Volgograd State Medical University

Research Center of Innovative Medicines

Laboratory for Information Technology in Pharmacology and Computer Modeling of Drugs

MULTI-TARGET NEURAL NETWORK MODEL OF ANXIOLYTIC ACTIVITY OF CHEMICAL COMPOUNDS BASED ON CORRELATION CONVOLUTION OF ENERGY SPECTRA OF MULTIPLE DOCKING

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Research Center of Innovative Medicines

WHO – Anxiety disorders

World Health Organization | Health Topics | Countries | Newsroom | Emergencies | Data | About WHO

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Anxiety disorders

27 September 2023

301 million people

Key facts

- **Anxiety disorders are the world's most common mental disorders, affecting 301 million people in 2019.**
- **More women are affected by anxiety disorders than men.**
- **Symptoms of anxiety often have onset during childhood or adolescence.**
- **There are highly effective treatments for anxiety disorders.**
- **Approximately 1 in 4 people with anxiety disorders receive treatment for this condition.**

Overview

Everyone can feel anxious sometimes, but people with anxiety disorders often experience fear and worry that is both intense and excessive. These feelings are typically accompanied by physical tension and other behavioural and cognitive symptoms. They are difficult to control, cause significant distress and can last a long time if untreated. Anxiety disorders interfere with daily activities and can impair a person's family, social and school or working life.

An estimated 4% of the global population currently experience an anxiety disorder *(1)*. In 2019, 301 million people in the world had an anxiety disorder, making anxiety disorders the most common of all mental disorders *(1)*.

Although highly effective treatments for anxiety disorders exist, only about 1 in 4 people in need (27.6%) receive any treatment *(2)*. Barriers to care include lack of awareness that this is a treatable health condition, lack of investment in mental health services, lack of trained health care providers, and social stigma.

Related

Comprehensive mental health action plan 2013–2030 >

Mental Health Gap Action Programme (mhGAP) >

More on mental health >

Fact sheets

Mental disorders
8 June 2022

Depressive disorder

Purpose

To construct a multi-target model of the dependence of the anxiolytic activity of chemical compounds on their multiple docking energies using correlation convolution and artificial neural networks

Tasks

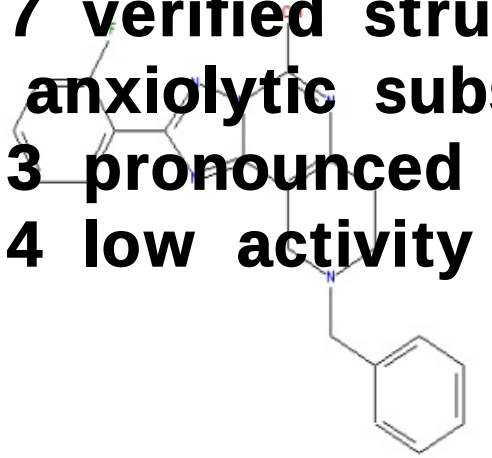
- Construction of optimized 3D models of ligands
- Selection and validation of relevant biotargets
- Formation of spaces for multiple docking
- Performing multiple ensemble docking to relevant biotargets
- Correlation convolution of multiple docking energy spectra
- Formation of training set
- Training of neural networks and selection of the best model

Verified database of anxiolytic substances

Anxiolytic Substances v11 - Corrected

24 January 2022

Structure



537 verified structures of anxiolytic substances:
273 pronounced activity
264 low activity

Activity

Standard Type: ED50

pChEMBL Value:

Assay

Assay ChEMBL ID: CHEMBL779993

Assay Description: Anxiolytic response measur
stimuli in rats.

