Protein-Conditioned QSAR Report

Targets: EGFR, KCNH2, CYP3A4, CYP2D6, HTR2B

Primary: EGFR

Model: xgb_ensemble (N=5)

Date: 2025-12-18 17:16

Benchmark Summary

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Within-Target Scaffold Split (Spearman):
features
ligand_only            0.523398
protein_conditioned    0.523398

Leave-One-Target-Out (Spearman):
features
ligand_only            0.047701
protein_conditioned    0.039187

Enrichment@10% (mean):
features
ligand_only            4.064997
protein_conditioned    4.064997
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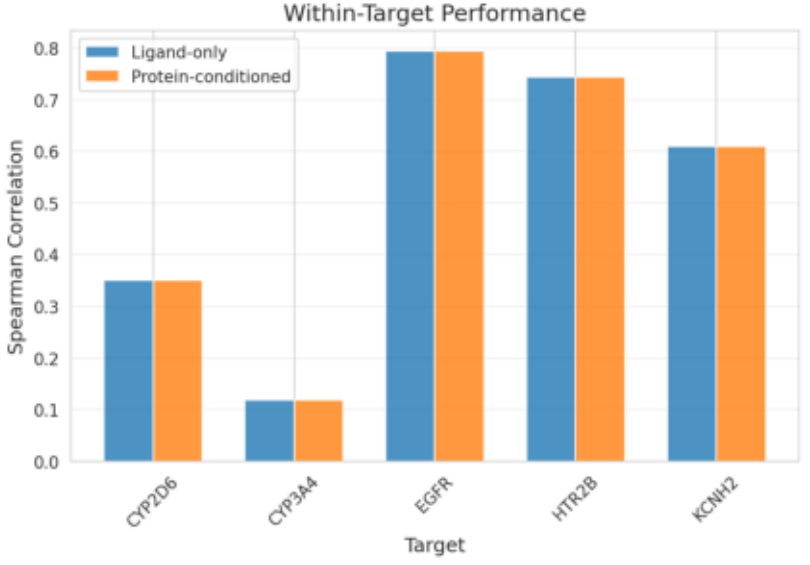
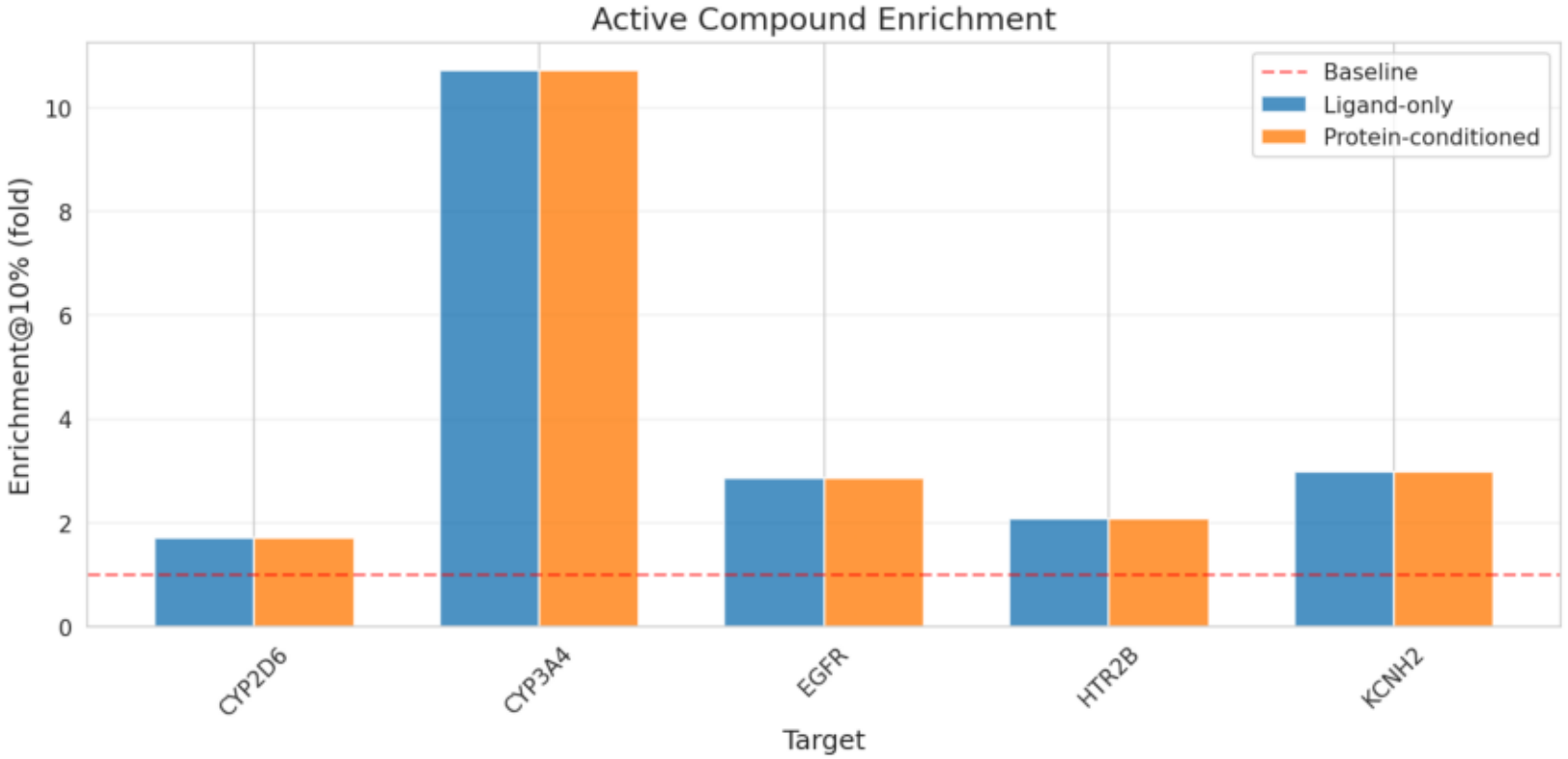

