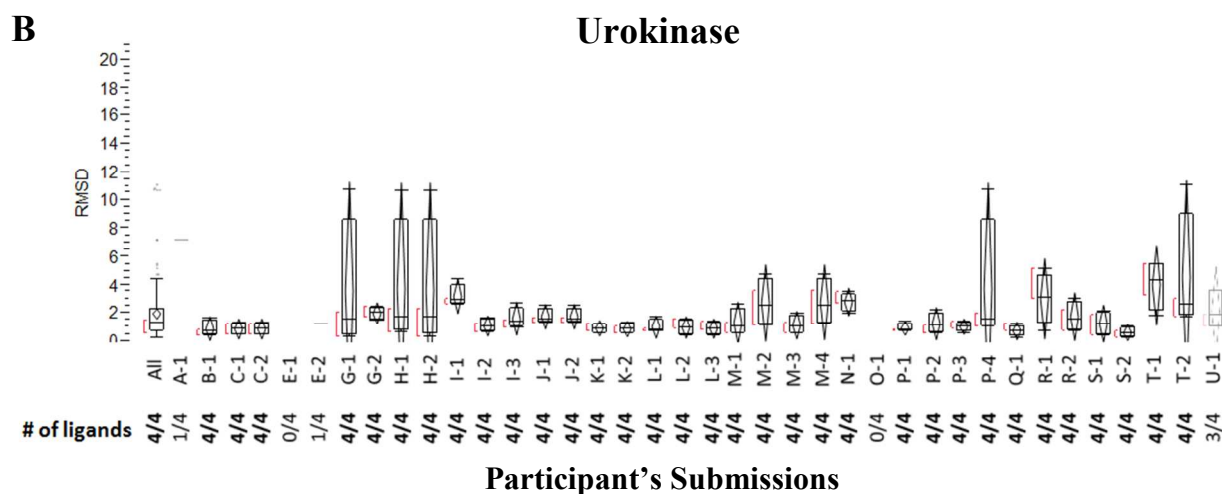
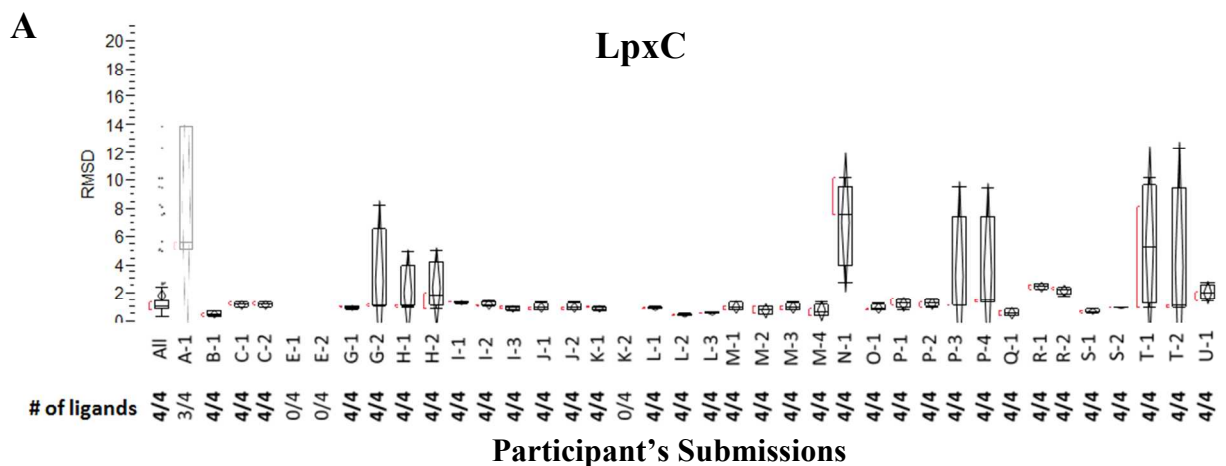


Supporting Information

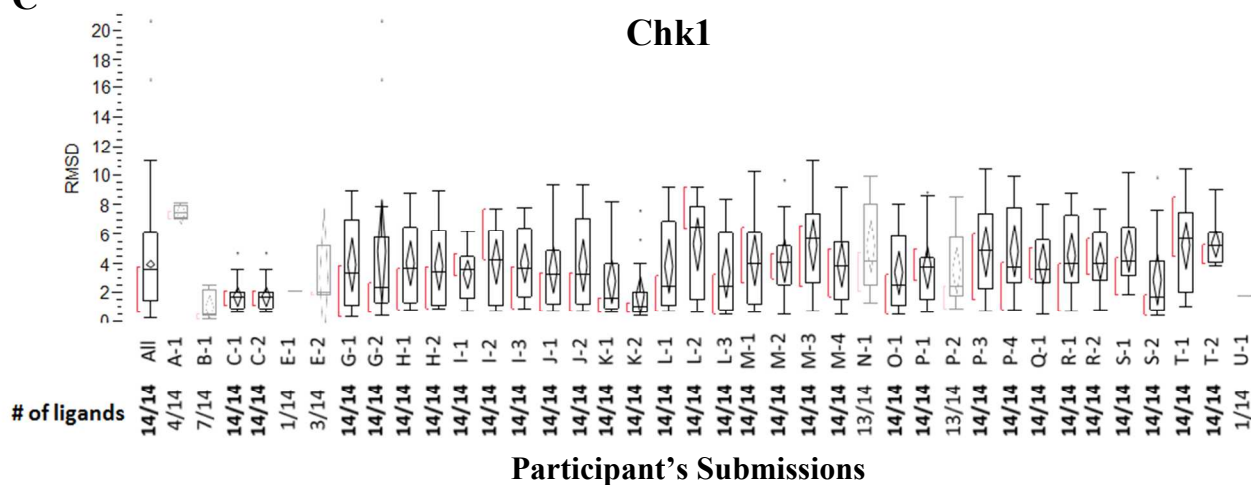
Damm-Ganamet *et al.* CSAR Benchmark Exercise 2011-2012: Evaluation of Results from Docking and Relative Ranking of Blinded Congeneric Series.

- S1.** RMSD box plot of the best pose for each protein-ligand complex broken down by group-method for each protein target.
- S2.** Percent of %Total contacts within various RMSD bins and broken down by various %Total contact cut-offs.
- S3.** Number of raw Het-Het contacts in co-crystal versus number of raw Het-Het contacts in prediction.
- S4.** Number of raw C-C contacts in co-crystal versus number of raw C-C contacts in prediction.
- S5.** Number of raw packing contacts in co-crystal versus number of raw packing contacts in prediction.
- S6.** Pearson, Spearman, and Kendall correlations between ligand descriptors and pose prediction metrics (RMSD and % Native contacts correct).
- S7.** Pearson r parametric correlation between the predicted scores and experimental binding affinities by protein for all group-methods.
- S8.** Spearman ρ nonparametric correlation between the predicted scores and experimental binding affinities by protein for all group-methods.
- S9.** Kendall τ nonparametric correlation between the predicted scores and experimental binding affinities by protein for all group-methods.
- S10.** Pearson r parametric correlation between the predicted scores and experimental binding affinities by chemical series for all group-methods.
- S11.** Spearman ρ nonparametric correlation between the predicted scores and experimental binding affinities by chemical series for all group-methods.
- S12.** Kendall τ nonparametric correlation between the predicted scores and experimental binding affinities by chemical series for all group-methods.
- S13.** AUC values derived from ROC curves by protein for all group-methods.
- S14.** AUC values derived from ROC curves by all series of Chk1 for all group-methods.

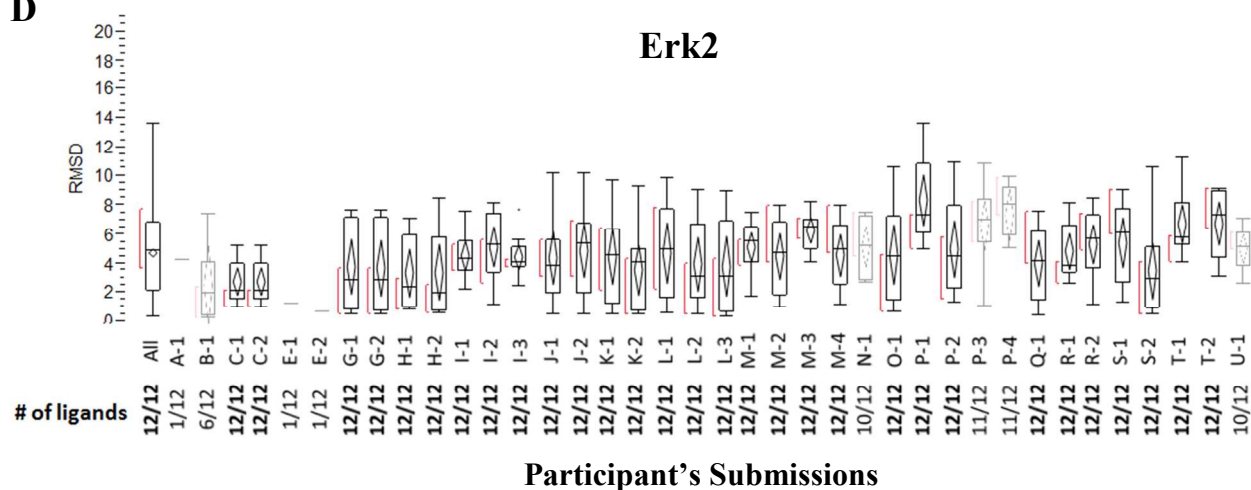
S1. RMSD box plot of the best pose for each protein-ligand complex broken down by group-method for each protein target. The rectangular box indicates the interquartile range (25-75%) and the bars 1.5x interquartile range. The median is shown by the line in the box and the diamond denotes the mean and 95% confidence interval around the mean. The red bracket signifies the shortest interval which contains 50% of the data, and outliers are indicated by squares above the bars. A) LpxC, B) Urokinase, C) Chk1, and D) Erk2.



