Supplemental Information:

Lessons Learned in Empirical Scoring with `smina` from the CSAR 2011 Benchmarking Exercise

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Figures

Figures 1-40 are scatter plots of the error in predicted binding affinity (predicted - actual) vs RMSD to the crystal pose. See the legend in Figure 6 in the main text for the key. They are sorted by target, then by crossdocking/redocking, then by docking method, followed by scoring method. Table 1 summarizes the average and standard deviation of the difference in predicted affinities of the crystal pose of the ligand in the reference and cocrystal receptors. Figures 41 and 42 show the same data as Figures 4 and 5 in the main text, but for docking with `--exhaustiveness=50`.

*To whom correspondence should be addressed

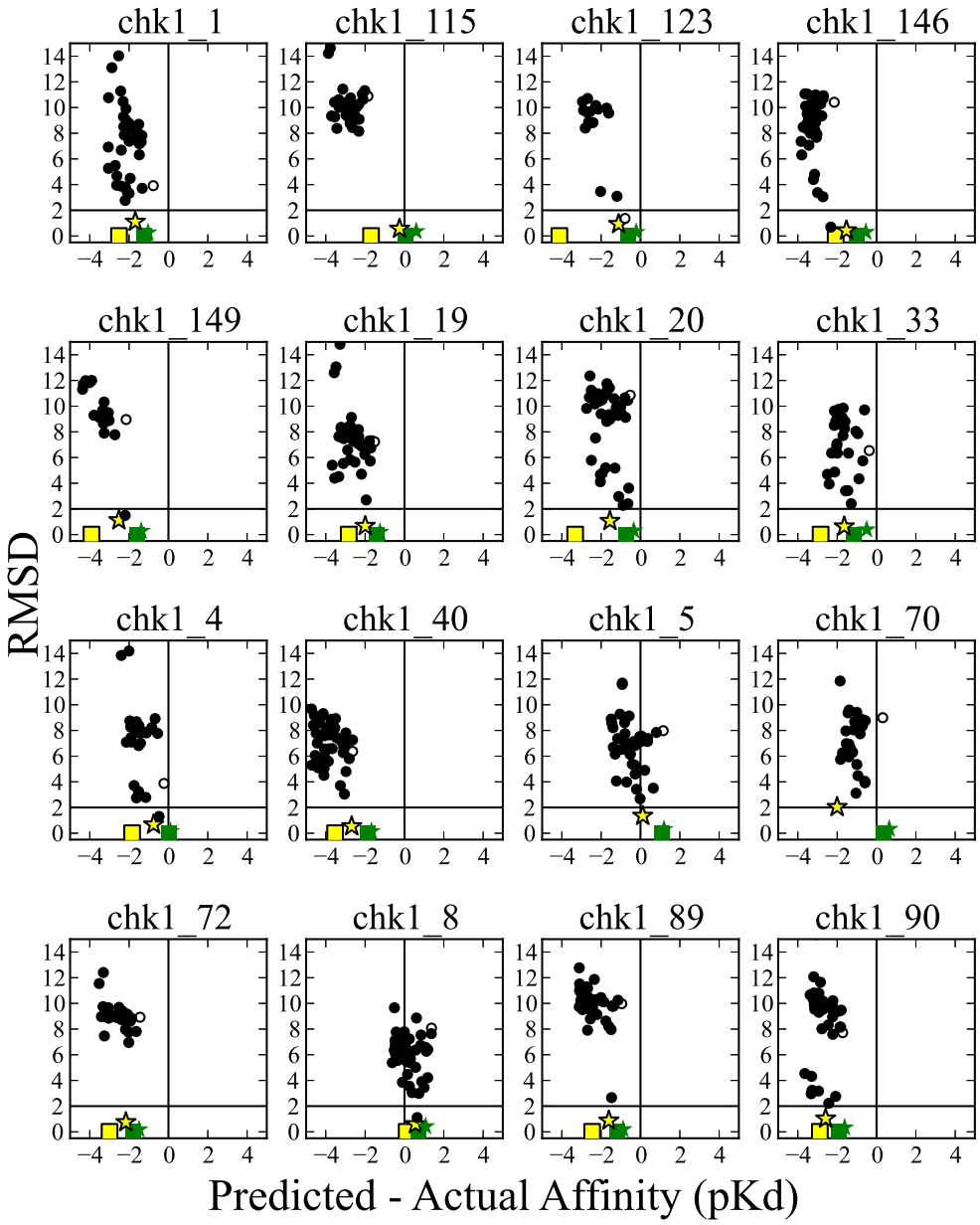


Figure 1: Chk1 Crossdocking Vina-Vina

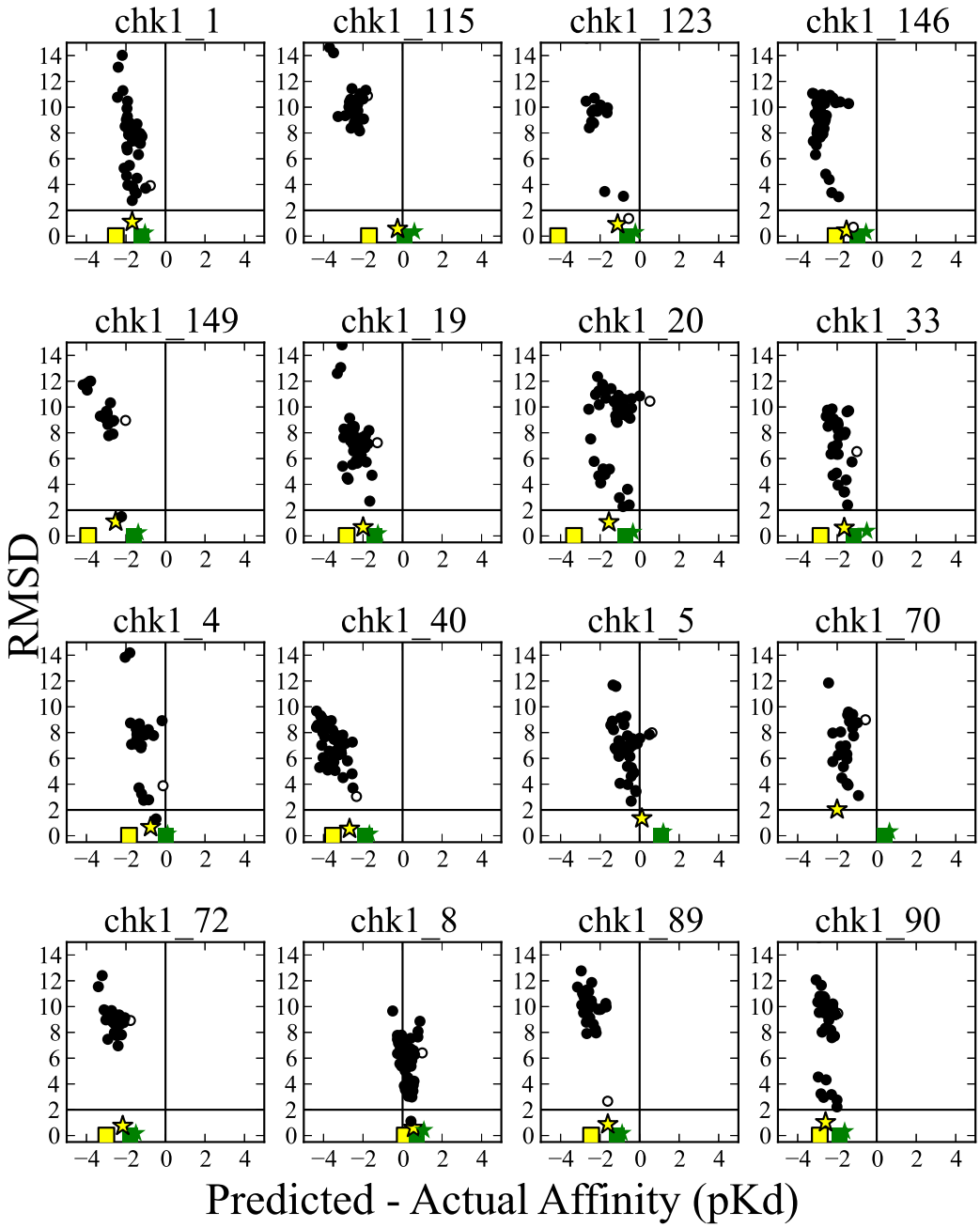


Figure 2: Chk1 Crossdocking Vina-Custom

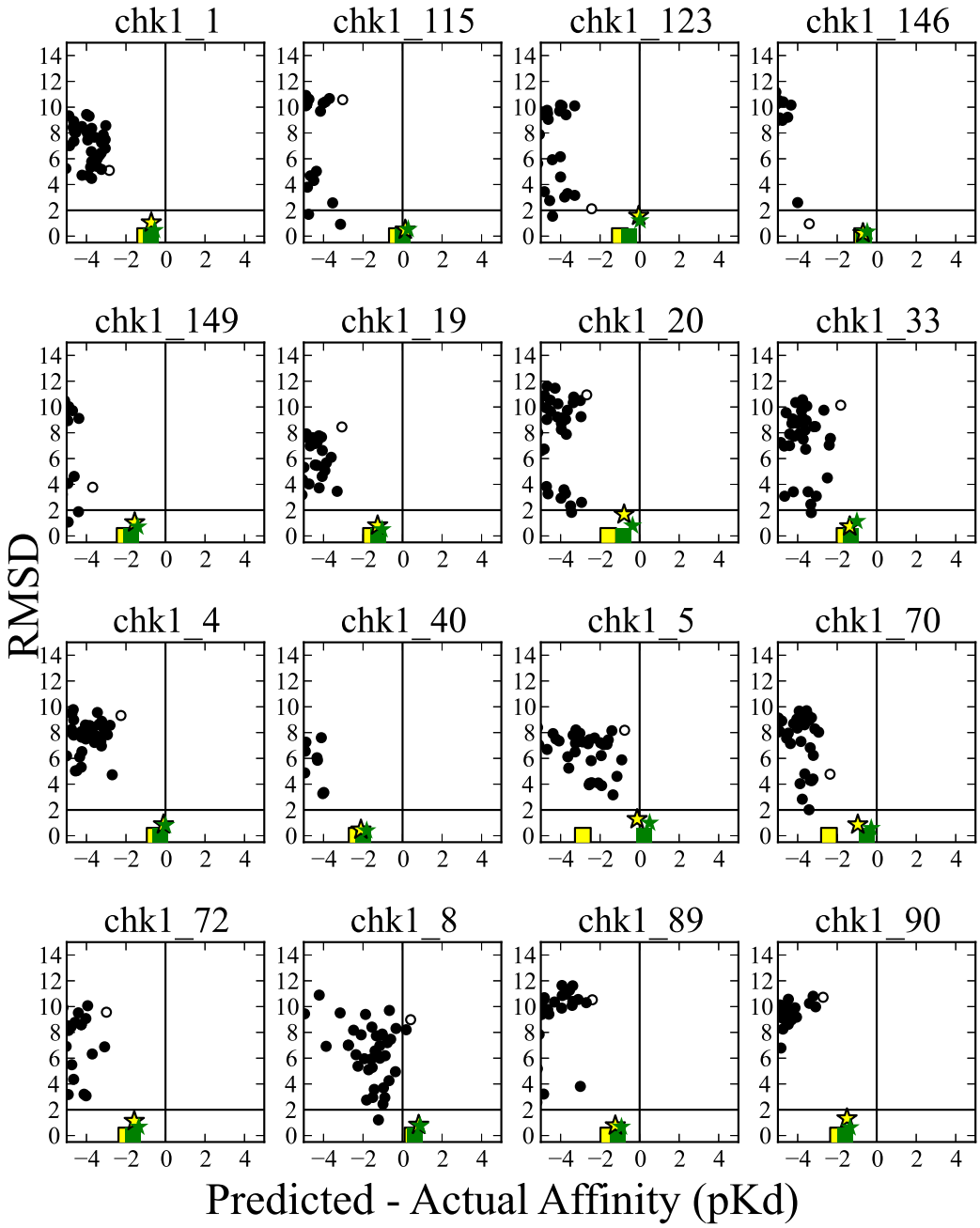


Figure 3: Chk1 Crossdocking Custom-Vina

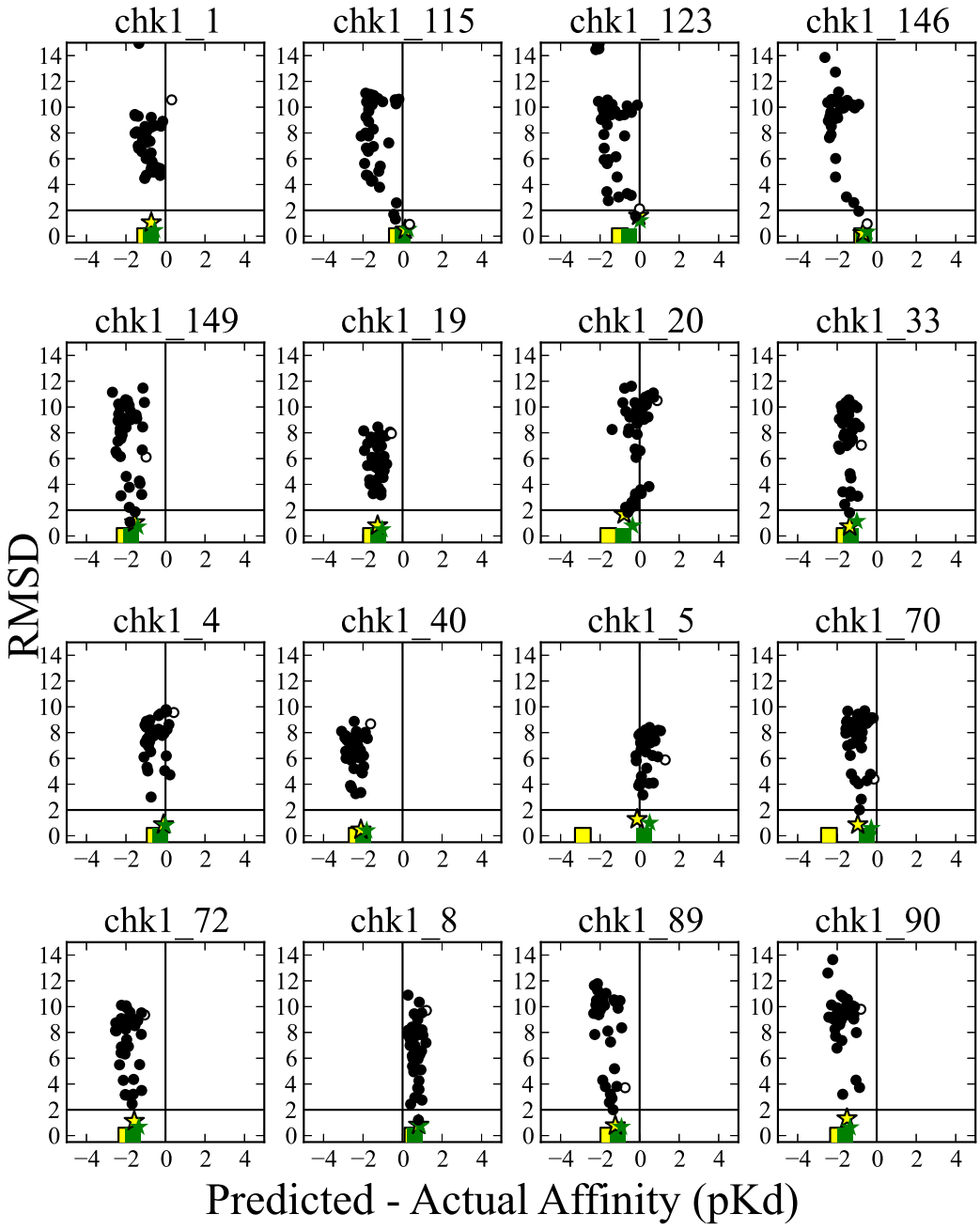


Figure 4: Chk1 Crossdocking Custom-Custom

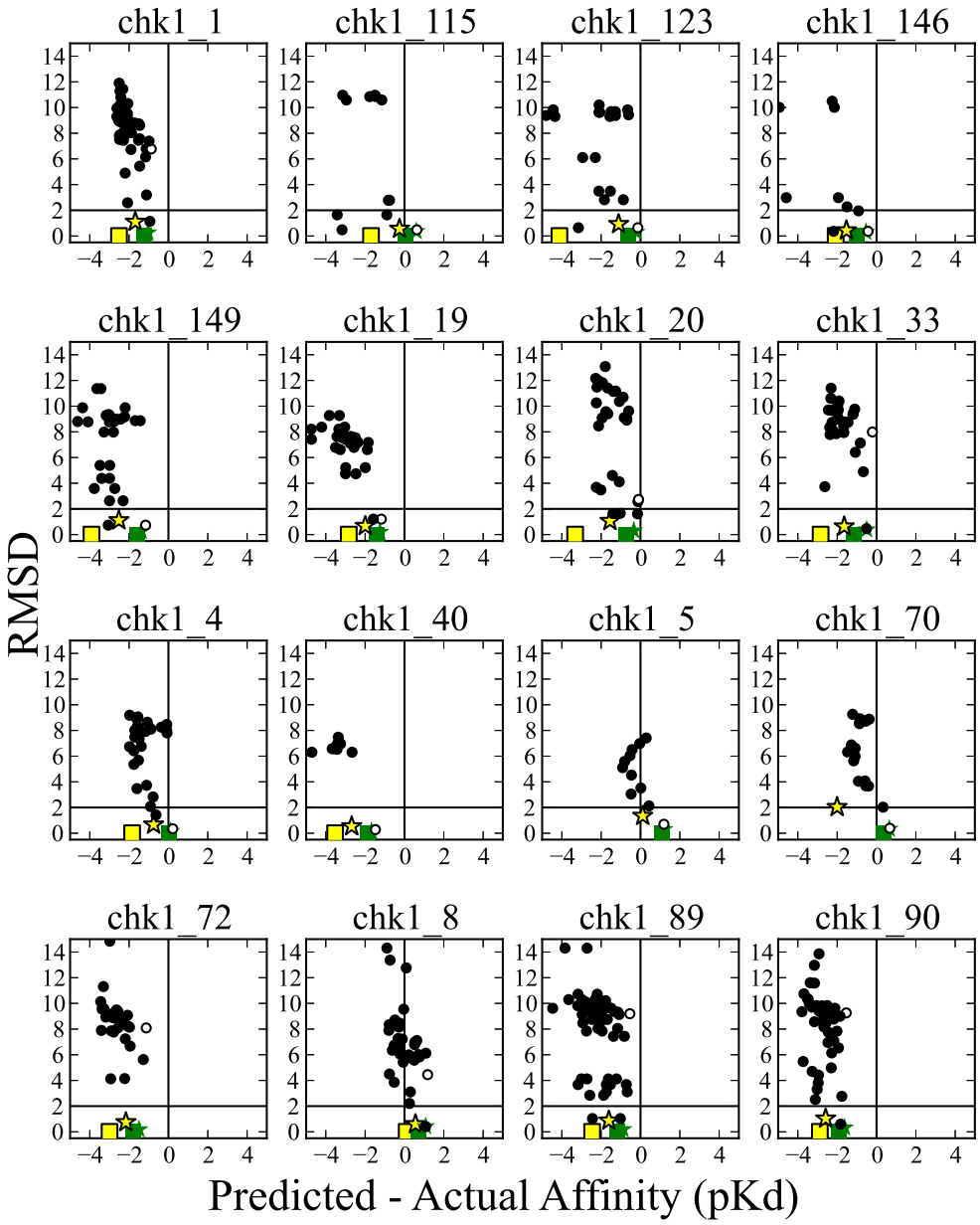


Figure 5: Chk1 Redock Vina-Vina

