

Figure 2: a) The R2 and Q2 values of internal cross-validation of the different COMBINE models were plotted in dependency of the number of latent variables (LV). (For more details see legend of table 1).

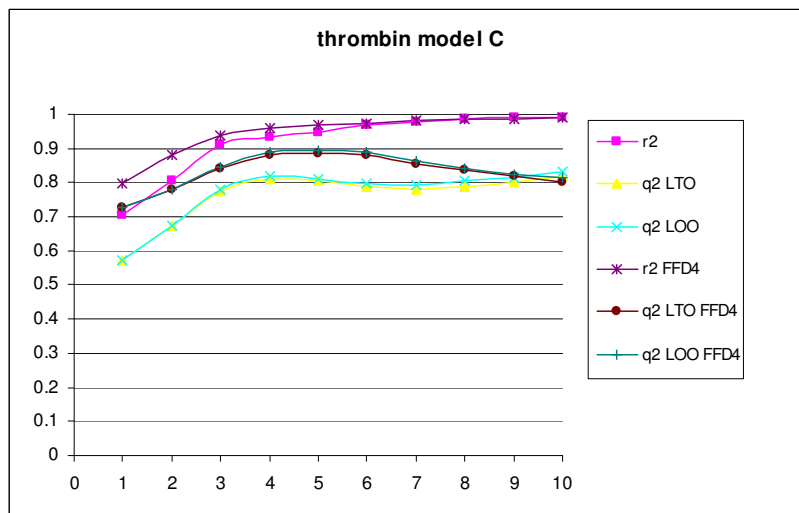
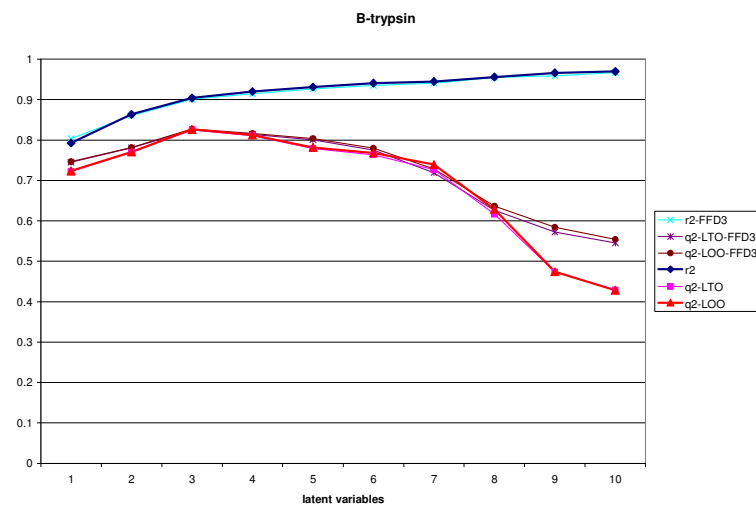
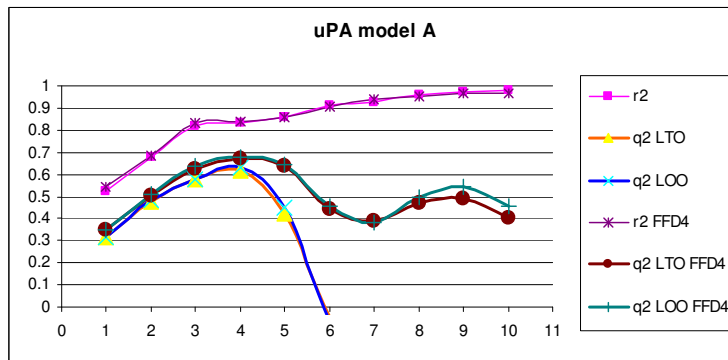
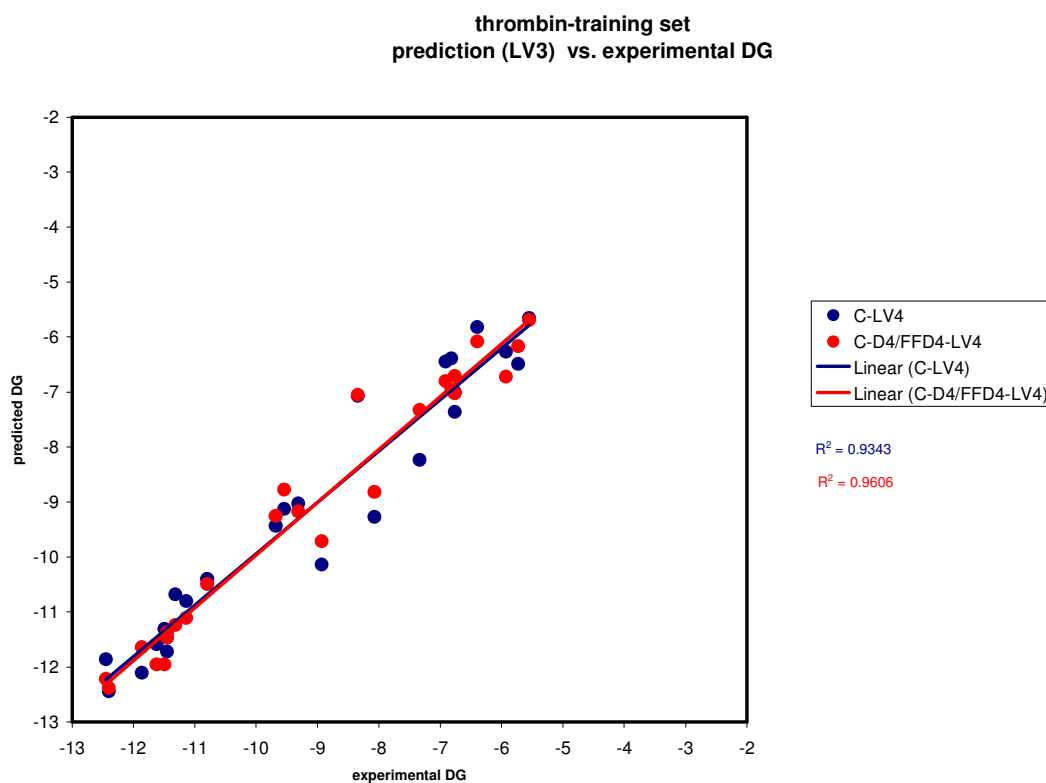
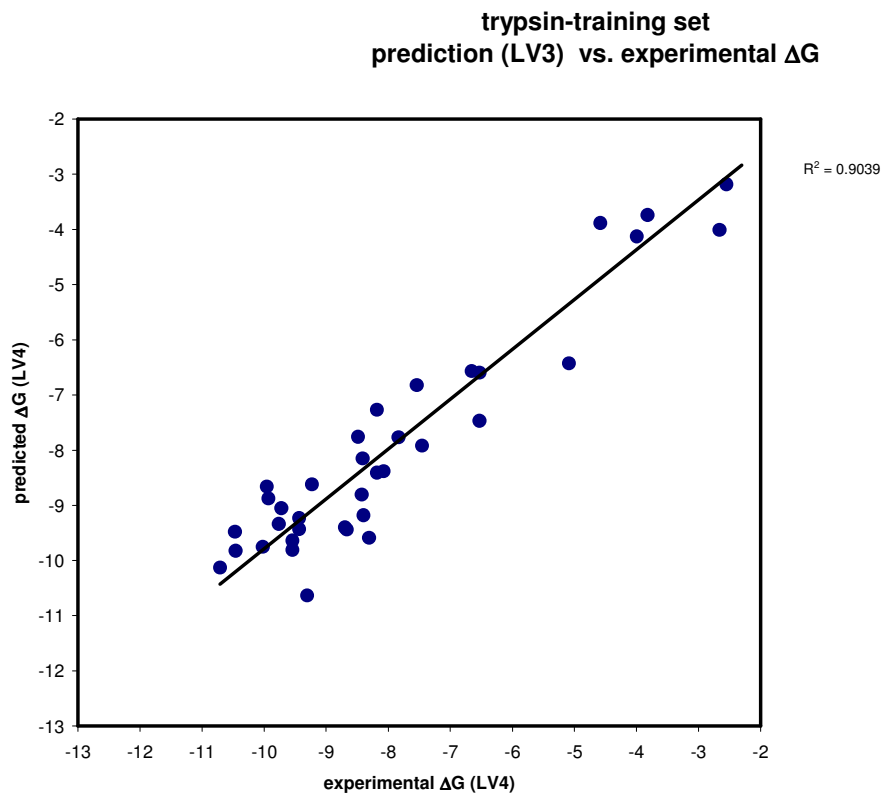


Figure 2: b) Predicted versus experimental binding free energy ΔG in kcal/mol. For the COMBINE models of urokinase and thrombin latent variable 4 were chosen before (blue dots) and after variable selection (red dots). For trypsin the best model could be reached at latent variable 3 without any variable selection. The R2 values based on the plots are given in the figures and in table 1.

b1) thrombin



b2) trypsin



b3) urokinase

