Protein-Conditioned QSAR Report

Targets: EGFR, ERBB2, ERBB4

Primary: EGFR

Model: rf_ensemble (N=5)

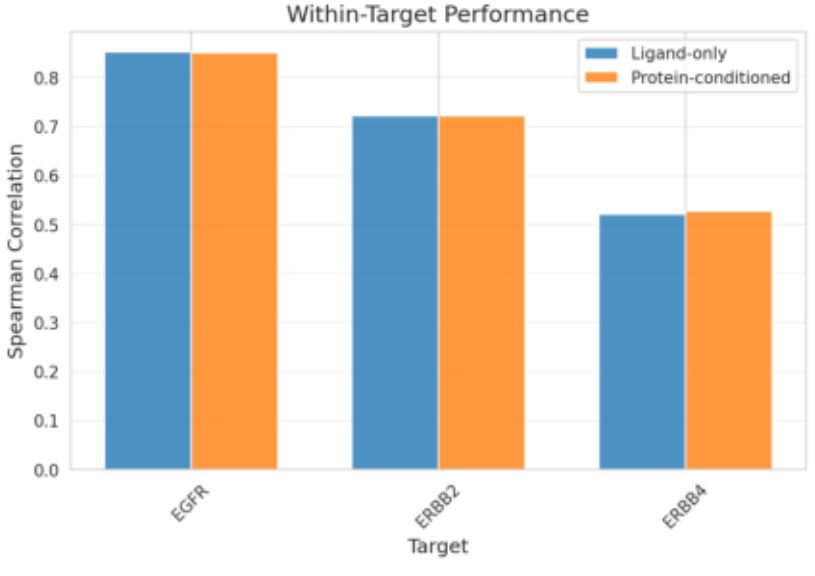
Date: 2025-12-18 16:47

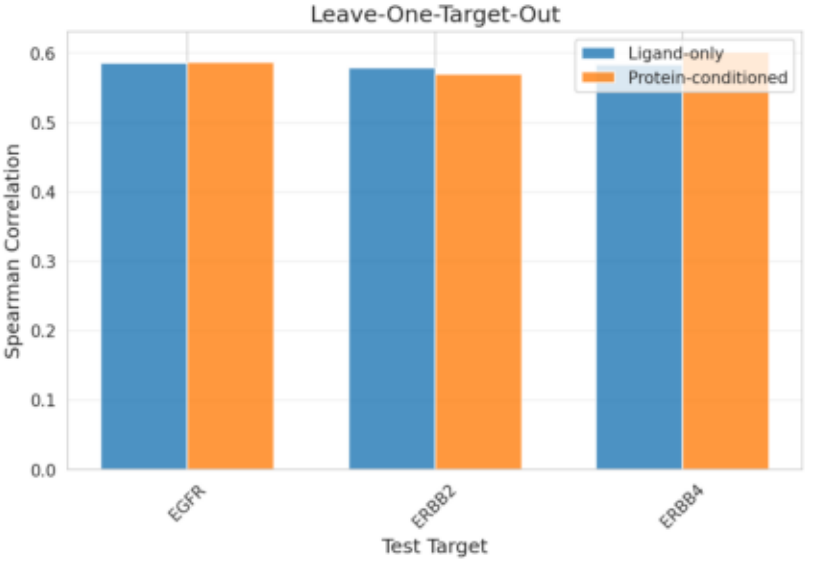
Benchmark Summary

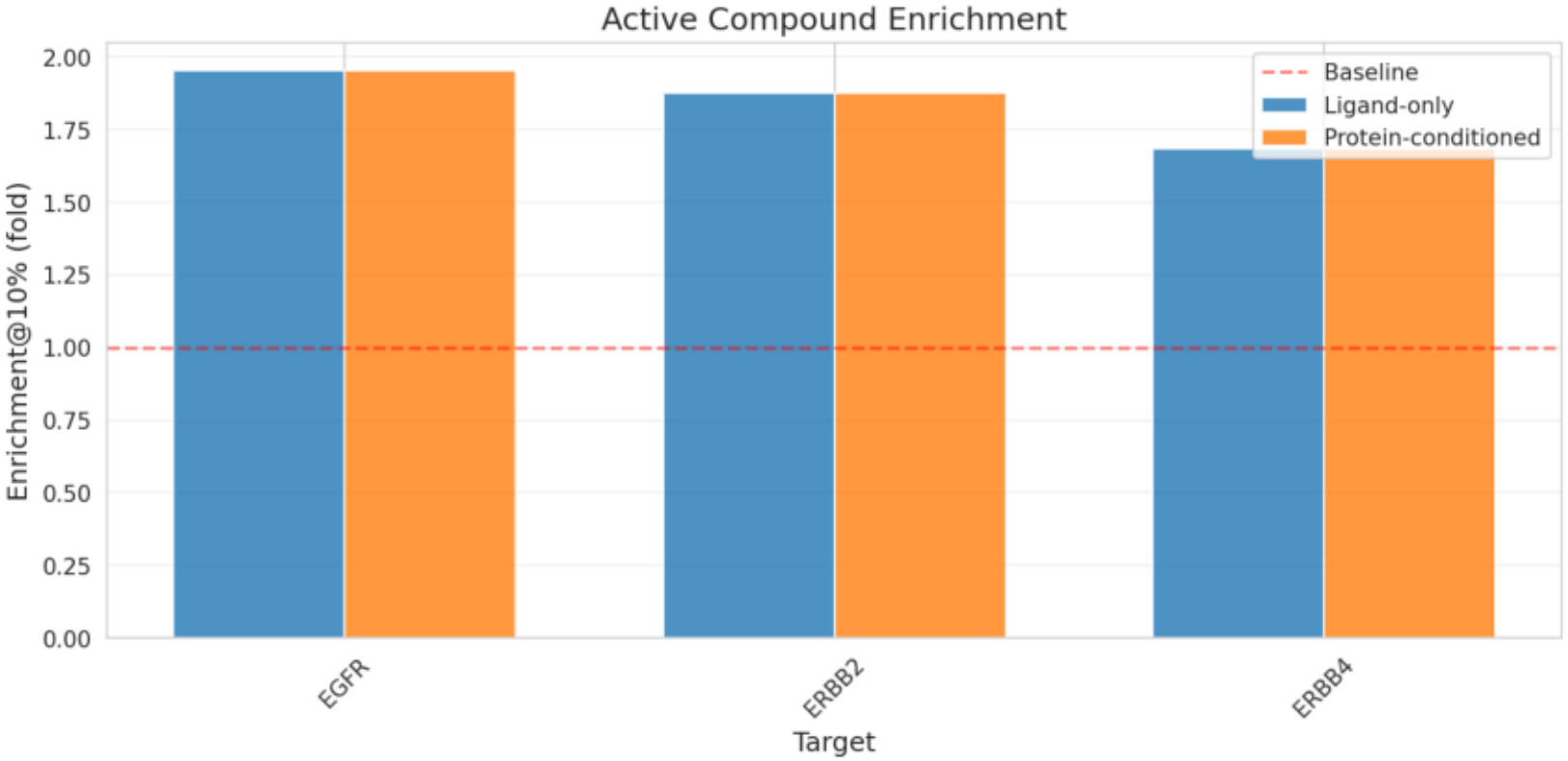
```
Within-Target Scaffold Split (Spearman):
features
ligand_only            0.698071
protein_conditioned    0.700220

Leave-One-Target-Out (Spearman):
features
ligand_only            0.582562
protein_conditioned    0.585747

Enrichment@10% (mean):
features
ligand_only            1.837808
protein_conditioned    1.837808
```


Within-Target Performance
Ligand-only
Protein-conditioned
Spearman Correlation
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
EGFR
ERBB2
ERBB4
Target

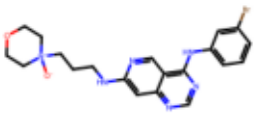

Leave-One-Target-Out
Ligand-only
Protein-conditioned
Spearman Correlation
0.0
0.1
0.2
0.3
0.4
0.5
0.6
EGFR
ERBB2
ERBB4
Test Target


Active Compound Enrichment
Enrichment@10% (fold)
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
Baseline
Ligand-only
Protein-conditioned
EGFR
ERBB2
ERBB4
Target