C



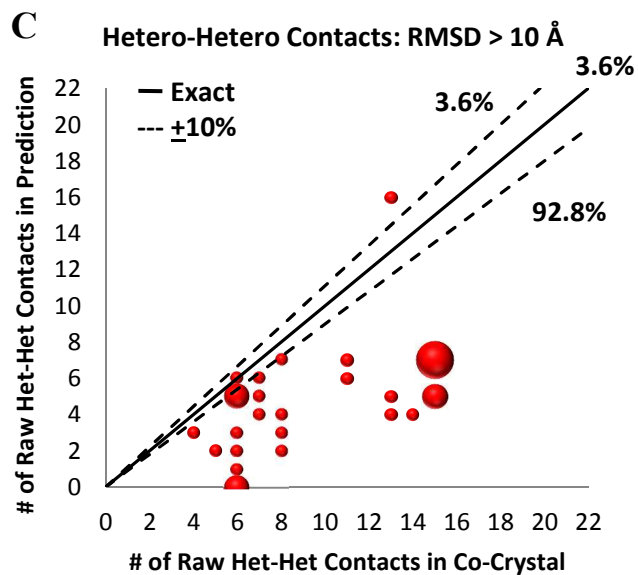
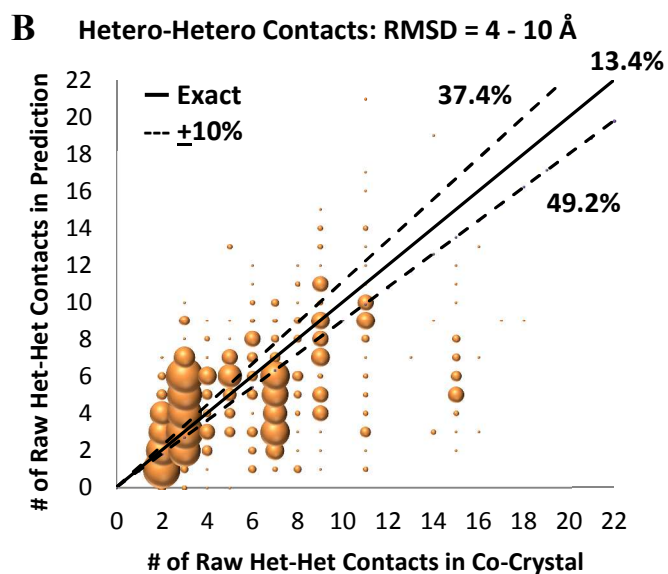
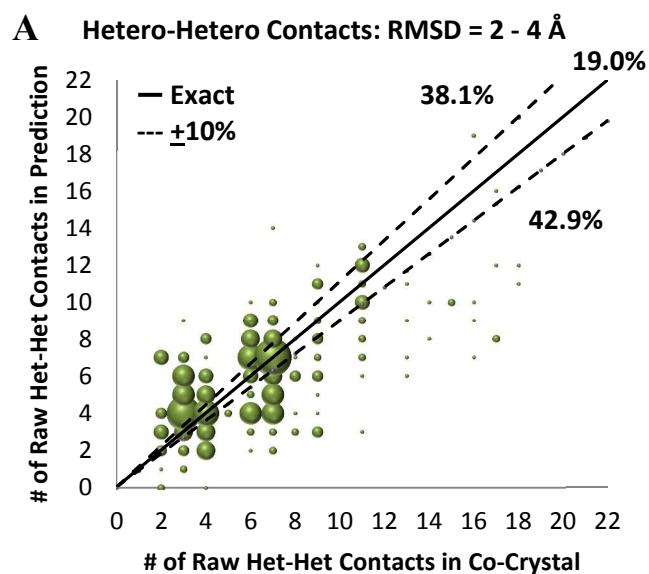
D



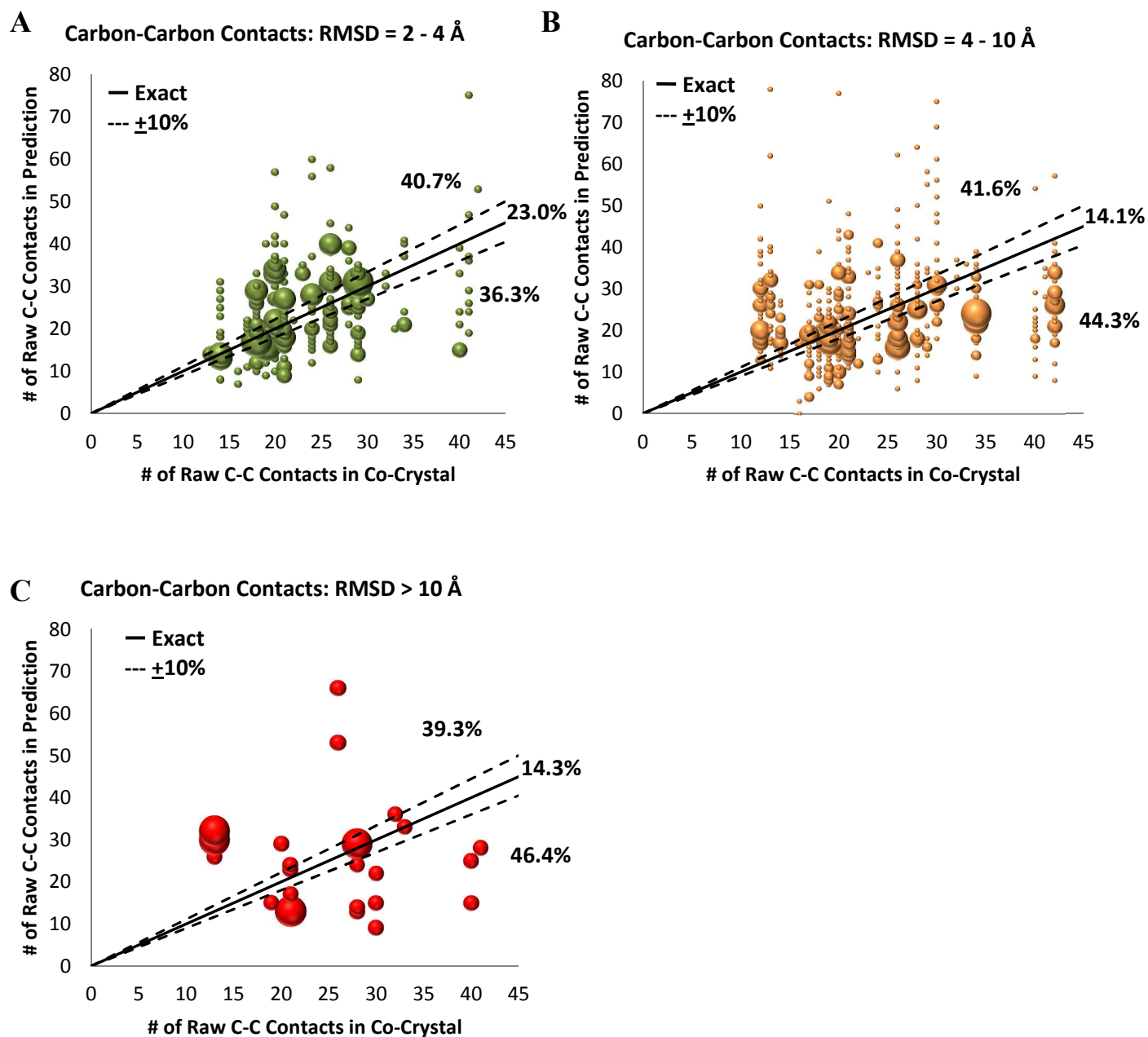
S2. Percent of %Total contacts within various RMSD bins and broken down by various %Total contact cut-offs.

RMSD CUT-OFF (Å)	TOTAL #	RANGE (%)	%Total Contacts								Median
			< 20%	< 30%	< 40%	< 50%	< 60%	< 70%	< 80%	< 90 %	
1.5	415	24 - 86%	0.0%	3.4%	13.7%	32.5%	56.4%	83.4%	96.4%	100%	57%
2.0	498	14 - 86%	0.4%	5.2%	17.3%	37.1%	61.8%	85.7%	97.0%	100%	55%
2.5	559	14 - 86%	0.7%	6.4%	19.3%	40.8%	64.2%	86.9%	97.3%	100%	53%
3.0	602	5 - 86%	1.7%	9.3%	23.1%	44.0%	66.4%	87.7%	97.5%	100%	52%
3.5	661	0 - 86%	4.5%	15.1%	28.7%	48.9%	69.4%	88.8%	97.7%	100%	50%

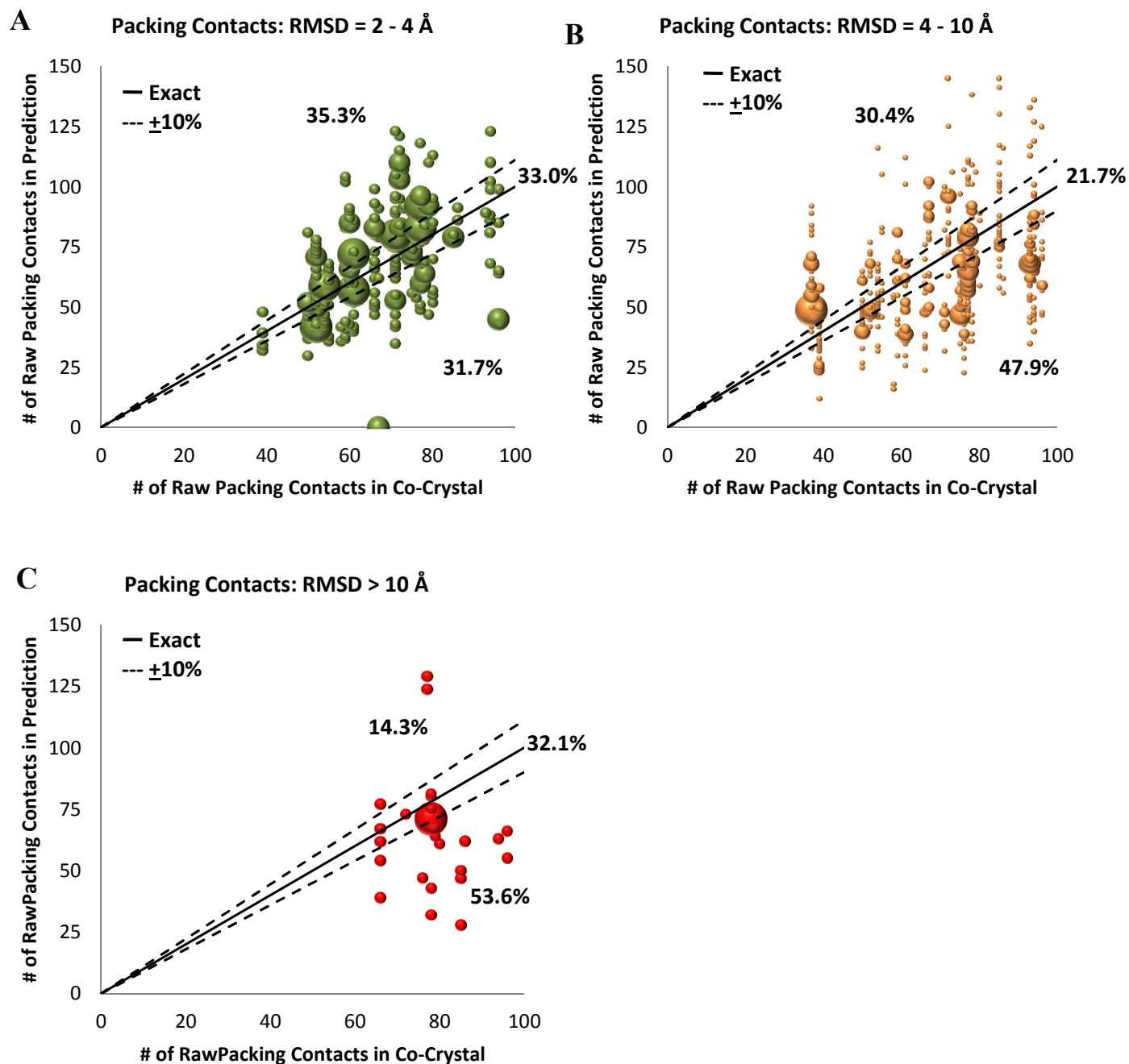
S3. Number of Native Het-Het contacts versus Number of Predicted Het-Het contacts. The solid line illustrates a perfect match while the dotted lines show a $\pm 10\%$ range. A) RMSD = 2 - 4 Å bin. B) RMSD = 4 - 10 Å bin. C) RMSD > 10 Å bin.



