

Supporting Information

K_{DEEP} : Protein-ligand absolute binding affinity prediction via 3D-convolutional neural networks.

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1 Compounds in the PDBbind v.2016 *refined* training set

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2cej, 3ryz, 4bf1, 4fcf, 4hf4, 4jx9, 5egm, 3f17, 1g45, 1mue, 1r1j, 1t31, 2qry, 3hkw, 3s71, 4pft, 4zyf, 5e8f, 6std, 2oax, 1i9n, 3d1x, 3nox, 2qd6, 2q55, 1bcd, 1g4j, 1hfs, 1jgl, 1jyq, 1lnm, 1ohr, 1pxo, 1t7j, 1w13, 1xap, 2b7d, 2f8g, 2fmb, 2h4n, 2jh0, 2ojj, 2pcp, 2uwo, 2vj8, 2wgj, 2wyg, 2y5f, 2y7z, 2y81, 3brn, 3d9z, 3eqr, 3hvj, 3i5z, 3i60, 3s73, 4a7i, 4bah, 4eo6, 4hy1, 4r5a, 4rwj, 4yth, 4zwx, 4zwz, 5e2o, 3ckz, 3p8o, 3ts4, 4ish, 4x6o, 1b6k, 1mjj, 1sdv, 3rz1, 4ei4, 4gii, 1bnv, 1d4l, 1qft, 1x38, 1zp8, 2wkz, 3qdd, 4e4l, 4m0f, 4yhq, 1fkn, 1g46, 1w5w, 3d1z, 3oaf, 3rt4, 5cau, 5e2p, 1ork, 1g54, 1m0b, 2zxx, 3fvk, 3nu4, 4i5c, 4ks1, 4x6n, 1lhu, 3mxd, 1d4i, 2avo, 2obf, 3b67, 4gj3, 5cas, 2xej, 1n3i, 1nfy, 1nt1, 2idw, 2y7x, 3ekp, 3vhc, 3zze, 4cst, 4yc9, 3egt, 4bak, 1ec1, 1kzn, 1r1h, 3k37, 4e6d, 4heg, 4bam, 1j37, 1nfw, 2p4j, 3dcc, 3i9g, 3rz7, 3v5p, 4ag8, 1apv, 1e3g, 1fm9, 1k27, 1mq5, 1mu8, 1y0l, 2j4i, 2wyj, 3jrx, 3u6h, 3u6i, 4c2v, 4h3f, 4x5q, 2q54, 4baq, 4jh0, 4xtw, 1ec3, 1g53, 3m37, 3vfb, 1ebw, 1ezq, 1kdk, 1s63, 3hb4, 3nu9, 4e4n, 4i72, 1nw4, 2qd8, 3gba, 4cmo, 1bnw, 2rkf, 3a2o, 3ffg, 3sue, 3x00, 1d3d, 1msn, 2v58, 2w8y, 4zls, 2qd7, 3lea, 3lpk, 3mdz, 3o56, 3pwm, 3vf7, 4az6, 4hws, 1d9i, 4xu0, 3ttp, 1ta6, 2wb5, 3su3, 2qmg, 2xjx, 3d91, 3ibu, 4clj, 4p6w, 5aml, 8cpa, 1z71, 2fgu, 2xb7, 2xy9, 3ozg, 3vfa, 1mh5, 4xty, 1d4k, 1fcz, 1hpo, 1hps, 1hvp, 1uho, 1x39, 1zvx, 2cer, 