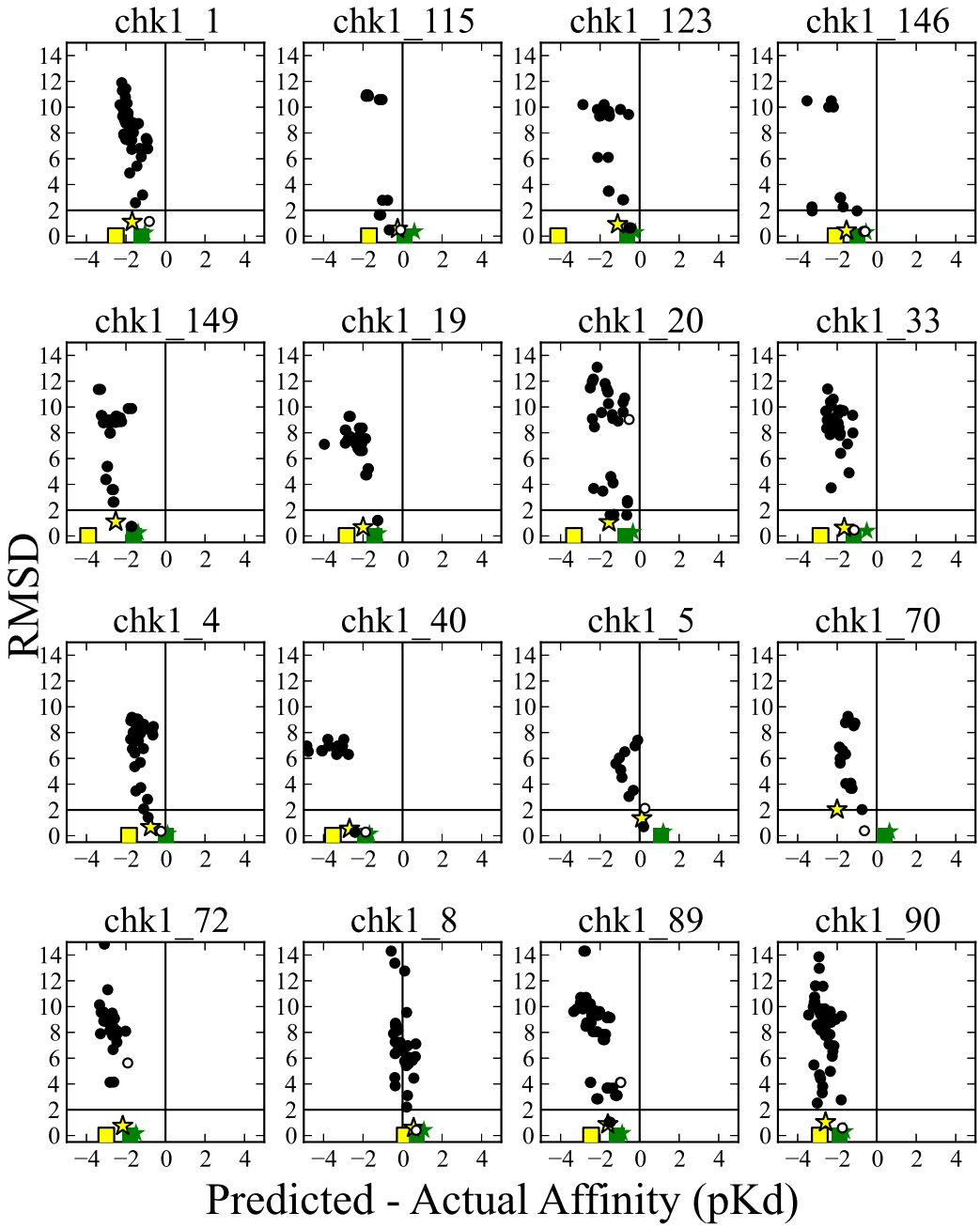


Figure 6: Chk1 Redock Vina-Custom

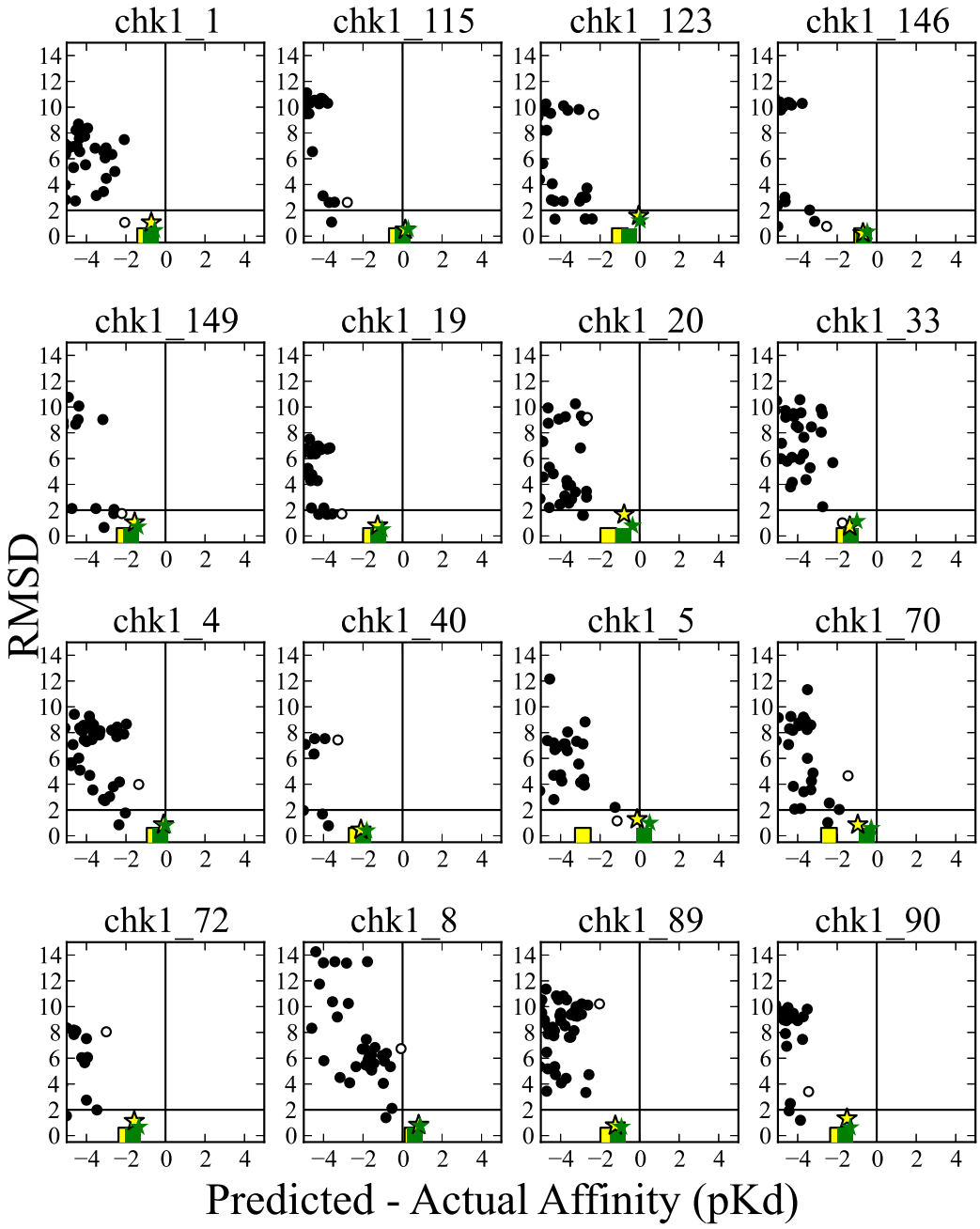


Figure 7: Chk1 Redock Custom-Vina

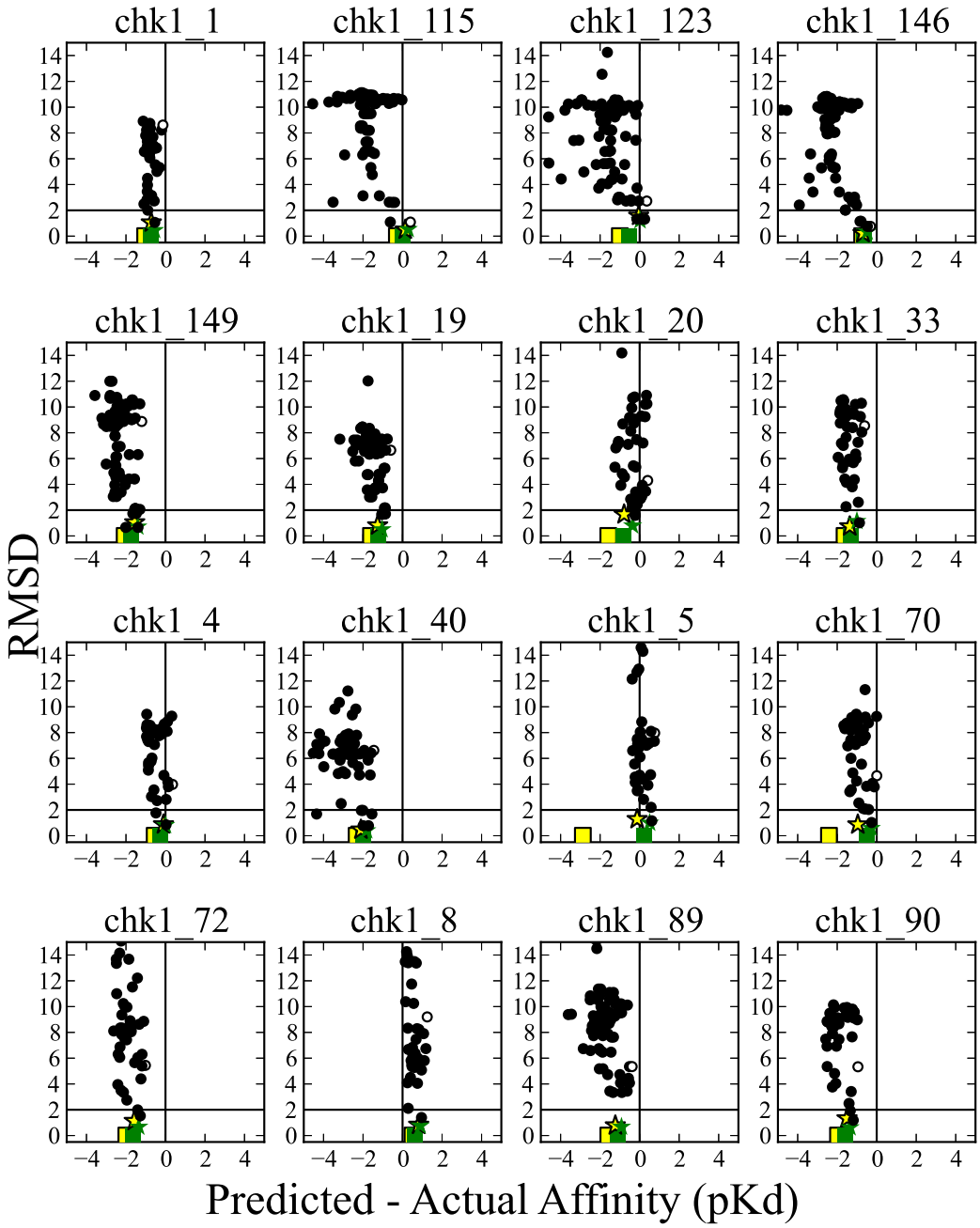


Figure 8: Chk1 Redock Custom-Custom

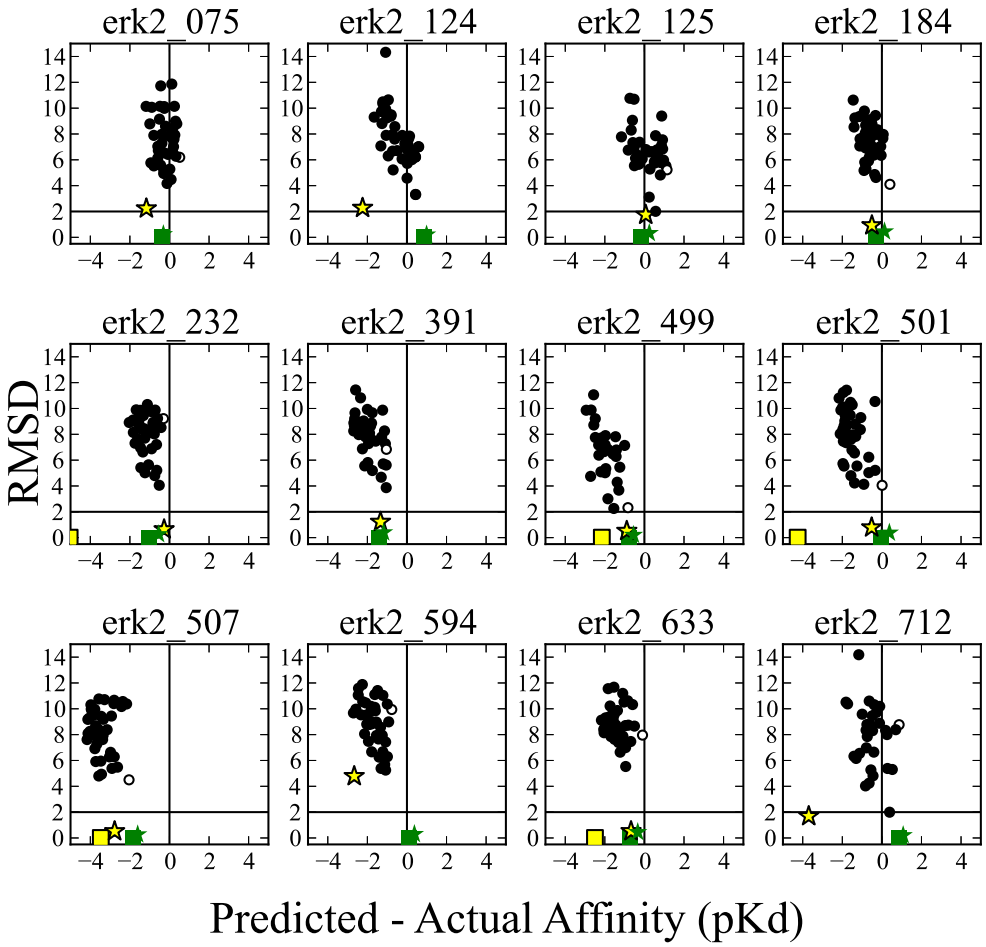


Figure 9: Erk2 Crossdocking Vina-Vina

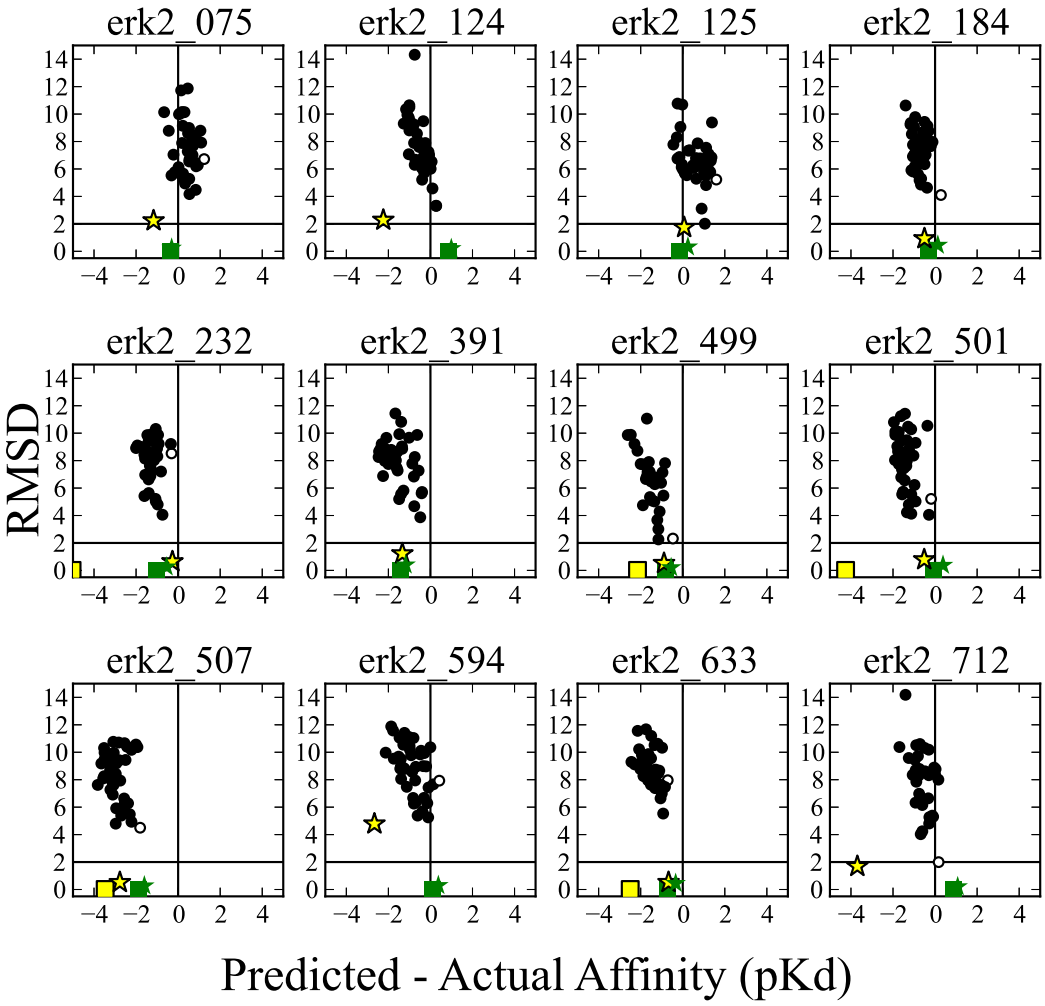


Figure 10: Erk2 Crossdocking Vina-Custom

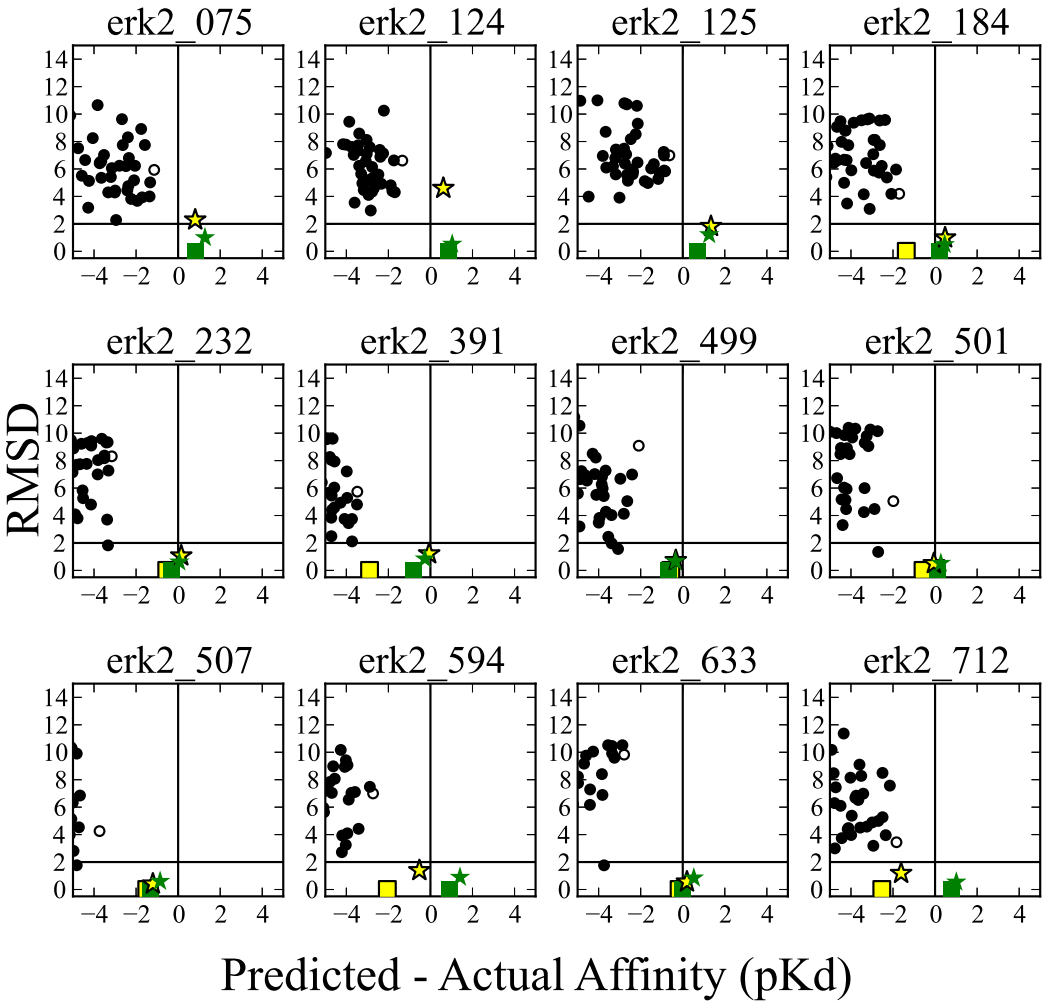


Figure 11: Erk2 Crossdocking Custom-Vina

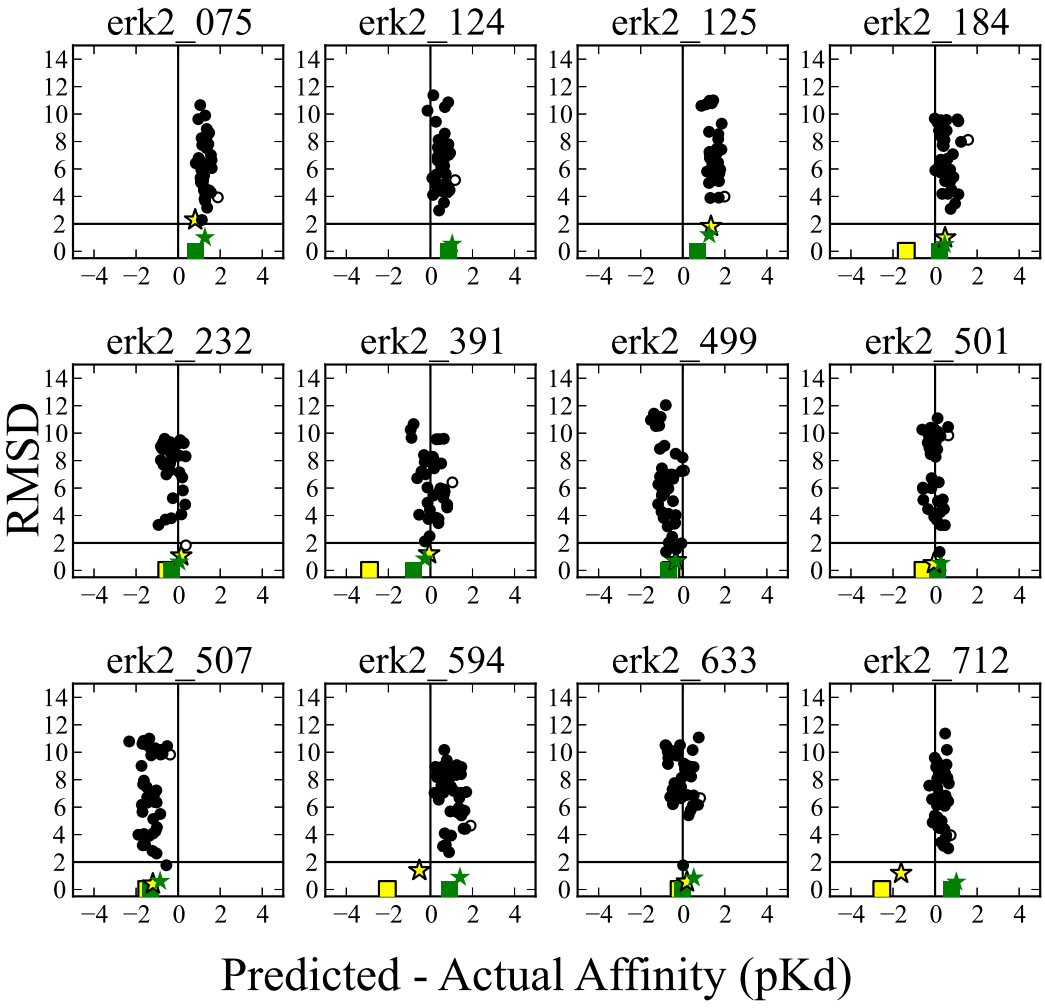


Figure 12: Erk2 Crossdocking Custom-Custom

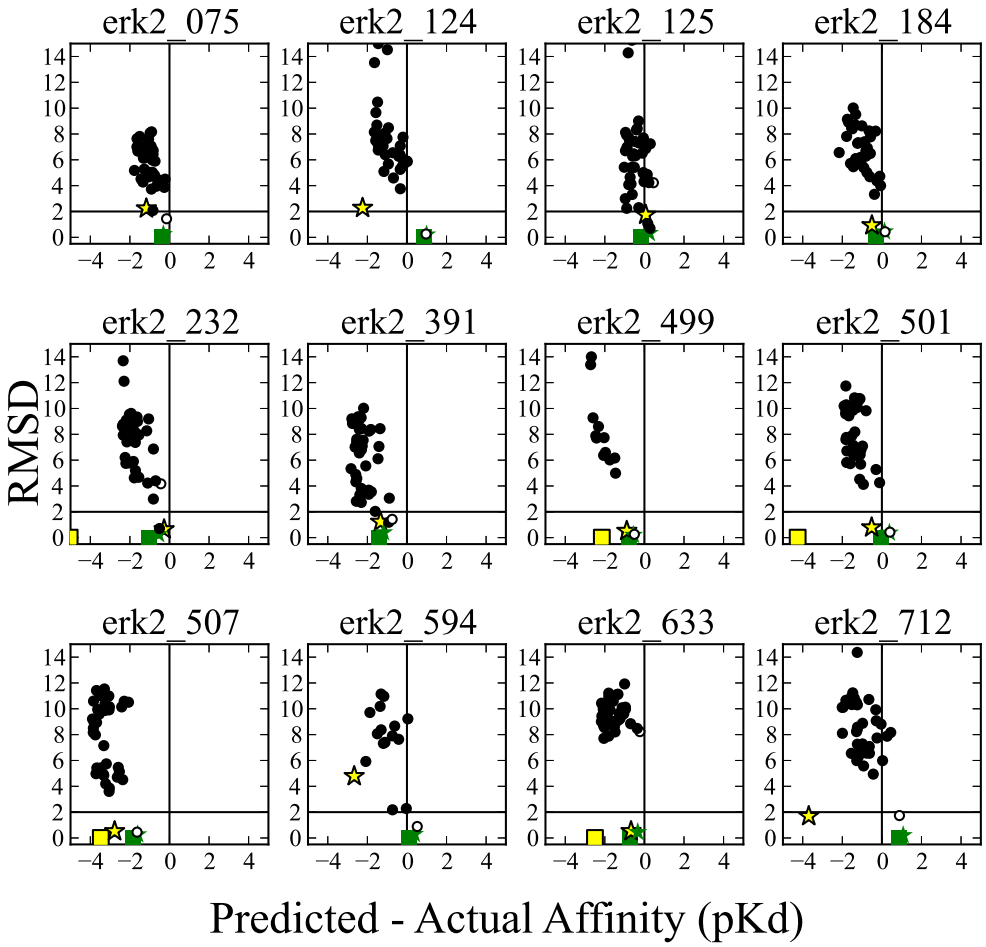


