IS THE „FUZZY OIL DROP" MODEL OF GENERAL CHARACTER?

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„Fuzzy Oil Drop" Model

◆ FOD assumes the hydrophobicity function in proteins to be accordant with 3D-Gauss function, differentiating the hydrophobicity density from the highest one in the center of the molecule and zero level on the surface.

◆ Are there many proteins representing the structure of „fuzzy oil drop" character in respect to hydrophobicity distribution?

◆ Data: The complete set of proteins present in PDB (December 2010)

  ◆ Files representing nucleic acid molecules were excluded

◆ Expected (Theoretical) hydrophobicity distribution

  ◆ Based on residues positions in 3-D space

◆ Observed hydrophobicity distribution was calculated according to Levitt function

  ◆ For all interacting residues (distance below cut-off value = 9A)

  ◆ Sum of interacting resiudes hydrophobicity (according to hydrophobicity scale)

◆ The similarity of expected and observed distribution was calculated according to Kullback-Leibler distance entropy

Experiment and results

- ◆ The structural unit was defined in two ways:
  - ◆ Protein complexes were taken as one unit
  - ◆ Each chain was taken separately
- ◆ Experiment was executed on ZEUS cluster
- ◆ Complete PDB database was split into 1050 subsets, each computing task operated on just one subset, communication was not required
- ◆ A SQL databases with results for every data set were created.
- ◆ The statistics for proteins with structure accordant to FOD model were collected
  - ◆ Source organism, length of polypeptide, enzyme characteristics

Chain / Complex — CHAINS: 96,41; COMPLEXES: 26,27

LENGTH OF POLYPEPTIDE — CHAINS: 86,8; 98,3; 98,4; 97,8; 99,0; 97,2; 86,4 — COMPLEX: 22,2; 27,8; 28,7; 23,7; 29,3; 20,5; 26,4. Residues: < 80; 80 – 120; 120 – 200; 200 – 250; 250 – 400; 400 – 600; > 600

ENZYME — CHAINS: Enzyme 98,2; Not Enzyme 95,0 — COMPLEX: Enzyme 28,8; Not Enzyme 24,3