KULLBACK-LEIBLER ENTROPY for FUZZY OIL DROP MODEL

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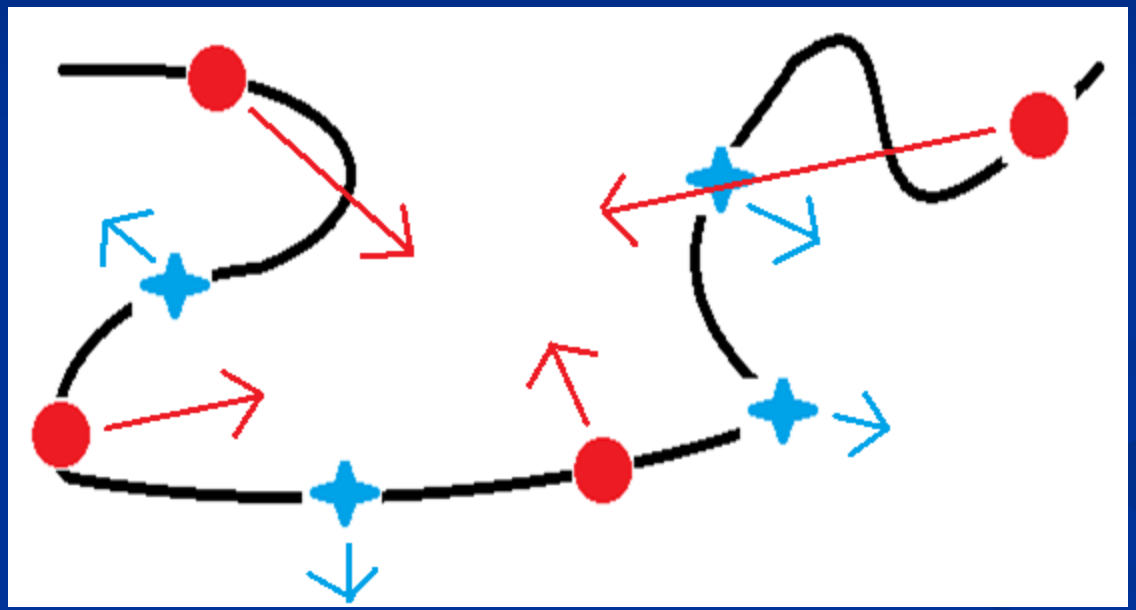
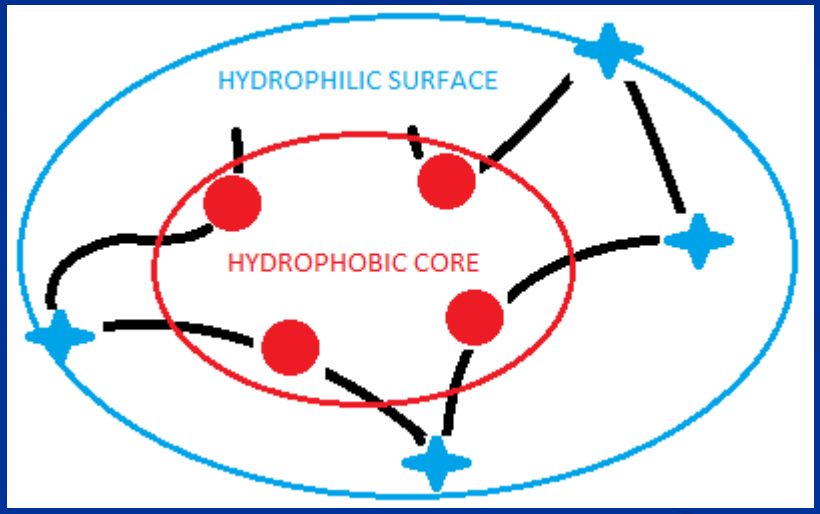
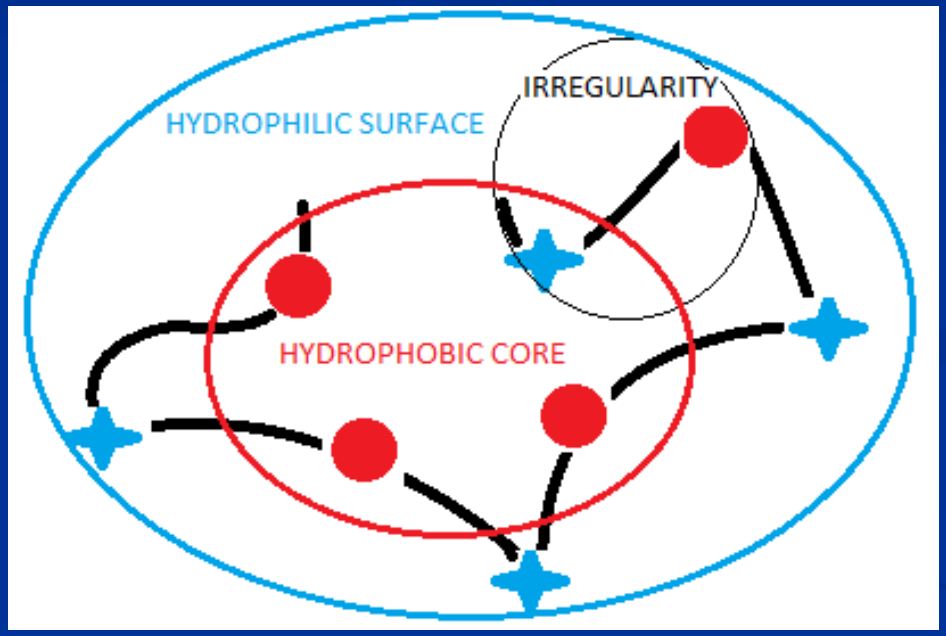
PROTEIN FOLDING