Within-Target Performance
Ligand-only
Protein-conditioned
Spearman Correlation
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
CYP2D6
CYP3A4
EGFR
HTR2B
KCNH2
Target

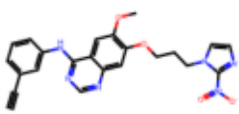

Leave-One-Target-Out
Ligand-only
Protein-conditioned
Spearman Correlation
−0.2
−0.1
0.0
0.1
0.2
0.3
CYP2D6
CYP3A4
EGFR
HTR2B
KCNH2
Test Target


Active Compound Enrichment
Baseline
Ligand-only
Protein-conditioned
Enrichment@10% (fold)
0
2
4
6
8
10
CYP2D6
CYP3A4
EGFR
HTR2B
KCNH2
Target

Top 20 Compounds (EGFR) — Ranked

SMILES	pred_pActivity	selectivity	makeability	combined_score
Nc2ncnc3cc(OCCCn4ccnc4[N+](=O)[	9.020999908447266	3.621999979019165	0.889	1.0260000228881836
Nc2ncnc3cc(OCCCCCn4ccnc4[N+](=	9.076000213623047	3.489000082015991	0.889	1.0169999599456787
c3cccc(Br)c3)ncnc2cc1OCCCn1ccnc1	9.032999992370605	3.371999979019165	0.889	1.0049999952316284
c3cccc(Br)c3)ncnc2cc1OCCCCCn1ccn	9.13599967956543	3.2739999294281006	0.889	1.0019999742507935
ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)C	8.76099967956543	2.99399995803833	0.889	0.9580000042915344
ccccc(Nc2ncnc3cnc(NCCN4CCOCC4)c	8.769000053405762	2.9769999980926514	0.889	0.9570000171661377
Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCn1ccn	8.873000144958496	2.871000051498413	0.889	0.953000009059906
Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCCCn1	8.873000144958496	2.8310000896453857	0.889	0.949999988079071
ccccc(Nc2ncnc3cnc(NCCN4CCOCC4)cc	8.649999618530273	2.8989999294281006	0.889	0.9449999928474426
CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)	8.321000099182129	2.9179999828338623	0.917	0.9340000152587891
ccccc(Nc2ncnc3cnc(NCCCN4CCOCC4)c	8.61299991607666	2.6410000324249268	0.889	0.9200000166893005
1ccccc(Nc2ncnc3cnc(NCCc4ccccn4)cc	8.583999633789062	2.5369999408721924	0.889	0.9100000262260437
NCc1ccc(-c2cc3nccc(Nc4ccc5[nH]ccc	8.369000434875488	2.681999921798706	0.861	0.9070000052452087
CNc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	8.166000366210938	2.6440000534057617	0.917	0.9020000100135803
Cc1ccc(-c2cc3nccc(Nc4ccc5[nH]ccc5	8.331000328063965	2.635999917984009	0.861	0.9010000228881836
ccc(Nc2ncnc3cnc(NCCCN4CCOCC4)c	8.656000137329102	2.4019999504089355	0.889	0.9010000228881836
c1ccc(-c2cc3nccc(Nc4ccc5[nH]ccc5c4	8.309000015258789	2.634000062942505	0.861	0.8999999761581421
Brc1cccc(Nc2ncnc3cc4[nH]ccc4cc23)	8.350000381469727	2.50600004196167	0.889	0.8949999809265137
Cn1ccc2cc3c(Nc4cccc(Br)c4)ncnc3cc	8.222999572753906	2.5160000324249268	0.889	0.8899999856948853
CC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3	8.17300033569336	2.3940000534057617	0.917	0.8809999823570251

Top 20 Molecules (EGFR) — Structures



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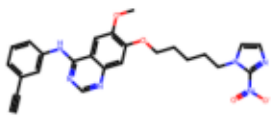

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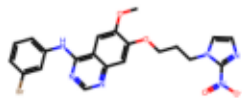

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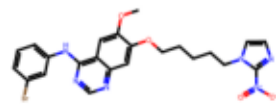

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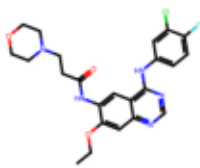

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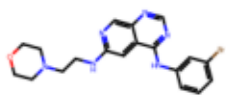

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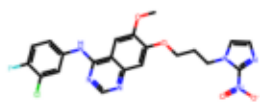

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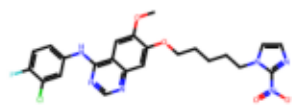

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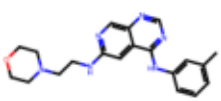

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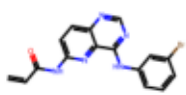

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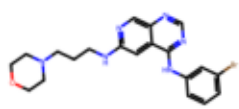

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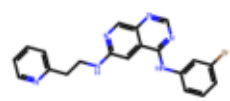

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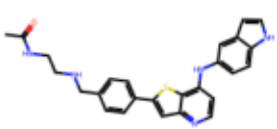

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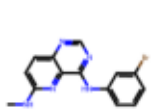

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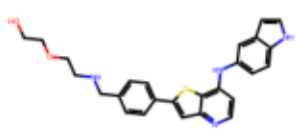

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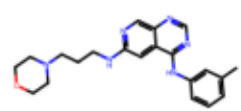
Sel 2.64 Mk 0.86



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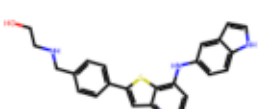

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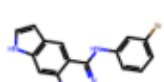

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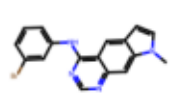

