KULLBACK-LEIBLER ENTROPY for FUZZY OIL DROP MODEL

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PROTEIN FOLDING
HYDROPHOBIC CORE
IRREGULARITY in HYDROPHOBIC CORE
IDEALIZED DISTRIBUTION of HYDROPHOBICITY

\[ \tilde{H}_{t_j} = \frac{1}{\tilde{H}_{t_{sum}}} \exp\left(-\frac{(x_j - \bar{x})^2}{2\sigma_x^2}\right) \exp\left(-\frac{(y_j - \bar{y})^2}{2\sigma_y^2}\right) \exp\left(-\frac{(z_j - \bar{z})^2}{2\sigma_z^2}\right) \]
OBSERVED DISTRIBUTION of HYDROPHOBICITY

\[ \hat{H}_{o_j} = \frac{1}{\hat{H}_{o_{sum}}} \sum_{i=1}^{N} (H'_i + H'_j) \begin{cases} 1 - \frac{1}{2} \left( 7 \left( \frac{r_{ij}}{c} \right)^2 - 9 \left( \frac{r_{ij}}{c} \right)^4 + 5 \left( \frac{r_{ij}}{c} \right)^6 - \left( \frac{r_{ij}}{c} \right)^8 \right) & \text{for } r_{ij} \leq c \\ 0 & \text{for } r_{ij} > c \end{cases} \]

INTER-RESIDUAL HYDROPHOBIC INTERACTION
UNIFIED DISTRIBUTION of HYDROPHOBICITY

\[ \tilde{H}r_j = \frac{1}{N} \]

NO DIFFERENTIATION OF HYDROPHOBIC DENSITY
DISTRIBUTIONS of HYDROPHOBICITY
KULLBACK-LEIBLER ENTROPY to MEASURE the DIFFERENCES

$$D_{KL}(p|p^0) = \sum_{i=1}^{N} p_i \log_2 \left( \frac{p_i}{p_i^0} \right)$$
OBSERVED DISTRIBUTION

versus

THEORETICAL DISTRIBUTION

\[ \frac{O}{T} = \sum_{i=1}^{N} O_i \log_2 \frac{O_i}{T_i} \]
OBSERVED DISTRIBUTION

versus

UNIFIED DISTRIBUTION

\[ O/R = \sum_{i=1}^{N} O_i \log_2 O_i / R_i \]
RELATIVE DISTANCE

\[ RD = \frac{O/T}{O/T + O/R} \]
RELATIVE DISTANCE

IDEALIZED DISTRIBUTION

PROTEIN UNDER CONSIDERATION

UNIFORM DISTRIBUTION

DISTANCE versus IDEALIZED DISTRIBUTION
IDEALIZED versus OBSERVED

O/T = 0.27
O/R = 0.58
RD = 0.31
ACCORDANT

O/T = 0.73
O/R = 0.45
RD = 0.62
DISCORDANT
ACTIVE SITE RECOGNITION

ANTIGEN BINDING
HUMAN LYSOZYME
CONCLUSIONS/1

- 3D-GAUSS FUNCTION REPRESENTS WELL THE STRUCTURE OF HYDROPHOBIC CORE

- DIVERGENCE ENTROPY ALLOWS MEASURE THE DIFFERENCES IN QUANTITATIVE FORM
CONCLUSIONS/2

- LOCAL DISCORDANCE BETWEEN OBSERVED AND IDEALIZED DISTRIBUTION VERY OFTEN RELATED TO AREA OF BIOLOGICAL ACTIVITY

- RELATION BETWEEN STABILIZATION ROLE OF HYDROPHOBIC CORE AND DISULPHIDE BONDS is the object of the paper submitted for conference
References:

MANY THANKS
for
YOUR ATTENTION

We shall be very glad for any comments