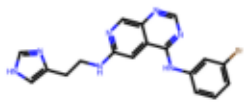
Top 20 Compounds (EGFR) — Ranked

SMILES	pred_pActivity	selectivity	makeability	combined_score
(CCCNc2cc3ncnc(Nc4cccc(Br)c4)c3c	8.799	1.804	0.889	0.832
cccc(Nc2ncnc3cnc(NCCc4c[nH]cn4)c	8.986	1.451	0.889	0.823
Brc1cccc(Nc2ncnc3cc4[nH]ncc4cc23)	8.807	1.641	0.889	0.822
Cn1ncc2cc3c(Nc4cccc(Br)c4)ncnc3cc	8.536	1.748	0.889	0.81
cccc(Nc2ncnc3cnc(NCCc4c[nH]cn4)c	8.845	1.073	0.889	0.79
ccc(Nc2ncnc3cc(NCCCCN4CCOCC4)n	8.378	1.395	0.889	0.781
CCOc1cc2ncnc(/C=C/c3ccccc3)c2cc1O	7.831	1.854	0.917	0.778
CNc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	8.12	1.508	0.917	0.775
COc1cc2ncnc(Sc3cccc(Cl)c3)c2cc1O	7.739	1.82	0.917	0.77
N(c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2	8.566	1.309	0.773	0.77
cccc(Nc2[nH]nc3ncnc(Nc4cccc(Cl)c4)	8.529	1.05	0.889	0.768
COc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	7.998	1.457	0.917	0.765
CN(C)c1ccc2ncnc(Nc3cccc(Br)c3)c2n	7.843	1.458	0.917	0.755
ccc(Nc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c	8.242	1.021	0.889	0.748
CCN1CCCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)	8.832	0.14	0.889	0.728
CCN1CCOCC1)Nc1cc2c(Nc3ccc(F)c(Cl)	8.9	-0.029	0.889	0.725
ccc(Nc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c	8.175	0.653	0.889	0.72
Nc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	7.954	0.819	0.917	0.719
CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)	8.374	0.318	0.917	0.717
CCN1CCOCC1)Nc1cc2c(Nc3ccc(F)c(Br	8.859	-0.138	0.889	0.715