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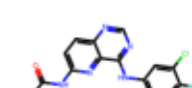
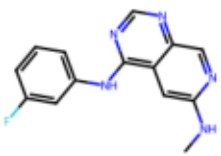


pAct 8.17 0.00
Sel 2.39 Mk 0.92

Top 20 Enumerated Compounds (EGFR) — Ranked

SMILES	Parent SMILES	pred_pActivity	selectivity	makeability	combined_score
CNc1cc2c(Nc3cccc(F)c3)ncnc2cc1OCC	CNc1cc2c(Nc3cccc(Br)c3)ncnc	8.685999870300293	2.934000015258789	0.917	0.9539999961853027
Nc1cc2c(Nc3cccc(C#N)c3)ncnc2cc1OCC(O)	CNc1cc2c(Nc3cccc(Br)c3)ncn	8.531999588012695	2.8289999961853027	0.917	0.9369999766349792
cc2c(Nc3cccc(S(C)(=O)=O)c3)ncnc2cc1NC(=O)C	CNc1cc2c(Nc3cccc(Cl)c3)ncnc2c	8.449000358581543	2.871000051498413	0.917	0.9359999895095825
1cc2c(Nc3cccc(S(C)(=O)=O)c3)ncnc2cc1NC(=O)CO	CNc1cc2c(Nc3cccc(Br)c3)ncn	8.192000389099121	2.743000030517578	0.917	0.9120000004768372
N(C)c1cc2c(Nc3cccc(Cl)c3)ncnc2cc1NC(=O)CO	CNc1cc2c(Nc3cccc(Br)c3)ncn	8.182000160217285	2.7219998836517334	0.917	0.9100000262260437
c1cccc(Nc2ncnc3cnc(N(C)C)cc23)c1	CNc1cc2c(Nc3cccc(Cl)c3)ncnc2c	8.357000350952148	2.5769999027252197	0.917	0.906000018119812
C)c1cc2c(Nc3cccc(C#N)c3)ncnc2cc1OCC	CNc1cc2c(Nc3cccc(Cl)c3)ncnc2c	8.168000221252441	2.5910000801086426	0.917	0.8980000019073486
#C)c1cc2ncnc(Nc3cccc(Br)c3OC)c2cc1OCC	CNc1cc2ncnc(Nc3cccc(Br)c3)c	8.246999740600586	2.5220000743865967	0.917	0.8960000276565552
cc2c(Nc3cccc(-c4ccccn4)c3)ncnc2cc1NC(=O)CO	CNc1cc2c(Nc3cccc(Br)c3)ncn	8.234000205993652	2.575000047683716	0.889	0.8949999809265137
c1cc2c(Nc3cccc(-c4cnccn4)c3)ncnc2cc1NC(=O)C	CNc1cc2c(Nc3cccc(Cl)c3)ncnc2c	8.062999725341797	2.6670000553131104	0.889	0.8949999809265137
CNc1cc2ncnc(Nc3cccc(F)c3OC)c2cc1OCC	CNc1cc2ncnc(Nc3cccc(Br)c3)c	8.204999923706055	2.453000068664551	0.917	0.8870000243186951
C)c1cccc(Nc2ncnc3cnc(N(C)C)cc23)c1OCC(O)	CNc1cc2c(Nc3cccc(Br)c3)ncn	8.050999641418457	2.4590001106262207	0.917	0.8799999952316284
Nc1cccc(Nc2ncnc3cc(NC)ncc23)c1OC	CNc1cc2ncnc(Nc3cccc(Br)c3)c	8.090999603271484	2.424999952316284	0.917	0.8790000081062317
CNc1cccc(Nc2ncnc3cnc(C)cc23)c1OCC(O)	CNc1cc2c(Nc3cccc(Br)c3)ncn	8.052000045776367	2.380000114440918	0.917	0.8730000257492065
Fc1ccc2c(Nc3cccc(Br)c3)ncnc2c1	NC1ccc2c(Nc3cccc(Br)c3)ncnc2	8.086000442504883	2.3459999561309814	0.917	0.871999979019165
Fc1cccc(Nc2ncnc3cc(Br)ncc23)c1	CNc1cc2ncnc(Nc3cccc(Br)c3)c	7.921000003814697	2.437999963760376	0.917	0.871999979019165
CO)c1ccc2c(Nc3cccc(Br)c3)ncnc2cc1NC(=O)CO	CNc1cc2ncnc(Nc3cccc(Br)c3)c2cc	7.986999988555908	2.3970000743865967	0.917	0.871999979019165
Cc1cccc(Nc2ncnc3cc(NC)ncc23)c1	CNc1cc2ncnc(Nc3cccc(Br)c3)c	8.10099983215332	2.3299999237060547	0.917	0.8709999918937683
CNc1cccc(Nc2ncnc3cnc(Cl)cc23)c1	CNc1cc2c(Nc3cccc(Cl)c3)ncnc2c	8.045000076293945	2.359999895095825	0.917	0.8709999918937683
Cc1ccc2c(Nc3cccc(Br)c3)ncnc2cc1NC(=O)CO	CNc1cc2ncnc(Nc3cccc(Br)c3)c2cc	8.010000228881836	2.378000020980835	0.917	0.8709999918937683