2o4l, 3rwp, 4s1g, 4xu2, 4dv8, 3zlr, 1sdt, 2xab, 3nzk, 4xtv, 1xow, 3kdc, 3p8n, 3rux, 3vhd, 4asd, 4n6h, 2ayr, 2iw4, 2yxj, 3nu6, 4crf, 4er2, 4qge, 1bn4, 3rdq, 2aqu, 3wha, 1bn1, 3vf5, 2e27, 2p95, 3nuj, 4ca5, 1ebz, 1fkf, 1ksn, 1met, 1pme, 2o4r, 2w26, 4a4q, 4erf, 3ekv, 3ekx, 1hsh, 3bgs, 3rbu, 1g1d, 4mc9, 4b7p, 1qbs, 4wko, 1xjd, 1bnq, 4xu1, 4xu3, 1hvr, 1s19, 2p4s, 1m4h, 2ax9, 2bys, 2g94, 2gvj, 2hoc, 3fv3, 3g5k, 1g52, 3ppm, 1dmp, 1ws1, 4wkp, 1i37, 1o86, 2z4o, 4ax9, 4gql, 4mc6, 5cjf, 4gqp, 3s56, 1if8, 2zx8, 3el1, 3s54, 4b7r, 3pe1, 3dp9, 4zip, 1bnu, 1df8, 1fkb, 1mrw, 2vh6, 3sm2, 4cd0, 4fk6, 4crl, 3fuc, 4wkn, 1nh0, 3dk1, 3p3g, 3pe2, 3ggg, 456c, 4x24, 1bnt, 3lxx, 3nuo, 1pvn, 3m36, 3nu3, 4eb8, 4wup, 4xtz, 4zo5, 2xef, 2std, 3kdb, 3rdo, 1bn3, 2drc, 1hxb, 1zsf, 2vnp, 3ies, 3rlb, 1hvl, 1bv9, 1fjs, 2xmy, 4m8y, 1bnn, 1bxo, 1d4h, 1ec2, 1flr, 1gar, 1igj, 1rjk, 3h5b, 4lhv, 3mxe, 1n4k, 1nm6, 3lzu, 1sdu, 1sr7, 2o4j, 2p16, 4f3k, 3ps1, 4ww8, 4ggz, 1ie9, 2qi3, 4m8x, 2qi7, 4ww6, 3t3c, 1qbu, 1rr6, 1bv7, 1c70, 1hvs, 4djg, 4std, 3i6o, 4ngm, 4q1y, 4lvt, 1c4u, 4ynb, 1kzk, 4wt2, 2qi4, 4ffs, 2o4k, 1msm, 2zx7, 5std, 2o4s, 1b8n, 1if7, 1n46, 2f81, 4yo8, 1g2o, 4djp, 1qbr, 2qi6, 4xtx, 3djk, 3ekt, 2zx6, 1qbt, 2xei, 4lch, 1b8o, 1dif, 3cs7, 2pk5, 2wva, 2xeg, 3o9a, 4agc, 5alb, 2o4p, 3o9d, 7std, 4omc, 3gi4, 4hla, 5c1m, 1hwx, 3o99, 2qi5, 3i7e, 2pk6, 4i8w, 1hvi, 1hvk, 1m7y, 3lzs, 4ase, 4kb9, 5bs4, 1q84, 4i8z, 5dgw, 1x1z, 3k8o, 1d4y, 3std, 4q1x, 2i4v, 3gi5, 3gi6, 3ok9, 4u8w, 1hpx, 4ryd, 3k8q, 1pro, 2q5k, 2xpk, 3o9e, 3st5, 4gbd, 2j62, 2hb3, 5dgu, 1hvj, 2i0a, 1lyb, 4djo, 4djr, 6cpa, 3qaa, 2i4u, 4ll3, 4wkb, 2i4w, 2i4d, 4jn2, 1y6q, 4q1w, 4wr7, 2i4x, 4dfg, 1duv, 5bry, 1sl3, 1ctu.