S4. Number of Native C-C contacts versus Number of Predicted C-C contacts. The solid line illustrates a perfect match while the dotted lines show a $\pm 10\%$ range. A) RMSD = 2 - 4 Å bin. B) RMSD = 4 - 10 Å bin. C) RMSD > 10 Å bin.



S5. Number of Native Packing contacts versus Number of Predicted Packing contacts. The solid line illustrates a perfect match while the dotted lines show a $\pm 10\%$ range. A) RMSD = 2 - 4 Å bin. B) RMSD = 4 - 10 Å bin. C) RMSD > 10 Å bin.



S6. Pearson, Spearman, and Kendall correlations between ligand descriptors and pose prediction metrics (RMSD and % Native contacts correct).

Pearson (r)	Molecular Weight	# Atoms	# Heavy Atoms	# Hetero Atoms	# H-phob Atoms	# Acceptors	# Donors	# Acceptors + Donors	# C	# N	# O
RMSD	0.187	0.159	0.210	0.246	0.137	0.075	0.109	0.108	0.144	0.308	-0.112
%Het-Het	-0.199	-0.132	-0.188	-0.329	-0.080	-0.179	-0.227	-0.236	-0.073	-0.321	0.053
%C-C	-0.114	-0.070	-0.116	-0.214	-0.044	0.014	-0.061	-0.027	-0.039	-0.306	0.175

Spearman (ρ)											
RMSD	0.157	0.157	0.201	0.256	0.134	0.052	0.037	0.038	0.136	0.315	-0.152
%Het-Het	-0.160	-0.120	-0.173	-0.275	-0.072	-0.126	-0.128	-0.127	-0.063	-0.339	0.134
%C-C	-0.129	-0.098	-0.145	-0.233	-0.063	-0.013	-0.023	0.001	-0.060	-0.314	0.182

Kendall (τ)											
RMSD	0.107	0.105	0.139	0.184	0.093	0.040	0.027	0.027	0.092	0.237	-0.115
%Het-Het	-0.115	-0.087	-0.126	-0.211	-0.050	-0.100	-0.099	-0.096	-0.044	-0.263	0.108
%C-C	-0.088	-0.065	-0.100	-0.168	-0.044	-0.012	-0.019	-0.002	-0.042	-0.236	0.134

S7. Pearson r parametric correlation between the predicted scores and experimental binding affinities by protein for all group-methods. Bolded groups submitted scores for all ligands and are included in the evaluation.

Group-Method	LpxC (n)	Urokinase (n)	Chk1 (n)	Erk2 (n)	Sum r (max value)
median	0.78, (3)	0.50, (15)	-0.01, (29)	0.37, (38)	1.64, (4.00)
Molecular Wt	0.37, (3)	0.42, (15)	-0.14, (29)	0.40, (38)	1.05, (4.00)
SlogP	-0.51, (3)	0.06, (15)	-0.33, (29)	-0.15, (38)	-0.93, (4.00)
Group A-1	-0.84, (3)	-0.28, (15)	0.01, (29)	0.11, (38)	-1.00, (4.00)
Group B-1	n/a	0.53, (14)	-0.26, (13)	0.21, (27)	0.48, (3.00)
Group C-1	0.76, (3)	0.71, (15)	0, (29)	0.30, (38)	1.77, (4.00)
Group C-2	0.73, (3)	0.71, (15)	-0.12, (29)	0.34, (38)	1.66, (4.00)
Group D-1	n/a	0.70, (15)	0.35, (29)	0.53, (38)	1.58, (3.00)
Group D-2	n/a	0.55, (15)	0.35, (29)	0.53, (38)	1.43, (3.00)
Group D-3	n/a	0.65, (15)	0.34, (29)	0.52, (38)	1.51, (3.00)
Group E-1	0.87, (3)	0.45, (15)	0.09, (29)	0.66, (38)	2.07, (4.00)
Group E-2	0.87, (3)	0.45, (15)	0.01, (29)	0.57, (38)	1.90, (4.00)
Group F-1	0.51, (3)	0.47, (15)	-0.22, (29)	0.41, (36)	1.17, (4.00)
Group F-2	-0.22, (3)	0.50, (15)	0.29, (29)	0.32, (36)	0.89, (4.00)
Group F-3	0.53, (3)	0.51, (15)	-0.20, (29)	0.40, (36)	1.24, (4.00)
Group F-4	0, (3)	0.47, (15)	0.28, (29)	0.32, (36)	1.07, (4.00)
Group G-1	1.00, (3)	0.09, (15)	0.16, (29)	0.41, (38)	1.66, (4.00)
Group G-2	0.99, (3)	0.09, (15)	0.09, (29)	n/a	1.17, (3.00)
Group H-1	0.99, (3)	0.32, (15)	0.02, (29)	0.46, (38)	1.79, (4.00)
Group H-2	0.92, (3)	0.23, (15)	0.02, (29)	0.47, (38)	1.64, (4.00)
Group I-1	0.94, (3)	0.48, (15)	-0.12, (29)	0.26, (38)	1.56, (4.00)
Group I-2	0.92, (3)	0.49, (15)	-0.09, (29)	0.31, (38)	1.63, (4.00)
Group J-1	1.00, (3)	0.35, (15)	0.30, (29)	-0.02, (38)	1.63, (4.00)
Group J-2	-0.47, (3)	0.61, (14)	-0.21, (26)	0.37, (38)	0.30, (4.00)
Group K-1	n/a	0.6, (15)	0.03, (29)	0.17, (38)	0.80, (3.00)
Group K-2	n/a	0.55, (15)	0.02, (29)	0.03, (38)	0.60, (3.00)
Group L-1	0.61, (3)	0.77, (15)	-0.02, (29)	-0.02, (38)	1.34, (4.00)
Group L-2	0.41, (3)	0.60, (15)	0.02, (29)	0.09, (38)	1.12, (4.00)
Group M-1	0.67, (3)	0.29, (15)	-0.15, (29)	0.23, (38)	1.04, (4.00)
Group M-2	0.31, (3)	0.33, (15)	-0.26, (29)	0.41, (38)	0.79, (4.00)
Group M-3	0.40, (3)	0.47, (15)	-0.13, (29)	0.16, (38)	0.90, (4.00)
Group M-4	0.20, (3)	0.43, (15)	-0.31, (29)	0.33, (38)	0.65, (4.00)
Group N-1	-0.56, (3)	0.22, (15)	-0.12, (29)	0.03, (38)	-0.43, (4.00)
Group O-1	0.90, (3)	n/a	0.14, (25)	n/a	1.04, (2.00)
Group O-2	n/a	n/a	-0.34, (25)	0.49, (34)	0.15, (2.00)
Group O-3	n/a	n/a	n/a	0.54, (34)	0.54, (100)
Group O-4	0.99, (3)	n/a	n/a	n/a	0.99, (1.00)
Group P-1	0.99, (3)	0.36, (15)	0, (29)	0.41, (38)	1.76, (4.00)
Group P-2	0.59, (3)	0.50, (15)	-0.22, (29)	0.63, (38)	1.50, (4.00)
Group P-3	0.99, (3)	0.68, (14)	-0.09, (29)	0.60, (37)	2.18, (4.00)

Group P-4	0.49, (3)	0.53, (14)	-0.09, (29)	0.62, (37)	1.55, (4.00)
Group P-5	0.99, (3)	0.72, (15)	-0.03, (29)	0.48, (38)	2.16, (4.00)
Group P-6	0.79, (3)	0.58, (15)	-0.14, (29)	0.55, (38)	1.78, (4.00)
Group R-1	0.89, (3)	0.54, (15)	-0.12, (29)	0.22, (38)	1.53, (4.00)
Group R-2	0.84, (3)	0.61, (15)	-0.11, (29)	0.15, (38)	1.49, (4.00)
Group S-1	0.92, (3)	0.57, (15)	0.38, (29)	0.12, (38)	1.99, (4.00)
Group S-2	0.77, (3)	0.60, (15)	0.16, (29)	0.44, (38)	1.97, (4.00)
Group T-1	-0.56, (3)	0.17, (15)	0.32, (29)	-0.07, (38)	-0.14, (4.00)
Group T-2	0.85, (3)	0.37, (15)	-0.17, (29)	0.40, (38)	1.45, (4.00)

S8. Spearman ρ nonparametric correlation between the predicted scores and experimental binding affinities by protein for all group-methods. Bolded groups submitted scores for all ligands and are included in the evaluation.

