

## Improved methods for modeling of the interaction between molecules and proteins

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**Background:** Accurate, descriptive and statistically valid models predicting interactions between molecules and proteins are of immense value in a number of important fields in biology and chemistry, e.g. functional genomics and drug development. Proteochemometrics (PCM) is a new approach to interaction analysis put forward by Jarl Wikberg's research group. PCM models are constructed by first adhering the molecules and the proteins with a mathematical description. That mathematical description is then correlated, by e.g. regression models or machine learning algorithms, to an experimentally determined value of the interaction strength between a given molecule and a given protein. The thus constructed models give insights to the inner workings of a given interaction and aid in making predictions about the interaction strength of an unknown (not experimentally determined) interaction.

**Aim:** PCM is under rapid development and a number of ideas about how to improve the modeling have been suggested. The overall aim of this project is to try out and implement (in R and/or Java) one of these ideas. Examples: 1) SIMEX modeling for controlling error-in variables, 2) improve the regression method to use the information in the dependent variable in a better way, 3) develop improved ways of using data produced by different labs.

**Misc:** This will be a modeling and simulation project. Datasets where the mathematical description of the molecules and the proteins already is done will be provided to the student. We are looking for a mathematics/statistics- or an engineer (civilingenjör) student with an interest in bio- or chemoinformatics.

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