2 Compounds in the PDBbind v.2016 *core* set

3ao4, 3gv9, 1uto, 1ps3, 4ddk, 4jsz, 3g2z, 3dxg, 3l7b, 3gr2, 3kgp, 3fcq, 3lka, 3zt2, 3udh, 3g31, 4llx, 4u4s, 4owm, 5aba, 2xdl, 4kz6, 2ymd, 3aru, 1bcu, 3zxs, 4ddh, 4mrw, 4eky, 4mrz, 4abg, 5a7b, 3dx1, 4bkt, 2v00, 4cig, 3n7a, 3d6q, 2hb1, 3twp, 4agn, 1c5z, 3nq9, 4msn, 2w66, 3kwa, 3g2n, 4cr9, 4ih5, 4de2, 3ozt, 3f3a, 1a30, 3ivg, 3u9q, 3rsx, 3pxf, 2wbg, 3rr4, 4w9c, 3mss, 4agp, 4mgd, 1vso, 4jxs, 1q8t, 3acw, 4lzs, 3r88, 4ciw, 2w4x, 2brb, 1p1q, 3d4z, 1bzc, 1nc3, 4agq, 4w9l, 2yge, 5c1w, 2r9w, 3gy4, 3syr, 3zso, 2br1, 1s38, 3b27, 4gkm, 4m0z, 1w4o, 3ueu, 4ih7,

4jfs, 3ozs, 3bv9, 1gpk, 1syi, 2cbv, 1ydr, 4de3, 3coz, 2wca, 3u5j, 4dli, 1z9g, 3arv, 3n86, 5c28, 4j28, 3jvr, 1o5b, 2y5h, 3qqs, 3wz8, 4dld, 3ehy, 3uev, 3ebp, 1o0h, 1q8u, 4de1, 4msc, 4w9i, 3ary, 3coy, 3f3c, 2fxs, 4kzq, 2qnq, 1nc1, 2wvt, 1yc1, 3bgz, 4wiv, 3k5v, 4eor, 3uew, 2wnc, 2zb1, 2qbr, 3arq, 2j78, 4ea2, 1r5y, 4m0y, 1gpn, 2weg, 4kzu, 4mme, 3cj4, 3uo4, 3wtj, 3jvs, 1k1i, 2yfe, 4k77, 2xj7, 2iwx, 4f09, 4djv, 4w9h, 4ogj, 1p1n, 3dx2, 2xnb, 3n76, 3pyy, 2zcr, 3oe5, 3jya, 3gbb, 3uex, 4f9w, 2wer, 1lpg, 3zdg, 1z95, 1pxn, 3arp, 3f3d, 3tsk, 2j7h, 2xii, 4cra, 4gfm, 1oyt, 3p5o, 3gc5, 2vvn, 1qf1, 1ydt, 3pww, 1owh, 2zy1, 3up2, 4j21, 2xys, 2qbq, 3oe4, 3rlr, 2xb8, 2c3i, 4e5w, 3f3e, 1ulb, 3qgy, 3ryj, 4j3l, 3prs, 4pcs, 4hge, 1o3f, 2qe4, 3uu0, 3cyx, 3e92, 3fur, 2cet, 5tmn, 3ag9, 3kr8, 3nx7, 3fv2, 4eo8, 3e5a, 1nvq, 2v7a, 4x6p, 1h23, 4e6q, 2al5, 2qbp, 2zda, 3b68, 2xbv, 3b1m, 2fvd, 2vw5, 2wn9, 3ejr, 4qd6, 3u8k, 3ge7, 4crc, 4ivb, 2vkm, 2wtv, 3b5r, 2zcq, 3e93, 4k18, 2p4y, 3dd0, 3nw9, 3ui7, 3uri, 1qkt, 1h22, 3gnw, 1sqa, 4jia, 3b65, 3fv1, 4qac, 2yki, 3g0w, 4ivd, 4ty7, 2pog, 4gr0, 1eby, 1z6e, 1e66, 4ivc, 4twp, 4rfm, 1y6r, 3u8n, 4tmn, 2p15, 3myg, 4gid, 3utu, 5c2h, 1mq6, 5dwr, 4f2w, 2x00, 3o9i, 4f3c.