Figure 13: Erk2 Redock Vina-Vina

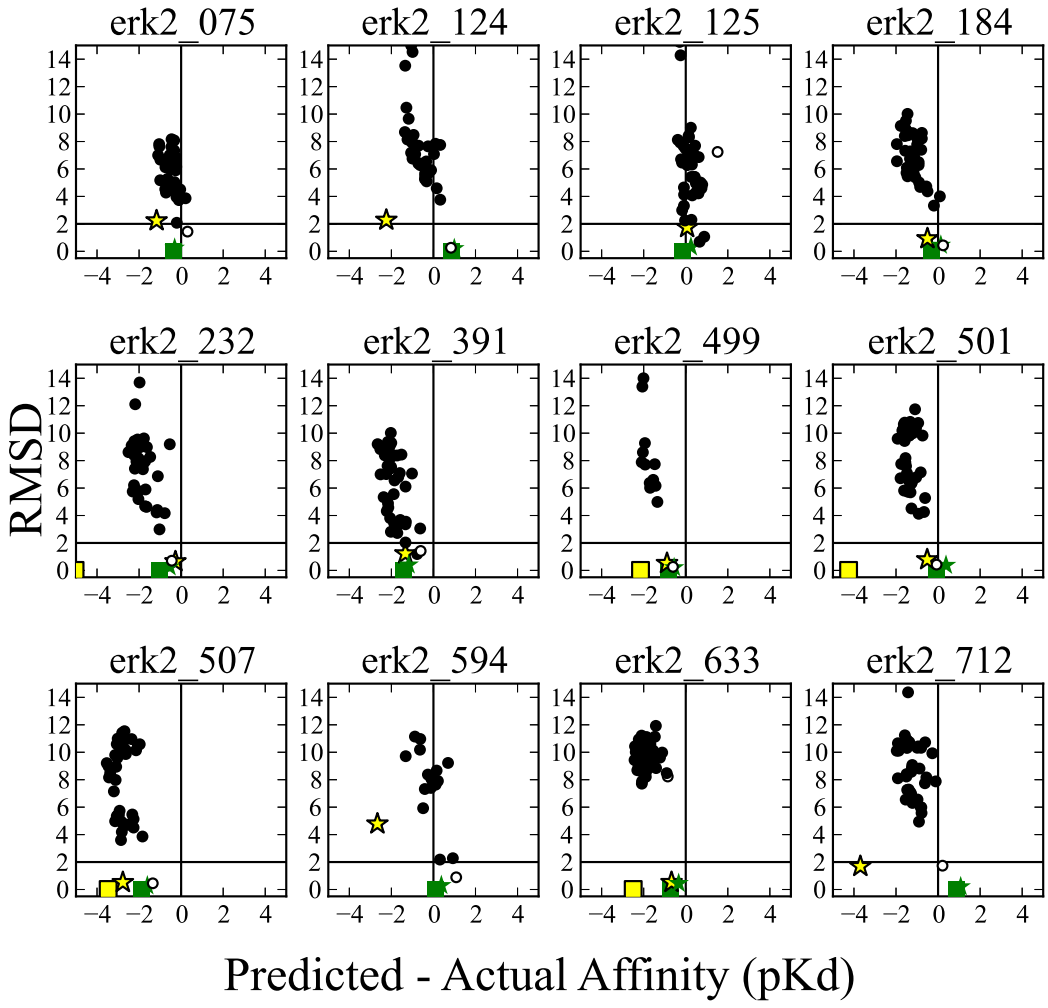


Figure 14: Erk2 Redock Vina-Custom

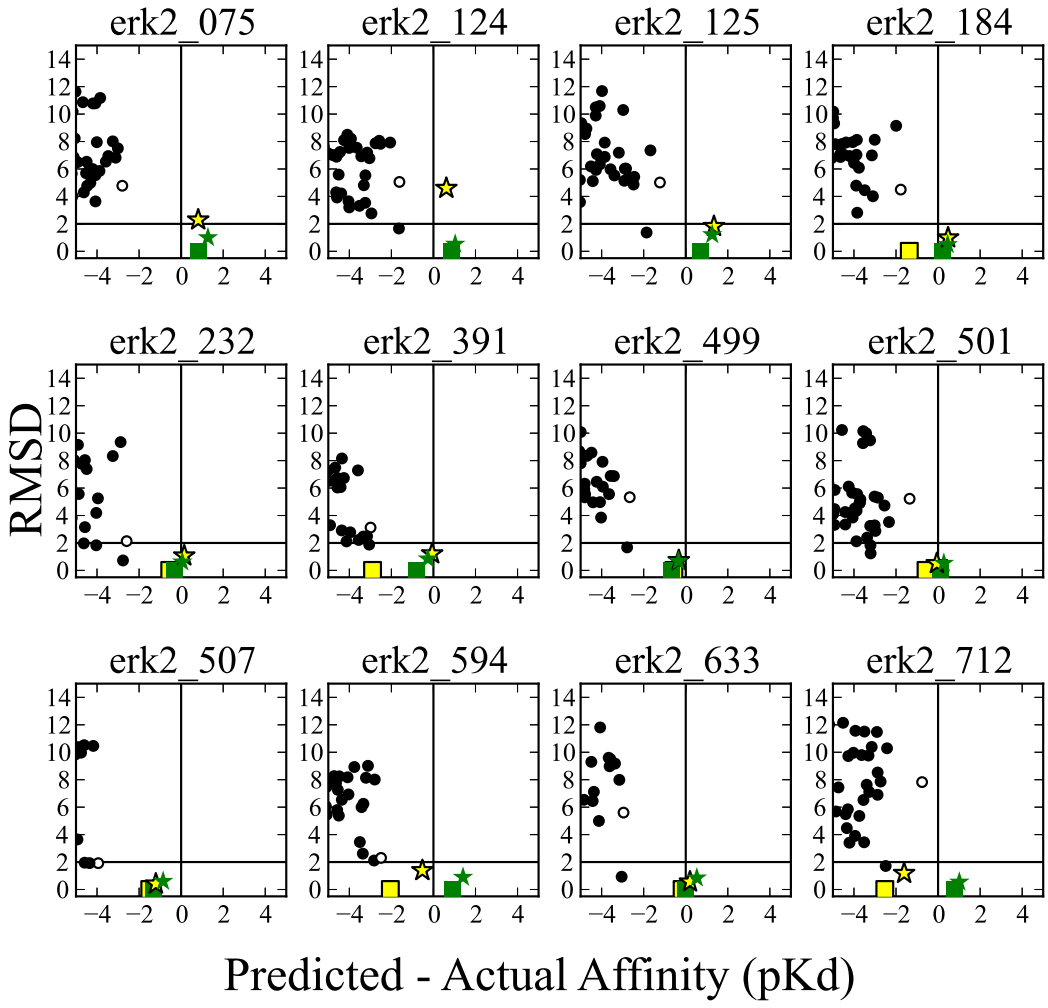


Figure 15: Erk2 Redock Custom-Vina

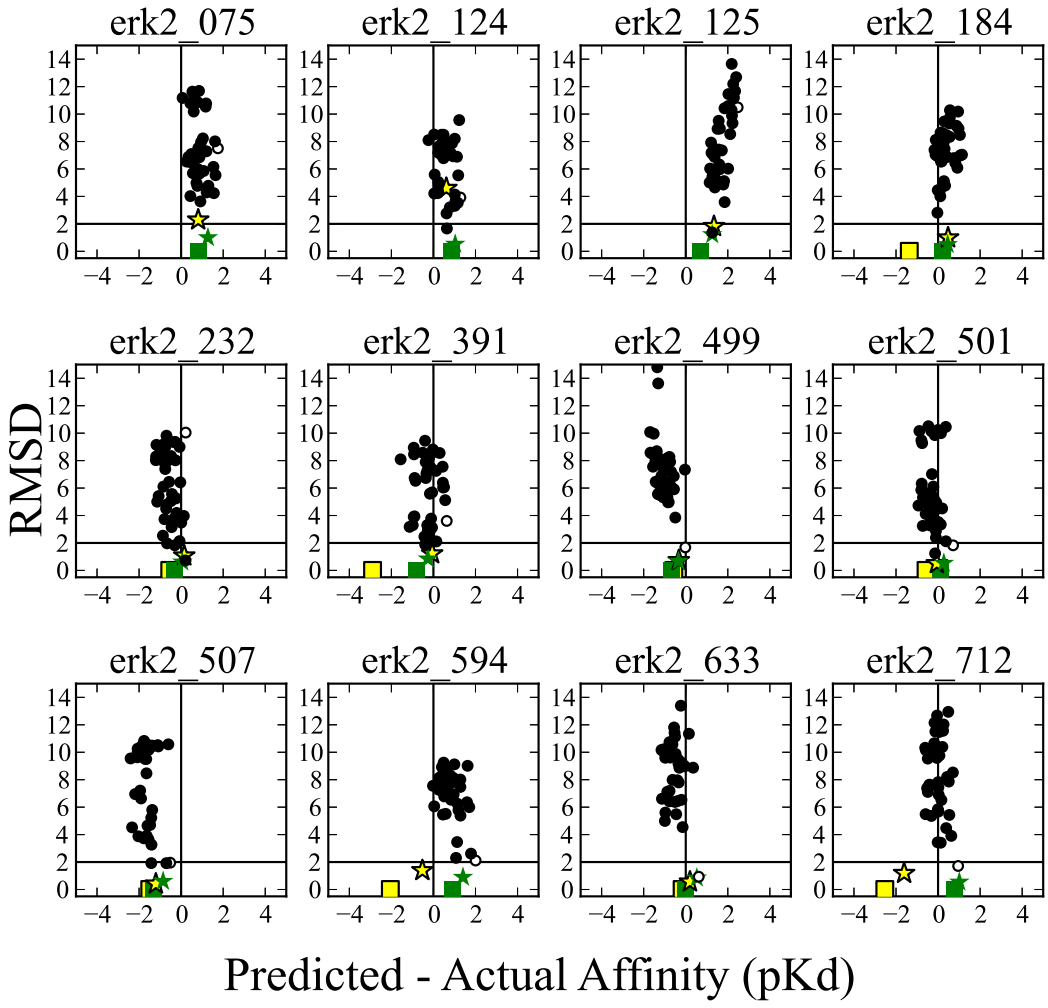


Figure 16: Erk2 Redock Custom-Custom

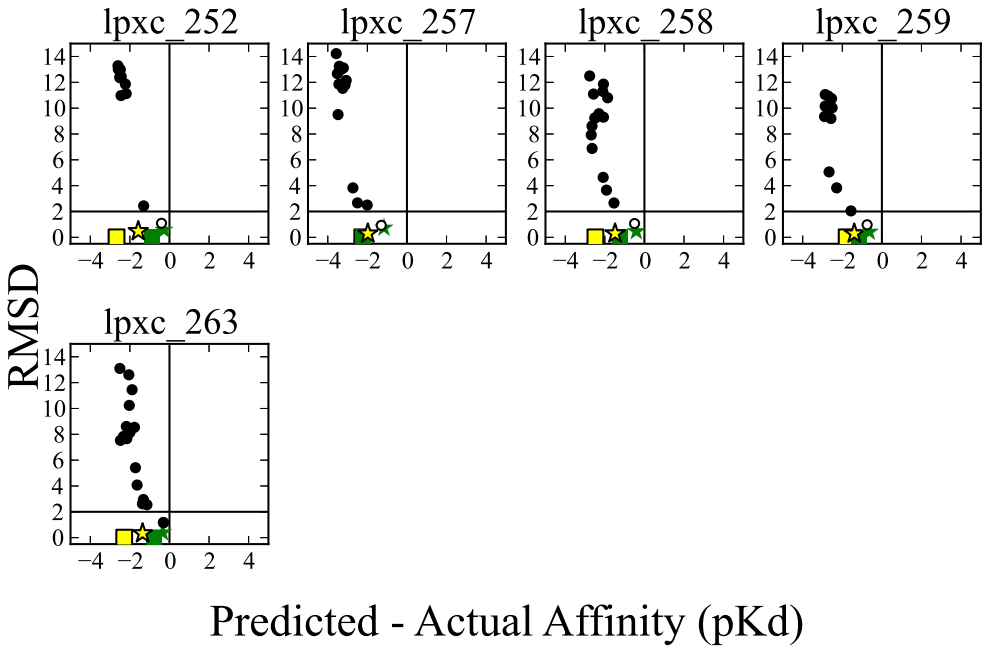


Figure 17: Lpxc Crossdocking Vina-Vina

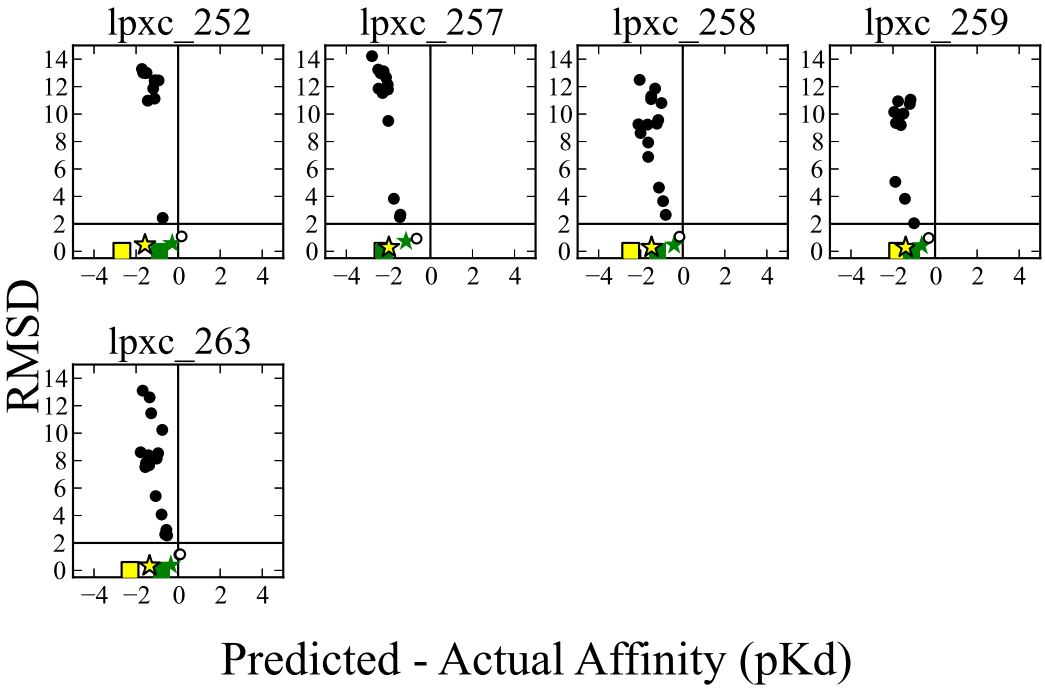


Figure 18: Lpxc Crossdocking Vina-Custom

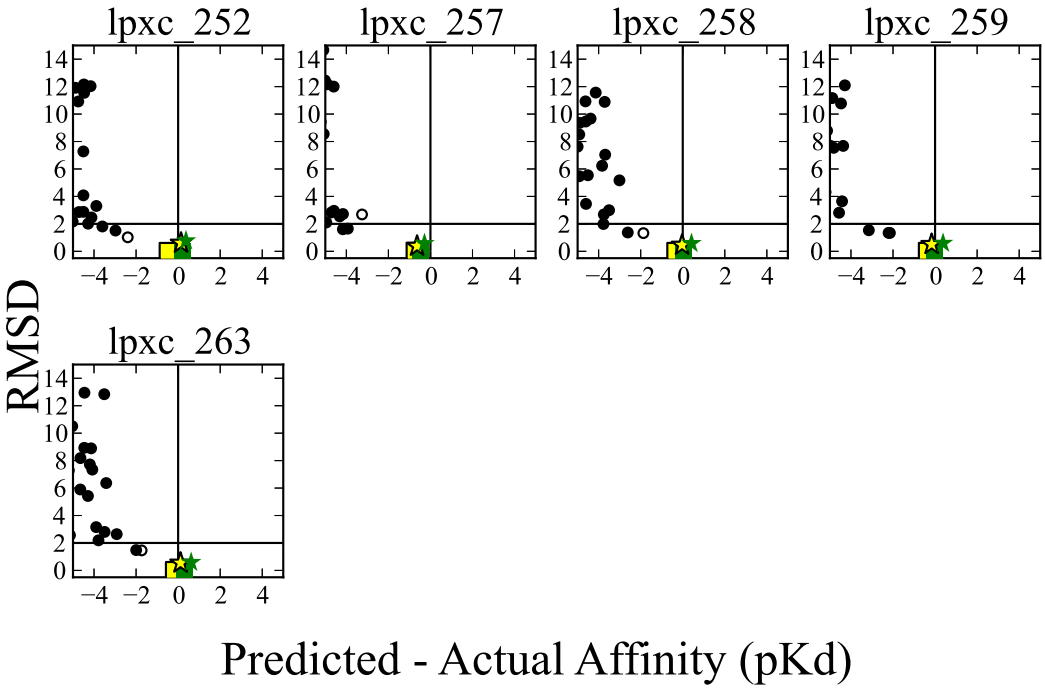


Figure 19: Lpxc Crossdocking Custom-Vina

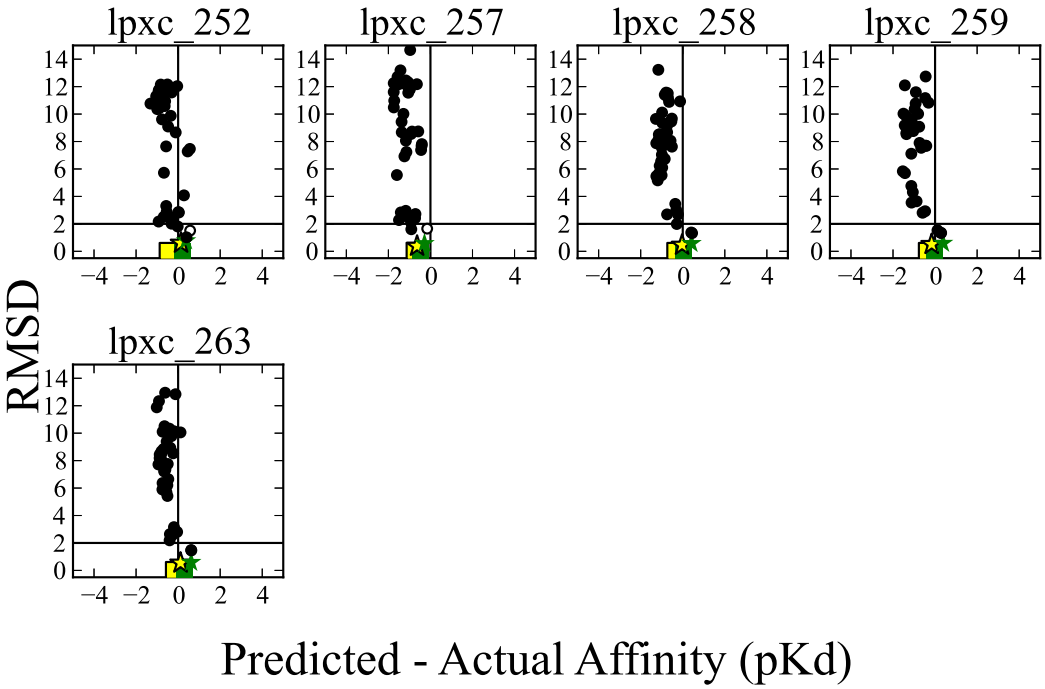
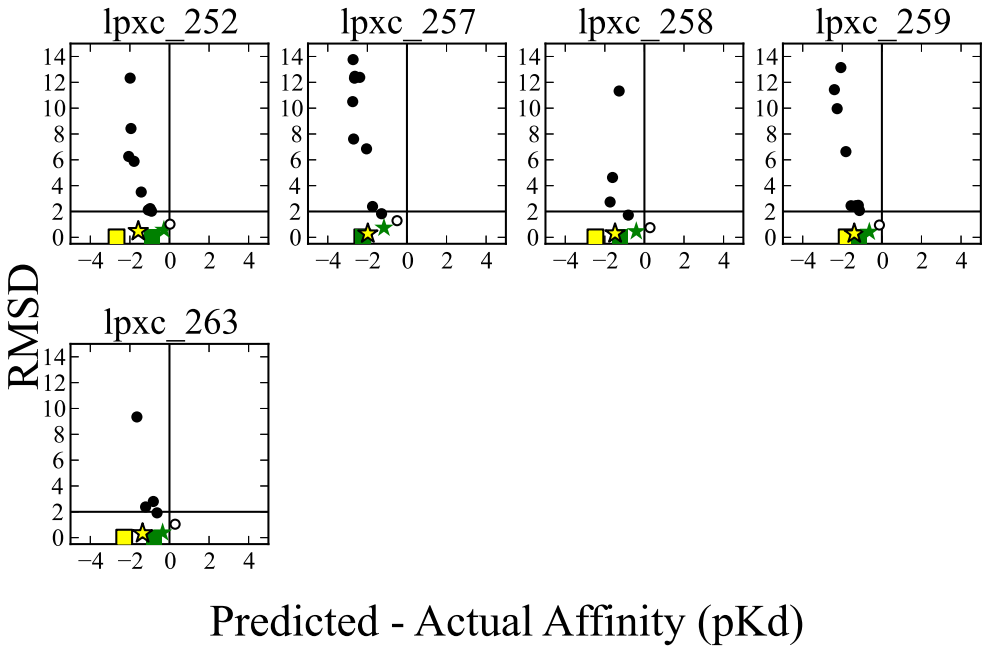


