Predicting kinetic constants of protein-protein interactions based on structural properties

Proteins

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• Most complexes in the PDB do not have known kinetic data, so an accurate predictor could aid protein interface design and the predicted values could also be used in systems biology models.

• The authors construct a new dataset of 62 protein complexes with experimentally determined kinetic data.

• Table 1 presents the 35 structure based features used in the work. Could be useful for anyone interested in protein-protein interactions.

• Leave one out cross validation results:
  • Association rate constant \((K_{on})\): Pearson correlation of .801
  • Dissociation rate constant \((K_{off})\): Pearson correlation of .732
  • Affinity / dissociation rate constant \((K_d)\): Pearson correlation of .770
Pre-calculated proteins structure alignments at the RCSB PDB website

Bioinformatics

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http://bioinformatics.oxfordjournals.org/content/26/23/2983.full

• Calculating all-versus-all structure alignments and sequence alignments takes a lot of CPU time, now the PDB has selected 16,000 representative chains and done all-vs-all comparison with results stored as xml files.

• This type of information is useful for analyzing structural variability within a fold, sequence structure relationships, and as data for protein structure prediction methods.

• The new web tools are useful for comparing a handful of proteins of interest with minimal effort.