One way of protein structure representation for determining protein structure similarity

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Algorithms, based on alignment of secondary structure elements

! ONE OF THE IMPORTANT ASPECTS IS THE APPROPRIATE PROTEIN STRUCTURE REPRESENTATION

ALGORITHMS, USING GRAPH

- VAST
- MWBM
- STOICHEV-MILUSHEVA METHOD

VAST

- NODES ->SSEs
- EDGES ->DISTANCE AND ANGLE WITHIN SOME THRESHOLD

MAXIMUM WEIGTH BIPARTITE GRAPH

- NODES -> SSEs
- EDGES -> DEGREE OF SIMILARITY BETWEEN TWO NODES, EACH FROM DIFFERENT PROTEIN

STOICHEV- MILUSHEVA METHOD

- NODES -> SSEs(CENTROIDS)
- EDGES -> DISTANCES BELOW GIVEN THRESHOLD

THE METHOD

- NODES ->SSEs OR SINGLE STRAND
- EDGES ->RULES

PARAMETRES CAN BE:

- DISTANCE BETWEEN SSEs;
- ANGLE BETWEEN SSEs;
- NUMBERS OF VISITS;
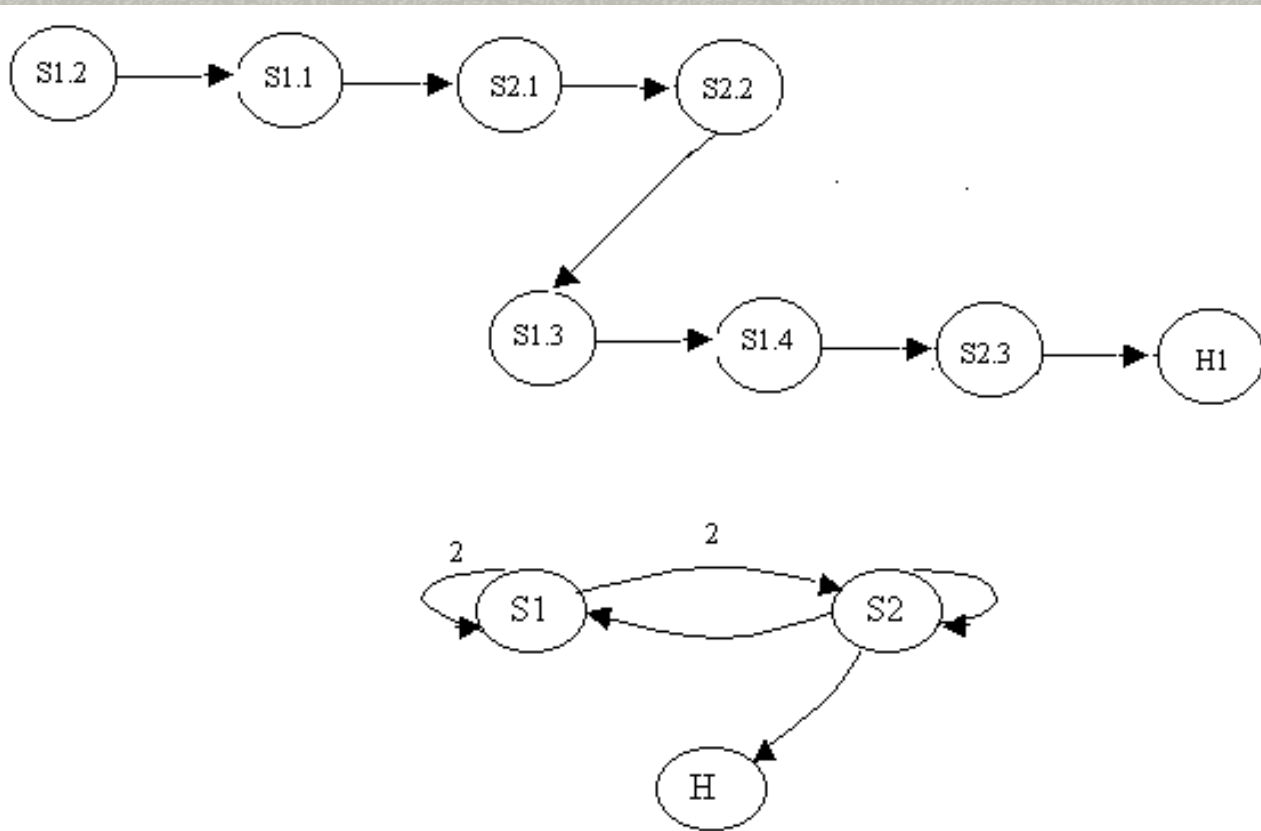- PARALLEL OR ANTIPARALLEL WAY OF CONNECTION

LEVELS OF INTEREST

- LOW LEVEL - ONLY NUMBERS OF VISITS;
- MEDIUM LEVEL – DISTANCES, ANGLES AND NUMBERS OF VISITS;
- HIGH LEVEL - DISTANCES, ANGLES, NUMBERS OF VISITS AND WAY OF CONNECTION

LOW LEVEL- ADDITIONAL RULES

- ALL STRANDS IN SHEET ARE REPRESENTED BY A SINGLE NODE;
- NODE CAN REPRESENT A SINGLE HELIX OR UNINTERRUPTED SEQUENCE OF HELICIES;

Structure of human immunodeficiency virus type 1

Virus Proteins