

PROTEINS WEBSITE USER MANUAL

Protein website (current functional website <http://binf.gmu.edu/srajamal/htdocs>) is designed to benefit students who are currently doing research under Dr.Vaisman using computational geometry analysis.

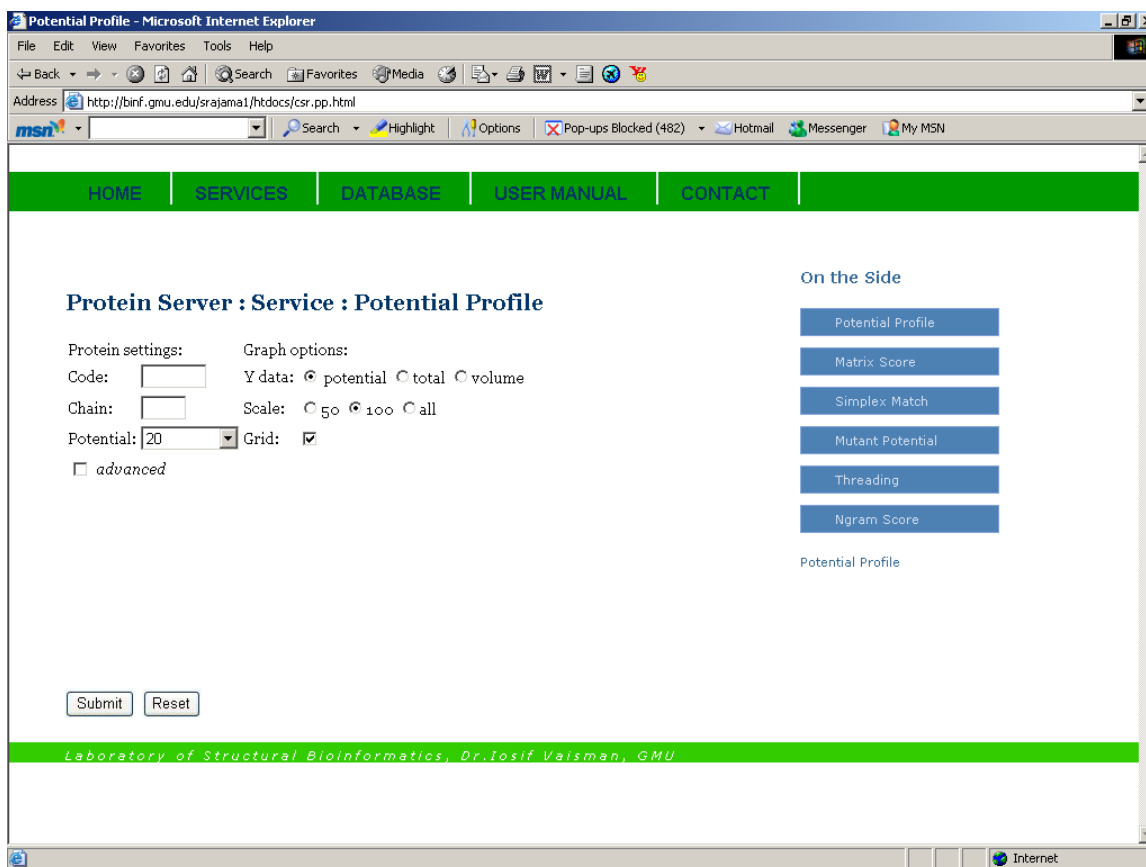
There are five main menus: Home, Services, Database, User Manual and Contact.

Interface to java programs Potential Profile, Matrix Score, Simplex Match, Mutant Potential, Threading and Ngram Score are in the Services menu. These java programs are useful for the study related to protein structures. They perform Delaunay tessellation and produce statistical values of the simplices of the protein structures using computational geometry approach.

In the current version, Services menu and the submenus Potential Profile, Matrix Score, Simplex Match, Mutant Potential and Threading are functional. All other functionality will be available in future.

Potential Profile:

This submenu is an interface for the java program PotentialProfile.java.



Usage: java PotentialProfile [-5] [-v] -p <potential file> -e <pdbEntry>|{-f <pdb file name> [-c chain]} [-o <output file>] [-c <code file>]

User can enter the PDB id, can chose one of the options from the potential combo box for the -p argument, and can provide definition file by clicking the “advanced” textbox. When the checkbox is selected, definition textbox appears. User can type the needed code definition in the textbox and can click submit button. Reset button is used to reset all values. If the PDB entry is not a valid entry, error message will be displayed. User can reenter the correct PDB id. For example, if a PDB id requires a chain, it has to be entered, otherwise, error message will be displayed.

