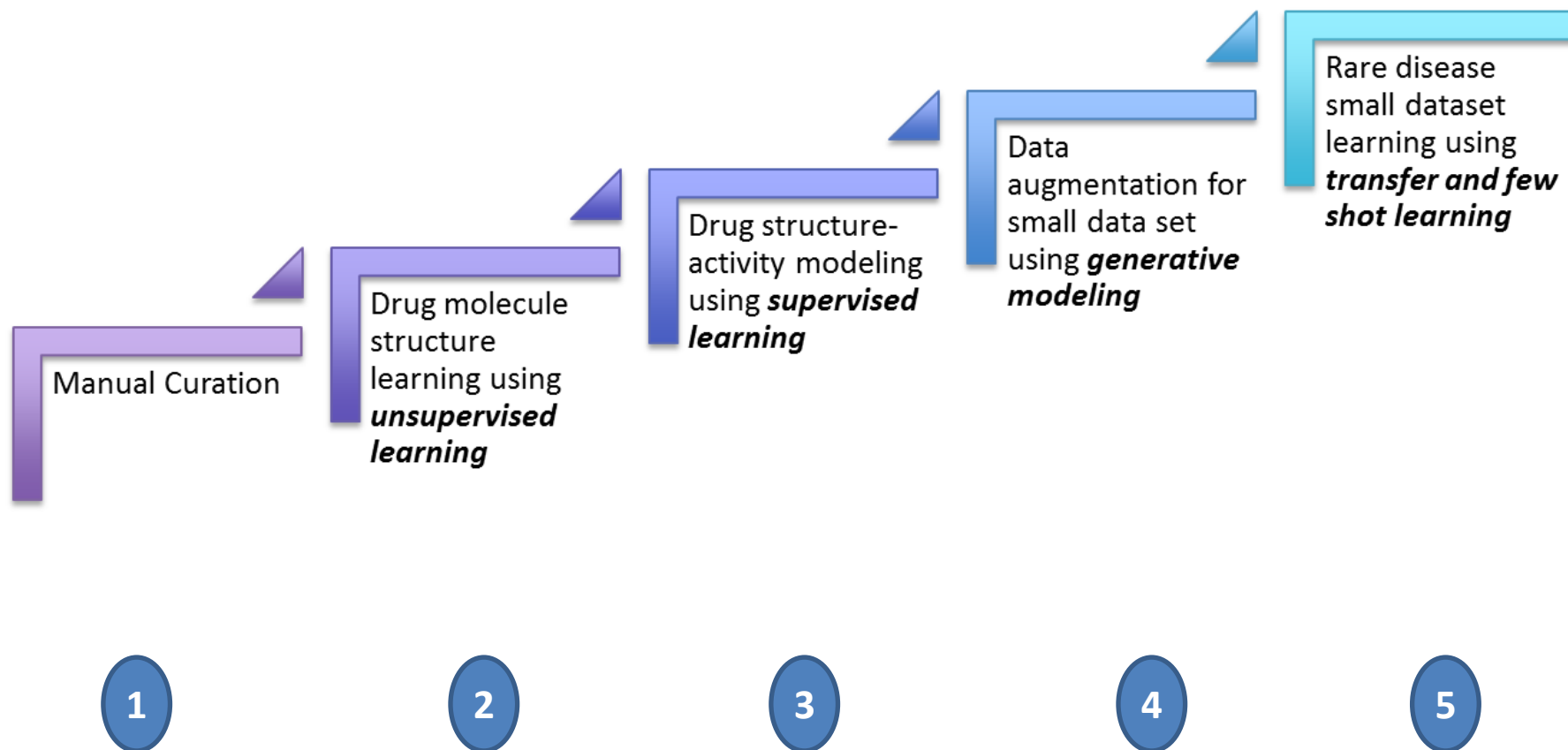


The Technology

Various Components and Subsystems



Manual Curation

Extracting biochemical information from unstructured literature (patents/journal article) into structured format (by semi-automation). ChEMBL open source database will be helpful for extracting Protease inhibitors .