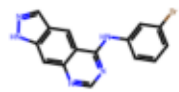
Top 20 Molecules (EGFR) — Structures



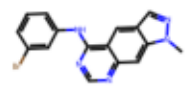
pAct 8.80 0.04
Sel 1.80 Mk 0.89



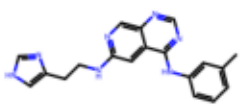
pAct 8.99 0.00
Sel 1.45 Mk 0.89



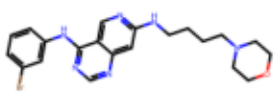
pAct 8.81 0.03
Sel 1.64 Mk 0.89



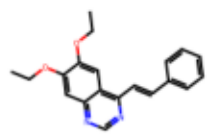
pAct 8.54 0.08
Sel 1.75 Mk 0.89



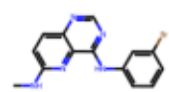
pAct 8.84 0.02
Sel 1.07 Mk 0.89



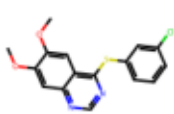
pAct 8.38 0.02
Sel 1.39 Mk 0.89



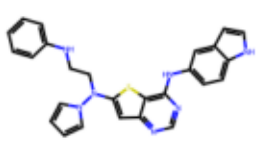
pAct 7.83 0.04
Sel 1.85 Mk 0.92



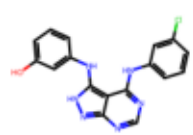
pAct 8.12 0.03
Sel 1.51 Mk 0.92



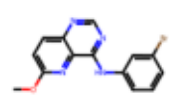
pAct 7.74 0.04
Sel 1.82 Mk 0.92



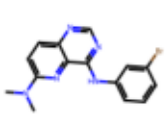
pAct 8.57 0.02
Sel 1.31 Mk 0.77



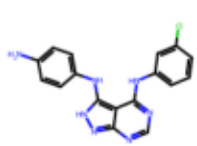
pAct 8.53 0.03
Sel 1.05 Mk 0.89



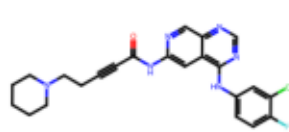
pAct 8.00 0.03
Sel 1.46 Mk 0.92



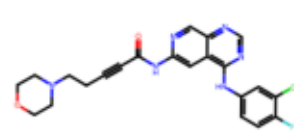
pAct 7.84 0.02
Sel 1.46 Mk 0.92



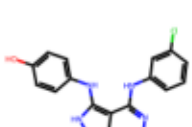
pAct 8.24 0.03
Sel 1.02 Mk 0.89



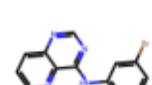
pAct 8.83 0.07
Sel 0.14 Mk 0.89



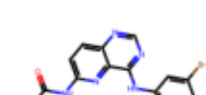
pAct 8.90 0.01
Sel -0.03 Mk 0.89



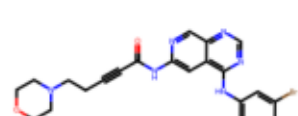
pAct 8.18 0.04
Sel 0.65 Mk 0.89



pAct 7.95 0.08
Sel 0.82 Mk 0.92



pAct 8.37 0.03
Sel 0.32 Mk 0.92

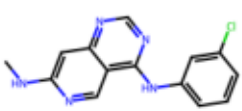


pAct 8.86 0.01
Sel -0.14 Mk 0.89

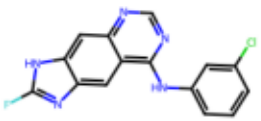
Top 20 Enumerated Compounds (EGFR) — Ranked

SMILES	Parent SMILES	pred_pActivity	selectivity	makeability	combined_score
CNc1cc2ncnc(Nc3cccc(Cl)c3)c2cc1C(=O)N	CCCNc1cc2ncnc(Nc3cccc(Br)c	8.798	2.223	0.917	0.861
c2cc3c(Nc4cccc(Cl)c4)ncnc3cc1C(=O)N	Cc1cc2cc3c(Nc4cccc(Br)c4)ncnc3cc	8.808	1.84	0.889	0.835
Nc1cc2ncnc(Nc3cccc(OC)c3)c2cc1C(=O)N	CCCNc1cc2ncnc(Nc3cccc(Br)c	8.479	1.951	0.917	0.825
Cc1cccc(Nc2ncnc3cc(NC(=O)C	CCCNc1cc2ncnc(Nc3cccc(Br)c	8.441	1.855	0.917	0.817
CNc1cc2c(Nc3cccc(F)c3)ncnc2cc1C(=O)N	CN(C)C(=O)c1cc2c(Nc3cccc(Br)c3)ncn	8.981	1.307	0.917	0.816
CNc1ccc2cncnc2c1	Nc1ccc2cncnc2c1	8.189	1.961	0.944	0.813
N#Cc1ccc2c(Nc3cccc(Br)c3)ncnc2cc1OCCO	COCCOc1cc2ncnc(Nc3cccc(Br)c3)c2cc	8.442	1.73	0.917	0.809
Nc1cc2c(Nc3cccc(C#N)c3)ncnc2cc1OC	COc1cc2c(Nc3cccc(Br)c3)ncnc	8.944	1.217	0.917	0.808
N#Cc1cccc(Nc2ncnc3cc(F)ccc23)c1	N#Cc1ccc2c(Nc3cccc(Br)c3)ncnc2	8.28	1.832	0.917	0.805
CCc1cccc(Nc2ncnc3cnc(NC(=O)C	CCCNc1cc2c(Nc3cccc(Br)c3)nc	8.839	1.275	0.917	0.805
c1cccc(Nc2ncnc3cc4[nH]ccc4cc23)c1	Brc1cc2cc3c(Nc4cccc(Br)c4)ncnc3cc	8.475	1.722	0.889	0.804
Cc1cccc(Nc2ncnc3cc(C#N)ccc23)c1	CCCc1cc2ncnc(Nc3cccc(Br)c3)c2cc	8.25	1.859	0.917	0.803
CN(C)c1cc2ncnc(Nc3cccc(Cl)c3)c2cc1OC	COCCNc1cc2ncnc(Nc3cccc(Br)c3)c	8.281	1.794	0.917	0.802
N#Cc1ccc2c(Nc3cccc(F)c3)ncnc2cc1OCCO	COCCOc1cc2ncnc(Nc3cccc(Br)c3)c2cc	8.26	1.822	0.917	0.802
N#Cc1cccc(Nc2ncnc3cc(Cl)ccc23)c1	Cc1cc2ncnc(Nc3cccc(Br)c3)c2cc	8.277	1.814	0.917	0.802
CN(C)c1ccc2c(Nc3cccc(Cl)c3)ncnc2cc1	Nc1cc2ncnc(Nc3cccc(Br)c3)c2cc	8.104	1.903	0.917	0.799
Cc1ccc2cncnc2c1	Nc1ccc2cncnc2c1	8.047	1.886	0.944	0.798
CN(C)c1cccc(Nc2ncnc3cc(Cl)ccc23)c1	Cc1cc2ncnc(Nc3cccc(Br)c3)c2cc	8.098	1.909	0.917	0.798
Fc1ccc2cncnc2c1	Nc1ccc2cncnc2c1	8.122	1.817	0.944	0.796
CCc1ccc2cncnc2c1	Nc1ccc2cncnc2c1	7.917	1.921	0.944	0.792