Graphs are displayed in the output screen. There are many graph options which users can select. Potential Profile output file contains residue numbers, values of potential, total and volume. There is a link in the output page to either view the results or to store the output file in user’s local directory. For the graphs, Y data can be potential, total or volume. User can select Y data option from this submenu. Residue scale can also be chosen by the user for x-axis. User can chose for 50 residues in one graph, 100 residues or all residues in one graph. The graphs can be displayed with or without grid. User can click grid checkbox, if he wants the graphs to be displayed with grid.

Limitations:

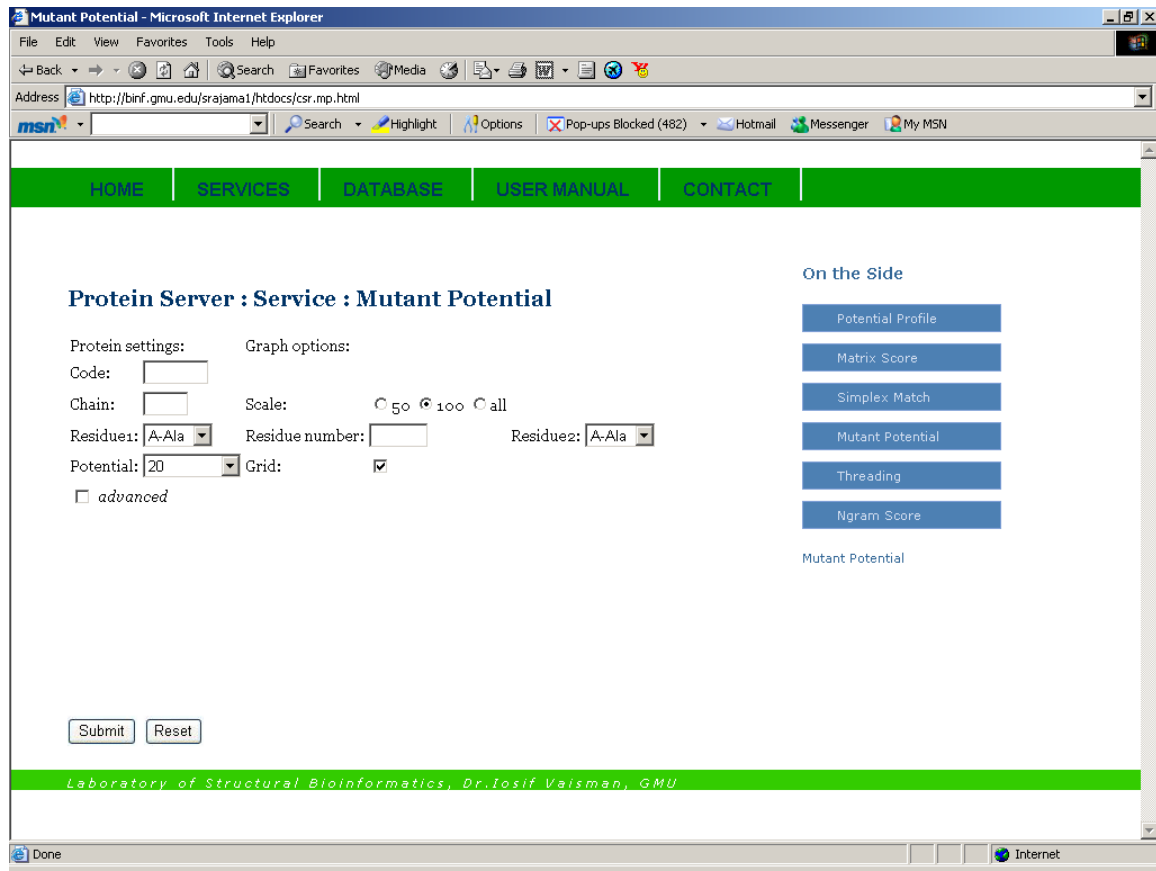
1. -f option in the PotentialProfile.java program will be enhanced later. Instead of PDB entry, if the user likes to upload a file, he will be able to do it with this feature. Current version doesn’t support this feature.
2. For the -p option, right now, user can only chose the 20 option. The corresponding file potential_20.out for the 20 option in the potential combo-box is stored in the server. Other respective files, potential_20_5.out, potential_BT.out, potential_BT_5.out, potential_BT_cut7.out and potential_BT_5_cut7.out need to be stored in the server in order to use those options from the combo-box.

