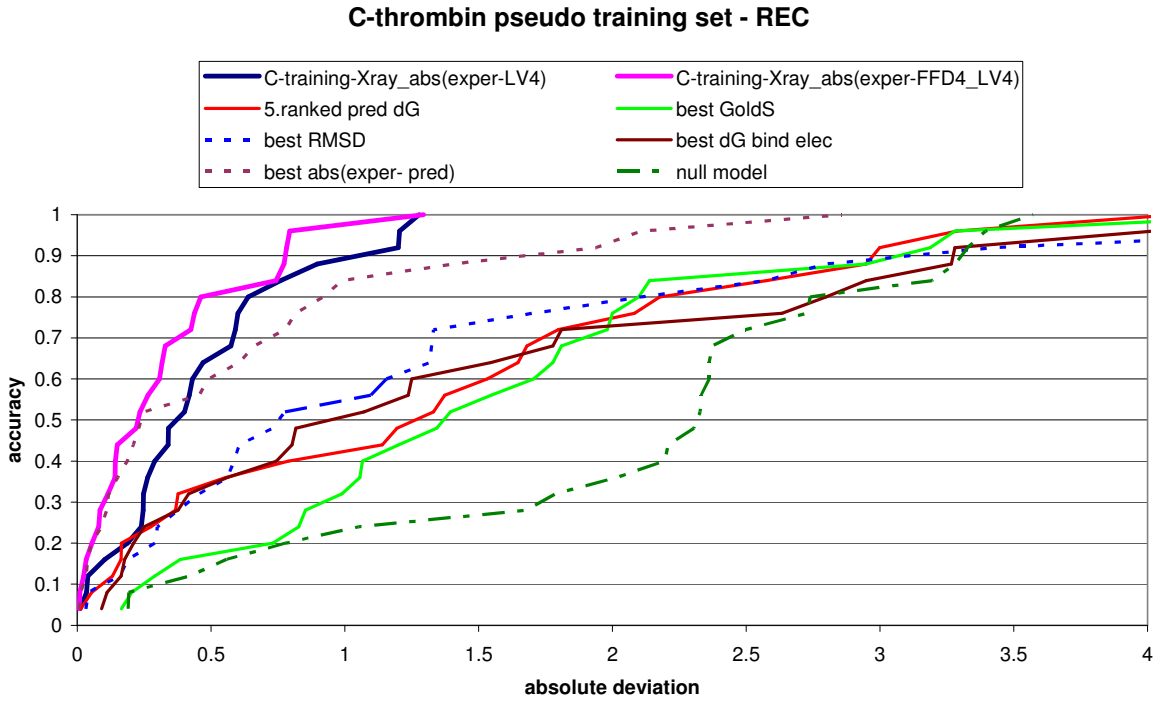
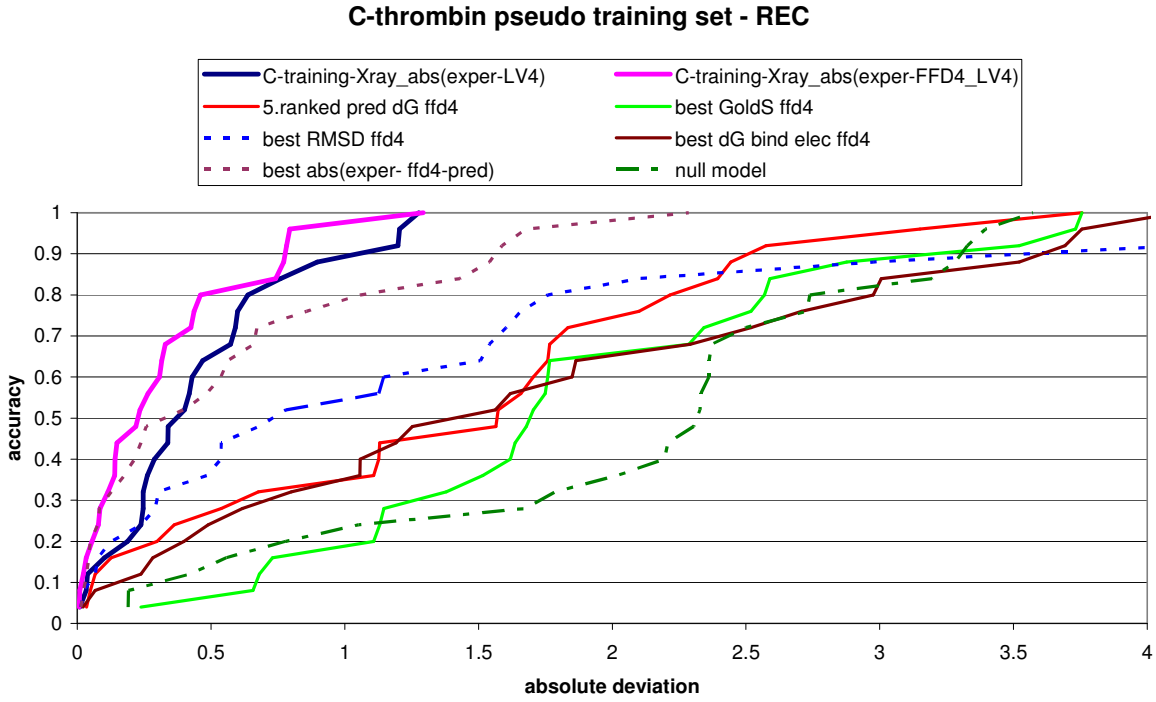
Figure 3: In the Regression Error Characteristic (REC) curves the cumulative proportion were plotted versus the error tolerance of the absolute difference between the experimental and predicted ΔG values. Ligands of the 'pseudo' test set were docked ten times in the corresponding receptor models of thrombin, trypsin and urokinase. For each docking solution a ΔG value were predicted and were ranked according to RMSD, GoldS, $\Delta\Delta G_{exper\text{-}pred}$, (best abs(exper-pred)), $\Delta\Delta G_{desolv}$ (best dG bind elec) and ΔG_{pred} (for more details see results).
a) The different curves shows the cumulative distribution of best RMSD (dotted blue line), GoldS (green line), $\Delta\Delta G_{exper\text{-}pred}$ (dotted dark red), $\Delta\Delta G_{desolv}$ (brown) ranked and the 5th ranked (red) ΔG values against the error of prediction in kcal/mol. In addition, curves based predicted ΔG values of ligand conformations taken from X-ray structures before (blue) and after (purple) variable selection are given.
b) The same ranking was used to plot the cumulative proportion versus the RMSD (in Å) of the docking solutions.

