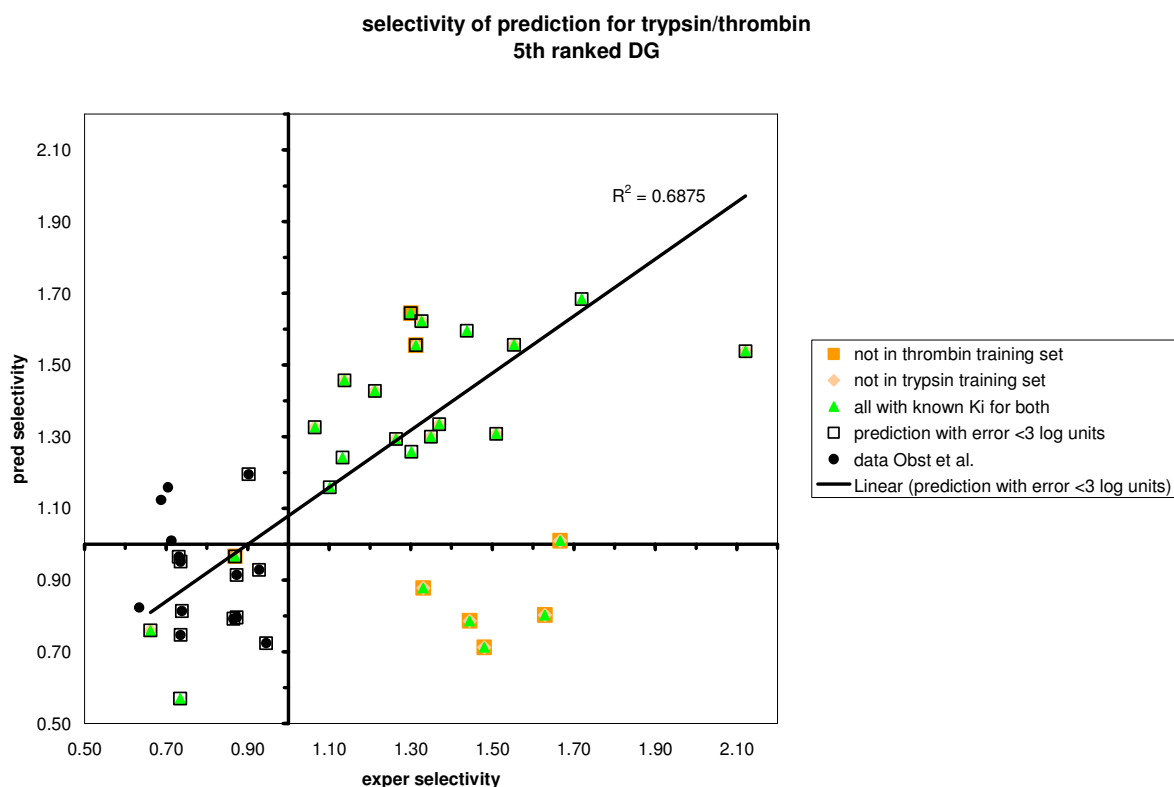


Selectivity between trypsin and thrombin



The 5th ranked predicted ΔG value of the docking solution for trypsin was divided by the 5th ranked predicted ΔG value of the docking solution for thrombin, which gives the predicted selectivity. The predicted selectivity was plotted against the experimental selectivity (experimental ΔG of trypsin/ experimental ΔG of thrombin). The inhibitors of the Klebe data set were not used. The five points in the lower right part were not used for calculating the R^2 , because the absolute difference between the experimental and predicted ΔG values for thrombin were greater than 3 log units. Although the prediction for the Klebe data set was quite good, the experimental ΔG values were within the noise of the prediction. No prediction for selectivity could be given.

selectivity of prediction for $K_i(\text{trypsin})/K_i(\text{thrombin})$
of 5th ranked ΔG