3 Compounds in the CSAR datasets

3.1 CSAR NRC HiQ set 1

2ou0, 1w6o, 2hr6, 2idz, 2c1q, 1ax1, 2v8y, 2vhw, 2v7u, 2ihk, 2r3d, 2bbf, 2qmj, 3ene, 2v7v, 2jff, 2j4k, 2arb, 1iup, 3f4j, 3c7i, 1vot, 1ukb, 2jj3, 2cjp, 2p98, 2jbj, 2b1q, 2are, 2z4b, 2otz, 2zlj, 2qeh, 2p3t, 2z8f, 2pjo, 2ilz, 2rca, 2rde, 2q3c, 2r6w, 2jgb, 2qv0, 2nnq, 2d2v, 2p3v, 2v8q, 3d2r, 2b3f, 1swk, 2q6m, 2cem, 2jdy, 2add, 2v7t.

3.2 CSAR NRC HiQ set 2

1z3t, 1b6m, 1rdn, 1q6e, 2hj4, 1tr7, 1ax2, 1q4w, 1rdi, 1x9d, 2f5t, 1q6g, 1uld, 1bky, 1xl5, 2hdq, 1w2g, 1yxd, 2fv5, 1q0y, 2cji, 2fai, 1zhx, 1urg, 1gi9, 1y1m, 1ha2, 1gzc, 1gww, 2dm5, 1uzv, 2hdr, 1xw6, 1s7y, 1bcj, 1s50, 1y93, 2ff1, 2a3c, 4ubp, 1gz9, 2i0d, 2hd6, 1s9t, 1txf, 1gx0, 1ow4, 1lhw, 1tt1.

3.3 CSAR12

Downloaded from <https://drugdesigndata.org/about/datasets>

Targets: Urokinase, CDK2-Kinase, CDK2-CyclinA, CHK1-Kinase, ERK2, LpXc.

3.4 CSAR14

Downloaded from <https://drugdesigndata.org/about/datasets>

Targets: SYK, tRMD, HSP90.

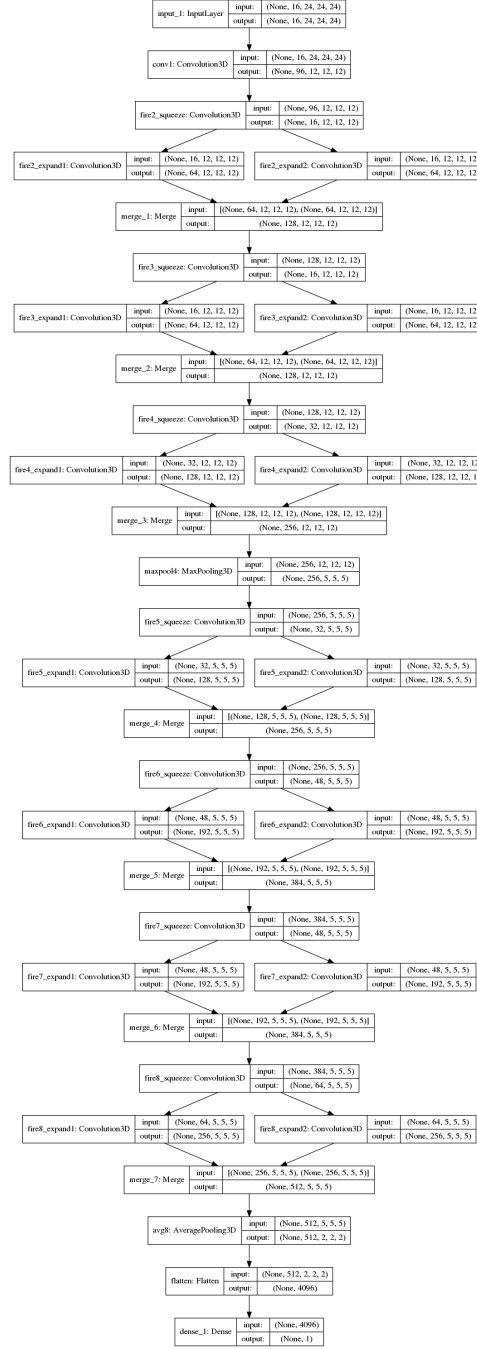


Figure S1: CNN model used for all tests, heavily inspired by SqueezeNet. Layers of convolution operation are followed by max and average pooling operations, heavily reducing the number of learnable parameters and encouraging generalization. All model activations are ReLU-based ($f(x) = \max\{0, x\}$), except for the last one, which is linear.