Manual Curation

Structure and Physico-chemical Properties

2D Structure

Calculated Physico-chemical Properties

Hydrogen bond acceptors	22
Hydrogen bond donors	5
Rotatable bonds	15
Topological polar surface area	285.69
Molecular weight	959.49
XLogP	3.89
No. Lipinski's rules broken	2

Molecular properties generated using the CDK

Summary Biological activity References Structure

Classification

Compound class Natural product or derivative

IUPAC Name

[(1R)-1-[(3S,6S,9S,12S,16R,21S,22R)-21-acetamido-3-[(1R)-1-methoxyethyl]-4,9,10,12,16,22-hexamethyl-15-methyldiene-2,5,8,11,14,17,20-hepta-oxo-18-phenylmethyl)-1,19-dioxo-4,7,10,13,16-pentazacyclodocos-8-yl]-2-methylpropyl] (2S,3R)-2-acetamido-3-hydroxy-4-methylpentanoate

Synonyms

YM254890

Database Links

PubChem CID 9919454

Search Google for chemical match using the InChIKey QVYLWCAYZGFGNF-WBWCVBTSAN

Search Google for chemicals with the same backbone QVYLWCAYZGFGNF

Comments

The natural product YM-254890 from *Chromobacterium* sp. Q53666 is a selective inhibitor of Gq signalling. The first total synthesis of this and analogues with SAR are reported [1]. Note that PubChem substances with assay results are indexed in the Nature Chemistry article. An earlier PDB entry 3AH8 shows a bovine G-protein complex with YM-254890.

ChEMBL database

EMBL-EBI ChEMBL

Services Research Train

Search ChEMBL...

Compounds Targets Assays Documents Cells Tissues Exact Match Activity Source Filter

Ligand Search Target Search Browse Targets Browse Drugs Browse Drug Targets Browse Drug Indications About

Approved Drug Data Freeze: March 2017

10 records per page Search

Molecule	Molecule Type	First Approval	USAN Stem	Mechanism of Action	Target Name	Action Type	Organism	Target Type
Avelumab	Antibody	2017	-mab	Programmed cell death 1 ligand 1 other	Programmed cell death 1 ligand 1	OTHER	Homo sapiens	SINGLE PROTEIN
Brodalumab	Antibody	2017	-mab	Interleukin-17 receptor A antagonist	Interleukin-17 receptor A	ANTAGONIST	Homo sapiens	SINGLE PROTEIN
Deflazacort	Small molecule	2017	N/A	Glucocorticoid receptor agonist	Glucocorticoid receptor	AGONIST	Homo sapiens	SINGLE PROTEIN
Deflazacort	Antibody	2017	-mab	Interleukin-4 receptor subunit alpha antagonist	Interleukin-4 receptor subunit alpha	ANTAGONIST	Homo sapiens	SINGLE PROTEIN

ChEMBL Statistics

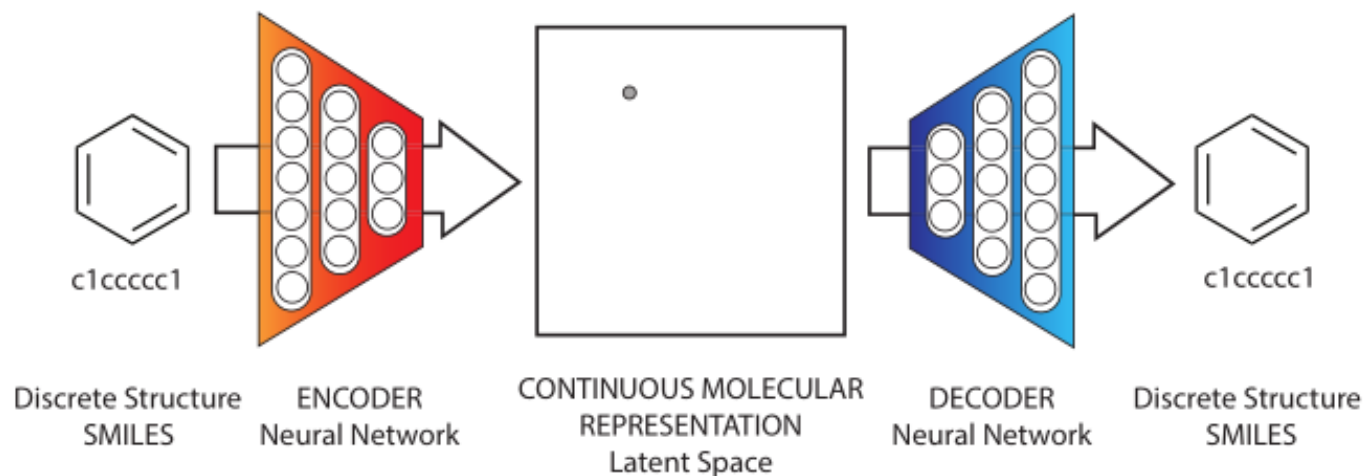
- DB ChEMBL_23
- Targets 11,538
- Compound records 2,101,843
- Distinct compounds 1,758,442
- Activities 14,676,320
- Publications 67,722
- Release Notes

