

Improving Quantitative Structure-Activity Relationships through Multi-Objective Optimization

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External predictions based on trade-off models derived through MOO. Thrombin test set.

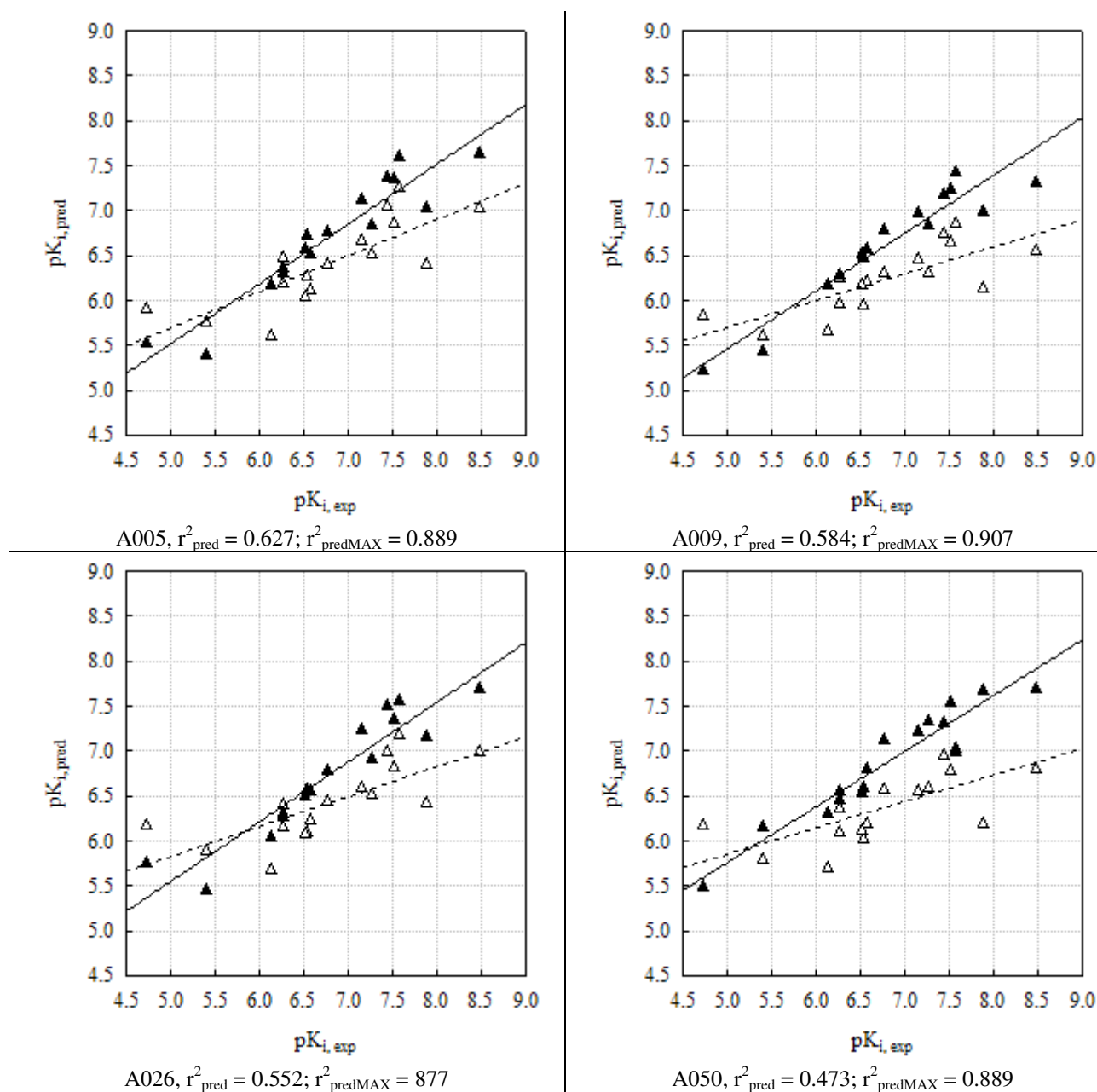


Figure 1. Thrombin test set compounds predicted on the basis of four different trade-off models derived through MOO. Empty triangles represent projections obtained through consensus by mean over the entire family of docking solutions while solid triangles indicated the docking pose retrospectively identified as the one having the smallest residual. The values of r^2_{pred} and r^2_{predMAX} indicated the predictive squared correlation coefficient for empty and solid series, respectively.