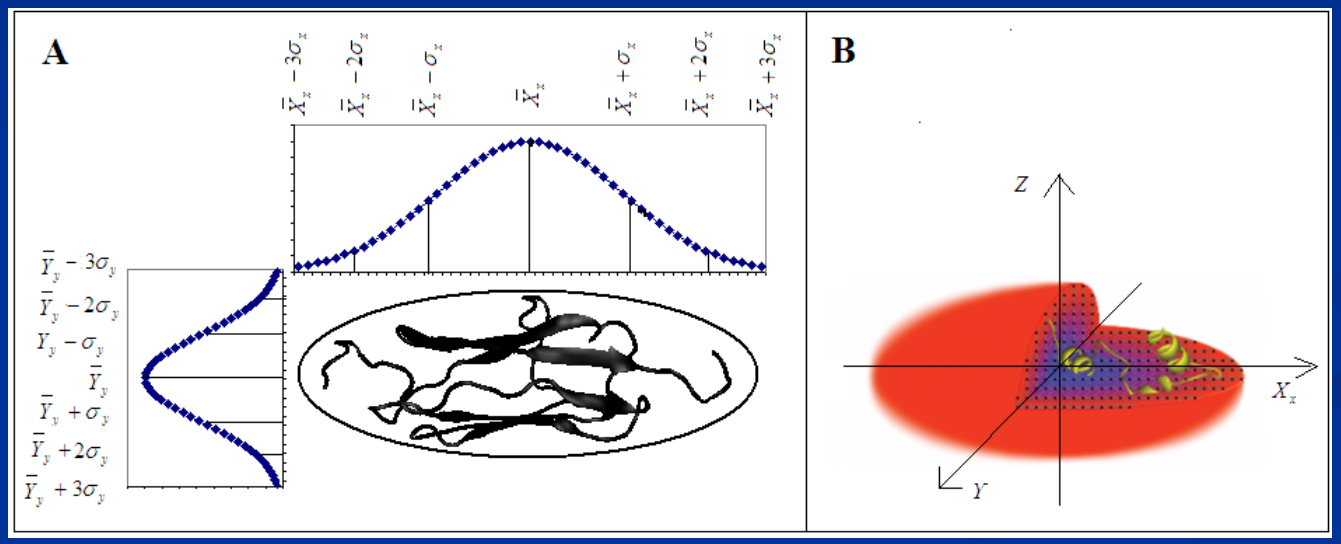
HYDROPHOBIC CORE



IRREGULARITY in HYDROPHOBIC CORE



IDEALIZED DISTRIBUTION of HYDROPHOBICITY



$$\widetilde{Ht}_j = \frac{1}{\widetilde{Ht}_{sum}} \exp\left(\frac{-\left(x_j - \bar{x}\right)^2}{2\sigma_x^2}\right) \exp\left(\frac{-\left(y_j - \bar{y}\right)^2}{2\sigma_y^2}\right) \exp\left(\frac{-\left(z_j - \bar{z}\right)^2}{2\sigma_z^2}\right)$$