ChEMBL Blog

- Using autoencoders for molecule generation
- ChEMBL web services webinar - April 12th 2017

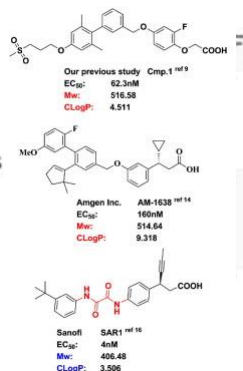
Drug Molecule Structure Learning:

From the curated database, we extract the molecules and encode chemical structures as features. This is how we inject the drug molecules knowledge into Neural Networks



Drug Structure Activity Modelling using Supervised Learning

SAR data
+ Molecular descriptors



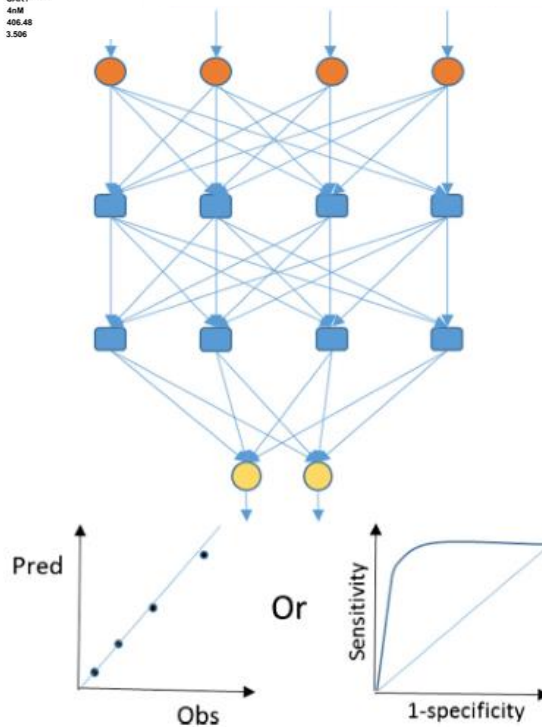
Title	ALogP	ALogP2	AMR	BCUTp-1	BCUTp-1h	fragC	apol	naAromAt	nAtom
Acabutozol	-2.1004	4.41168	67.0727	4.75506	9.76616	2152.06	55.7582	6	52
Amoxitollin	-1.874	3.51168	63.3964	4.78119	12.1043	1516.09	51.0391	6	44
Benzofurumethazide	-0.8075	0.65206	99.6471	4.24449	12.8541	1147.12	49.7141	12	41
Benzocaine	-0.4883	0.23844	20.5043	4.54796	6.52863	397.03	25.8767	6	23
Benzthiazide	-1.3398	1.79506	50.9651	6.69282	12.9721	1114.11	53.1231	10	40
Clozapine	0.0092	8.46E-05	45.0577	5.92358	11.5903	1519.05	50.9291	12	42
Dibucaine	-0.5602	0.31382	57.7981	5.09923	10.5046	2425.05	59.441	10	54
Diethylstilbestrol	-0.2302	0.05299	33.7086	4.85094	11.5338	1301.02	46.6199	12	40
Diffunisal	0.2593	0.06724	11.5289	4.03982	9.84339	423.05	31.7343	12	26
Dipyridamole	-3.3772	11.4055	95.8664	4.30728	11.5724	4981.12	80.9197	10	76
Folic Acid	-3.3182	11.0105	52.3095	3.83215	9.33155	1817.13	58.6211	12	51
Furosemide	-0.9949	0.98983	33.6078	4.6696	12.2524	669.09	39.7447	11	32
Hydrochlorothiazide	-1.5436	2.3827	35.4327	7.26833	12.8018	404.1	32.1423	6	25
Imipramine	0.091	0.00828	39.2562	5.70631	11.5894	1789.02	51.643	12	45
Indomethacin	0.2922	0.08538	37.8739	4.12177	11.086	1249.06	50.5967	12	41
Ketoprofen	-0.2088	0.0436	21.9194	4.29006	9.91827	814.03	39.9011	12	33
Lidocaine	1.166	1.35956	45.8867	5.09304	9.98654	1249.03	42.3114	6	39
Meclofenamic acid	1.4704	2.16208	27.2526	4.4468	11.3886	619.05	39.0367	12	30