Figure 20: Lpxc Crossdocking Custom-Custom



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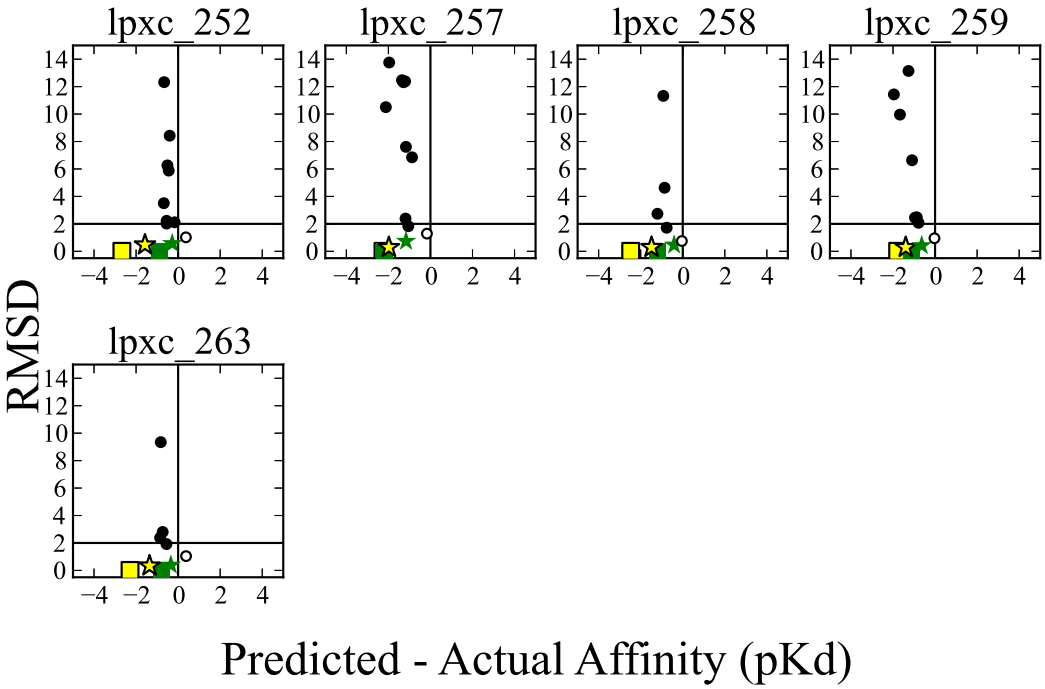

