Visualization tool for comparison of a single amino acid change in protein simulation

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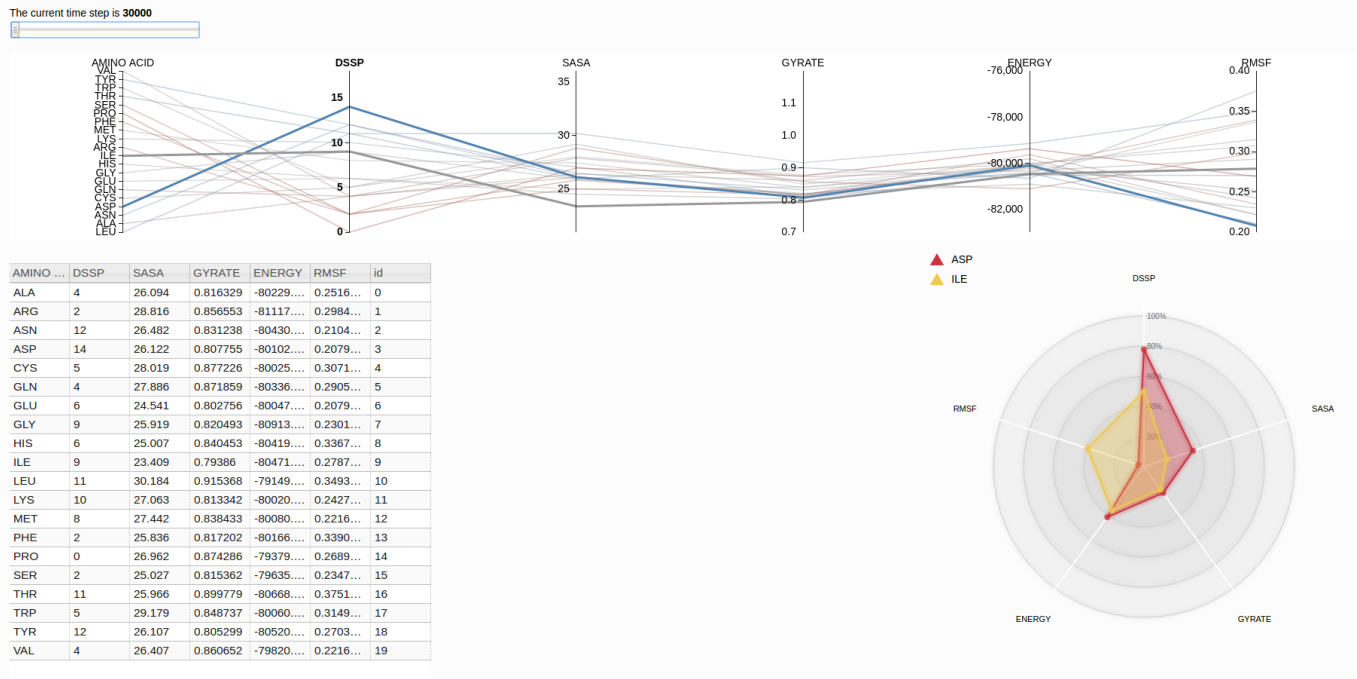

AMINO …	DSSP	SASA	GYRATE	ENERGY	RMSF	id
ALA	4	26.094	0.816329	-80229.…	0.2516…	0
ARG	2	28.816	0.856553	-81117.…	0.2984…	1
ASN	12	26.482	0.831238	-80430.…	0.2104…	2
ASP	14	26.122	0.807755	-80102.…	0.2079…	3
CYS	5	28.019	0.877226	-80025.…	0.3071…	4
GLN	4	27.886	0.871859	-80336.…	0.2905…	5
GLU	6	24.541	0.802756	-80047.…	0.2079…	6
GLY	9	25.919	0.820493	-80913.…	0.2301…	7
HIS	6	25.007	0.840453	-80419.…	0.3367…	8
ILE	9	23.409	0.79386	-80471.…	0.2787…	9
LEU	11	30.184	0.915368	-79149.…	0.3493…	10
LYS	10	27.063	0.813342	-80020.…	0.2427…	11
MET	8	27.442	0.838433	-80080.…	0.2216…	12
PHE	2	25.836	0.817202	-80166.…	0.3390…	13
PRO	0	26.962	0.874286	-79379.…	0.2689…	14
SER	2	25.027	0.815362	-79635.…	0.2347…	15
THR	11	25.966	0.899779	-80668.…	0.3751…	16
TRP	5	29.179	0.848737	-80060.…	0.3149…	17
TYR	12	26.107	0.805299	-80520.…	0.2703…	18
VAL	4	26.407	0.860652	-79820.…	0.2216…	19

Fig. 1. Image of the tool with all elements presented.