/report/COMBINE-paper/final-row/thrombin-all_040706-add.xls

a1) Thrombin: without variable selection

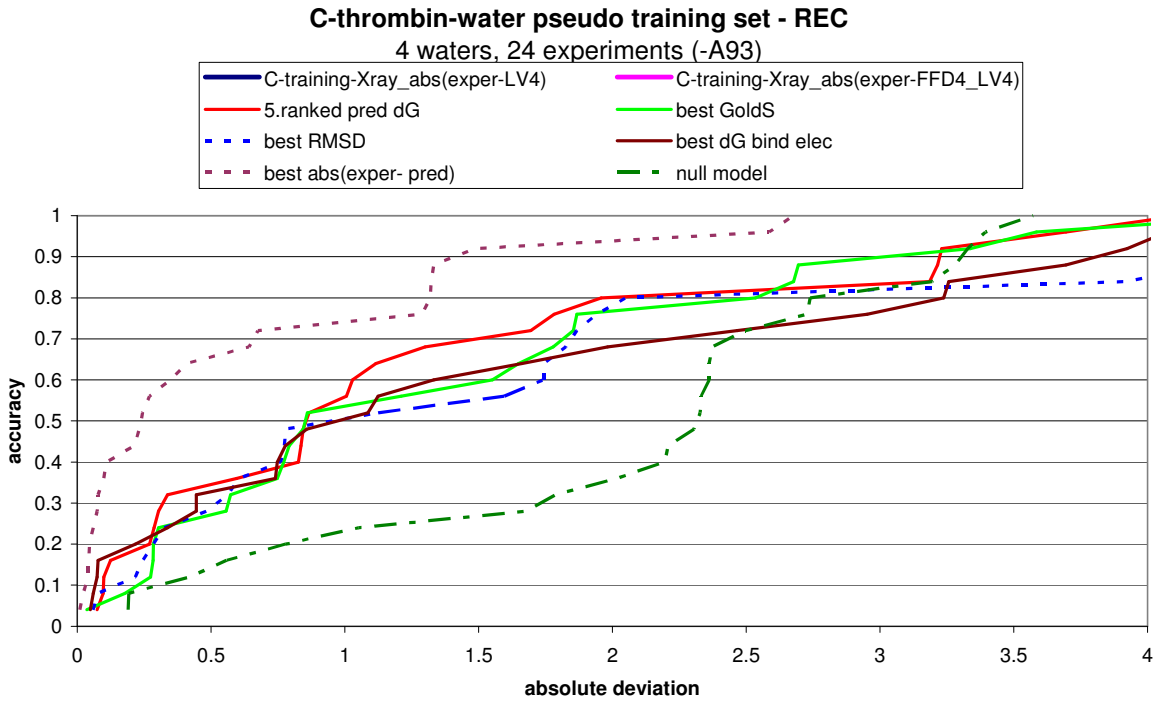


a1) Thrombin: with variable selection

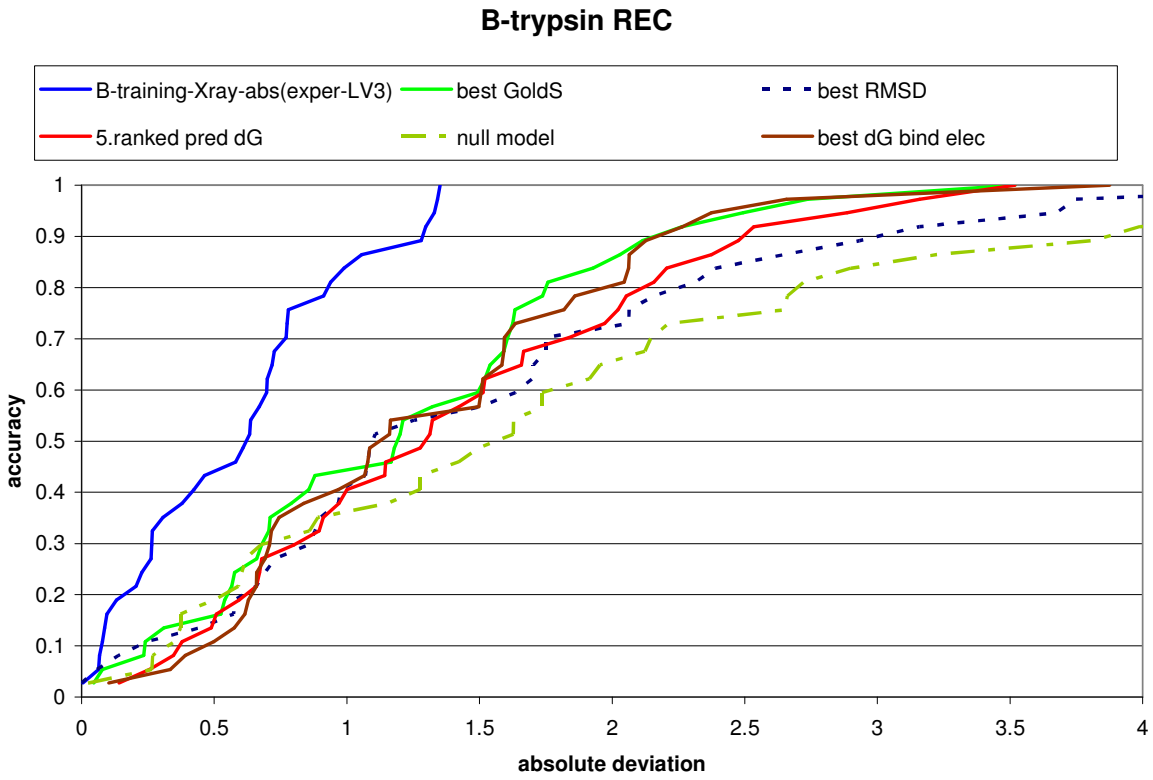


