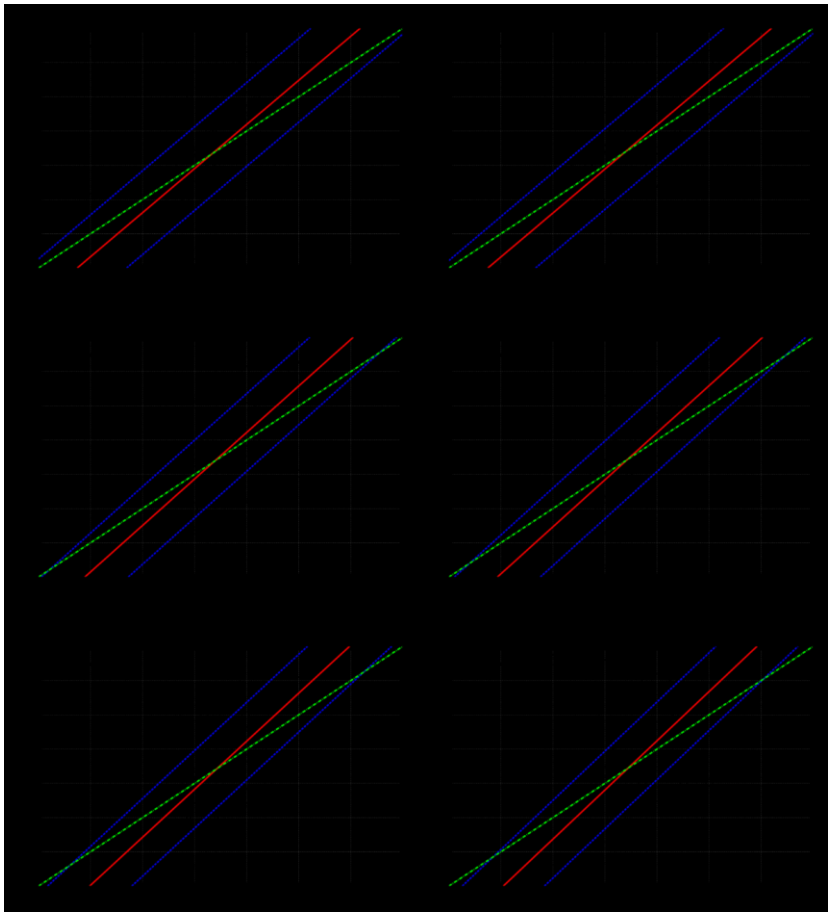

Table 9. Performances of the nonlinear scoring functions trained with machine learning techniques on the test sets. For the general scoring functions the test set is the curated v2013 core set, while the target-class scoring functions were validated on their respective independent test sets. R is the Pearson correlation coefficient on training (R training), 10-fold cross-validation (R cross), independent test set (R test) and RMSE is the root mean squared error (in kcal/mol).

	Scoring functions	**R training**	**R cross**	**R test**	**RMSE**
LWL	General::random	0.7964	0.6358	0.6159	2.4263
	General::all	0.7739	0.6308	0.6375	2.3940
	Proteases				

	Kinases_oneSolv				
	iPPIs_oneSolv				
KStar	General::random	0.9490	0.6418		
	General::all	0.9518	0.6475		
	Proteases				
	Kinases_oneSolv				
	iPPIs_oneSolv				
SMOReg	General::random	0.9998	0.6526		
	General::all	1.0000	0.6472		
	Proteases				
	Kinases_oneSolv				
	iPPIs_oneSolv				
RF	General::random	0.9750	0.6551		
	General::all	0.9739	0.6565		
	Proteases				
	Kinases_oneSolv				
	iPPIs_oneSolv				

Redocking with DockThor

The large-scale study of redocking performed on DockThor program provides a large amount of complexes with successfully predicted binding mode for the respective native ligand. We evaluated the docking performance using several criterions for RMSD values as previously suggested in the literature (JAIN; NICHOLLS, 2008), considering the best solution, top-2, top-3 and top-10 poses, and the solution with the lowest RMSD value (Figure 8, **Erro! Fonte de referência não encontrada.**). Using a strict but broadly applied criterion of 2.0 Angstroms between the predicted pose and the experimentally observed conformation of the native ligand, DockThor was succeeded on 1.835 complexes, which corresponds to almost 67% of the entire dataset when considering the top-energy solution. DockThor finds at least one binding mode near the experimental one using the