Group-Method	LpxC (n)	Urokinase (n)	Chk1 (n)	Erk2 (n)	Sum ρ (max value)
median	0.50 (3)	0.52 (15)	-0.03 (29)	0.31 (38)	1.30 (4.00)
Molecular Wt	0.50 (3)	0.41 (15)	-0.14 (29)	0.40 (38)	1.17 (4.00)
SlogP	-0.50 (3)	0.14 (15)	-0.29 (29)	-0.15 (38)	-0.80 (4.00)
Group A-1	-0.87 (3)	-0.28 (15)	0.02 (29)	0.06 (38)	-1.07 (4.00)
Group B-1	n/a	0.43 (14)	-0.19 (13)	0.09 (27)	0.33 (3.00)
Group C-1	0.50 (3)	0.64 (15)	-0.02 (29)	0.32 (38)	1.44 (4.00)
Group C-2	0.50 (3)	0.63 (15)	-0.09 (29)	0.34 (38)	1.38 (4.00)
Group D-1	n/a	0.56 (15)	0.32 (29)	0.58 (38)	1.46 (3.00)
Group D-2	n/a	0.58 (15)	0.32 (29)	0.58 (38)	1.48 (3.00)
Group D-3	n/a	0.53 (15)	0.33 (29)	0.59 (38)	1.45 (3.00)
Group D-4	n/a	0.67 (15)	0.18 (29)	0.49 (38)	1.34 (3.00)
Group D-5	n/a	0.62 (15)	0.17 (29)	0.49 (38)	1.28 (3.00)
Group D-6	n/a	0.58 (15)	0.19 (29)	0.48 (38)	1.25 (3.00)
Group E-1	0.50 (3)	0.50 (15)	0.03 (29)	0.67 (38)	1.70 (4.00)
Group E-2	0.50 (3)	0.50 (15)	0.05 (29)	0.58 (38)	1.63 (4.00)
Group F-1	0.50 (3)	0.55 (15)	-0.25 (29)	0.40 (36)	1.20 (4.00)
Group F-2	-0.50 (3)	0.56 (15)	0.35 (29)	0.38 (36)	0.79 (4.00)
Group F-3	0.50 (3)	0.53 (15)	-0.25 (29)	0.39 (36)	1.17 (4.00)
Group F-4	-0.50 (3)	0.56 (15)	0.36 (29)	0.35(36)	0.77 (4.00)
Group G-1	1.00 (3)	0.29 (15)	0.18 (29)	0.42 (38)	1.89 (4.00)
Group G-2	1.00 (3)	0.29 (15)	0.10 (29)	n/a	1.39 (3.00)
Group H-1	1.00 (3)	0.20 (15)	0.06 (29)	0.45 (38)	1.71 (4.00)
Group H-2	1.00 (3)	0.24 (15)	0.01 (29)	0.50 (38)	1.75 (4.00)
Group I-1	1.00 (3)	0.56 (15)	-0.09 (29)	0.22 (38)	1.69 (4.00)
Group I-2	1.00 (3)	0.51 (15)	-0.14 (29)	0.30 (38)	1.67 (4.00)
Group J-1	1.00 (3)	0.44 (15)	0.10 (29)	-0.08 (38)	1.46 (4.00)
Group J-2	-0.50 (3)	0.58 (14)	-0.20 (26)	0.42 (38)	0.30 (4.00)
Group K-1	n/a	0.48 (15)	0.02 (29)	0.13 (38)	0.63 (3.00)
Group K-2	n/a	0.15 (15)	0.02 (29)	0.03 (38)	0.20 (3.00)
Group L-1	0.50 (3)	0.76 (15)	0.01 (29)	-0.04 (38)	1.23 (4.00)
Group L-2	0.50 (3)	0.72 (15)	0.08 (29)	0.05 (38)	1.35 (4.00)
Group M-1	0.50 (3)	0.31 (15)	-0.16 (29)	0.21 (38)	0.86 (4.00)
Group M-2	0.50 (3)	0.37 (15)	-0.24 (29)	0.39 (38)	1.02 (4.00)
Group M-3	0.50 (3)	0.50 (15)	-0.05 (29)	0.14 (38)	1.09 (4.00)
Group M-4	0.50 (3)	0.50 (15)	-0.30 (29)	0.28 (38)	0.98 (4.00)
Group N-1	-0.50 (3)	0.22 (15)	-0.10 (29)	0.17 (38)	-0.21 (4.00)
Group O-1	1.00 (3)	n/a	0.08 (25)	n/a	1.08 (2.00)
Group O-2	n/a	n/a	-0.33 (25)	0.45 (34)	0.12 (2.00)
Group O-3	n/a	n/a	n/a	0.52 (34)	0.52 (1.00)
Group O-4	1.00 (3)	n/a	n/a	n/a	1.00 (1.00)

Group P-1	1.00 (3)	0.38 (15)	-0.04 (29)	0.41 (38)	1.75 (4.00)
Group P-2	0.50 (3)	0.52 (15)	-0.22 (29)	0.64 (38)	1.44 (4.00)
Group P-3	1.00 (3)	0.52 (14)	-0.11 (29)	0.65 (37)	2.06 (4.00)
Group P-4	0.50 (3)	0.45 (14)	-0.12 (29)	0.68 (37)	1.51 (4.00)
Group P-5	1.00 (3)	0.55 (15)	-0.02 (29)	0.45 (38)	1.98 (4.00)
Group P-6	0.50 (3)	0.49 (15)	-0.11 (29)	0.56 (38)	1.44 (4.00)
Group R-1	0.50 (3)	0.60 (15)	-0.17 (29)	0.24 (38)	1.17 (4.00)
Group R-2	0.50 (3)	0.62 (15)	-0.15 (29)	0.14 (38)	1.11 (4.00)
Group S-1	1.00 (3)	0.63 (15)	0.30 (29)	0.12 (38)	2.05 (4.00)
Group S-2	0.50 (3)	0.57 (15)	0.13 (29)	0.40 (38)	1.60 (4.00)
Group T-1	-0.50 (3)	0.32 (15)	0.28 (29)	-0.02 (38)	0.08 (4.00)
Group T-2	0.50 (3)	0.40 (15)	-0.14 (29)	0.40 (38)	1.16 (4.00)

S9. Kendall τ nonparametric correlation between the predicted scores and experimental binding affinities by protein for all group-methods. Bolded groups submitted scores for all ligands and are included in the evaluation.

Group-Method	LpxC (n)	Urokinase (n)	Chk1 (n)	Erk2 (n)	Sum τ (max value)
median	0.33 (3)	0.36 (15)	-0.04 (29)	0.26 (38)	0.92 (4.00)
Molecular Wt	0.33 (3)	0.30 (15)	-0.09 (29)	0.27 (38)	0.82 (4.00)
SlogP	-0.33 (3)	0.17 (15)	-0.20 (29)	-0.08 (38)	-0.44 (4.00)
Group A-1	-0.82 (3)	-0.20 (15)	0.02 (29)	0.04 (38)	-0.96 (4.00)
Group B-1	n/a	0.31 (14)	-0.12 (13)	0.07 (27)	0.26 (3.00)
Group C-1	0.33 (3)	0.50 (15)	0.00 (29)	0.20 (38)	1.04 (4.00)
Group C-2	0.33 (3)	0.54 (15)	-0.05 (29)	0.21 (38)	1.04 (4.00)
Group D-1	n/a	0.43 (15)	0.23 (29)	0.41 (38)	1.08 (3.00)
Group D-2	n/a	0.43 (15)	0.23 (29)	0.42 (38)	1.09 (3.00)
Group D-3	n/a	0.39 (15)	0.24 (29)	0.41 (38)	1.05 (3.00)
Group D-4	n/a	0.52 (15)	0.13 (29)	0.33 (38)	0.98 (3.00)
Group D-5	n/a	0.46 (15)	0.12 (29)	0.33 (38)	0.91 (3.00)
Group D-6	n/a	0.42 (15)	0.14 (29)	0.31 (38)	0.87 (3.00)
Group E-1	0.33 (3)	0.34 (15)	0.02 (29)	0.51 (38)	1.21 (4.00)
Group E-2	0.33 (3)	0.34 (15)	0.02 (29)	0.43 (38)	1.12 (4.00)
Group F-1	0.33 (3)	0.38 (15)	-0.18 (29)	0.25 (36)	0.79 (4.00)
Group F-2	-0.33 (3)	0.42 (15)	0.24 (29)	0.28 (36)	0.61 (4.00)
Group F-3	0.33 (3)	0.38 (15)	-0.18 (29)	0.25 (36)	0.78 (4.00)
Group F-4	-0.33 (3)	0.42 (15)	0.24 (29)	0.26 (36)	0.59 (4.00)
Group G-1	1.00 (3)	0.21 (15)	0.12 (29)	0.29 (38)	1.62 (4.00)
Group G-2	1.00 (3)	0.21 (15)	0.07 (29)	n/a	1.28 (3.00)
Group H-1	1.00 (3)	0.17 (15)	0.06 (29)	0.31 (38)	1.54 (4.00)
Group H-2	1.00 (3)	0.21(15)	0.01 (29)	0.35 (38)	1.56 (4.00)
Group I-1	1.00 (3)	0.38(15)	-0.04 (29)	0.12 (38)	1.46 (4.00)
Group I-2	1.00 (3)	0.36 (15)	-0.10 (29)	0.17 (38)	1.43 (4.00)
Group J-1	1.00 (3)	0.30 (15)	0.08 (29)	-0.07 (38)	1.31 (4.00)
Group J-2	-0.33 (3)	0.44 (14)	-0.15 (26)	0.27 (38)	-0.22 (4.00)
Group K-1	n/a	0.38 (15)	0.02 (29)	0.10 (38)	0.50 (3.00)
Group K-2	n/a	0.11 (15)	0.01 (29)	0.03 (38)	0.15 (3.00)
Group L-1	0.33 (3)	0.56 (15)	0.00 (29)	-0.01 (38)	0.88 (4.00)
Group L-2	0.33 (3)	0.54 (15)	0.06 (29)	0.04 (38)	0.97 (4.00)
Group M-1	0.33 (3)	0.26 (15)	-0.11 (29)	0.13 (38)	0.62 (4.00)
Group M-2	0.33 (3)	0.25 (15)	-0.18 (29)	0.27 (38)	0.67 (4.00)
Group M-3	0.33 (3)	0.44 (15)	-0.04 (29)	0.09 (38)	0.83 (4.00)
Group M-4	0.33 (3)	0.36 (15)	-0.22 (29)	0.19 (38)	0.66 (4.00)
Group N-1	-0.33 (3)	0.19 (15)	-0.06 (29)	0.12(38)	-0.08 (4.00)
Group O-1	1.00 (3)	n/a	0.05 (25)	n/a	1.05 (2.00)
Group O-2	n/a	n/a	-0.22 (25)	0.32 (34)	0.10 (2.00)
Group O-3	n/a	n/a	n/a	0.36 (34)	0.36 (1.00)
Group O-4	1.00 (3)	n/a	n/a	n/a	1.00 (1.00)

Group P-1	1.00 (3)	0.28 (15)	-0.04 (29)	0.30 (38)	1.54 (4.00)
Group P-2	0.33 (3)	0.38 (15)	-0.15 (29)	0.47 (38)	1.03 (4.00)
Group P-3	1.00 (3)	0.39 (14)	-0.08 (29)	0.45 (37)	1.76 (4.00)
Group P-4	0.33 (3)	0.35 (14)	-0.06 (29)	0.48 (37)	1.10 (4.00)
Group P-5	1.00 (3)	0.44 (15)	-0.01 (29)	0.33 (38)	1.76 (4.00)
Group P-6	0.33 (3)	0.36 (15)	-0.08 (29)	0.41 (38)	1.03 (4.00)
Group R-1	0.33 (3)	0.44 (15)	-0.13 (29)	0.16 (38)	0.81 (4.00)
Group R-2	0.33 (3)	0.46 (15)	-0.11 (29)	0.10 (38)	0.78 (4.00)
Group S-1	1.00 (3)	0.40 (15)	0.21 (29)	0.10 (38)	1.71 (4.00)
Group S-2	0.33 (3)	0.36 (15)	0.11 (29)	0.28 (38)	1.09 (4.00)
Group T-1	-0.33 (3)	0.26 (15)	0.21 (29)	-0.02 (38)	0.12 (4.00)
Group T-2	0.33 (3)	0.30 (15)	-0.08 (29)	0.28 (38)	0.84 (4.00)

S10. Pearson r parametric correlation between the predicted scores and experimental binding affinities by chemical series for all group-methods. Bolded groups submitted scores for all ligands and are included in the evaluation.