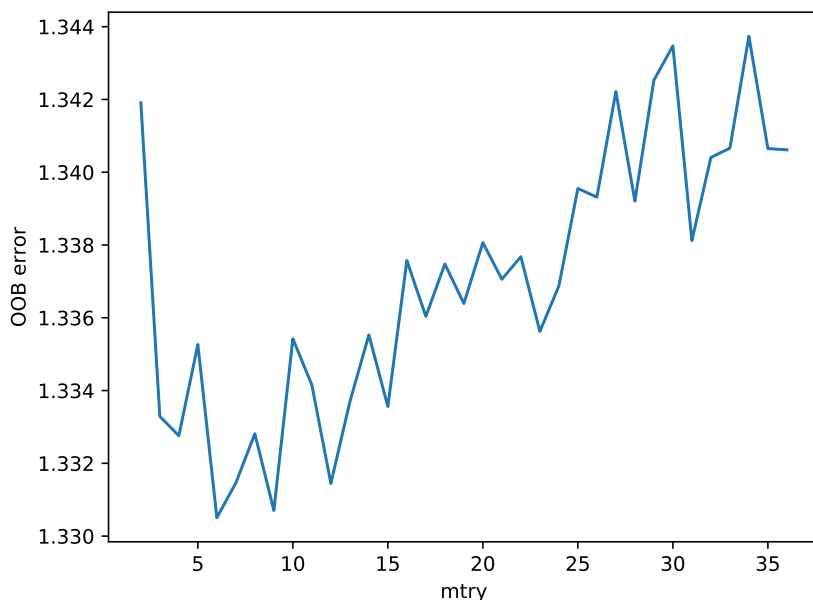


Figure S2: Out-of-bag error for RF-Score in the PDBbind v.2016 *refined* set, excluding complexes in the *core* set. Minimum error is found for $m_{\text{try}} = 6$

Table S1: RMSE results for the CSAR datasets.

	CNN	RF-Score	cyScore	X-Score
CSAR NRC-HiQ set 1	2.08	1.99	2.33	2.31
CSAR NRC-HiQ set 2	1.91	1.66	2.2	1.84
CSAR12	1.59	1.00	2.08	0.93
CSAR14	1.75	0.87	1.49	1
Weighted average	1.83	1.39	2.04	1.53
Simple average	1.83	1.38	2.02	1.52

Table S2: Spearman correlation (ρ) results for the CSAR datasets.

	CNN	RF-Score	cyScore	X-Score	$\log P$	mol. weight
CSAR NRC-HiQ set 1	0.7	0.77	0.71	0.63	0.28	0.31
CSAR NRC-HiQ set 2	0.54	0.85	0.55	0.71	0.39	0.31
CSAR12	0.29	0.48	0.22	0.54	0.23	0.47
CSAR14	0.5	0.69	0.62	0.76	0.18	0.66
Weighted average	0.5	0.69	0.52	0.65	0.27	0.43
Simple average	0.5	0.7	0.52	0.66	0.27	0.44



Figure S3: Dissaggregated Spearman’s correlation coefficient (ρ) for the $m = 58$ targets in the PDBbind v.2016 *core* set, in descending order (higher is better).