Mutant Potential:

Usage: java MutantPotential [-5] [-v] -p <potential file> -e <pdbEntry> -m <mutant data file> [-o <output file>] [-c <code file>]

User has to enter a valid pdb entry (otherwise, error message is displayed). Potential option can be chosen from the potential combo-box. In the residue 1 combo-box, user can select the residue which he wants to replace with another residue. Corresponding residue number can be given in the respective textbox and in the residue 2 combo-box, user can select the residue which will be replaced with the residue 1 in the given residue number. If the residue number and residue 1 do not match, error message is displayed. User has to reenter the correct residue number and residue combination. If information is valid in the form, output is produced. Link to output file is given in the output screen. The graph, residue vs. potential and the graph, residue vs. difference potential between mutant and wild types, are displayed. Both graphs are of the same scale. User can select the scale option for x-axis, graphs with first 50 residues (both graphs potential and difference), and second 50 residues and so on, first 100 residues, second 100 residues and

so on and all residues in one graph, can be produced depending upon the user's choice. Default is 100 residues per graph. Each set of graphs (potential and difference) will have their own y axis scale depending upon their maximum and minimum value. Grid option is available in this submenu.



Limitation:

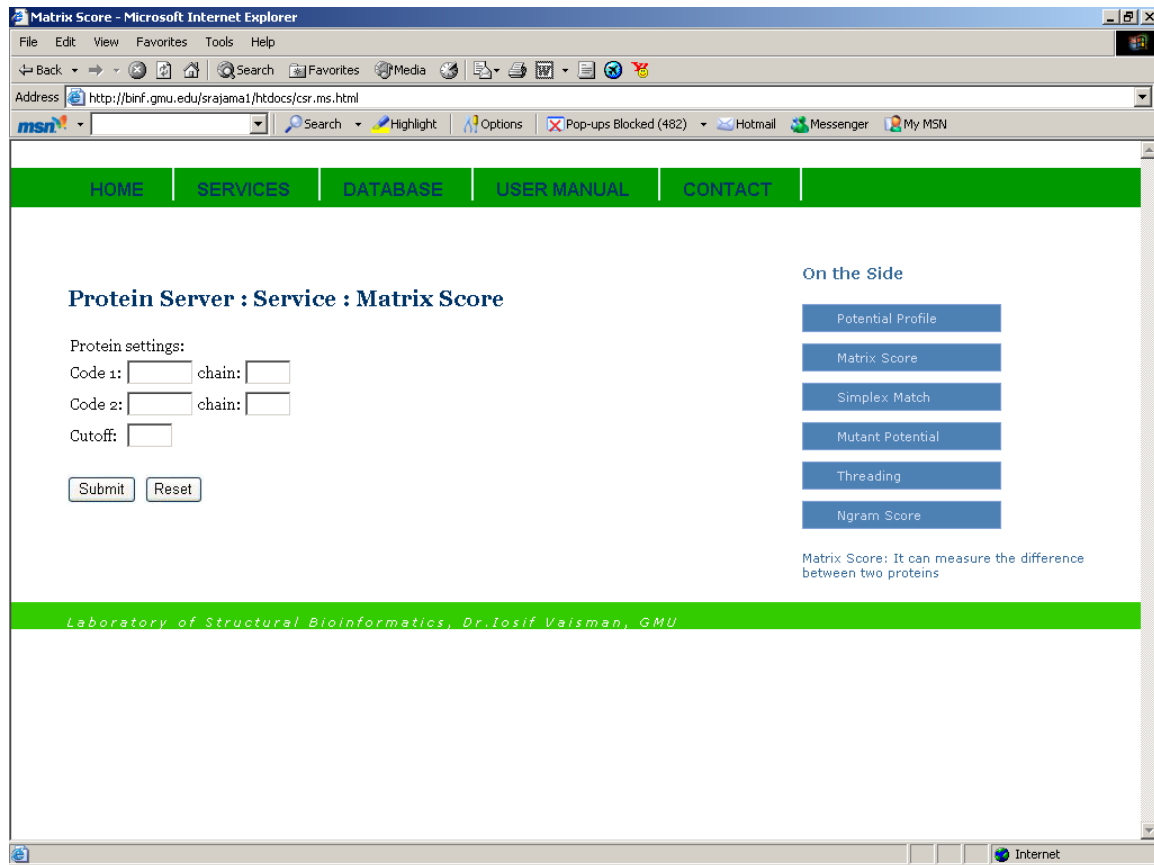
1. For the potential combo box, only potential_20.out can be chosen [-5 option doesn't work in the current version].
2. "Advanced" checkbox interface is working in this submenu, but since the java program has some problem with the -c option, the values given in the definition box which appears when selecting the advanced checkbox, is not used in the program. The program works without the -c option. This error can be rectified in future.