a1) Thrombin: with 4 water molecules and without variable selection

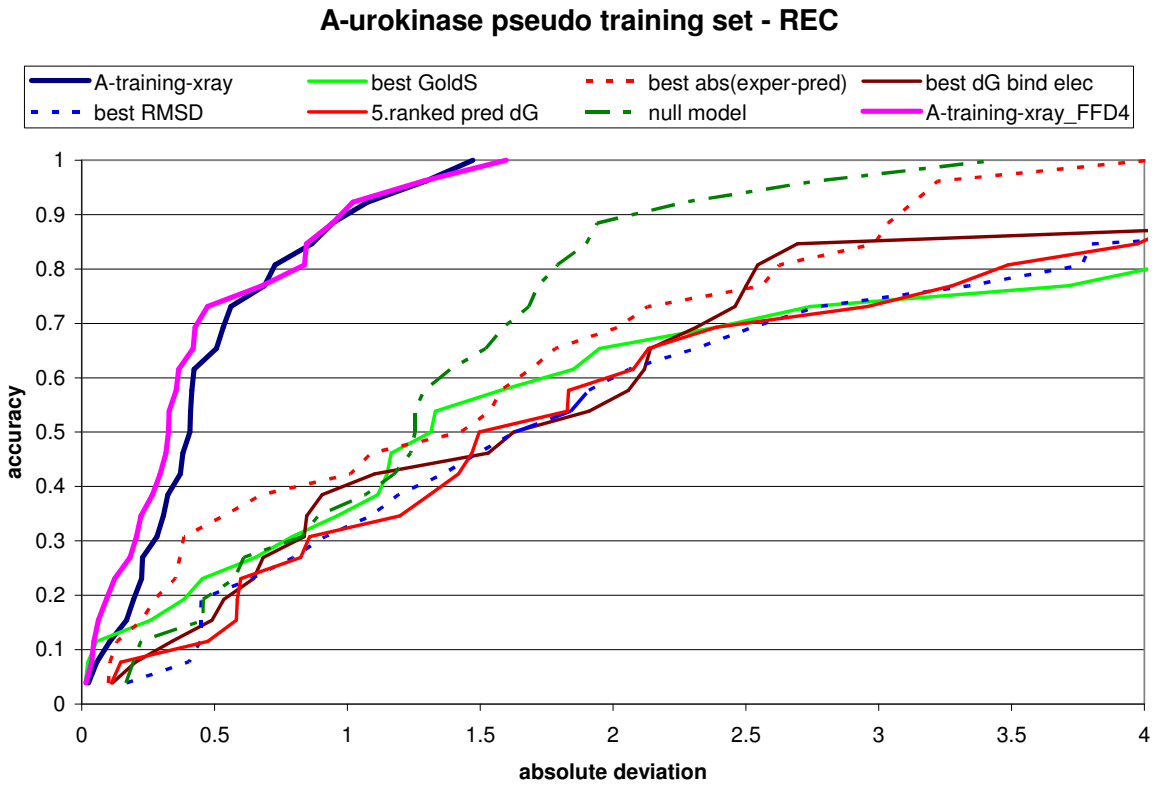
This model based just on 24 experiments, because there were some mistakes with ligand A93 in minimization of the xray structure and the interaction energy calculation!



