The 36 cocaine-addiction related datasets are collected from ChEMDL database (https://www.ebi.ac.uk/chembl/) and literature [1, 2], which involve 32 cocaine-addiction protein targets. The labels are binding affinities to these targets.

Dataset	Target ChEMBLID	Dataset size	Binding affinity range (kcal/mol)
DAT binding	CHEMBL238	1189	[-14.18, -2.90]
DAT uptake	CHEMBL238	350	[-12.52, -5.33]
Extended DAT	CHEMBL238	2877	[-14.18, -2.90]
D_3R	CHEMBL234	4685	[-14.59, -5.64]
D_2R from Ref. [2]	CHEMBL217	3721	active or inactive
Extended D_2R	CHEMBL217	6923	[-14.41, -5.45]
D_4R	CHEMBL219	2411	[-14.64, -5.52]
HDAC	CHEMBL2093865	1925	[-14.04, -5.86]
Sigma1	CHEMBL287	2388	[-14.23, -5.90]
Activin receptor 1	CHEMBL5903	257	[-12.57, -5.45]
VMAT2	CHEMBL4828	248	[-13.21, -5.73]
CDK1	CHEMBL308	1253	[-13.36, -5.86]
CACNA1D	CHEMBL2095229	137	[-15.40, -5.86]
CAPN1	CHEMBL3891	639	[-12.02, -5.79]
CNR1	CHEMBL218	3922	[-14.70, -5.45]
CNR2	CHEMBL253	4336	[-14.79, -5.48]
EGFR	CHEMBL203	6693	[-15.41, -5.67]
EPHA2	CHEMBL2068	490	[-12.98, -5.86]
GRM2	CHEMBL5137	748	[-12.62, -5.56]
GRM3	CHEMBL2888	114	[-12.72, -5.83]
HGF	CHEMBL3717	529	[-13.63, -5.59]
IGF1R	CHEMBL1957	2450	[-14.45, -5.45]
ITGB7	CHEMBL2095184	416	[-12.84, -5.86]
LRRK2	CHEMBL1075104	1871	[-13.78, -5.45]
MET	CHEMBL3717	3347	[-13.89, -5.59]
MMP3	CHEMBL283	1909	[-14.61, -5.45]
MMP7	CHEMBL4073	482	[-13.55, -5.48]
MMP9	CHEMBL321	2523	[-15.40, -5.45]
PSEN1	CHEMBL2473	117	[-11.97, -6.43]
SPR	CHEMBL3988583	1026	[-12.68, -6.41]
SRC	CHEMBL267	3268	[-13.93, -3.54]
SSTR5	CHEMBL1792	788	[-13.89, -6.09]
YES1	CHEMBL2073	121	[-13.22, -5.90]
GRK5	CHEMBL5678	262	[-10.36, -5.45]
hERG	CHEMBL240	2043	[-12.83, -3.27]
Extended hERG	CHEMBL240	6298	[-13.84, -3.27]

References

[1] Andrew D Fant, Soren Wacker, Joslyn Jung, Jiqing Guo, Ara M Abramyan, Henry J Duff, Amy H New- man, Sergei Y Noskov, and Lei Shi. Toward reducing herg affinities for dat inhibitors with a combinedmachine learning and molecular modeling approach. *Biophysical Journal*, 116(3):562a, 2019.

[2] Dawid Warszyckia, Łukasz Struskib, Marek Śmiejab, Rafał Kafela, and Rafał Kurczaba. Pharmacoprint – a combination of pharmacophore fingerprint and artificial intelligence as a tool for computeraided drug design. 2021.