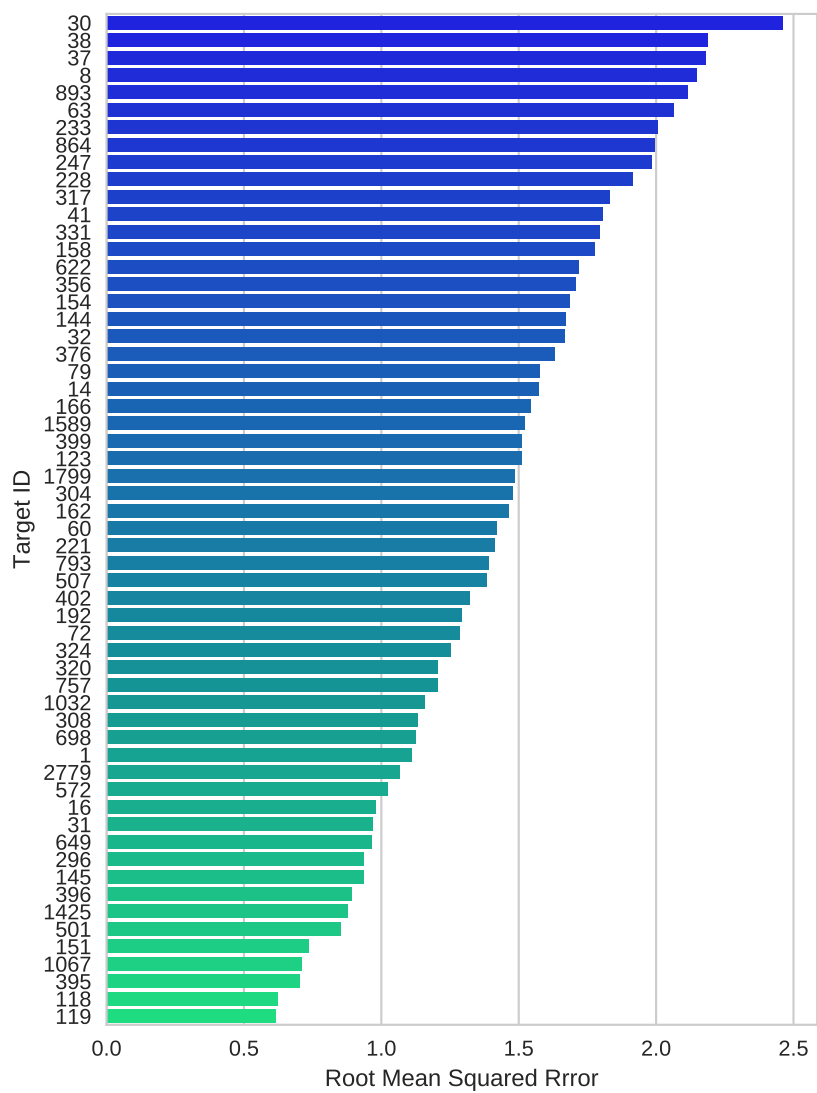


Figure S4: Dissagregated Root Mean Squared Error (RMSE) for the $m = 58$ targets in the PDBbind v.2016 *core* set, in descending order (lower is better).

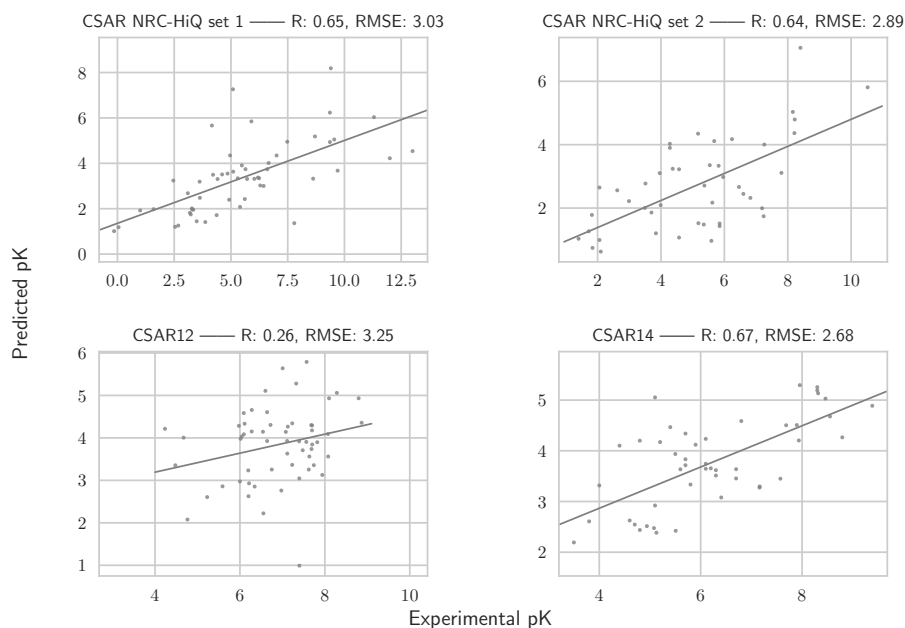


Figure S5: Disaggregated results for cyScore in each of the CSAR datasets considered in the study.