External predictions based on trade-off models derived through MOO. Trypsin test set.

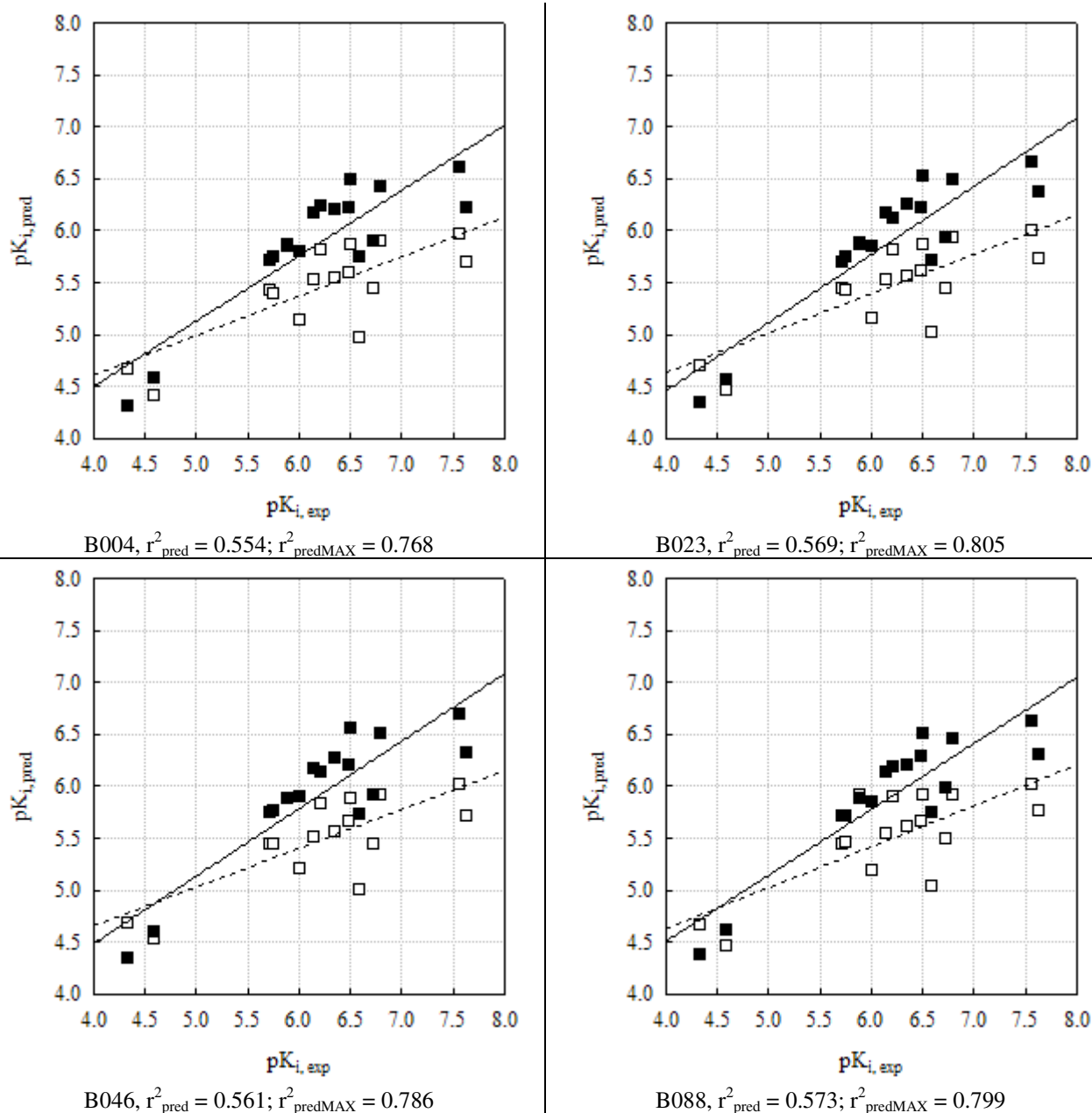


Figure 2. Trypsin test set compounds predicted on the basis of four different trade-off models derived through MOO. Empty squares represent projections obtained through consensus by mean over the entire family of docking solutions while solid squares indicated the docking pose retrospectively identified as the one having the smallest residual. The values of r^2_{pred} and $r^2_{predMAX}$ indicated the predictive squared correlation coefficient for empty and solid series, respectively.