***Abstract*—**

***Keywords*-one or two words; separated by semicolon; from specific; to generic fields;**

I. Introduction

Proteins are polymers formed by a sequence of 20 different possible amino acids that under physiological conditions fold into a precise shape known as its native state [1]. Each amino acid has an alpha carbon (CA) with bonds to amino (NH2) and carboxyl (COOH) groups and a variable side-chain (R) that determines the particular physicochemical properties of each residue. A peptide is a molecule composed of two or more amino acids chained by a chemical bond called the *peptide bond*. This bond is formed when the carboxyl group of one residue reacts with the amino group of the other residue, releasing a water molecule. The interaction between amino acids in a protein causes the polypeptide chain to fold, usually in a proper configuration, as α-helix, β-sheet, coil or turn. These local folding patterns represent the secondary structure of a protein. The topology or fold is given by the succession of secondary structures connected in a 3D space. The specific characteristics of the peptide bond have significant implications for the 3D fold that can be adopted by polypeptides. The peptide bond (C-N) has a double bond, and it is not allowed rotation of the molecule around this bond. The rotation is only permitted around the bonds N-Cα and C$_\alpha$-C. The analysis of experimental protein structures (X-ray data) reveals that amino acid residues can assume many conformations in proteins [2]. Each amino acid has a set of physiochemical properties which contributes to its intrinsic conformational preference [3]. Amino acids in a secondary structure usually adopt a particular set of backbone torsion angles [2].

AMINO ...	DSSP	SASA	GYRATE	ENERGY	RMSF	id
ALA	4	26.094	0.816329	-80229....	0.2516...	0
ARG	2	28.816	0.856553	-81117....	0.2984...	1
ASN	12	26.482	0.831238	-80430....	0.2104...	2
ASP	14	26.122	0.807755	-80102....	0.2079...	3
CYS	5	28.019	0.877226	-80025....	0.3071...	4
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MET	8	27.442	0.838433	-80080....	0.2216...	12
PHE	2	25.836	0.817202	-80166....	0.3390...	13
PRO	0	26.962	0.874286	-79379....	0.2689...	14
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Fig. 2. Overview of the used grid.

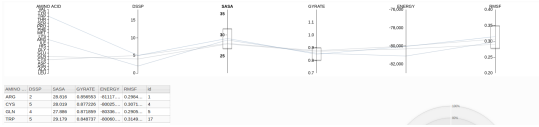

Fig. 3. Example of the use of brush.

A. Related work

II. Data characterization

A. Data dimensions

DSSP:

SASA: Solvent-accessible surface area is the surface area of the protein that is accessible to the solvent.

GYRATE: The radius of gyration can be used as a measurement of the compactness of a protein structure. It describes the overall spread of the molecule and is calculated taking the root mean square distance of the atoms from their common centre of gravity.

ENERGY:

RMSF: The root mean square fluctuation of atomic positions is the measure of the average distance between the atoms of the simulated protein and a well-defined average position.

III. Technical background

IV. Technique overview

A. Grid

Item highlighting:
Item selection:

B. Parallel Coordinates

Axis brushing: Fig. 3
Axis sorting:
Axis reordering:
Recoloring by axis selection:

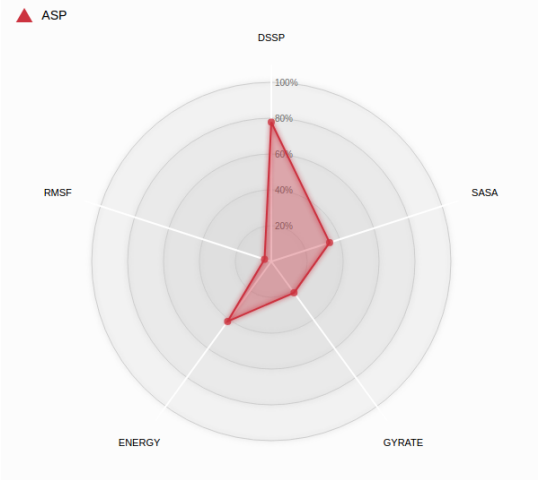

Fig. 4. Example of one amino acid being visualized in the radar plot.

C. Radar Plot

Item highlighting:

D. Slider

V. Experiments

VI. Results and Discussion

A. Future work

VII. Conclusion

A demo can be tested at: http://inf.ufrgs.br/ bigrisci/parallel-coordinates/

Acknowledgment

References

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[3] V. Mathura and D. Kolippakkam, "Apdbase: Amino acid physicochemical properties database," *Bioinformation*, vol. 1, no. 1, pp. 2–4, 2005.