Group-Method	Chk1 (n)	Chk1- Series 1 (n)	Chk1- Series 2 (n)	Chk1- Series 3 (n)	Erk2 (n)	Erk2- Series 1 (n)	Erk2- Series 2 (n)	Erk2- Series 3 (n)
median	-0.01, (29)	0.21, (6)	0.32, (11)	-0.20, (12)	0.37, (38)	0.25, (20)	0.51, (13)	0.53, (5)
Molecular Wt	-0.14, (29)	-0.13, (6)	0.44, (11)	-0.52, (12)	0.40, (38)	0.38, (20)	0.69, (13)	0.21, (5)
SlogP	-0.33, (29)	-0.83, (6)	0.41, (11)	-0.49, (12)	-0.15, (38)	0.14, (20)	0.19, (13)	0.31, (5)
Group A-1	0.01, (29)	0.20, (6)	0.42, (11)	-0.34, (12)	0.11, (38)	0, (20)	0.42, (13)	-0.05, (5)
Group B-1	-0.26, (13)	-0.28, (5)	n/a	-0.53, (8)	0.21, (27)	0.2, (20)	0.82, (7)	n/a
Group C-1	0, (29)	0.12, (6)	0.64, (11)	-0.54, (12)	0.30, (38)	-0.03, (20)	0.68, (13)	0.57, (5)
Group C-2	-0.12, (29)	-0.11, (6)	0.56, (11)	-0.66, (12)	0.34, (38)	0.12, (20)	0.70, (13)	0.50, (5)
Group D-1	0.35, (29)	0.77, (6)	0.40, (11)	0.06, (12)	0.53, (38)	0.49, (20)	0.51, (13)	0.33, (5)
Group D-2	0.35, (29)	0.88, (6)	0.40, (11)	0.06, (12)	0.53, (38)	0.56, (20)	0.58, (13)	0.33, (5)
Group D-3	0.34, (29)	0.90, (6)	0.41, (11)	0.11, (12)	0.52, (38)	0.56, (20)	0.55, (13)	0.39, (5)
Group E-1	0.09, (29)	0.7, (6)	0.32, (11)	0.24, (12)	0.66, (38)	0.63, (20)	0.83, (13)	0.80, (5)
Group E-2	0.01, (29)	0.47, (6)	0.38, (11)	0.13, (12)	0.57, (38)	0.63, (20)	0.60, (13)	0.35, (5)
Group F-1	-0.22, (29)	-0.43, (6)	0.24, (11)	-0.35, (12)	0.41, (36)	0.33, (18)	0.46, (13)	0.54, (5)
Group F-2	0.29, (29)	0.65, (6)	0.56, (11)	-0.16, (12)	0.32, (36)	0.27, (18)	0.51, (13)	0.28, (5)
Group F-3	-0.20, (29)	-0.44, (6)	0.22, (11)	-0.31, (12)	0.40, (36)	0.30, (18)	0.47, (13)	0.53, (5)
Group F-4	0.28, (29)	0.62, (6)	0.57, (11)	-0.19, (12)	0.32, (36)	0.27, (18)	0.51, (13)	0.31, (5)
Group G-1	0.16, (29)	0.5, (6)	0.32, (11)	0.03, (12)	0.41, (38)	0.17, (20)	0.58, (13)	0.61, (5)
Group G-2	0.09, (29)	0.34, (6)	0.28, (11)	-0.05, (12)	n/a	n/a	n/a	n/a
Group H-1	0.02, (29)	0.05, (6)	0.51, (11)	-0.20, (12)	0.46, (38)	0.34, (20)	0.37, (13)	0.98, (5)
Group H-2	0.02, (29)	-0.76, (6)	0.63, (11)	-0.05, (12)	0.47, (38)	0.42, (20)	0.23, (13)	0.94, (5)
Group I-1	-0.12, (29)	-0.22, (6)	0.27, (11)	-0.31, (12)	0.26, (38)	0.02, (20)	0.56, (13)	0.51, (5)
Group I-2	-0.09, (29)	0.31, (6)	0.06, (11)	-0.36, (12)	0.31, (38)	0.02, (20)	0.49, (13)	0.64, (5)
Group J-1	0.30, (29)	0.30, (6)	0.12, (11)	0.85, (12)	-0.02, (38)	0.10, (20)	-0.19, (13)	-0.24, (5)
Group J-2	-0.21, (26)	-0.16, (6)	0.34, (11)	-0.40, (9)	0.37, (38)	0.26, (20)	0.62, (13)	0.64, (5)
Group K-1	0.03, (29)	-0.17, (6)	0.03, (11)	0.05, (12)	0.17, (38)	-0.19, (20)	0.65, (13)	0.55, (5)
Group K-2	0.02, (29)	0.01, (6)	0.21, (11)	0.05, (12)	0.03, (38)	-0.19, (20)	0.33, (13)	0.13, (5)
Group L-1	-0.02, (29)	0.64, (6)	0.01, (11)	0.17, (12)	-0.02, (38)	-0.20, (20)	0.15, (13)	0.19, (5)
Group L-2	0.02, (29)	0.42, (6)	0.32, (11)	-0.03, (12)	0.09, (38)	0.08, (20)	0.25, (13)	-0.03, (5)
Group M-1	-0.15, (29)	-0.06, (6)	-0.11, (11)	-0.09, (12)	0.23, (38)	0.14, (20)	0.52, (13)	0.43, (5)
Group M-2	-0.26, (29)	0.21, (6)	0.32, (11)	-0.71, (12)	0.41, (38)	0.03, (20)	0.62, (13)	0.45, (5)
Group M-3	-0.13, (29)	-0.09, (6)	0.13, (11)	-0.14, (12)	0.16, (38)	0.07, (20)	0.44, (13)	0.25, (5)
Group M-4	-0.31, (29)	0.39, (6)	-0.03, (11)	-0.6, (12)	0.33, (38)	0.19, (20)	0.59, (13)	0.54, (5)
Group N-1	-0.12, (29)	-0.43, (6)	-0.07, (11)	-0.29, (12)	0.03, (38)	-0.21, (20)	-0.14, (13)	0.72, (5)
Group O-1	0.14, (25)	0.80, (6)	0.27, (9)	-0.48, (10)	n/a	n/a	n/a	n/a
Group O-2	-0.34, (25)	0.32, (6)	-0.53, (9)	-0.47, (10)	0.49, (34)	0.53, (20)	0.46, (11)	0.75, (3)
Group O-3	n/a	n/a	n/a	n/a	0.54, (34)	0.59, (20)	0.47, (11)	0.89, (3)
Group P-1	0, (29)	0.13, (6)	0.43, (11)	-0.23, (12)	0.41, (38)	0.11, (20)	0.84, (13)	0.68, (5)
Group P-2	-0.22, (29)	0, (6)	0.2, (11)	-0.54, (12)	0.63, (38)	0.53, (20)	0.82, (13)	0.77, (5)
Group P-3	-0.09, (29)	0.35, (6)	0.43, (11)	-0.65, (12)	0.60, (37)	0.57, (20)	0.63, (13)	0.80, (4)

Group P-4	-0.09, (29)	0.31, (6)	0.50, (11)	-0.63, (12)	0.62, (37)	0.61, (20)	0.68, (13)	0.90, (4)
Group P-5	-0.03, (29)	0.21, (6)	0.39, (11)	-0.38, (12)	0.48, (38)	0.25, (20)	0.72, (13)	0.73, (5)
Group P-6	-0.14, (29)	-0.06, (6)	0.32, (11)	-0.41, (12)	0.55, (38)	0.48, (20)	0.46, (13)	0.75, (5)
Group R-1	-0.12, (29)	-0.36, (6)	0.10, (11)	0, (12)	0.22, (38)	0.18, (20)	0.31, (13)	0.56, (5)
Group R-2	-0.11, (29)	0, (6)	0.28, (11)	-0.36, (12)	0.15, (38)	-0.02, (20)	0.49, (13)	0.23, (5)
Group S-1	0.38, (29)	0.07, (6)	0.50, (11)	0.75, (12)	0.12, (38)	-0.09, (20)	0.54, (13)	0.06, (5)
Group S-2	0.16, (29)	0.76, (6)	-0.08, (11)	0.49, (12)	0.44, (38)	0.32, (20)	0.58, (13)	0.40, (5)
Group T-1	0.32, (29)	0.26, (6)	0.49, (11)	0.42, (12)	-0.07, (38)	-0.10, (20)	-0.09, (13)	0.37, (5)
Group T-2	-0.17, (29)	-0.71, (6)	0.02, (11)	0.03, (12)	0.40, (38)	0.44, (20)	-0.12, (13)	0.73, (5)

S11. Spearman ρ nonparametric correlation between the predicted scores and experimental binding affinities by chemical series for all group-methods. Bolded groups submitted scores for all ligands and are included in the evaluation.