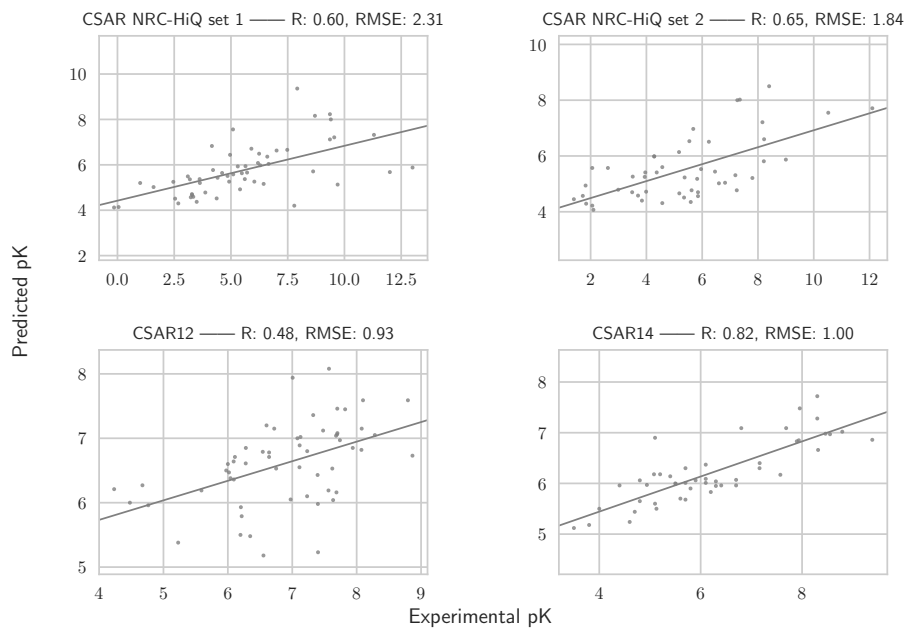


Figure S6: Disaggregated results for X-Score in each of the CSAR datasets considered in the study.

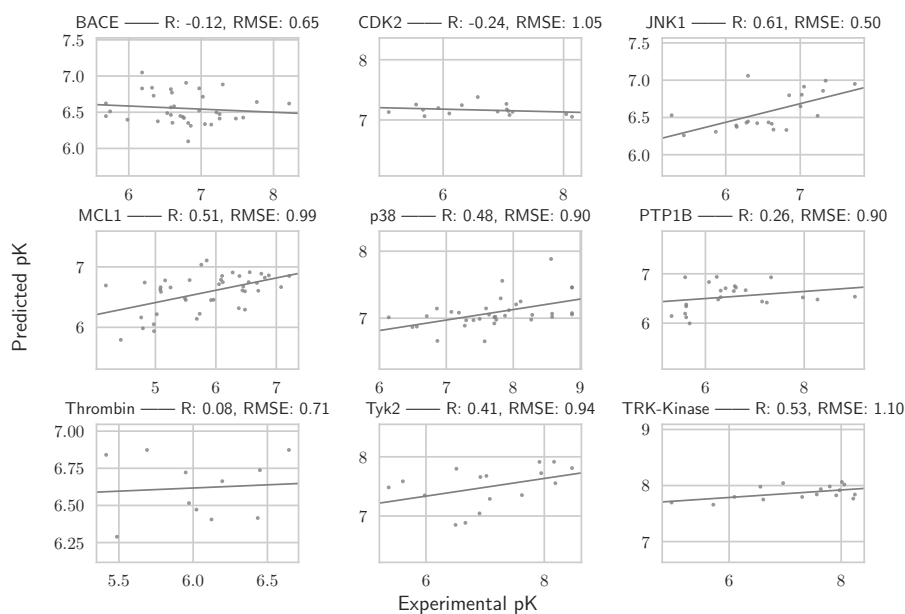


Figure S7: Disaggregated results for RF-Score in the rest of the datasets considered in the study.