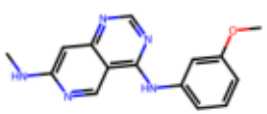
Top 20 Enumerated Molecules (EGFR) — Structures



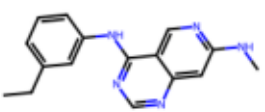
pAct 8.80 0.05
Sel 2.22 Mk 0.92



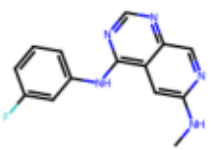
pAct 8.81 0.03
Sel 1.84 Mk 0.89



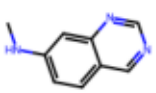
pAct 8.48 0.04
Sel 1.95 Mk 0.92



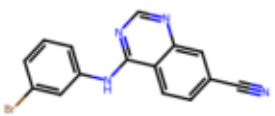
pAct 8.44 0.03
Sel 1.85 Mk 0.92



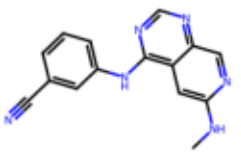
pAct 8.98 0.04
Sel 1.31 Mk 0.92



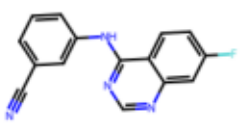
pAct 8.19 0.02
Sel 1.96 Mk 0.94



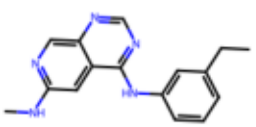
pAct 8.44 0.03
Sel 1.73 Mk 0.92



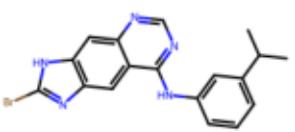
pAct 8.94 0.05
Sel 1.22 Mk 0.92



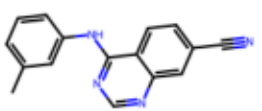
pAct 8.28 0.04
Sel 1.83 Mk 0.92



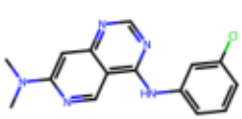
pAct 8.84 0.04
Sel 1.28 Mk 0.92



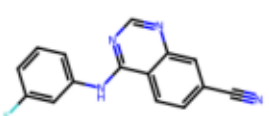
pAct 8.47 0.08
Sel 1.72 Mk 0.89



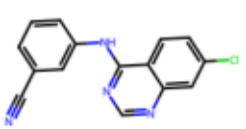
pAct 8.25 0.08
Sel 1.86 Mk 0.92



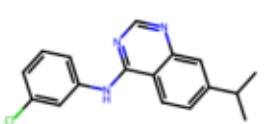
pAct 8.28 0.05
Sel 1.79 Mk 0.92



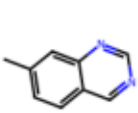
pAct 8.26 0.06
Sel 1.82 Mk 0.92



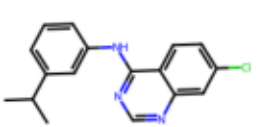
pAct 8.28 0.08
Sel 1.81 Mk 0.92



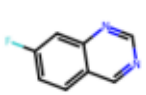
pAct 8.10 0.04
Sel 1.90 Mk 0.92



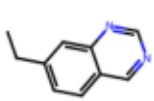
pAct 8.05 0.04
Sel 1.89 Mk 0.94



pAct 8.10 0.05
Sel 1.91 Mk 0.92



pAct 8.12 0.09
Sel 1.82 Mk 0.94



pAct 7.92 0.04
Sel 1.92 Mk 0.94