Matrix Score:

Usage: java MatrixScore <pdbEntry1> <pdbEntry2> [-c <cutoff>]

This submenu has a straightforward interface. User needs to give two PDB entries as input in the respective textboxes and the cutoff of the edge length in the cutoff textbox. If valid PDB entry is not given, error message is displayed. User can reenter the correct PDB id.

Output is displayed in the output screen.



Threading:

Usage: java Threading [-5] [-v] -p <potential file> -e <pdbEntry> -m <mutant data file> [-o <output file>] [-c <code file>]

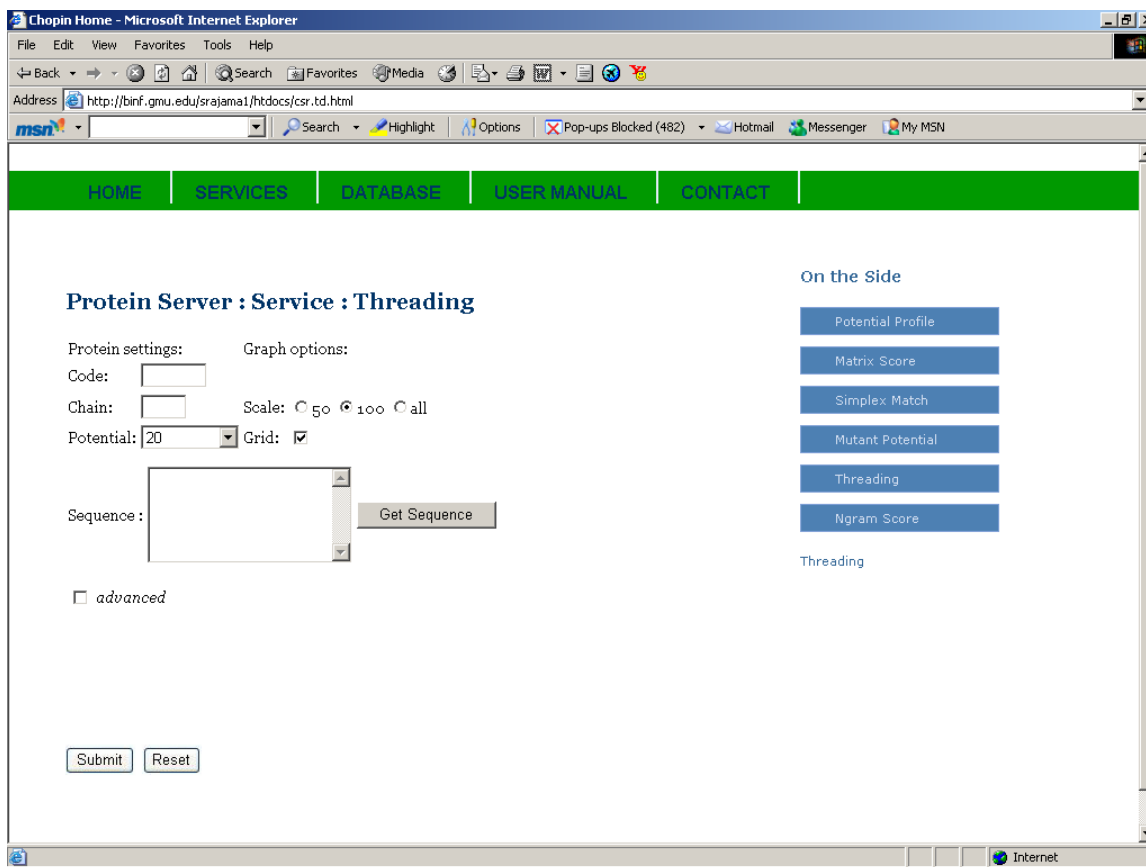
User needs to enter valid PDB id (otherwise error message is displayed). Potential option can be chosen from the potential combo-box (current version support option “20”). Scale option and grid option can be chose for the graph outputs.