Group-Method	Chk1 (n)	Chk1- Series 1 (n)	Chk1- Series 2 (n)	Chk1- Series 3 (n)	Erk2 (n)	Erk2- Series 1 (n)	Erk2- Series 2 (n)	Erk2- Series 3 (n)
median	-0.03 (29)	0.20, (6)	0.47, (11)	-0.20, (12)	0.31 (38)	0.26, (20)	0.57, (13)	0.50, (5)
Molecular Wt	-0.14 (29)	-0.06, (6)	0.70, (11)	-0.44, (12)	0.40 (38)	0.36, (20)	0.77, (13)	-0.10, (5)
SlogP	-0.29 (29)	-0.67, (6)	0.49, (11)	-0.52, (12)	-0.15 (38)	-0.16, (20)	0.32, (13)	-0.10, (5)
Group A-1	0.02 (29)	0.31, (6)	0.44, (11)	-0.45, (12)	0.06 (38)	-0.11, (20)	0.53, (13)	0.21, (5)
Group B-1	-0.19 (13)	-0.2, (5)	n/a	-0.45, (8)	0.09 (27)	0.09, (20)	0.87, (7)	n/a
Group C-1	-0.02 (29)	-0.06, (6)	0.76, (11)	-0.56, (12)	0.32 (38)	0.05, (20)	0.71, (13)	0.30, (5)
Group C-2	-0.09 (29)	0.03, (6)	0.59, (11)	-0.61, (12)	0.34 (38)	0.04, (20)	0.77, (13)	0.30, (5)
Group D-1	0.32 (29)	0.75, (6)	0.51, (11)	0.06, (12)	0.58 (38)	0.56, (20)	0.63, (13)	0.30, (5)
Group D-2	0.32 (29)	0.70, (6)	0.51, (11)	0.06, (12)	0.58 (38)	0.56, (20)	0.67, (13)	0.30, (5)
Group D-3	0.33 (29)	0.55, (6)	0.51, (11)	0.10, (12)	0.59 (38)	0.55, (20)	0.74, (13)	0.30, (5)
Group D-4	0.18 (29)	0.70, (6)	0.67, (11)	0.17, (12)	0.49 (38)	0.32, (20)	0.74, (13)	0.30, (5)
Group D-5	0.17 (29)	0.70, (6)	0.67, (11)	0.17, (12)	0.49 (38)	0.32, (20)	0.75, (13)	0.10, (5)
Group D-6	0.19 (29)	0.70, (6)	0.73, (11)	0.15, (12)	0.48 (38)	0.29, (20)	0.74, (13)	0.50, (5)
Group E-1	0.03 (29)	0.38, (6)	0.36, (11)	0.18, (12)	0.67 (38)	0.71, (20)	0.83, (13)	0.90, (5)
Group E-2	0.05 (29)	0.46, (6)	0.66, (11)	0.1, (12)	0.58 (38)	0.71, (20)	0.6, (13)	0.10, (5)
Group F-1	-0.25 (29)	-0.46, (6)	0.13, (11)	-0.41, (12)	0.40 (36)	0.29, (18)	0.45, (13)	0.30, (5)
Group F-2	0.35 (29)	0.58, (6)	0.71, (11)	-0.20, (12)	0.38 (36)	0.38, (18)	0.51, (13)	0, (5)
Group F-3	-0.25 (29)	-0.38, (6)	0.03, (11)	-0.44, (12)	0.39 (36)	0.32, (18)	0.43, (13)	0.30, (5)
Group F-4	0.36 (29)	0.64, (6)	0.71, (11)	-0.21, (12)	0.35(36)	0.36, (18)	0.52, (13)	0, (5)
Group G-1	0.18 (29)	0.41, (6)	0.61, (11)	-0.14, (12)	0.42 (38)	0.14, (20)	0.62, (13)	0.70, (5)
Group G-2	0.10 (29)	0.20, (6)	0.17, (11)	-0.06, (12)	n/a	n/a	n/a	n/a
Group H-1	0.06 (29)	0.03, (6)	0.60, (11)	-0.19, (12)	0.45 (38)	0.24, (20)	0.36, (13)	0.90, (5)
Group H-2	0.01 (29)	-0.93, (6)	0.80, (11)	-0.27, (12)	0.50 (38)	0.40, (20)	0.33, (13)	0.90, (5)
Group I-1	-0.09 (29)	-0.23, (6)	0.34, (11)	-0.27, (12)	0.22 (38)	-0.07, (20)	0.49, (13)	0.40, (5)
Group I-2	-0.14 (29)	0.50, (6)	-0.14, (11)	-0.51, (12)	0.30 (38)	0.02, (20)	0.55, (13)	0.40, (5)
Group J-1	0.10 (29)	0.46, (6)	-0.30, (11)	0.75, (12)	-0.08 (38)	0.01, (20)	-0.28, (13)	-0.20, (5)
Group J-2	-0.20 (26)	-0.17, (6)	0.27, (11)	-0.18, (9)	0.42 (38)	0.42, (20)	0.64, (13)	0.90, (5)
Group K-1	0.02 (29)	0.03, (6)	0.71, (11)	-0.14, (12)	0.13 (38)	-0.37, (20)	0.75, (13)	0.60, (5)
Group K-2	0.02 (29)	0.03, (6)	0.67, (11)	-0.02, (12)	0.03 (38)	-0.21, (20)	0.49, (13)	0.50, (5)
Group L-1	0.01 (29)	0.67, (6)	0.03, (11)	0.38, (12)	-0.04 (38)	-0.21, (20)	0.58, (13)	0.60, (5)
Group L-2	0.08 (29)	0.26, (6)	0.22, (11)	0, (12)	0.05 (38)	-0.05, (20)	0.42, (13)	-0.10, (5)
Group M-1	-0.16 (29)	-0.2, (6)	0.14, (11)	-0.16, (12)	0.21 (38)	0.04, (20)	0.50, (13)	-0.20, (5)
Group M-2	-0.24 (29)	-0.12, (6)	0.16, (11)	-0.69, (12)	0.39 (38)	0.29, (20)	0.59, (13)	0.30, (5)
Group M-3	-0.05 (29)	-0.03, (6)	0.36, (11)	-0.15, (12)	0.14 (38)	0.03, (20)	0.36, (13)	0.10, (5)
Group M-4	-0.30 (29)	0.32, (6)	-0.12, (11)	-0.61, (12)	0.28 (38)	0.20, (20)	0.57, (13)	0.60, (5)
Group N-1	-0.10 (29)	-0.41, (6)	-0.03, (11)	-0.23, (12)	0.17 (38)	-0.01, (20)	0.07, (13)	0.60, (5)
Group O-1	0.08 (25)	0.64, (6)	0.65, (9)	-0.53, (10)	n/a	n/a	n/a	n/a
Group O-2	-0.33 (25)	0.41, (6)	-0.1, (9)	-0.55, (10)	0.45 (34)	0.50, (20)	0.38, (11)	0.50, (3)

Group O-3	n/a	n/a	n/a	n/a	0.52 (34)	0.60, (20)	0.38, (11)	0.50, (3)
Group P-1	-0.04 (29)	0.03, (6)	0.5, (11)	-0.35, (12)	0.41 (38)	0.04, (20)	0.94, (13)	0.40, (5)
Group P-2	-0.22 (29)	-0.23, (6)	0.31, (11)	-0.53, (12)	0.64 (38)	0.45, (20)	0.82, (13)	0.80, (5)
Group P-3	-0.11 (29)	0.32, (6)	0.67, (11)	-0.68, (12)	0.65 (37)	0.55, (20)	0.7, (13)	0.80, (4)
Group P-4	-0.12 (29)	0.23, (6)	0.72, (11)	-0.59, (12)	0.68 (37)	0.60, (20)	0.71, (13)	0.80, (4)
Group P-5	-0.02 (29)	-0.06, (6)	0.73, (11)	-0.43, (12)	0.45 (38)	0.11, (20)	0.71, (13)	0.70, (5)
Group P-6	-0.11 (29)	-0.06, (6)	0.51, (11)	-0.49, (12)	0.56 (38)	0.41, (20)	0.48, (13)	0.80, (5)
Group R-1	-0.17 (29)	-0.35, (6)	0.15, (11)	-0.11, (12)	0.24 (38)	0.23, (20)	0.28, (13)	0.30, (5)
Group R-2	-0.15 (29)	0.06, (6)	0.36, (11)	-0.46, (12)	0.14 (38)	-0.11, (20)	0.65, (13)	0.40, (5)
Group S-1	0.30 (29)	0.17, (6)	0.23, (11)	0.63, (12)	0.12 (38)	-0.13, (20)	0.47, (13)	0.30, (5)
Group S-2	0.13 (29)	0.75, (6)	-0.17, (11)	0.57, (12)	0.40 (38)	0.27, (20)	0.60, (13)	0.30, (5)
Group T-1	0.28 (29)	0.23, (6)	0.54, (11)	0.30, (12)	-0.02 (38)	-0.08, (20)	-0.01, (13)	0.70, (5)
Group T-2	-0.14 (29)	-0.67, (6)	0.21, (11)	0.08, (12)	0.40 (38)	0.46, (20)	-0.09, (13)	0.60, (5)

S12. Kendall τ nonparametric correlation between the predicted scores and experimental binding affinities by chemical series for all group-methods. Bolded groups submitted scores for all ligands and are included in the evaluation.

