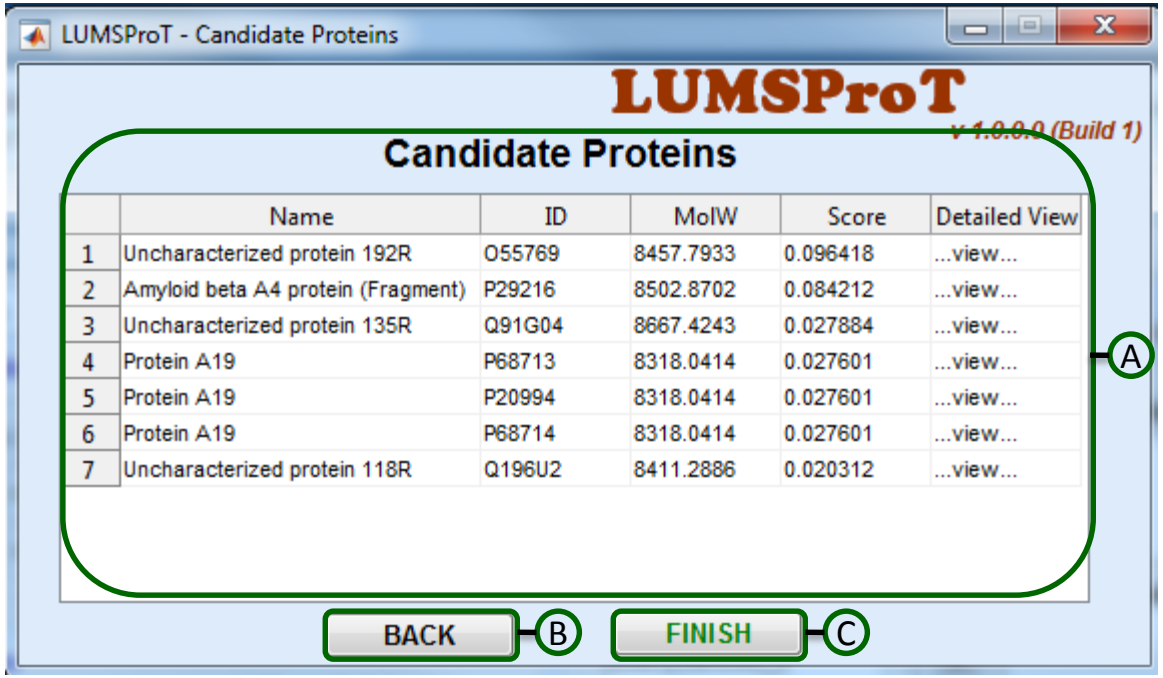


Window 6: LUMSProT- Candidate proteins

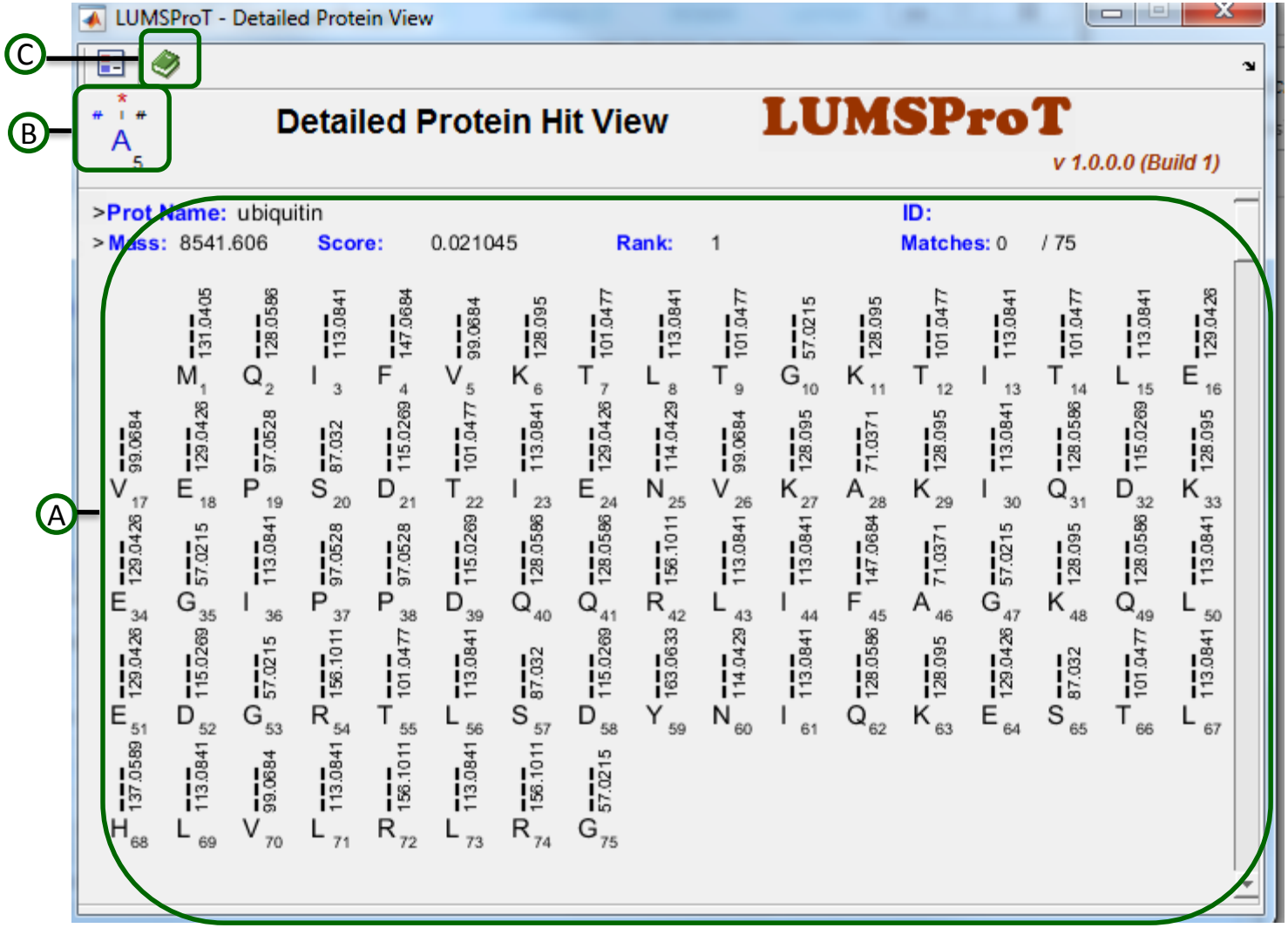
A. Name of the resultant protein along with molecular weight, score and detailed view according to the uploaded and selected data is represented under the list of 'Candidate Proteins'.