OBSERVED DISTRIBUTION of HYDROPHOBICITY

$$\tilde{H}o_j = \frac{1}{\tilde{H}o_{sum}} \sum_{i=1}^{N} (H_i^r + H_j^r) \begin{cases} \left[1 - \frac{1}{2}\left(7\left(\frac{r_{ij}}{c}\right)^2 - 9\left(\frac{r_{ij}}{c}\right)^4 + 5\left(\frac{r_{ij}}{c}\right)^6 - \left(\frac{r_{ij}}{c}\right)^8\right)\right] & \text{for } r_{ij} \le c \\ 0 \text{ for } r_{ij} > c \end{cases}$$

INTER-RESIDUAL HYDROPHOBIC INTERACTION

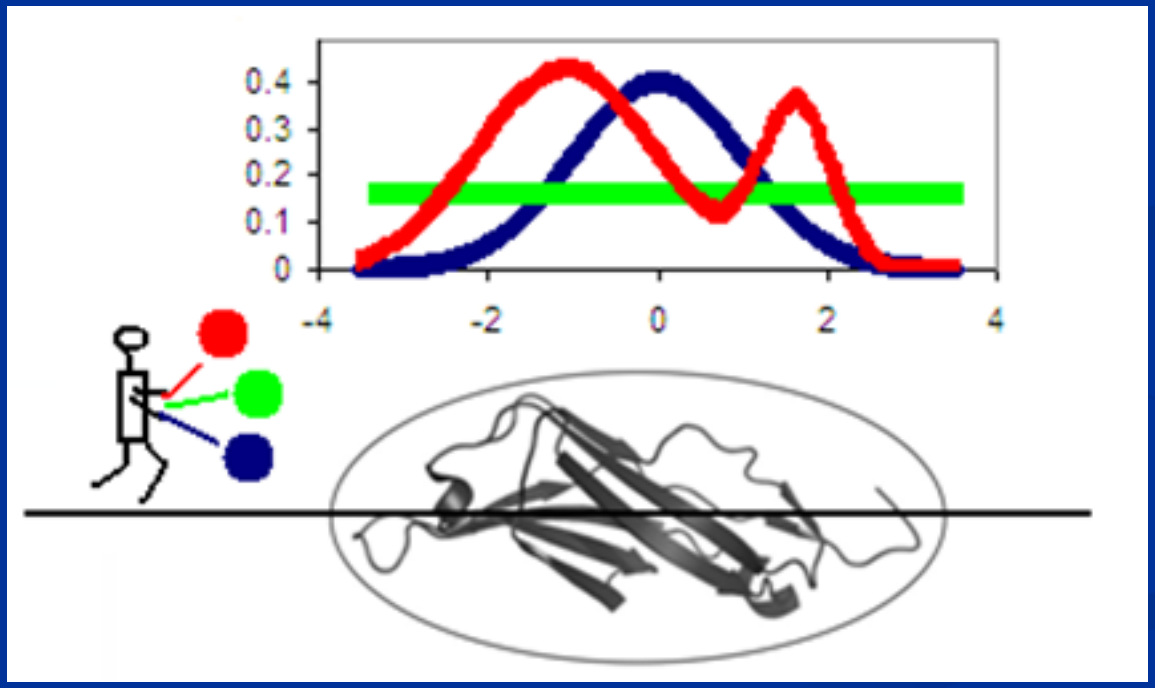
UNIFIED DISTRIBUTION of HYDROPHOBICITY

$$\tilde{H} r_j = \frac{1}{N}$$

NO DIFFERENTIATION

OF HYDROPHOBIC DENSITY

DISTRIBUTIONS of HYDROPHOBICITY



observed
unified
theoretical

KULLBACK-LEIBLER ENTROPY

to

