Proteins: Properties and Surface Patches

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Since the introduction of the first recombinant protein therapeutic 25 years ago the number of protein therapeutics has increased dramatically. [1] Getting experimental data on solubility, hydrodynamic and electrophoretic properties is laborious as it requires a significant amount of purified protein. Thus an in-silico method for protein property prediction is desirable. In this talk we will discuss the theoretical background and results obtained by an algorithm as implemented in MOE 2012 [2].

However looking at whole molecule properties is not sufficient to explain protein aggregation behavior in all cases. Therefore we implemented a surface patch analysis and visualization tool that allows getting further insights in the solubility behavior of proteins and gives hints mutants might lead to improved protein therapeutics.

Another new tool to apply site directed mutagenesis to wild type proteins completes the toolbox of protein design applications.

[1] Leader, B.; Baca, Q. J. et al.; Nature Reviews Drug design; 7, 21-29, 2008
[2] Long, W.; Labute, P.; J. Comput Aided Mol Des; 24, 907-916, 2010