Figure 22: Lpxc Redock Vina-Custom

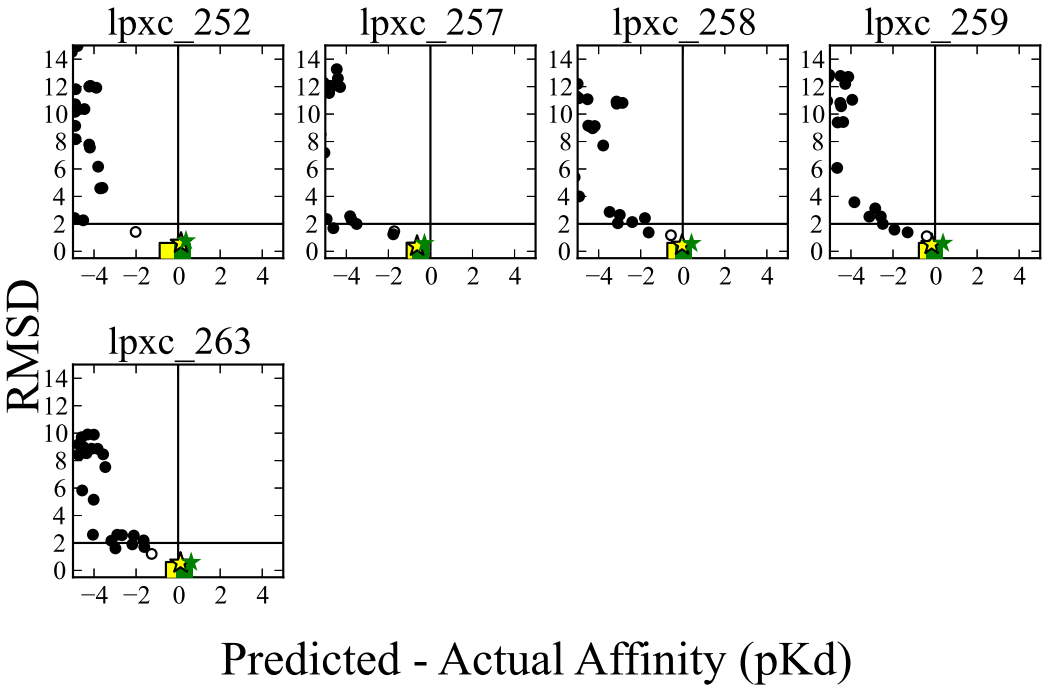

Figure 23: Lpxc Redock Custom-Vina

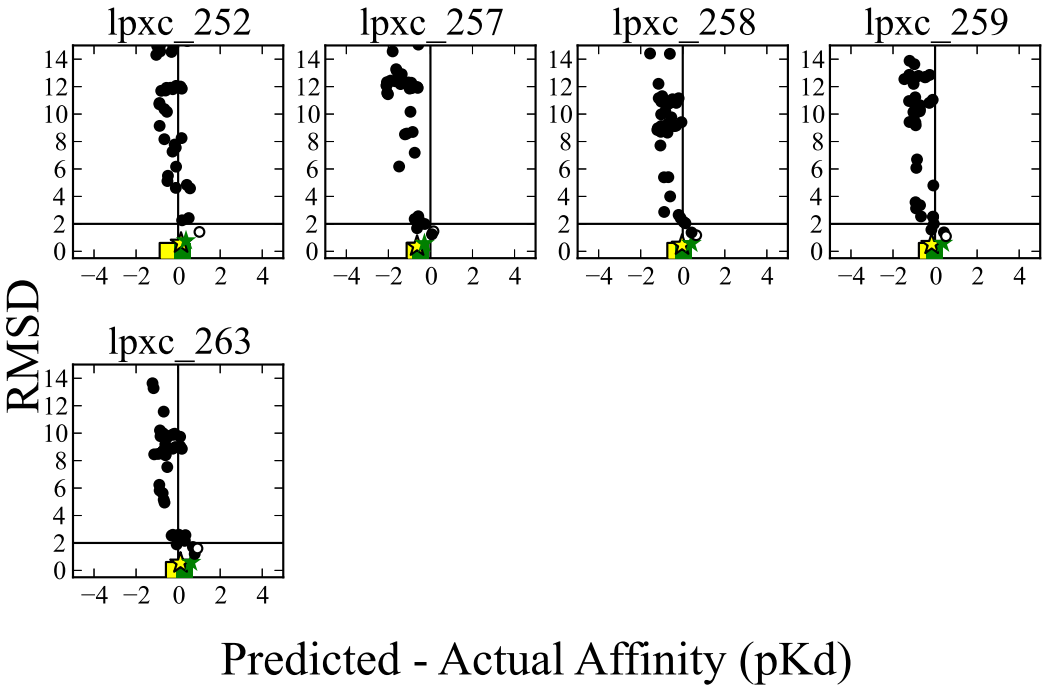

Figure 24: Lpxc Redock Custom-Custom

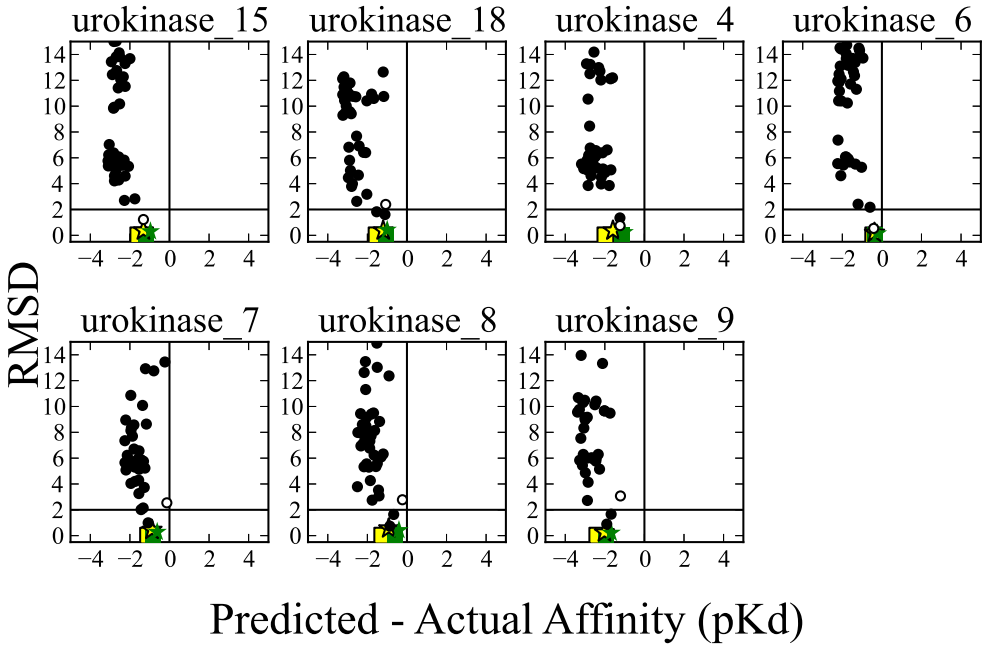

Figure 25: Urokinase Crossdocking Vina-Vina

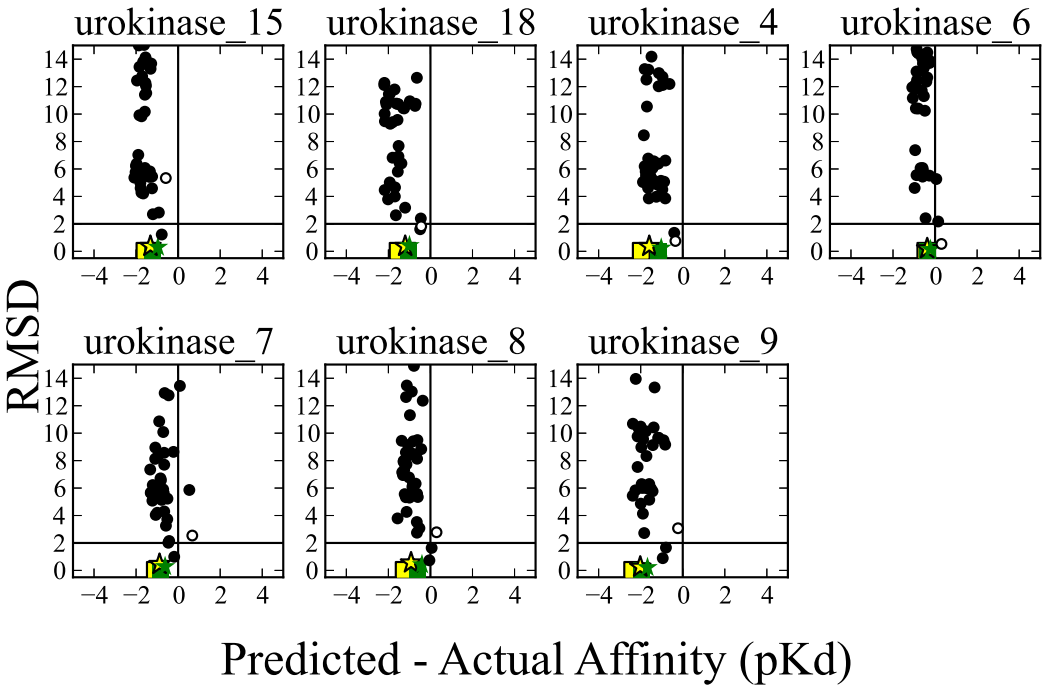

Figure 26: Urokinase Crossdocking Vina-Custom

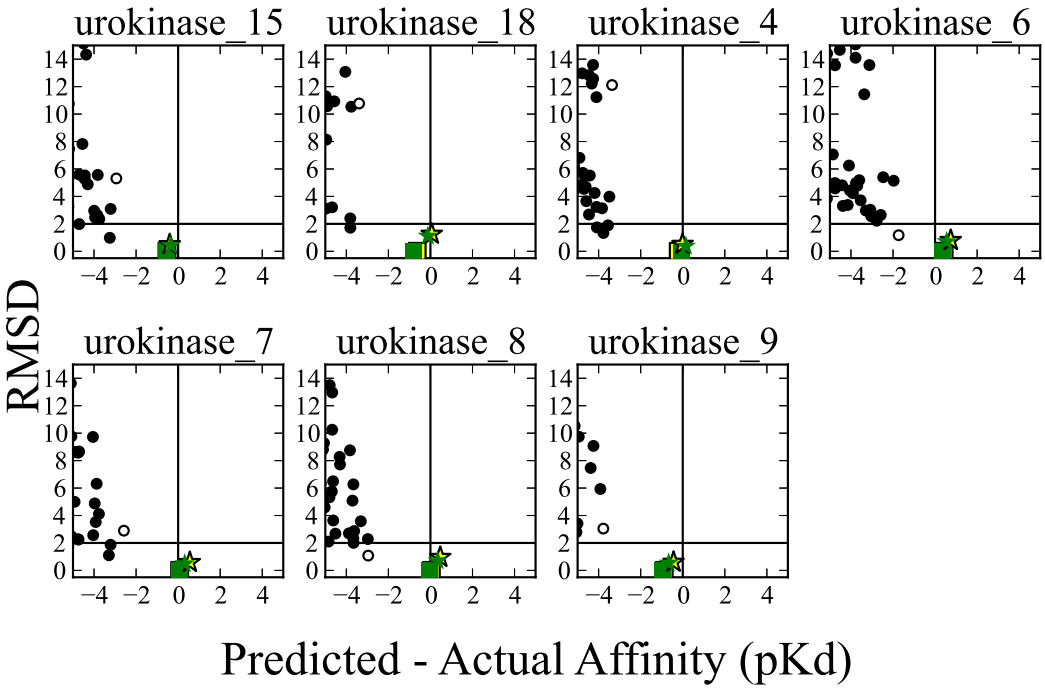

Figure 27: Urokinase Crossdocking Custom-Vina

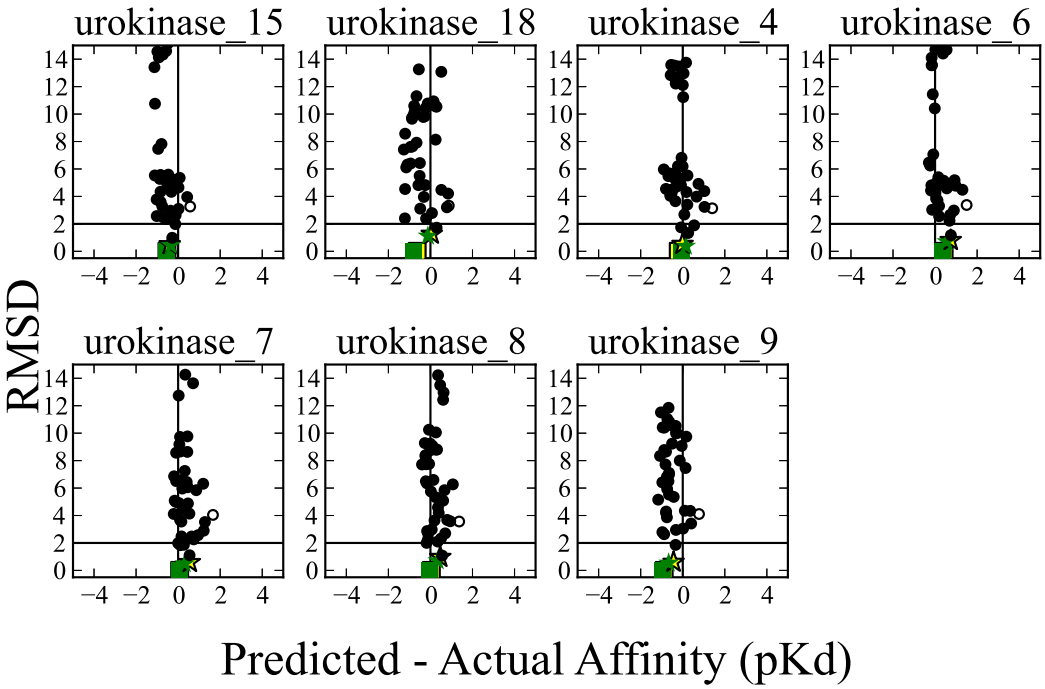

Figure 28: Urokinase Crossdocking Custom-Custom

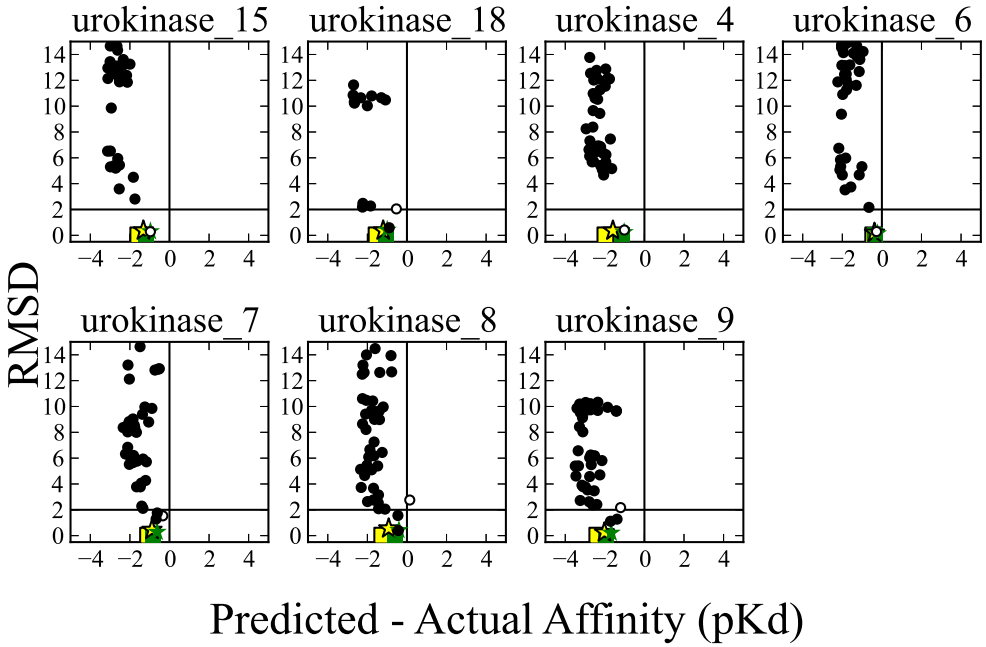

Figure 29: Urokinase Redock Vina-Vina

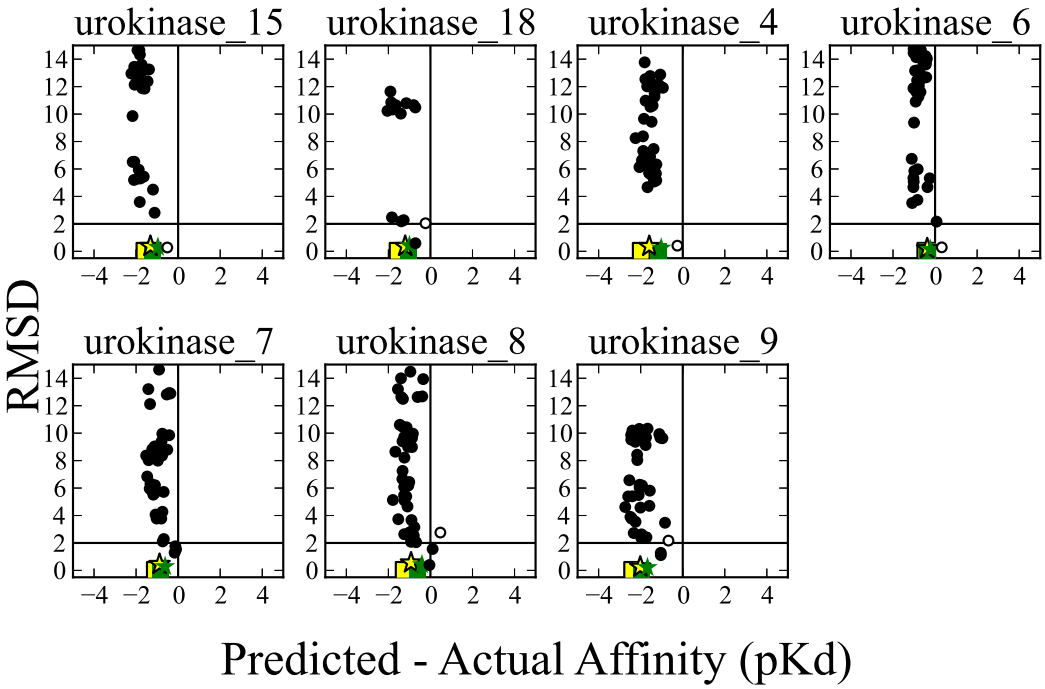

Figure 30: Urokinase Redock Vina-Custom

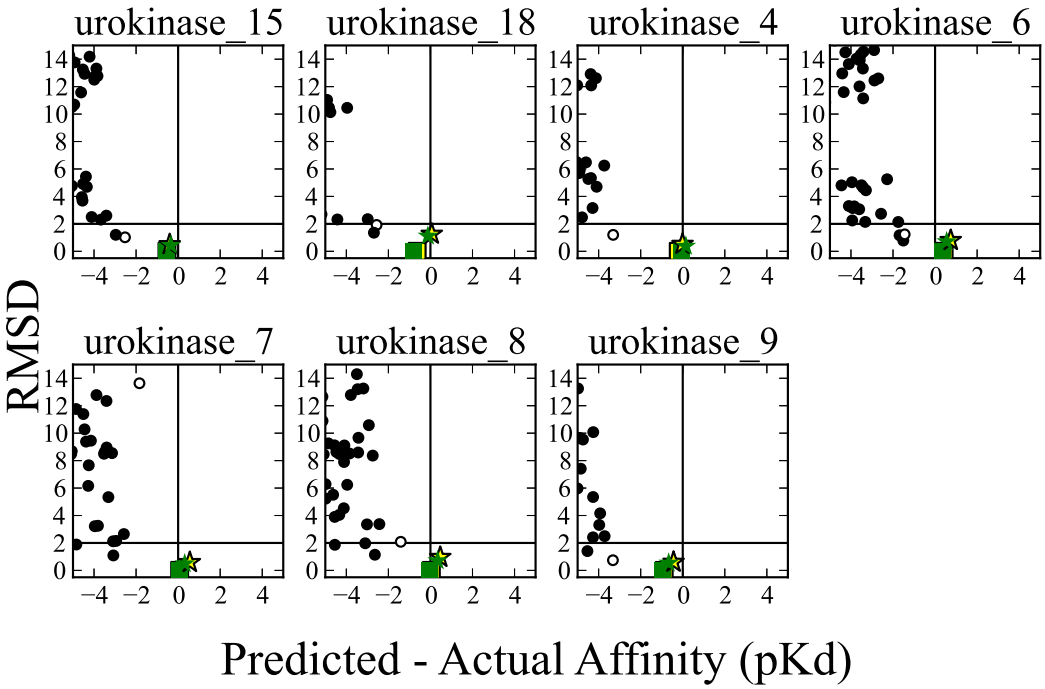

Figure 31: Urokinase Redock Custom-Vina

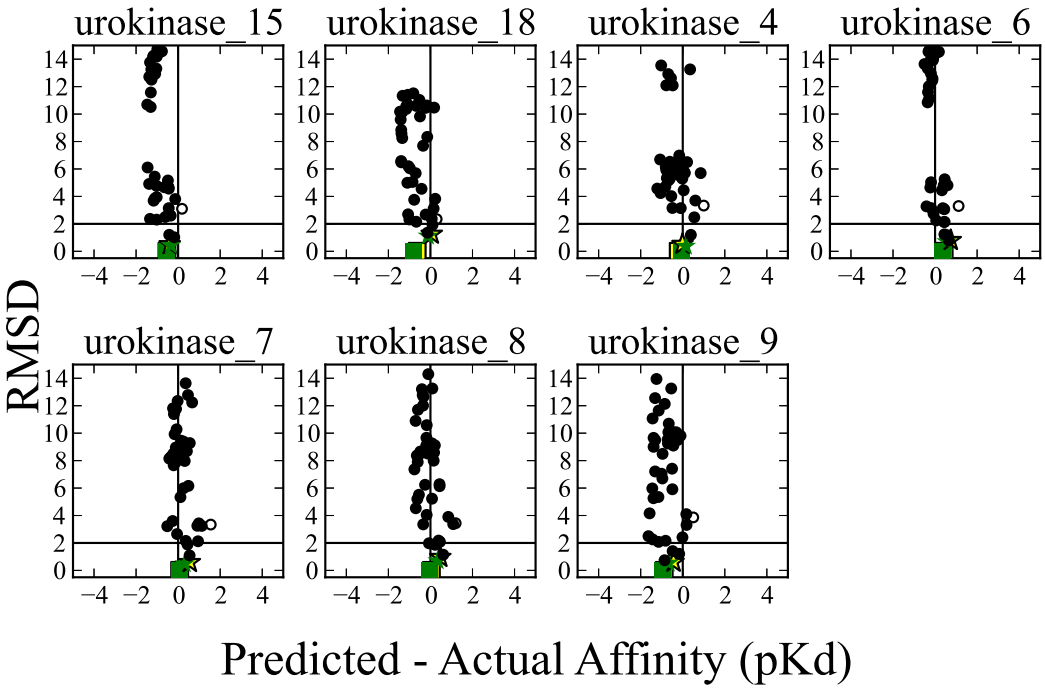

Figure 32: Urokinase Redock Custom-Custom

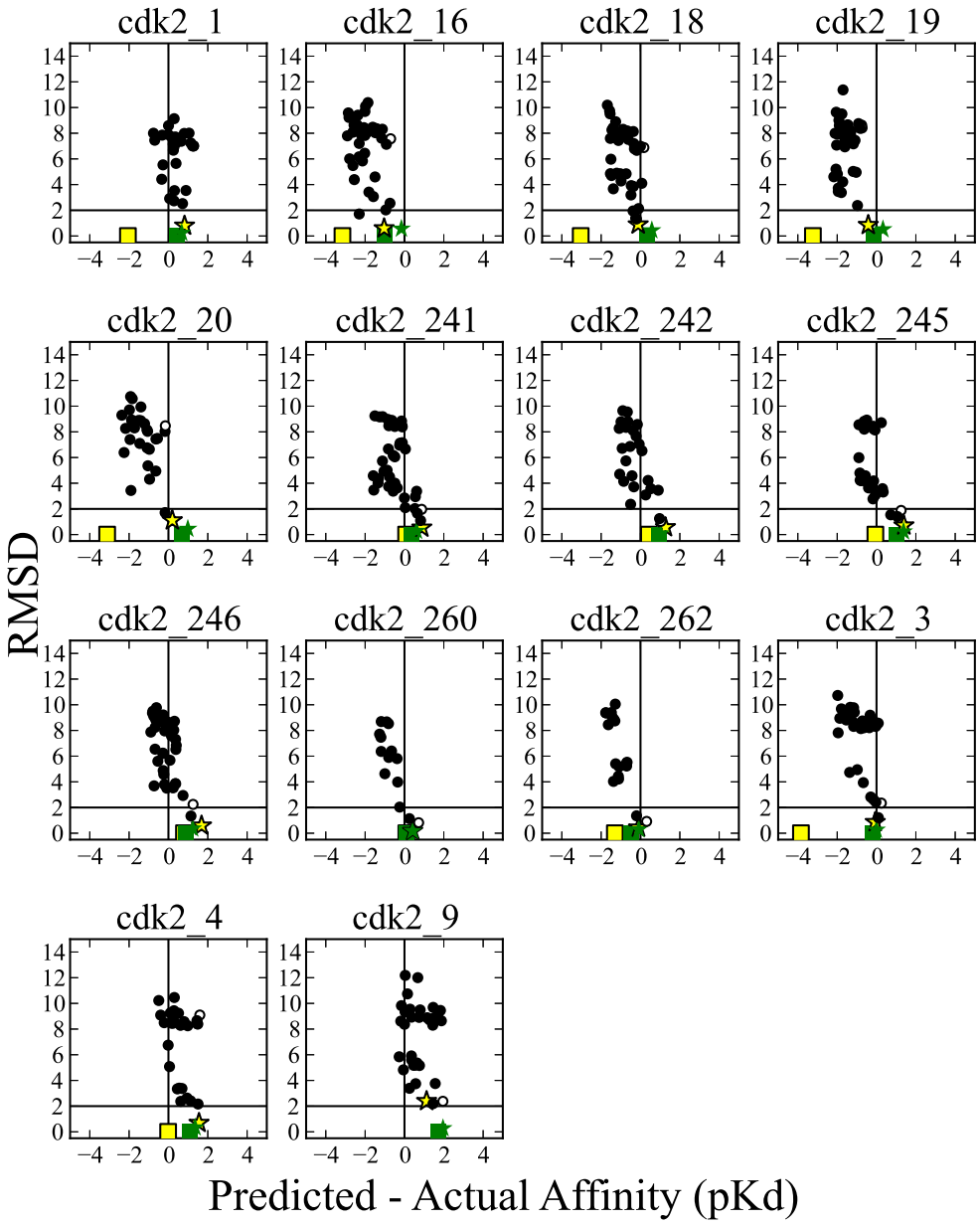

Figure 33: Cdk2 Crossdocking Vina-Vina

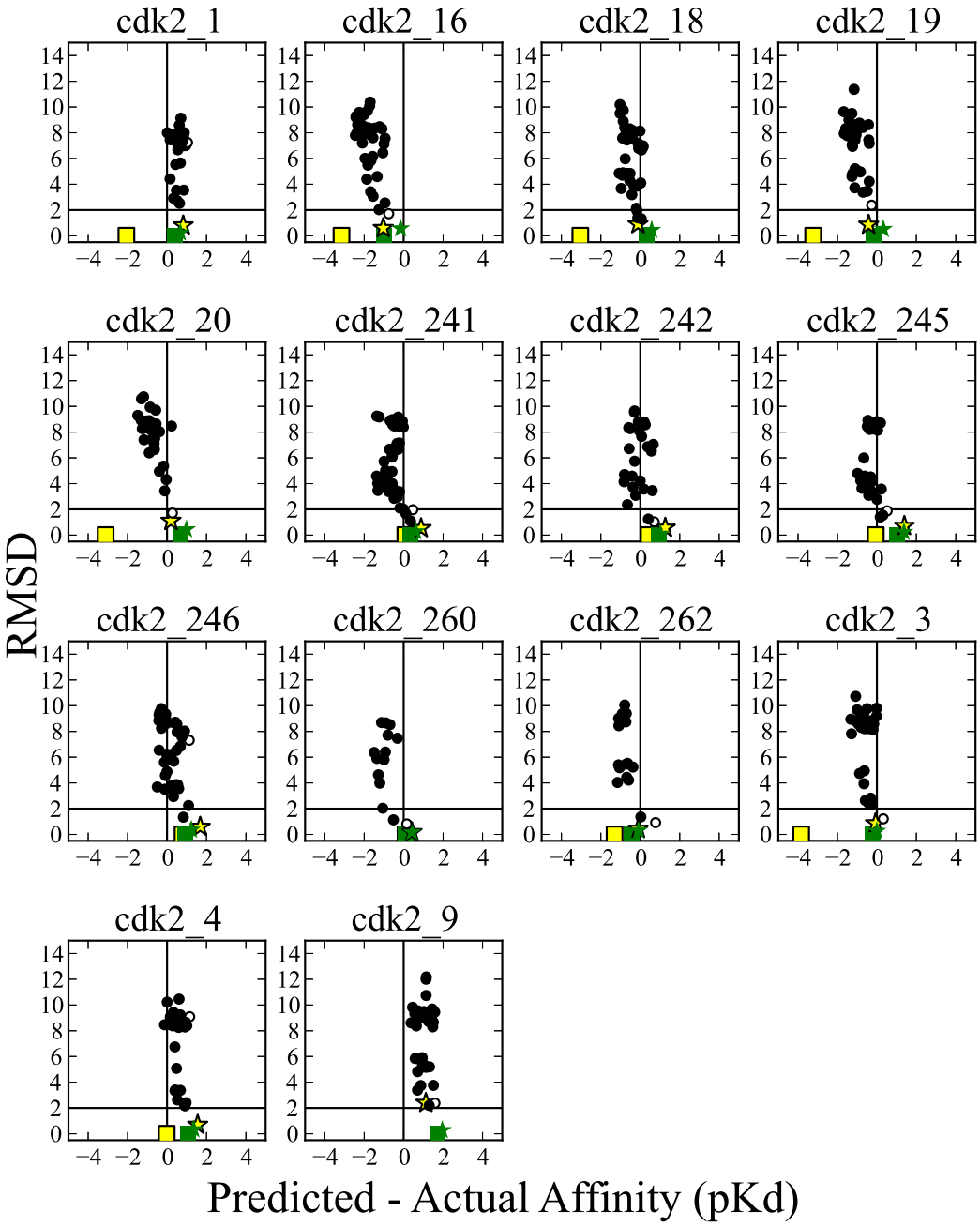

Figure 34: Cdk2 Crossdocking Vina-Custom