Input Layer

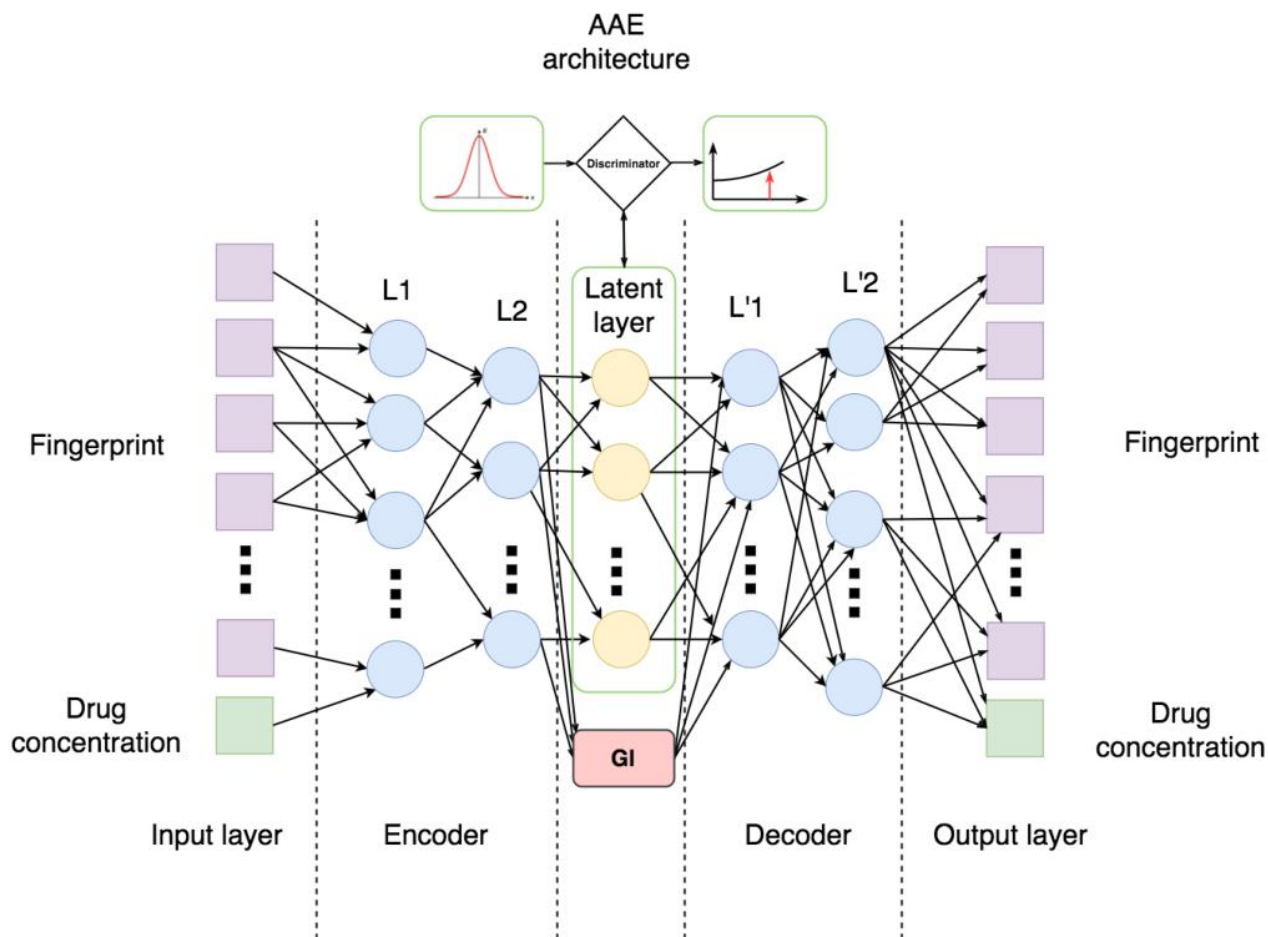
Hidden
Layers

Output layer

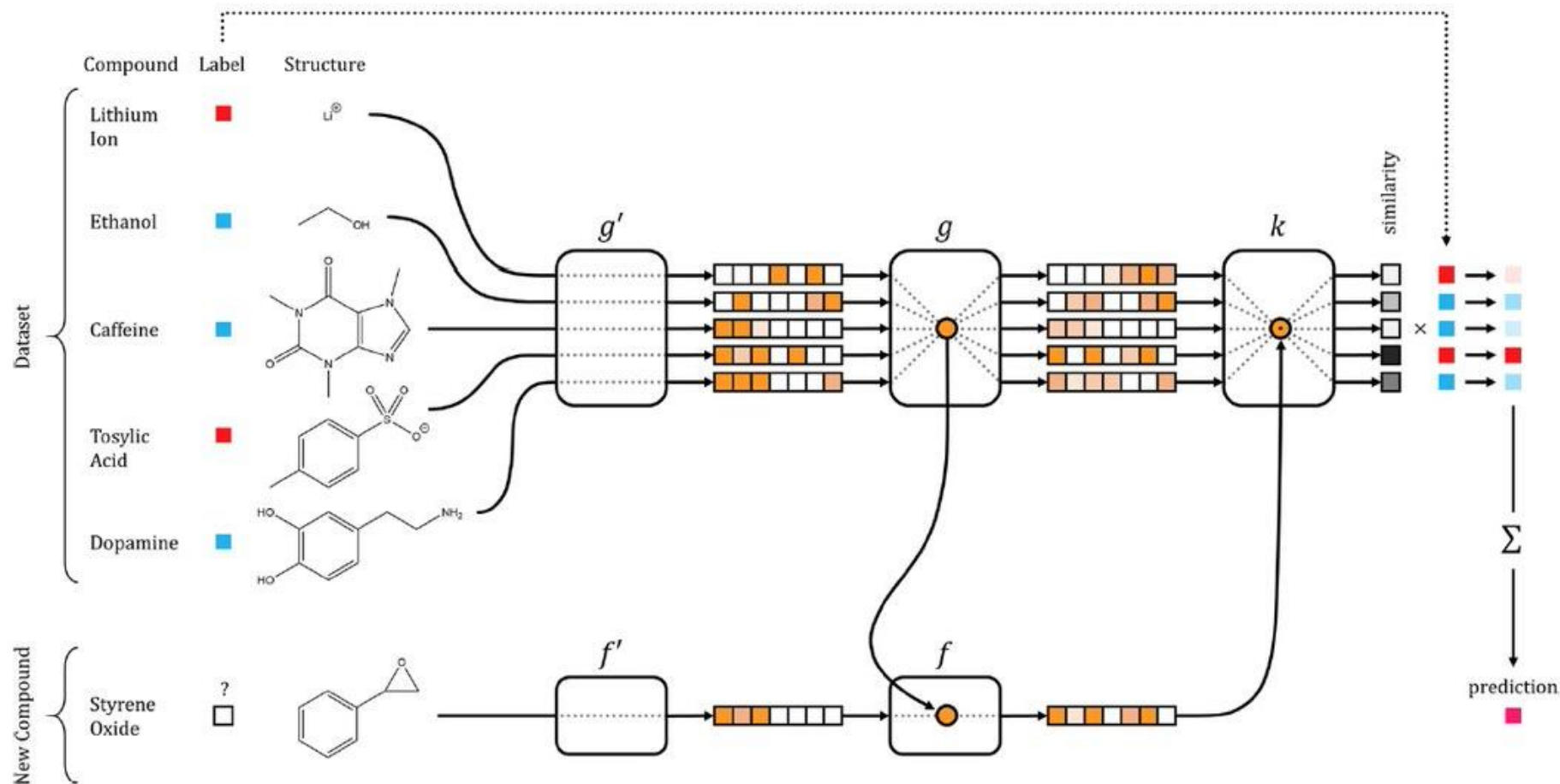
Correlation