Top 20 Enumerated Molecules (EGFR) — Structures



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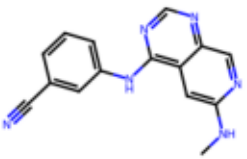

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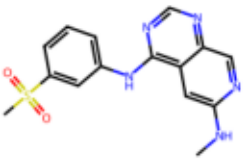

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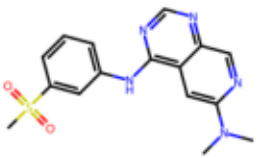

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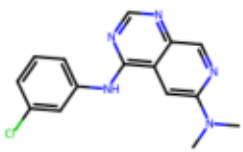

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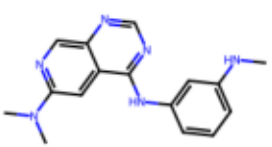

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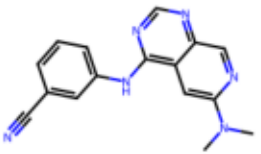

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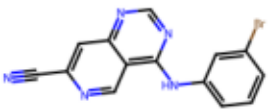

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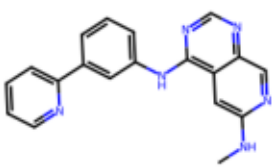

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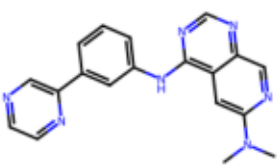

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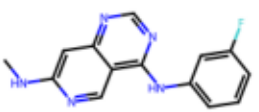

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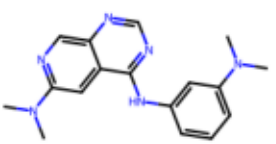

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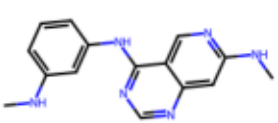

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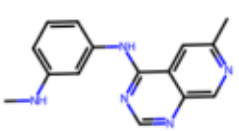

pAct 8.05 0.00
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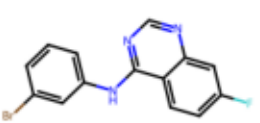

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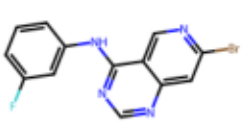

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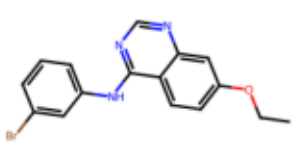
Sel 2.44 Mk 0.92



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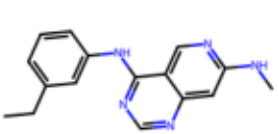

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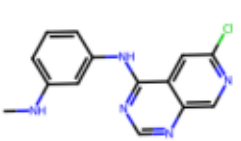

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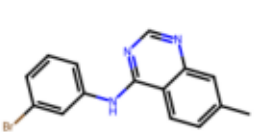

pAct 8.01 0.00
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