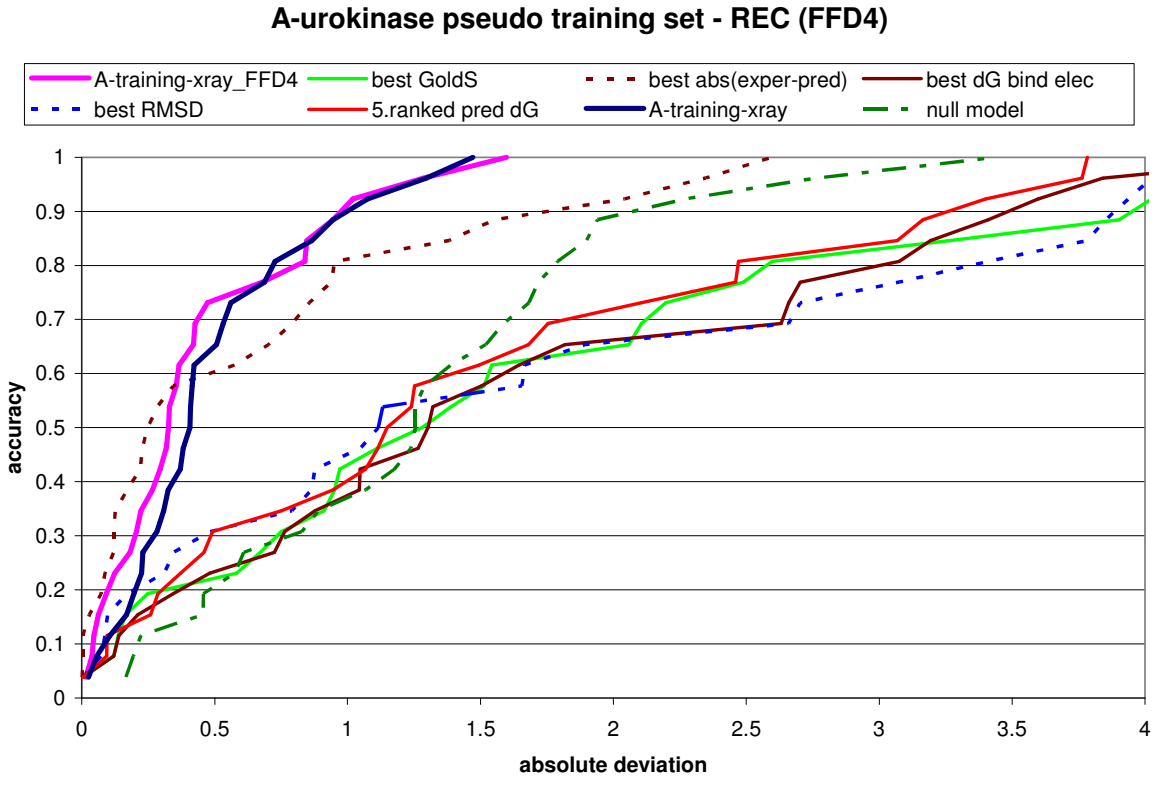
a2) Trypsin: without variable selection



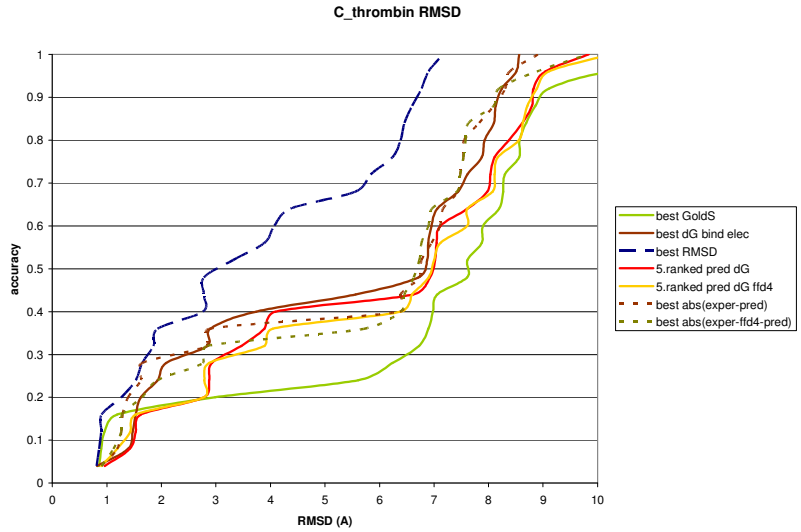
a3) Urokinase: without variable selection



a3) Urokinase: with variable selection (FFD4)

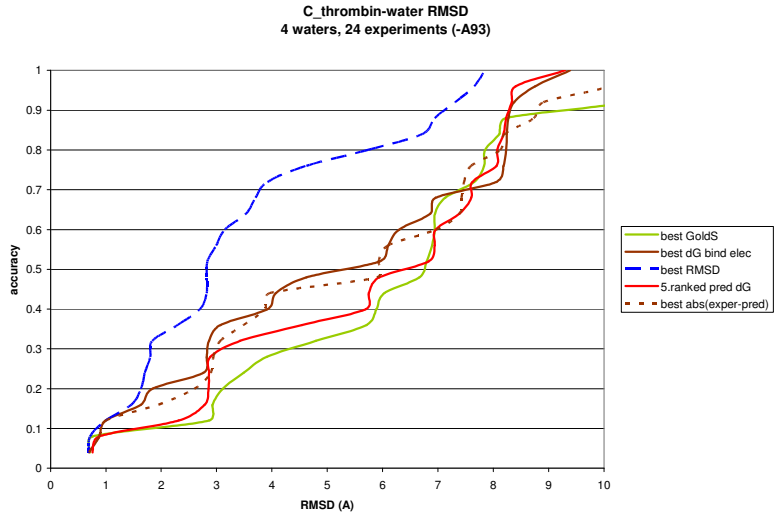


b1) Thrombin: RMSD