MEASURE the DIFFERENCES

$$D_{KL}(p|p^0) = \sum_{i=1}^{N} p_i \log_2(p_i / p_i^0)$$

OBSERVED DISTRIBUTION

versus

THEORETICAL DISTRIBUTION

$$O/T = \sum_{i=1}^{N} O_i \log_2 O_i / T_i$$

OBSERVED DISTRIBUTION

versus

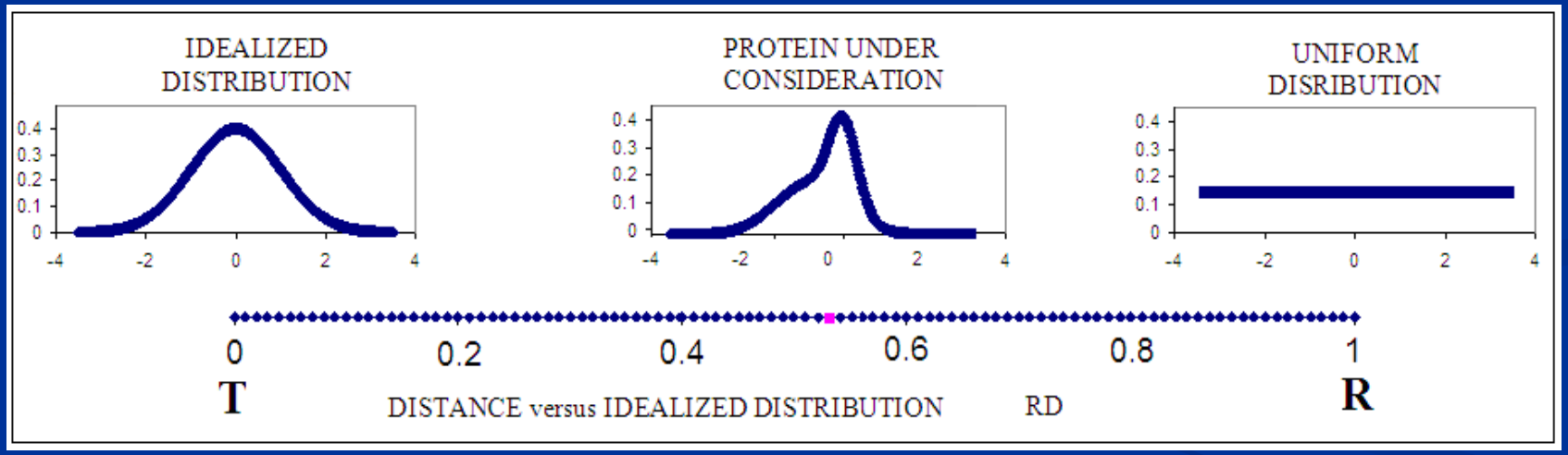
UNIFIED DISTRIBUTION

$$O/R = \sum_{i=1}^{N} O_i \log_2 O_i / R_i$$

RELATIVE DISTANCE