Group-Method	Chk1 (n)	Chk1- Series 1 (n)	Chk1- Series 2 (n)	Chk1- Series 3 (n)	Erk2 (n)	Erk2- Series 1 (n)	Erk2- Series 2 (n)	Erk2- Series 3 (n)
median	-0.04 (29)	0.14, (6)	0.34, (11)	-0.15, (12)	0.26 (38)	0.17, (20)	0.43, (13)	0.33, (5)
Molecular Wt	-0.09 (29)	0, (6)	0.54, (11)	-0.31, (12)	0.27 (38)	0.22, (20)	0.61, (13)	0, (5)
SlogP	-0.20 (29)	-0.55, (6)	0.35, (11)	-0.34, (12)	-0.08 (38)	-0.11, (20)	0.18, (13)	0, (5)
Group A-1	0.02 (29)	0.23, (6)	0.29, (11)	-0.33, (12)	0.04 (38)	-0.12, (20)	0.39, (13)	0.11, (5)
Group B-1	-0.12 (13)	-0.20, (5)	n/a	-0.36, (8)	0.07 (27)	0.05, (20)	0.75, (7)	n/a
Group C-1	0 (29)	0, (6)	0.56, (11)	-0.43, (12)	0.20 (38)	0.03, (20)	0.56, (13)	0.20, (5)
Group C-2	-0.05 (29)	0.14, (6)	0.45, (11)	-0.49, (12)	0.21 (38)	0.01, (20)	0.59, (13)	0.20, (5)
Group D-1	0.23 (29)	0.69, (6)	0.41, (11)	0, (12)	0.41 (38)	0.39, (20)	0.48, (13)	0.20, (5)
Group D-2	0.23 (29)	0.55, (6)	0.41, (11)	0, (12)	0.42 (38)	0.39, (20)	0.55, (13)	0.20, (5)
Group D-3	0.24 (29)	0.41, (6)	0.41, (11)	-0.05, (12)	0.41 (38)	0.33, (20)	0.59, (13)	0.20, (5)
Group D-4	0.13 (29)	0.55, (6)	0.52, (11)	0.18, (12)	0.33 (38)	0.20, (20)	0.56, (13)	0.20, (5)
Group D-5	0.12 (29)	0.55, (6)	0.52, (11)	0.18, (12)	0.33 (38)	0.20, (20)	0.56, (13)	0, (5)
Group D-6	0.14 (29)	0.55, (6)	0.56, (11)	0.15, (12)	0.31 (38)	0.17, (20)	0.56, (13)	0.40, (5)
Group E-1	0.02 (29)	0.28, (6)	0.26, (11)	0.15, (12)	0.51 (38)	0.50, (20)	0.72, (13)	0.80, (5)
Group E-2	0.02 (29)	0.28, (6)	0.41, (11)	0.06, (12)	0.43 (38)	0.51, (20)	0.46, (13)	0, (5)
Group F-1	-0.18 (29)	-0.41, (6)	0.15, (11)	-0.28, (12)	0.25 (36)	0.16, (18)	0.33, (13)	0.20, (5)
Group F-2	0.24 (29)	0.41, (6)	0.49, (11)	-0.15, (12)	0.28 (36)	0.25, (18)	0.41, (13)	0.20, (5)
Group F-3	-0.18 (29)	-0.28, (6)	0.07, (11)	-0.34, (12)	0.25 (36)	0.18, (18)	0.27, (13)	0.20, (5)
Group F-4	0.24 (29)	0.55, (6)	0.49, (11)	-0.15, (12)	0.26 (36)	0.24, (18)	0.41, (13)	0.20, (5)
Group G-1	0.12 (29)	0.41, (6)	0.45, (11)	-0.09, (12)	0.29 (38)	0.10, (20)	0.51, (13)	0.60, (5)
Group G-2	0.07 (29)	0.14, (6)	0.15, (11)	0.06, (12)	n/a	n/a	n/a	n/a
Group H-1	0.06 (29)	0.14, (6)	0.49, (11)	-0.12, (12)	0.31 (38)	0.16, (20)	0.3, (13)	0.80, (5)
Group H-2	0.01 (29)	-0.83, (6)	0.67, (11)	-0.15, (12)	0.35 (38)	0.29, (20)	0.22, (13)	0.80, (5)
Group I-1	-0.04 (29)	-0.14, (6)	0.22, (11)	-0.12, (12)	0.12 (38)	-0.08, (20)	0.27, (13)	0.40, (5)
Group I-2	-0.10 (29)	0.36, (6)	-0.09, (11)	-0.41, (12)	0.17 (38)	0.02, (20)	0.31, (13)	0.40, (5)
Group J-1	0.08 (29)	0.28, (6)	-0.19, (11)	0.58, (12)	-0.07 (38)	-0.01, (20)	-0.20, (13)	-0.20, (5)
Group J-2	-0.15 (26)	-0.14, (6)	0.19, (11)	-0.08, (9)	0.27 (38)	0.23, (20)	0.51, (13)	0.80, (5)
Group K-1	0.02 (29)	0.14, (6)	0.52, (11)	-0.09, (12)	0.10 (38)	-0.25, (20)	0.56, (13)	0.40, (5)
Group K-2	0.01 (29)	0.14, (6)	0.49, (11)	-0.15, (12)	0.03 (38)	-0.10, (20)	0.30, (13)	0.20, (5)
Group L-1	0.00 (29)	0.55, (6)	0, (11)	0.25, (12)	-0.01 (38)	-0.20, (20)	0.48, (13)	0.40, (5)
Group L-2	0.06 (29)	0.28, (6)	0.19, (11)	0.06, (12)	0.04 (38)	-0.05, (20)	0.30, (13)	0, (5)
Group M-1	-0.11 (29)	-0.14, (6)	0.15, (11)	-0.15, (12)	0.13 (38)	0.04, (20)	0.41, (13)	-0.20, (5)
Group M-2	-0.18 (29)	0, (6)	0.07, (11)	-0.57, (12)	0.27 (38)	0.20, (20)	0.43, (13)	0.20, (5)
Group M-3	-0.04 (29)	-0.14, (6)	0.26, (11)	-0.12, (12)	0.09 (38)	0.02, (20)	0.30, (13)	0, (5)
Group M-4	-0.22 (29)	0.28, (6)	-0.07, (11)	-0.46, (12)	0.19 (38)	0.12, (20)	0.51, (13)	0.40, (5)
Group N-1	-0.06 (29)	-0.28, (6)	0.02, (11)	-0.15, (12)	0.12(38)	-0.02, (20)	0.08, (13)	0.40, (5)
Group O-1	0.05 (25)	0.41, (6)	0.54, (9)	-0.38, (10)	n/a	n/a	n/a	n/a
Group O-2	-0.22 (25)	0.14, (6)	-0.03, (9)	-0.42, (10)	0.32 (34)	0.36, (20)	0.31, (11)	0.33, (3)
Group O-3	n/a	n/a	n/a	n/a	0.36 (34)	0.43, (20)	0.31, (11)	0.33, (3)
Group O-4	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Group P-1	-0.04 (29)	0.14, (6)	0.37, (11)	-0.25, (12)	0.30 (38)	0.02, (20)	0.82, (13)	0.40, (5)
Group P-2	-0.15 (29)	-0.14, (6)	0.30, (11)	-0.40, (12)	0.47 (38)	0.26, (20)	0.67, (13)	0.60, (5)
Group P-3	-0.08 (29)	0.28, (6)	0.52, (11)	-0.52, (12)	0.45 (37)	0.36, (20)	0.51, (13)	0.67, (4)
Group P-4	-0.06 (29)	0.14, (6)	0.52, (11)	-0.43, (12)	0.48 (37)	0.43, (20)	0.54, (13)	0.67, (4)
Group P-5	-0.01 (29)	0, (6)	0.52, (11)	-0.31, (12)	0.33 (38)	0.09, (20)	0.56, (13)	0.60, (5)
Group P-6	-0.08 (29)	0, (6)	0.41, (11)	-0.40, (12)	0.41 (38)	0.29, (20)	0.38, (13)	0.60, (5)
Group R-1	-0.13 (29)	-0.28, (6)	0.19, (11)	-0.06, (12)	0.16 (38)	0.17, (20)	0.14, (13)	0.20, (5)
Group R-2	-0.11 (29)	0.14, (6)	0.26, (11)	-0.31, (12)	0.10 (38)	-0.07, (20)	0.46, (13)	0.40, (5)
Group S-1	0.21 (29)	0.14, (6)	0.22, (11)	0.43, (12)	0.10 (38)	-0.10, (20)	0.38, (13)	0.20, (5)
Group S-2	0.11 (29)	0.69, (6)	-0.07, (11)	0.43, (12)	0.28 (38)	0.20, (20)	0.43, (13)	0.20, (5)
Group T-1	0.21 (29)	0.14, (6)	0.41, (11)	0.22, (12)	-0.02 (38)	-0.05, (20)	-0.01, (13)	0.60, (5)
Group T-2	-0.08 (29)	-0.55, (6)	0.22, (11)	0.03, (12)	0.28 (38)	0.32, (20)	-0.09, (13)	0.40, (5)

S13. AUC values derived from ROC curves by protein for all group-methods. Bolded groups submitted scores for all ligands and are included in the evaluation.

Group-Method	LpxC (nactive, nnonactive)	Urokinase (nactive, nnonactive)	Chk1 (nactive, nnonactive)	Sum AUCs (max value)	Urokinase + Chk1 Sum AUCs (max value)
median	0.21 (3, 8)	0.83 (15, 4)	0.56 (30, 9)	1.60 (3.00)	1.39 (2.00)
Molecular Wt	0.83 (3, 8)	0.55 (15, 4)	0.69 (30, 9)	2.08 (3.00)	1.24 (2.00)
SlogP	0.13 (3, 8)	0.72 (15, 4)	0.49 (30, 9)	1.33 (3.00)	1.21 (2.00)
Group A-1	0.71 (3, 8)	0.25 (15, 4)	0.69 (30, 9)	1.64 (3.00)	0.94 (2.00)
Group B-1	1.00 (1, 7)	0.61 (14, 2)	0.72 (13, 5)	2.33 (3.00)	1.33 (2.00)
Group C-1	0.04 (3, 8)	0.97 (15, 4)	0.59 (30, 9)	1.60 (3.00)	1.56 (2.00)
Group C-2	0.04 (3, 8)	0.78 (15, 4)	0.60 (30, 9)	1.42 (3.00)	1.38 (2.00)
Group D-1	n/a	0.93 (15, 4)	0.76 (30, 9)	1.69 (2.00)	1.69 (2.00)
Group D-2	n/a	0.95 (15, 4)	0.76 (30, 9)	1.71 (2.00)	1.71 (2.00)
Group D-3	n/a	0.95 (15, 4)	0.73 (30, 9)	1.68 (2.00)	1.68 (2.00)
Group D-4	n/a	0.97 (15, 4)	0.69 (30, 9)	1.65 (2.00)	1.65 (2.00)
Group D-5	n/a	0.97 (15, 4)	0.70 (30, 9)	1.66 (2.00)	1.66 (2.00)
Group D-6	n/a	0.97 (15, 4)	0.70 (30, 9)	1.66 (2.00)	1.66 (2.00)
Group E-1	0.08 (3, 8)	0.83 (15, 4)	0.64 (30, 9)	1.55 (3.00)	1.47 (2.00)
Group E-2	0.08 (3, 8)	0.83 (15, 4)	0.54 (30, 9)	1.46 (3.00)	1.37 (2.00)
Group F-1	0.17 (3, 8)	0.83 (15, 4)	0.56 (30, 9)	1.56 (3.00)	1.40 (2.00)
Group F-2	0.04 (3, 8)	0.60 (15, 4)	0.65 (30, 9)	1.29 (3.00)	1.25 (2.00)
Group F-3	0.21 (3, 8)	0.85 (15, 4)	0.56 (30, 9)	1.62 (3.00)	1.41 (2.00)
Group F-4	0 (3, 8)	0.58 (15, 4)	0.64 (30, 9)	1.22 (3.00)	1.22 (2.00)
Group G-1	0.33 (3, 8)	0.63 (15, 4)	0.41 (30, 9)	1.38 (3.00)	1.04 (2.00)
Group G-2	0.04 (3, 8)	0.63 (15, 4)	0.49 (30, 9)	1.17 (3.00)	1.13 (2.00)
Group H-1	0.42 (3, 8)	0.83 (15, 4)	0.55 (30, 9)	1.80 (3.00)	1.38 (2.00)
Group H-2	0.25 (3, 8)	0.83 (15, 4)	0.56 (30, 9)	1.64 (3.00)	1.39 (2.00)
Group I-1	0 (3, 8)	0.68 (15, 4)	0.46 (30, 9)	1.14 (3.00)	1.14 (2.00)
Group I-2	0.33 (3, 8)	0.73 (15, 4)	0.38 (30, 9)	1.44 (3.00)	1.11 (2.00)
Group J-1	0.92 (3, 8)	0.97 (15, 4)	0.44 (30, 9)	2.32 (3.00)	1.41 (2.00)
Group J-2	0.17 (3, 8)	0.93 (14, 2)	0.68 (27, 8)	1.78 (3.00)	1.61 (2.00)
Group K-1	n/a	1 (15, 4)	0.69 (30, 9)	1.69 (2.00)	1.69 (2.00)
Group K-2	n/a	1 (15, 4)	0.57 (30, 9)	1.57 (2.00)	1.57 (2.00)
Group L-1	0.75 (3, 8)	0.98 (15, 4)	0.49 (30, 9)	2.22 (3.00)	1.47 (2.00)
Group L-2	1 (3, 8)	0.97 (15, 4)	0.47 (30, 9)	2.44 (3.00)	1.44 (2.00)
Group M-1	0.13 (3, 8)	0.8 (15, 4)	0.55 (30, 9)	1.48 (3.00)	1.35 (2.00)
Group M-2	0.42 (3, 8)	0.78 (15, 4)	0.43 (30, 9)	1.63 (3.00)	1.21 (2.00)
Group M-3	0.13 (3, 8)	0.82 (15, 4)	0.47 (30, 9)	1.41 (3.00)	1.29 (2.00)
Group M-4	0.42 (3, 8)	0.78 (15, 4)	0.42 (30, 9)	1.62 (3.00)	1.21 (2.00)
Group N-1	0.79 (3, 8)	0.82 (15, 4)	0.50 (30, 9)	2.11 (3.00)	1.32 (2.00)
Group O-1	0 (3, 8)	n/a	0.53 (25, 9)	0.53 (2.00)	-
Group O-2	n/a	n/a	0.41 (25, 9)	0.41 (1.00)	-
Group P-1	0.38 (3, 8)	0.72 (15, 4)	0.62 (30, 9)	1.71 (3.00)	1.34 (2.00)
Group P-2	0.21 (3, 8)	0.75 (15, 4)	0.72 (30, 9)	1.68 (3.00)	1.47 (2.00)

