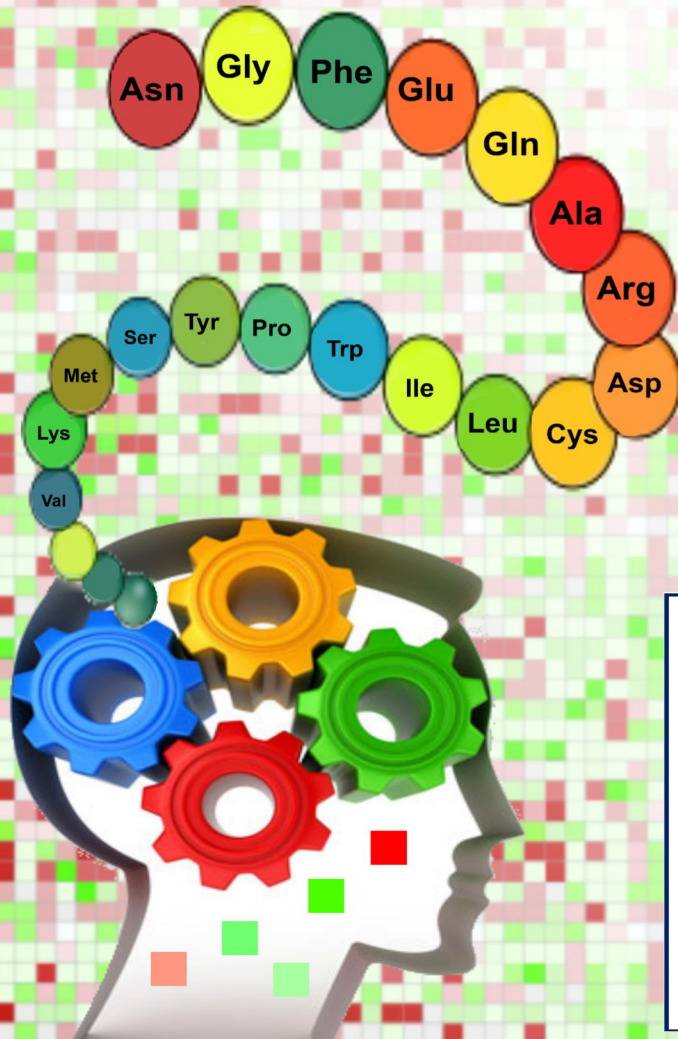


RAPHYD

Predictor of the Effect of Amino Acid Substitutions on Protein Function

Miloš Musil

Ing. Jaroslav Bendl



Conclusions & Outlook

The new predictor of the effect of amino acid substitutions on protein function was developed. The decision core is based on the complex phylogenetic analysis and the differences in the physico-chemical properties.

The combination of experiment based methods (forward selection & backward elimination) resulted in the set of 13 properties with the increase of accuracy about 2.4% on training dataset.

The extensive evaluation on the four datasets, compiled from 78,650 mutations, revealed that the best trade-off between normalized accuracy and time consumption is provided by CLUSTALΩ and FastTree launched on maximum 200 homologs sequences from nr90 database found by BLASTp with e-value threshold 10^{-12} . In this configuration 72.13% accuracy was reached.

Developed predictor will be embedded into existing integrative platform for protein engineering HotSpot Wizard available at <http://loschmidt.chemi.muni.cz/hotspotwizard/>

Schema