$$RD = \frac{O/T}{O/T + O/R}$$

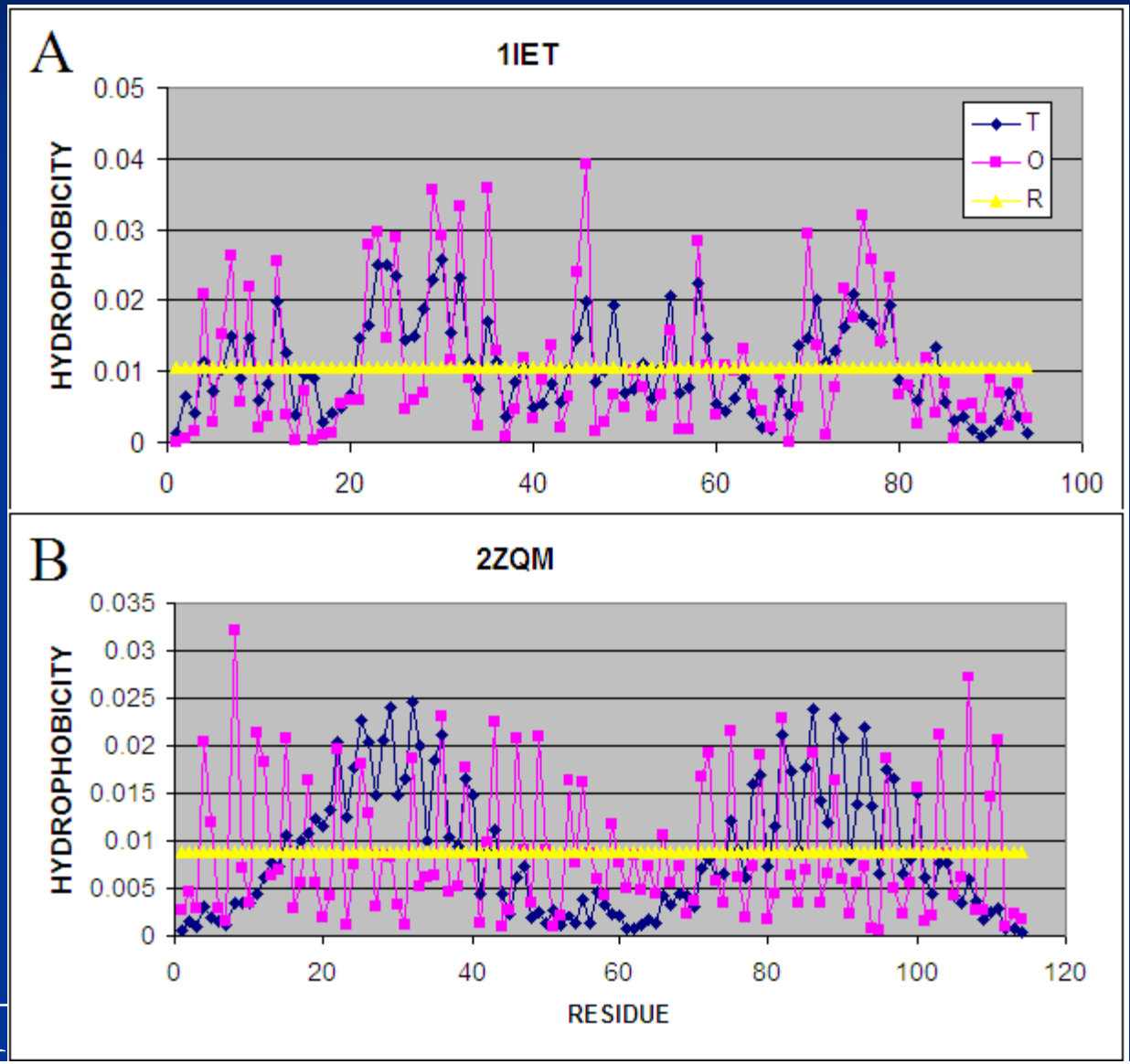
RELATIVE DISTANCE



IDEALIZED versus OBSERVED

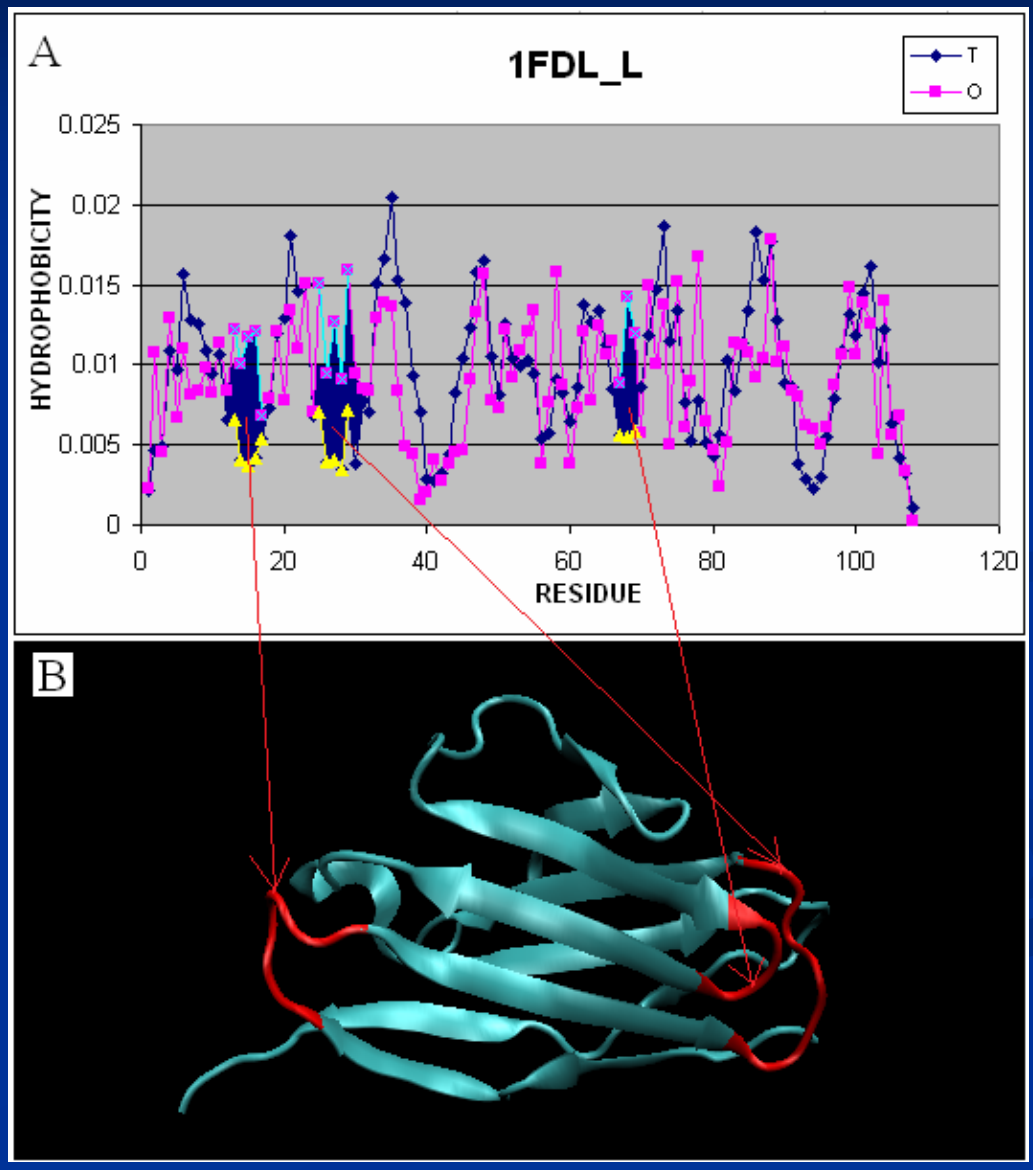
O/T=0.27
O/R=0.58
RD=0.31
ACCORDANT

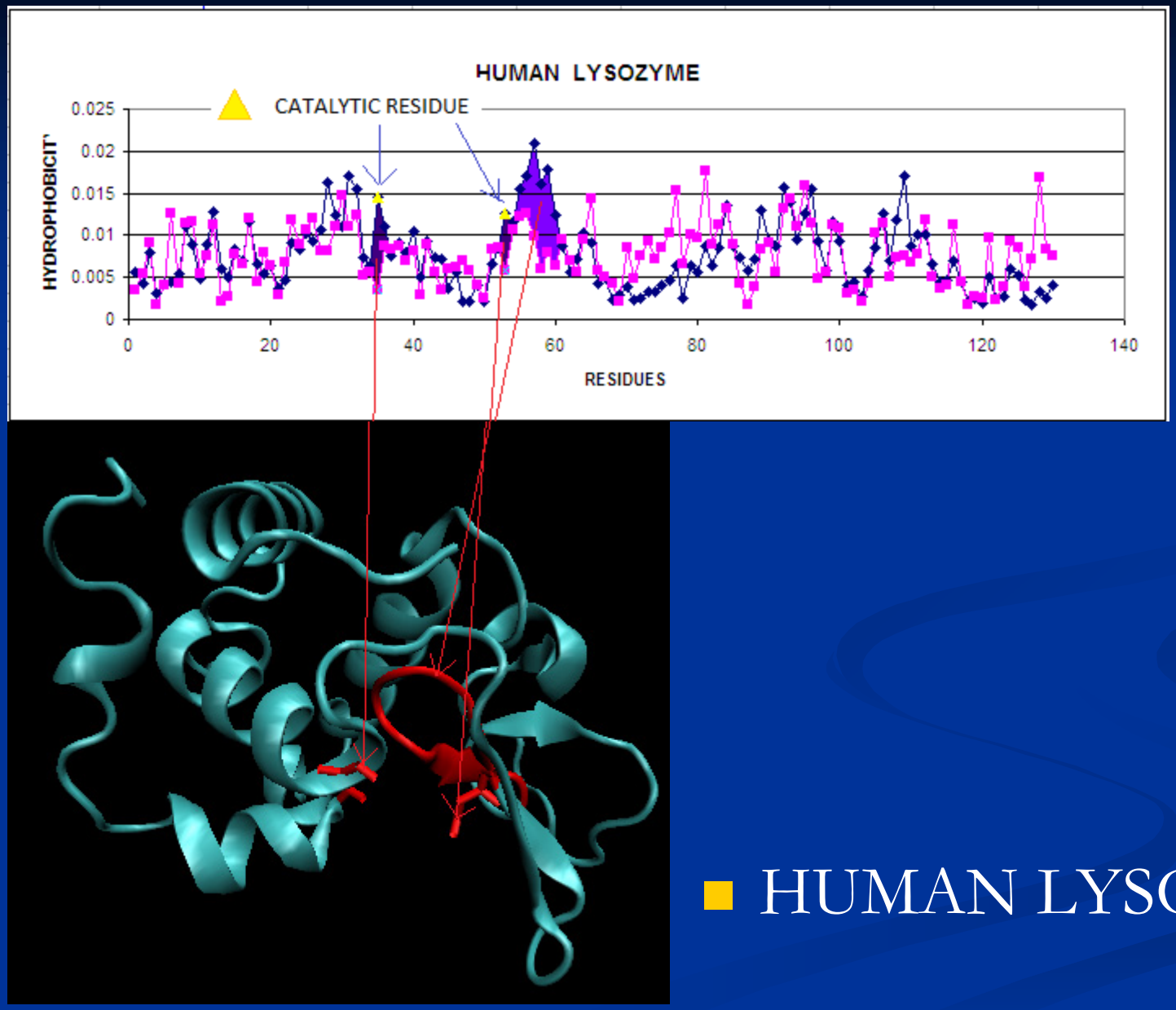
O/T=0.73
O/R=0.45
RD=0.62
DISCORDANT



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:

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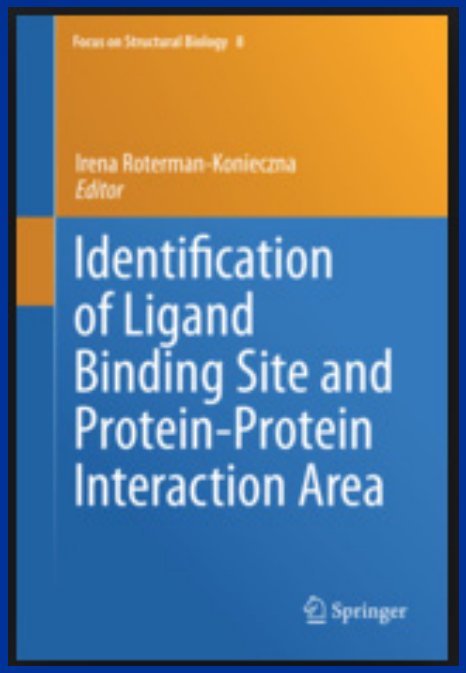
BOOKS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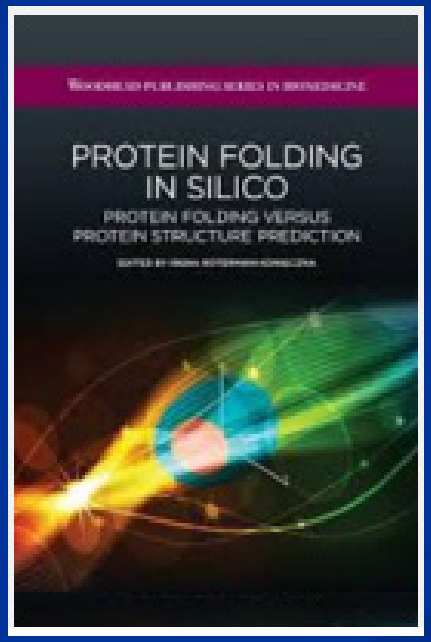
PROTEIN FOLDING IN SILICO
PROTEIN FOLDING VERSUS PROTEIN STRUCTURE PREDICTION

MANY THANKS
for
YOUR ATTENTION

We shall be very glad for any comments