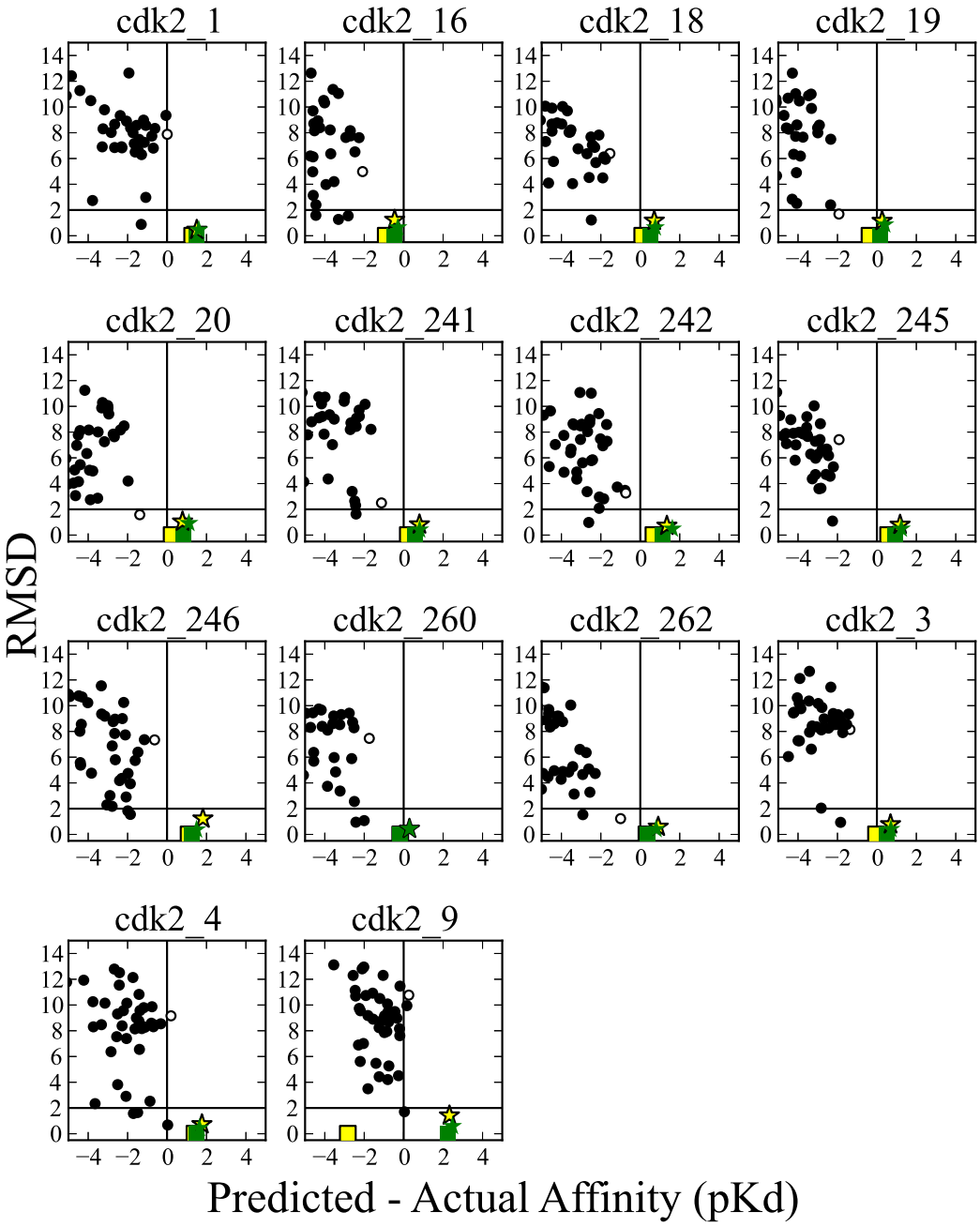

Figure 35: Cdk2 Crossdocking Custom-Vina

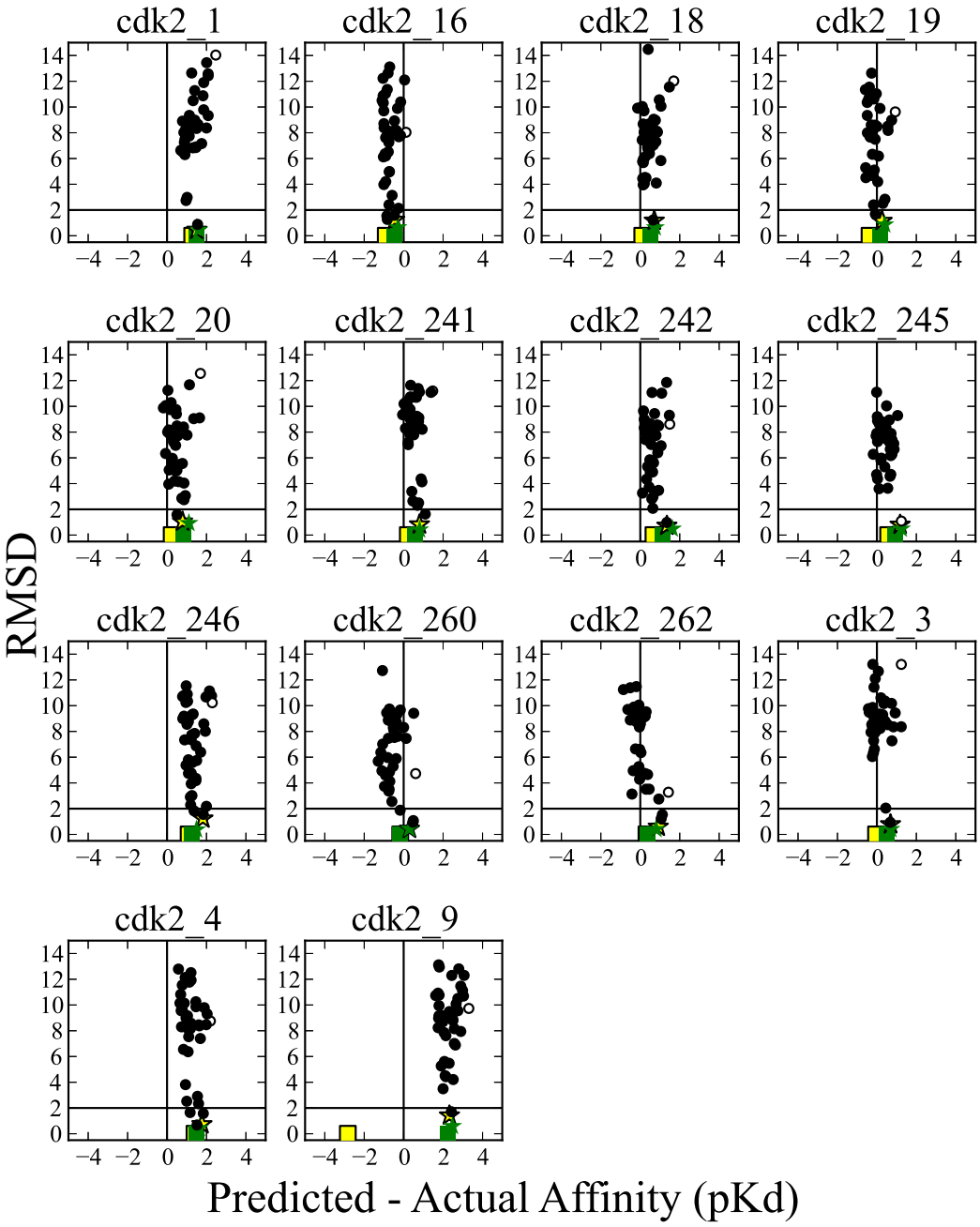

Figure 36: Cdk2 Crossdocking Custom-Custom

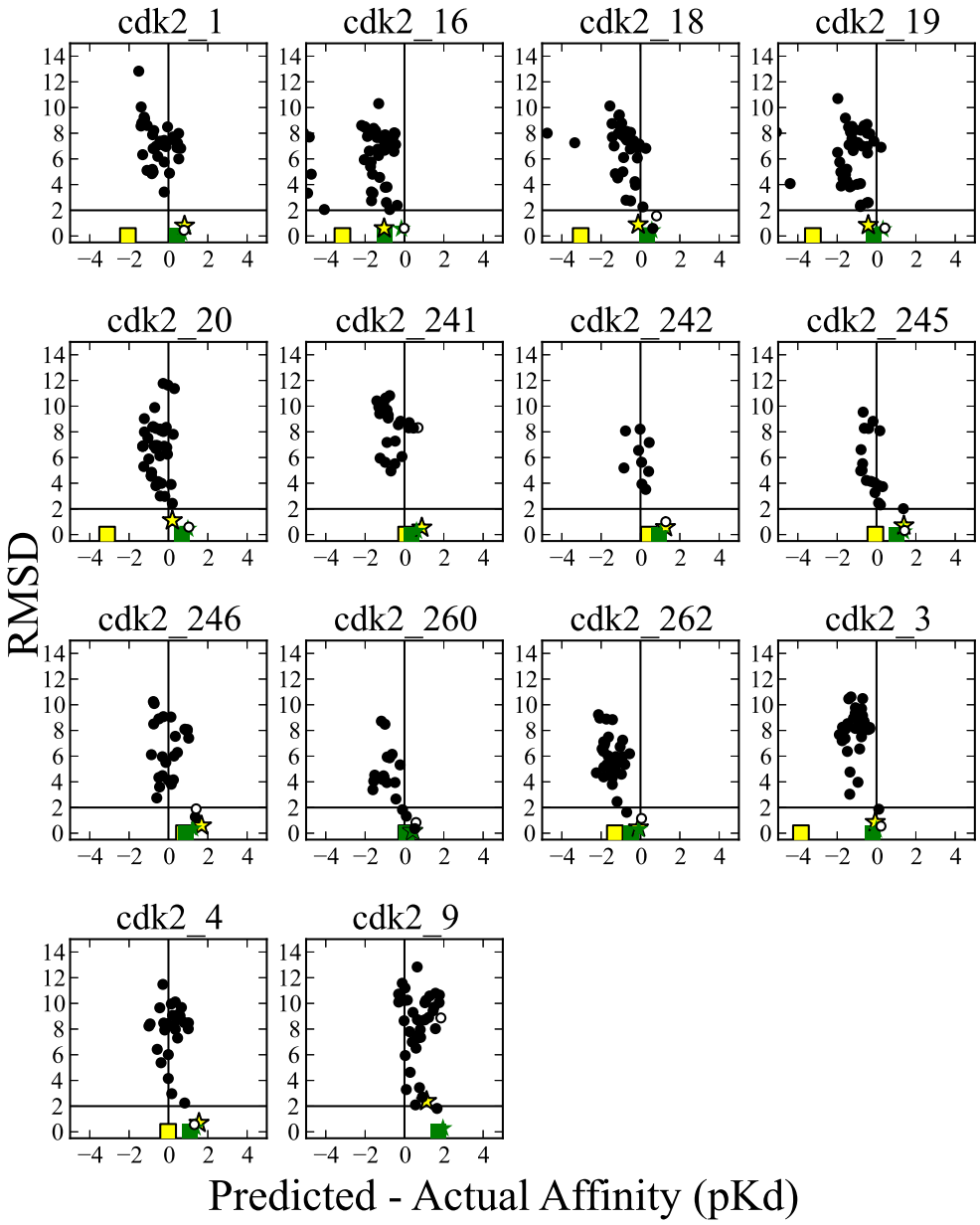

Figure 37: Cdk2 Redock Vina-Vina

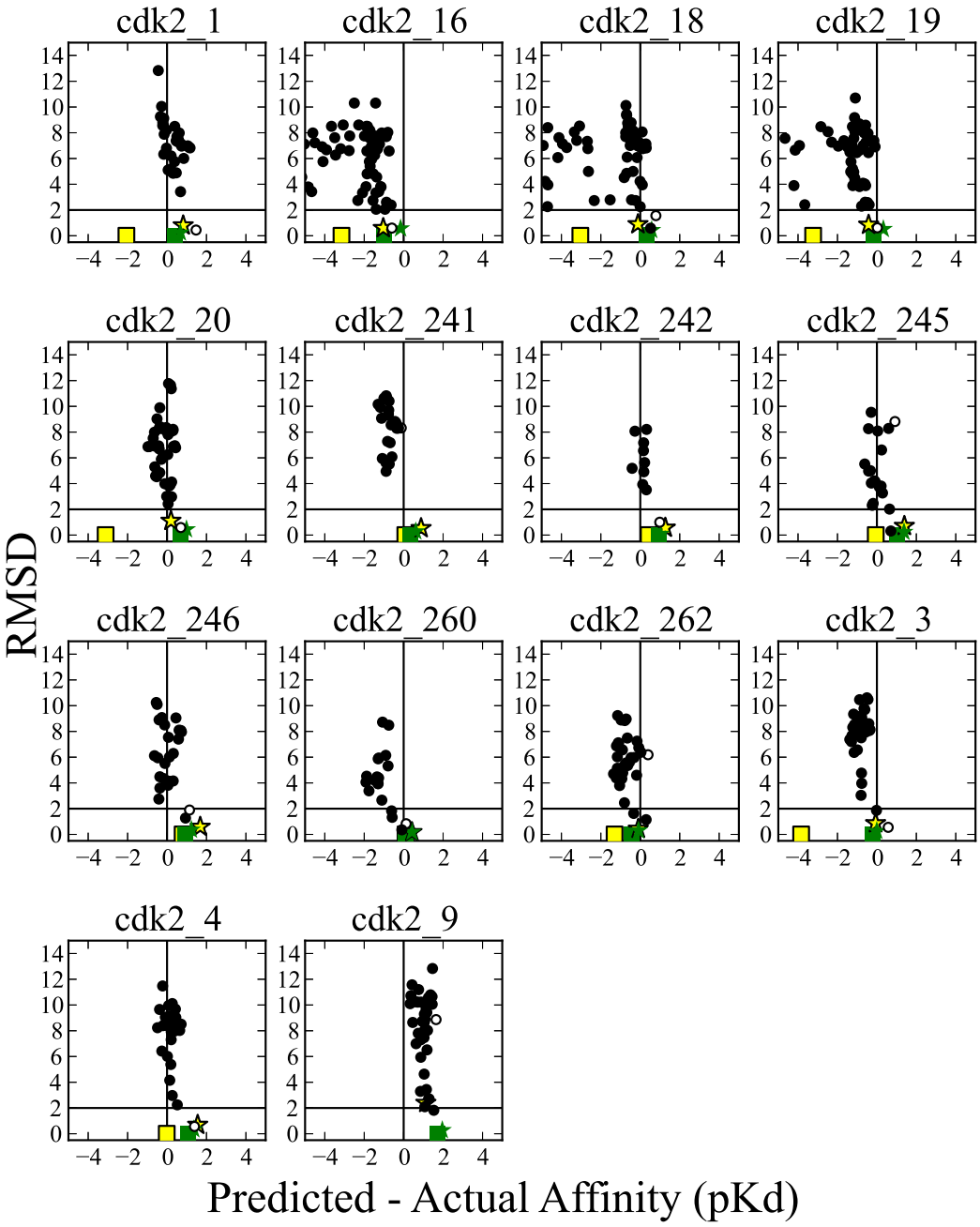

Figure 38: Cdk2 Redock Vina-Custom

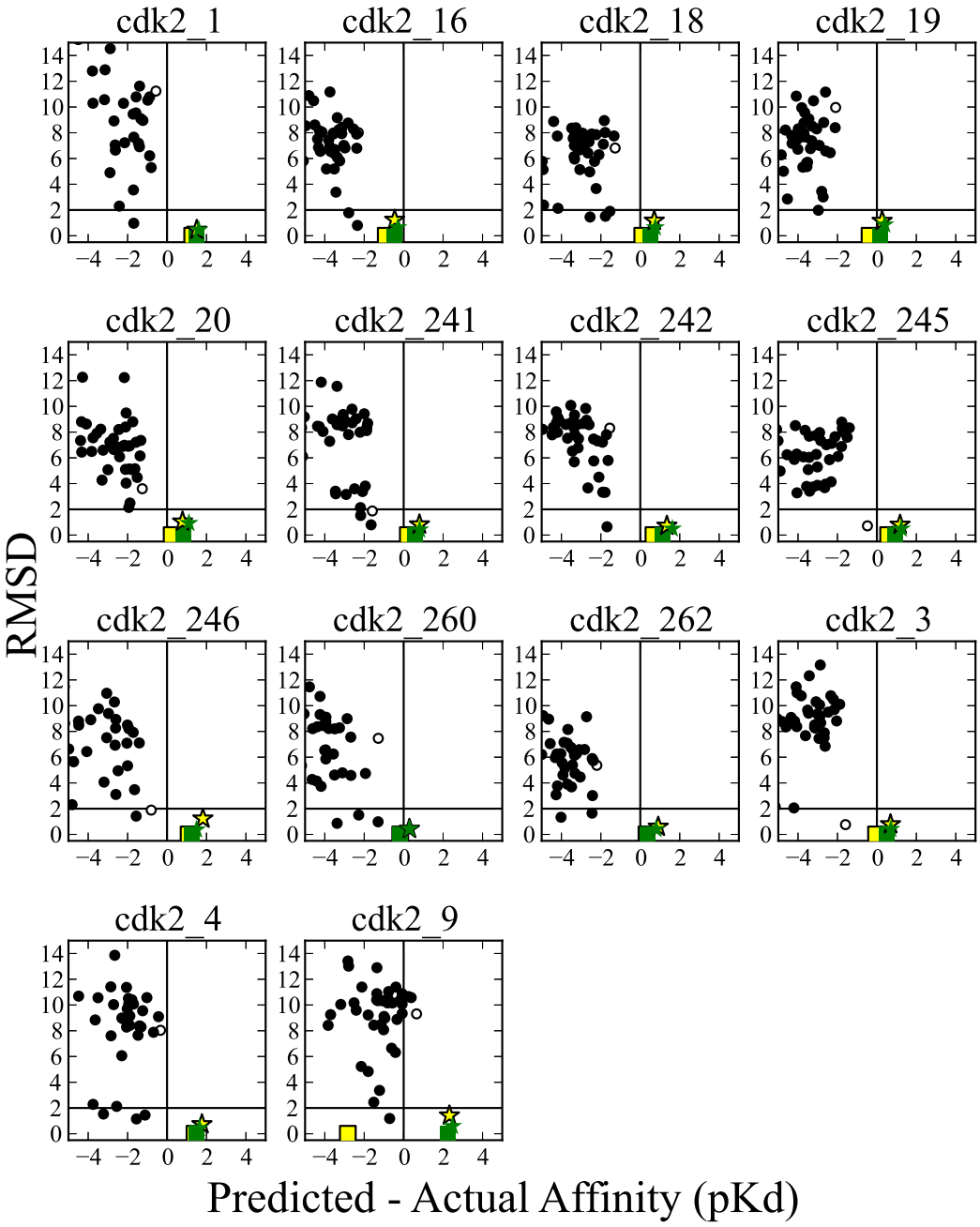

Figure 39: Cdk2 Redock Custom-Vina

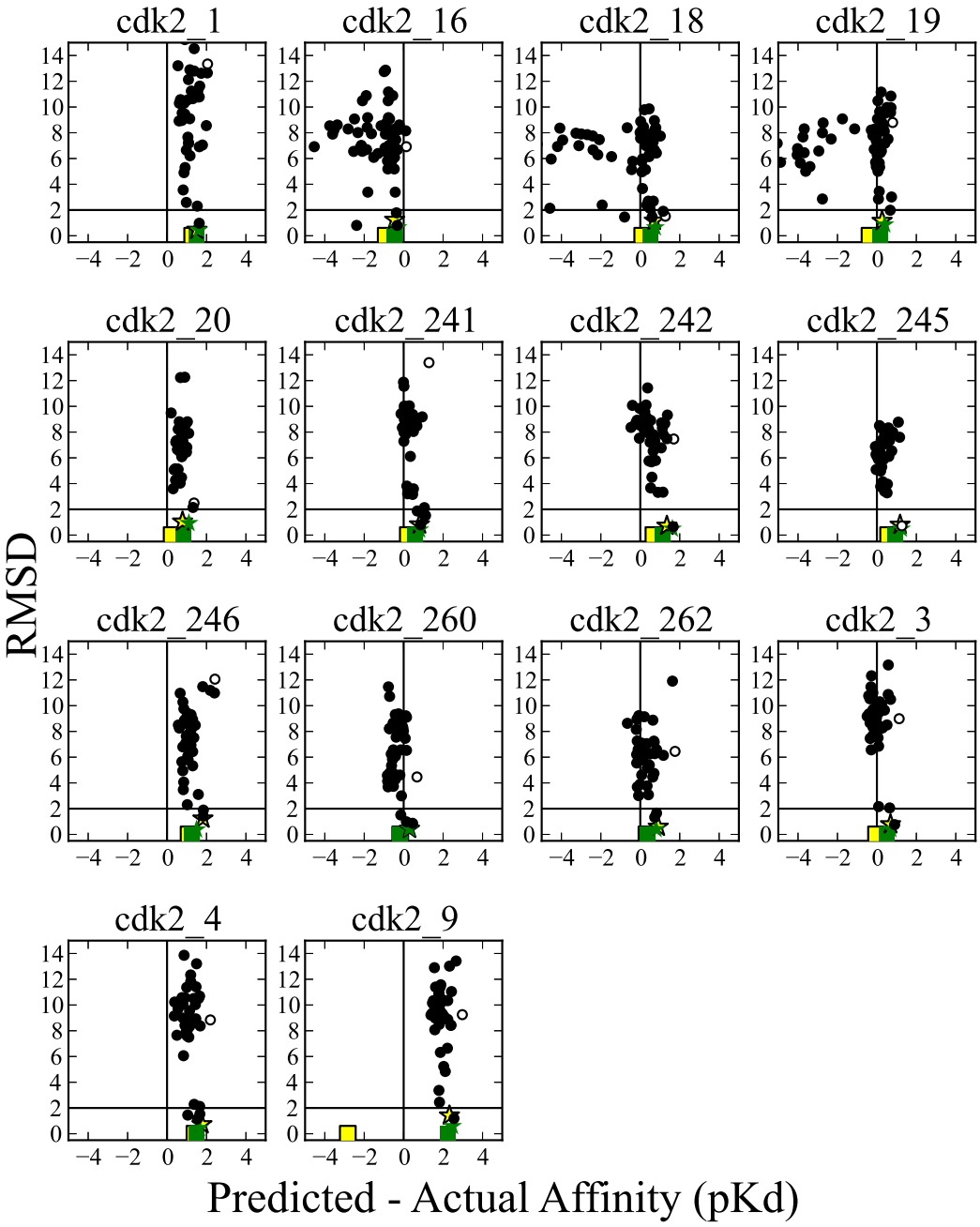

Figure 40: Cdk2 Redock Custom-Custom

Table 1: Difference in predicted affinity of the cross- and self-minimized and *un*minimized poses. Values reported are averages and standard deviations for minimizing and scoring with the specified function.

	Scored	Unminimized Difference Predicted Affinity	Minimized Difference Predicted Affinity
cdk2	Vina	2.388 ± 2.722	0.192 ± 0.464
	Custom	0.658 ± 1.237	0.052 ± 0.161
chk1	Vina	2.633 ± 2.723	1.007 ± 0.466
	Custom	0.615 ± 0.762	0.267 ± 0.177
erk2	Vina	11.439 ± 10.539	1.278 ± 1.487
	Custom	2.99 ± 3.251	0.503 ± 0.836