Group P-3	0.33 (3, 8)	0.91 (14, 4)	0.73 (30, 9)	1.98 (3.00)	1.64 (2.00)
Group P-4	0.08 (3, 8)	0.71 (14, 4)	0.74 (30, 9)	1.54 (3.00)	1.46 (2.00)
Group P-5	0.33 (3, 8)	0.97 (15, 4)	0.75 (30, 9)	2.05 (3.00)	1.71 (2.00)
Group P-6	0.21 (3, 8)	0.77 (15, 4)	0.74 (30, 9)	1.72 (3.00)	1.51 (2.00)
Group R-1	0.17 (3, 8)	0.53 (15, 4)	0.53 (30, 9)	1.23 (3.00)	1.06(2.00)
Group R-2	0.13 (3, 8)	0.57 (15, 4)	0.52 (30, 9)	1.21 (3.00)	1.08 (2.00)
Group S-1	0.79 (3, 8)	0.83 (15, 4)	0.47 (30, 9)	2.10 (3.00)	1.31 (2.00)
Group S-2	0.67 (3, 8)	0.90 (15, 4)	0.43 (30, 9)	1.99 (3.00)	1.33 (2.00)
Group T-1	0.92 (3, 8)	0.33 (15, 4)	0.53 (30, 9)	1.78 (3.00)	0.87 (2.00)
Group T-2	0 (3, 8)	0.72 (15, 4)	0.66 (30, 9)	1.38 (3.00)	1.38 (2.00)

S14. AUC values derived from ROC curves by all series of Chk1 for all group-methods. Bolded groups submitted scores for all ligands and are included in the evaluation.

Group-Method	Chk1 (nactive, nnonactive)	Chk1-Series 1 (nactive, nnonactive)	Chk1-Series 2 (nactive, nnonactive)	Chk1-Series 3 (nactive, nnonactive)
median	0.56 (30, 9)	0.61 (6, 3)	0.69 (12, 2)	0.56 (12, 4)
Molecular Wt	0.69 (30, 9)	0.33 (6, 3)	0.38 (12, 2)	0.52 (12, 4)
SlogP	0.49 (30, 9)	0.78 (6, 3)	0.75 (12, 2)	0.65 (12, 4)
Group A-1	0.69 (30, 9)	0.50 (6, 3)	0.92 (12, 2)	0.75 (12, 4)
Group B-1	0.72 (13, 5)	0.73 (5, 3)	n/a	0.81 (8, 2)
Group C-1	0.59 (30, 9)	0.33 (6, 3)	0.79 (12, 2)	0.65 (12, 4)
Group C-2	0.60 (30, 9)	0.33 (6, 3)	0.83 (12, 2)	0.56 (12, 4)
Group D-1	0.76 (30, 9)	0.72 (6, 3)	0.88 (12, 2)	0.73 (12, 4)
Group D-2	0.76 (30, 9)	0.72 (6, 3)	0.88 (12, 2)	0.73 (12, 4)
Group D-3	0.73 (30, 9)	0.78 (6, 3)	0.83 (12, 2)	0.73 (12, 4)
Group D-4	0.69 (30, 9)	0.56 (6, 3)	0.79 (12, 2)	0.73 (12, 4)
Group D-5	0.70 (30, 9)	0.61 (6, 3)	0.79 (12, 2)	0.73 (12, 4)
Group D-6	0.70 (30, 9)	0.61 (6, 3)	0.79 (12, 2)	0.73 (12, 4)
Group E-1	0.64 (30, 9)	0.78 (6, 3)	0.75 (12, 2)	0.75 (12, 4)
Group E-2	0.54 (30, 9)	0.67 (6, 3)	0.33 (12, 2)	0.73 (12, 4)
Group F-1	0.56 (30, 9)	0.61 (6, 3)	0.67 (12, 2)	0.60 (12, 4)
Group F-2	0.65 (30, 9)	0.56 (6, 3)	0.79 (12, 2)	0.44 (12, 4)
Group F-3	0.56 (30, 9)	0.56 (6, 3)	0.67 (12, 2)	0.60 (12, 4)
Group F-4	0.64 (30, 9)	0.56 (6, 3)	0.79 (12, 2)	0.44 (12, 4)
Group G-1	0.41 (30, 9)	0.50 (6, 3)	0.50 (12, 2)	0.33 (12, 4)
Group G-2	0.49 (30, 9)	0.39 (6, 3)	0.58 (12, 2)	0.48 (12, 4)
Group H-1	0.55 (30, 9)	0.39 (6, 3)	0.79 (12, 2)	0.48 (12, 4)
Group H-2	0.56 (30, 9)	0.39 (6, 3)	0.83 (12, 2)	0.52 (12, 4)
Group I-1	0.46 (30, 9)	0.72 (6, 3)	0.38 (12, 2)	0.40 (12, 4)
Group I-2	0.38 (30, 9)	0.61 (6, 3)	0.08 (12, 2)	0.35 (12, 4)
Group J-1	0.44 (30, 9)	0.17 (6, 3)	0.38 (12, 2)	0.44 (12, 4)
Group J-2	0.68 (27, 8)	0.92 (6, 2)	0.54 (12, 2)	0.64 (9, 4)
Group K-1	0.69 (30, 9)	0.83 (6, 3)	0.79 (12, 2)	0.56 (12, 4)
Group K-2	0.57 (30, 9)	0.50 (6, 3)	0.83 (12, 2)	0.46 (12, 4)
Group L-1	0.49 (30, 9)	0.67 (6, 3)	0.63 (12, 2)	0.54 (12, 4)
Group L-2	0.47 (30, 9)	0.22 (6, 3)	0.63 (12, 2)	0.44 (12, 4)
Group M-1	0.55 (30, 9)	0.72 (6, 3)	0.71 (12, 2)	0.48 (12, 4)
Group M-2	0.43 (30, 9)	0.56 (6, 3)	0.25 (12, 2)	0.48 (12, 4)
Group M-3	0.47 (30, 9)	0.67 (6, 3)	0.33 (12, 2)	0.42 (12, 4)
Group M-4	0.42 (30, 9)	0.56 (6, 3)	0.13 (12, 2)	0.46 (12, 4)
Group N-1	0.50 (30, 9)	0.5 (6, 3)	0.54 (12, 2)	0.40 (12, 4)
Group O-1	0.53 (25, 9)	0.44 (6, 3)	0.5 (9, 2)	0.55 (10, 4)
Group O-2	0.41 (25, 9)	0.22 (6, 3)	0.39 (9, 2)	0.53 (10, 4)
Group P-1	0.62 (30, 9)	0.67 (6, 3)	0.71 (12, 2)	0.63 (12, 4)
Group P-2	0.72 (30, 9)	0.89 (6, 3)	0.58 (12, 2)	0.71 (12, 4)
Group P-3	0.73 (30, 9)	0.83 (6, 3)	0.79 (12, 2)	0.73 (12, 4)

Group P-4	0.74 (30, 9)	0.83 (6, 3)	0.71 (12, 2)	0.75 (12, 4)
Group P-5	0.75 (30, 9)	0.89 (6, 3)	0.75 (12, 2)	0.69 (12, 4)
Group P-6	0.74 (30, 9)	0.83 (6, 3)	0.75 (12, 2)	0.73 (12, 4)
Group R-1	0.53 (30, 9)	0.61 (6, 3)	0.40 (12, 2)	0.50 (12, 4)
Group R-2	0.52 (30, 9)	0.61 (6, 3)	0.38 (12, 2)	0.50 (12, 4)
Group S-1	0.47 (30, 9)	0.28 (6, 3)	0.42 (12, 2)	0.56 (12, 4)
Group S-2	0.43 (30, 9)	0.56 (6, 3)	0.25 (12, 2)	0.65 (12, 4)
Group T-1	0.53 (30, 9)	0.44 (6, 3)	0.71 (12, 2)	0.48 (12, 4)
Group T-2	0.66 (30, 9)	0.78 (6, 3)	0.58 (12, 2)	0.67 (12, 4)