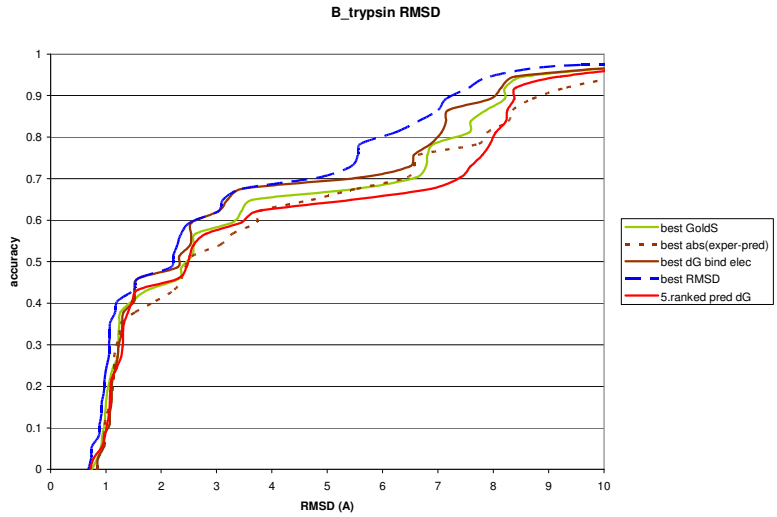


b1) Thrombin: with 4 water molecules, RMSD

<u>This model based just on 24 experiments, because there were some mistakes with ligand A93 in minimization of the xray structure and the interaction energy calculation!</u>



b2) Trypsin: RMSD



b3) Urokinase: RMSD