lpxc	Vina	1.048 ± 0.622	0.992 ± 0.192
	Custom	0.439 ± 0.146	0.417 ± 0.111
urokinase	Vina	0.442 ± 0.222	0.344 ± 0.144
	Custom	-0.042 ± 0.094	-0.109 ± 0.144

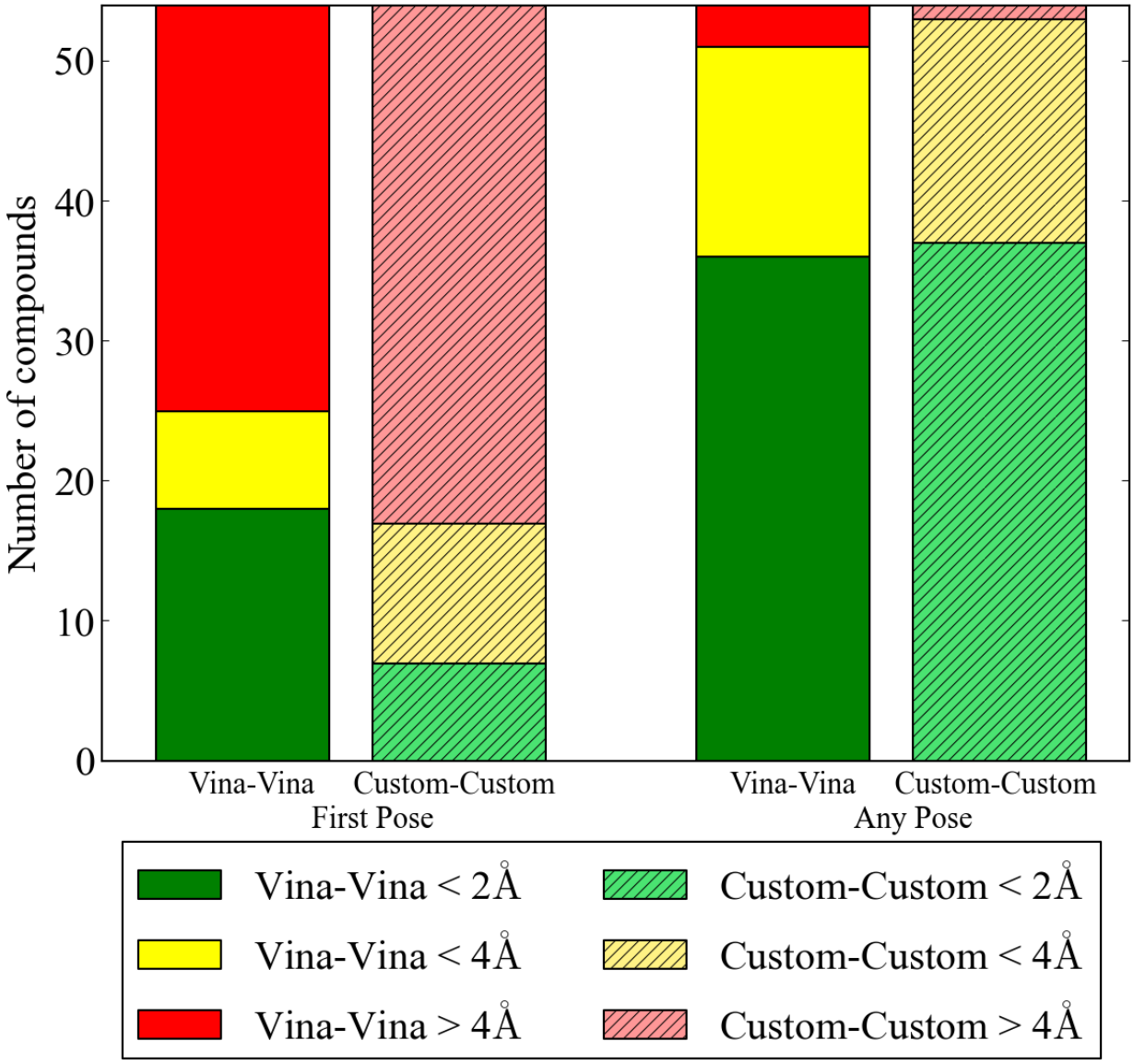

Figure 41: A summary of the scoring and sampling for Vina-Vina and custom-custom dock-rank methods docking with the parameter `--exhaustiveness=50`. Includes data summed over all 54 compounds for the five targets.

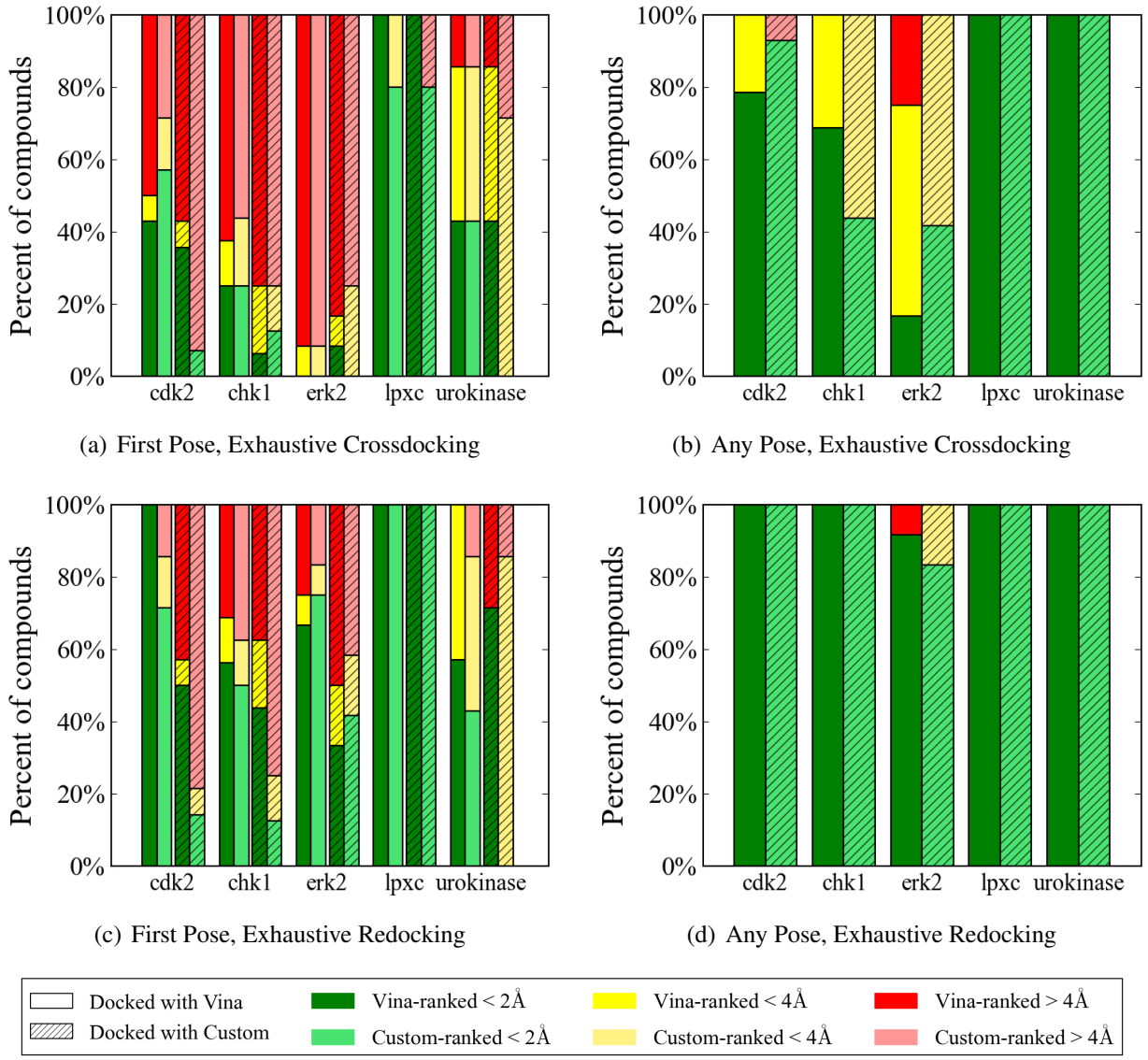

Figure 42: The docking results for all protein targets using Vina and our custom scoring function using docking parameter *--exhaustiveness=50*. In (a) and (c) there are four bars for each target, one for each dock-rank method. For each target, in order left to right: Vina-Vina, Vina-custom, custom-Vina, and custom-custom. (a) The RMSD for the top ranked (by predicted affinity) pose of each compound when crossdocking using each dock-rank method. (b) The RMSD of the lowest RMSD pose of all returned poses for a compound when crossdocking. (c) and (d) The same as (a) and (b) but for redocking.