Limitations:

1. Get sequence button gets the sequence and displays in the sequence text box. For some of the entries, only part of the sequence has structure. User needs to know the sequence numbering of the structure PDB file. Unwanted part should be removed from the sequence in the textbox before clicking on the submit button. For example, 1a12A has sequence from 1 – 413, but the structure file has entries from 21 – 421. First 12 residues from the sequence needs to be deleted before clicking the submit button. In future, this part might get automated so that the user need not worry about the sequence numbering.

Once the required sequence is placed in the textbox, the user can make any number of residue replacements (many mutations). Graphs are produced in the output screen. They are similar to Mutant Potential graphs, potential graph and the difference graph.

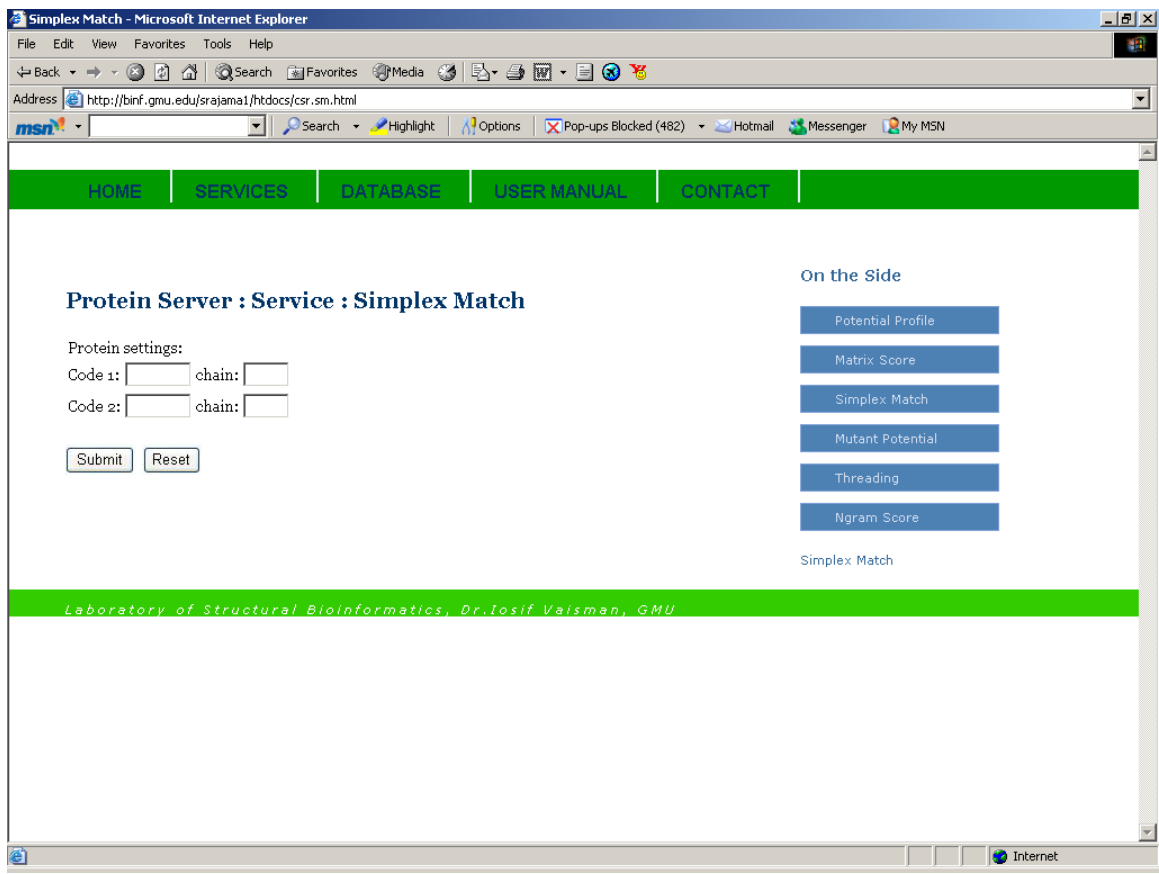
2. The same problem of the “Advanced” checkbox is present in this submenu. This feature can be improved through future enhancements.
3. Current version supports only potential_20.out for the -p option [potential combo box]



Simplex Match:

Usage: java SimplexMatch <pdbEntry1> <pdbEntry2>

This submenu is straightforward. User needs to enter two valid PDB ids (otherwise, error message is displayed). Output is displayed on the screen.



All output screen has links to home page, PDB website (PDB explore page for the corresponding PDB id) and output files.