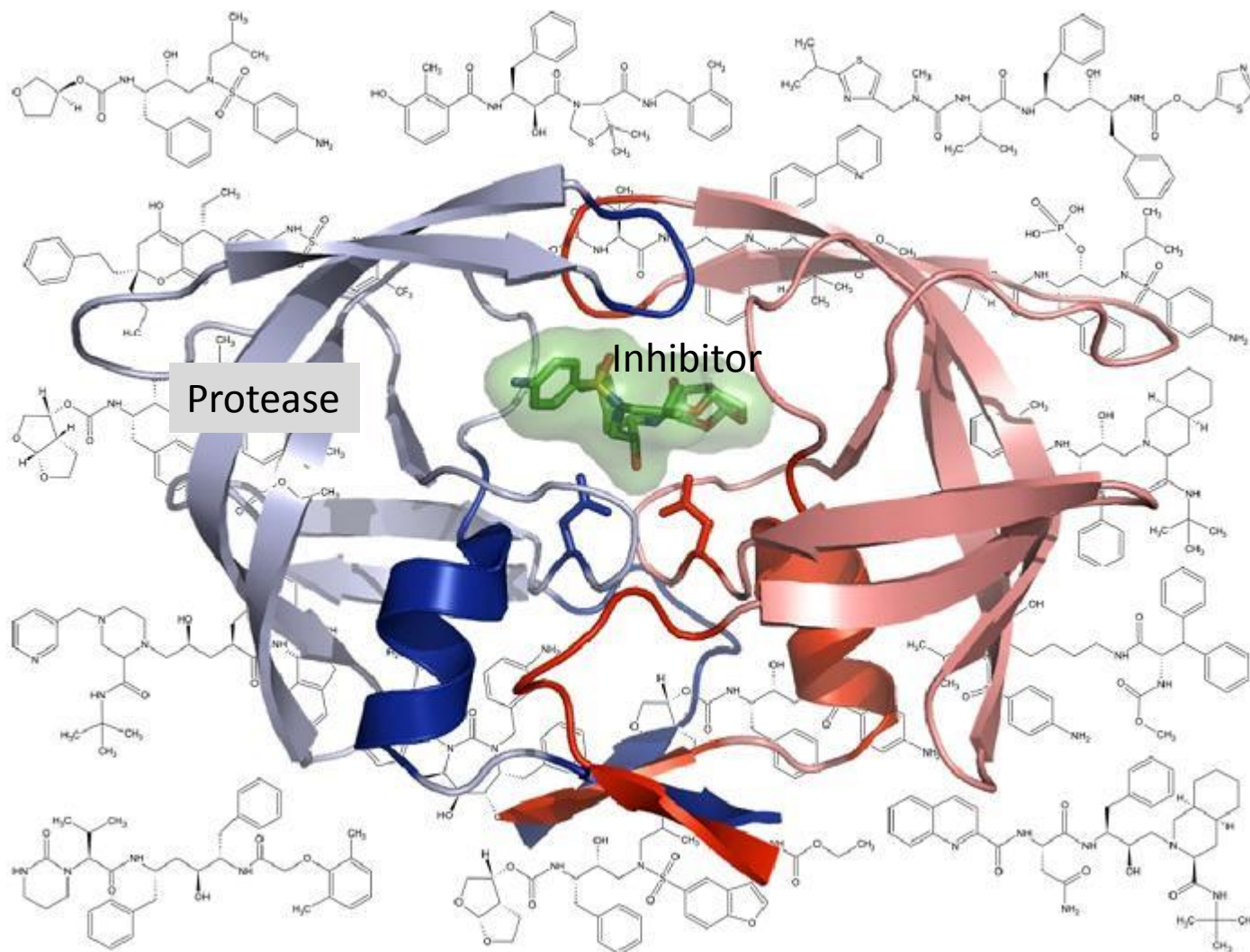
Data Augmentation using Generative Adversarial Networks



Network Architecture for One-Shot Learning in Drug Discovery



HIV Protease Inhibitors are Powerful anti-AIDS drugs



Quality Inhibitors for Quality Results