B. Click 'Back' to revert to the previous window

C. Click 'Finish' to end the process



Window 7: LUMSProT-Detailed Protein View

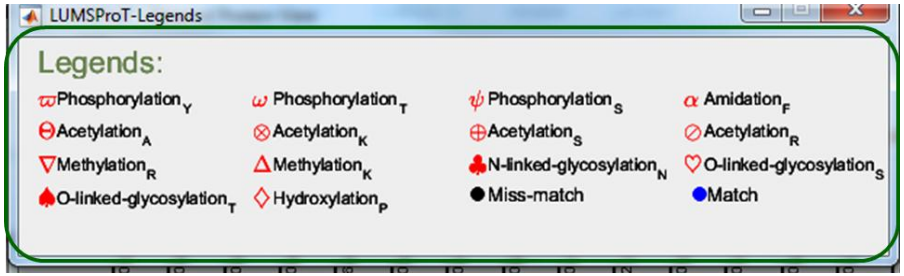


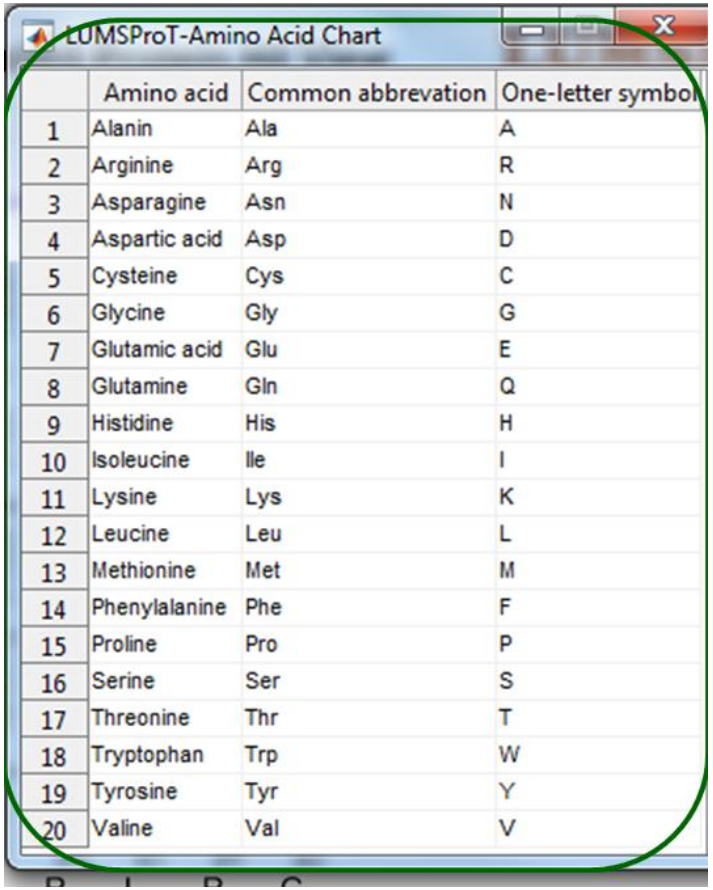
Window 7: LUMSProT-Detailed Protein View

A. ‘Detailed Protein View’ window shows proteins name, mass, score, rank, matches and amino acids (along the mass) present in the protein.

B. Leads to a window (i.e. LUMSProT-Amino acid Chart) containing list of full form of Amino acids along with abbreviations and one-letter symbol of protein to facilitate the user.

C. Open the window of legends (i.e. LUMSProT-Legends), which might be present in peptide sequence of candidate proteins.





	Amino acid	Common abbrevation	One-letter symbol
1	Alanin	Ala	A
2	Arginine	Arg	R
3	Asparagine	Asn	N
4	Aspartic acid	Asp	D
5	Cysteine	Cys	C
6	Glycine	Gly	G
7	Glutamic acid	Glu	E
8	Glutamine	Gln	Q
9	Histidine	His	H
10	Isoleucine	Ile	I
11	Lysine	Lys	K
12	Leucine	Leu	L
13	Methionine	Met	M
14	Phenylalanine	Phe	F
15	Proline	Pro	P
16	Serine	Ser	S
17	Threonine	Thr	T
18	Tryptophan	Trp	W
19	Tyrosine	Tyr	Y
20	Valine	Val	V