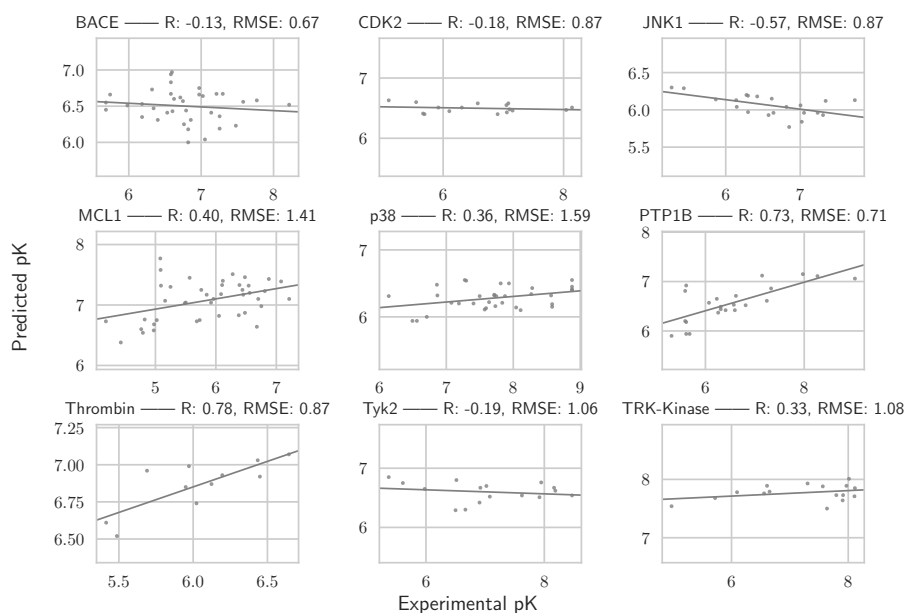


Figure S8: Disaggregated results for X-Score in the rest of the datasets considered in the study.

Table S3: RMSE results for the rest of the targets considered in the study.

	CNN model	RF-Score	cyScore	X-Score
BACE	0.84	0.65	4.65	0.67
CDK2	1.26	1.05	5	0.87
JNK1	1.18	0.5	4.26	0.87
MCL1	1.04	0.99	2.76	1.41
p38	1.57	0.9	5.74	1.59
pTP1B	0.93	0.9	3.96	0.71
Thrombin	0.44	0.71	2.63	0.87
Tyk2	1.13	0.94	4.47	1.06
TRK-Kinase	1.23	1.1	3.75	1.08
Weighted average	1.09	0.86	4.18	1.07
Simple average	1.07	0.86	4.14	1.01

Table S4: Spearman correlation (ρ) results for the rest of the targets considered in the study.

	CNN	RF-Score	cyScore	X-Score	$\log P$	mol. weight
BACE	-0.16	-0.18	0.06	-0.14	-0.09	-0.27
CDK2	0.64	-0.33	-0.52	-0.13	-0.84	0.56
JNK1	0.75	0.62	0.75	-0.59	-0.6	0.31
MCL1	0.32	0.51	0.43	0.41	0.52	0.51
p38	0.39	0.53	-0.11	0.31	0.4	0.56
pTP1B	0.49	0.29	0.35	0.65	0.44	0.67
Thrombin	0.58	0.11	0.85	0.66	0.92	0.65
Tyk2	-0.32	0.51	0.81	-0.18	-0.33	0.05
TRK-Kinase	0.5	0.4	0.26	0.23	-0.33	0.29
Weighted average	0.31	0.29	0.27	0.15	0.07	0.35
Simple average	0.31	0.29	0.27	0.15	0.01	0.37