In this presentation Olga Obrezanova talks about Gaussian Processes - a powerful computational method for QSAR modelling. Olga starts by describing the main ideas of this technique.

We are mostly interested in the application of this technique to predictive modelling of ADME properties. The importance of optimising ADME properties of potential drug molecules is now widely recognised. Considering the ADME properties early in the drug discovery process can reduce the costs of the drug development and decrease the attrition rate of drug candidates. We have developed new techniques for finding parameters of the Gaussian Processes method which I will present. I will also show examples of application of these techniques to ADME and QSAR datasets and compare Gaussian Processes methods with other known techniques. The demand of modern drug discovery for fast model (re)building whenever new data becomes available gave rise to a trend to develop computational algorithms for automatic model generation. I will demonstrate how we use Gaussian Processes in an automatic modelling process. (The purpose of such algorithms is to save scientists' time, explore more modelling possibilities and make the process of QSAR model building accessible to non-experts.)

This presentation was given at the American Chemical Society conference in Boston, 2007.

The following slides were given for Olga's presentation:

A copy of Olga's slides are available as a PDF file.