Mol_ID	Brutto formula	Mol weight	Salt Component
1	$C_{21}H_{18}FN_5O$	375.3	

Activity Processing

Gen_Assay_IDs: Rat-07a

Gen_Assay_CHEMBLID: CHEMBL3256343 CHEMBL
CHEMBL784521 CHEMBL8

Compound Codes & Names

MolFileName: CHEMBL99259

CODE - Molecule ChEMBL ID: CHEMBL99259

Molecule Name:

Compound Key: 8g

References

Document_ChEMBL_ID	Document Journal	Document_Year
CHEMBL1125833	J. Med. Chem.	1991

15.07.2022

РОССИЙСКАЯ ФЕДЕРАЦИЯ

СВИДЕТЕЛЬСТВО

о государственной регистрации базы данных

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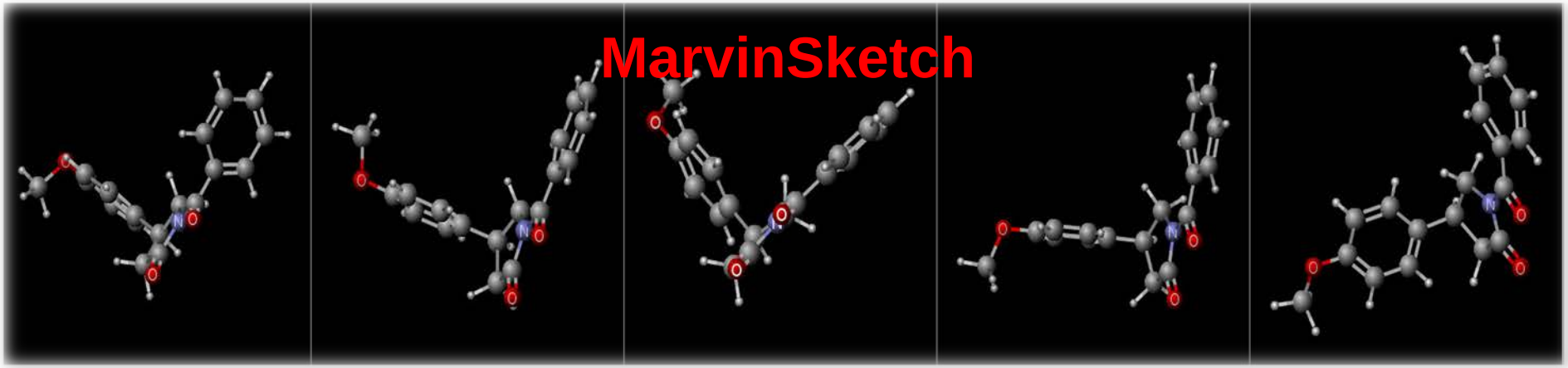
Руководитель Федеральной службы по интеллектуальной собственности

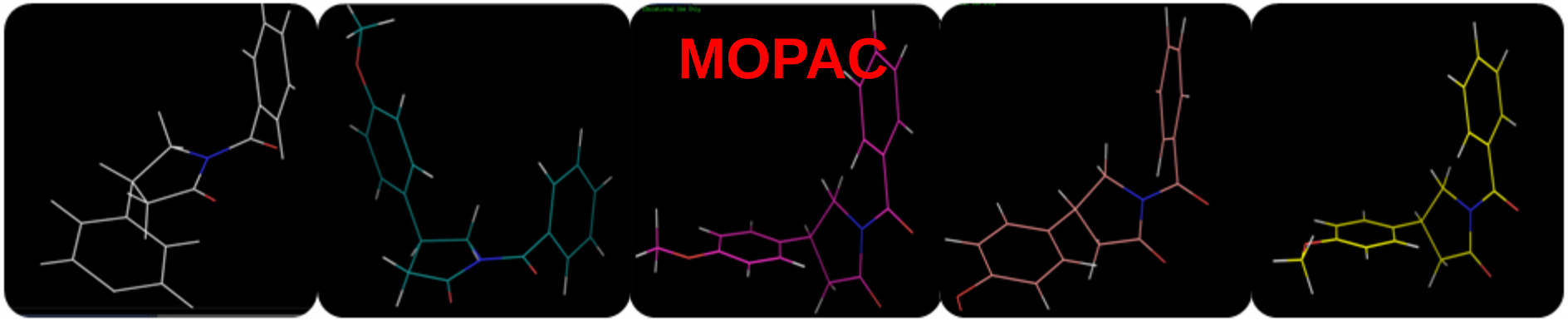
Ю.С. Зубов

Construction of optimized 3D models of ligands

Molecular mechanics 10 conformers

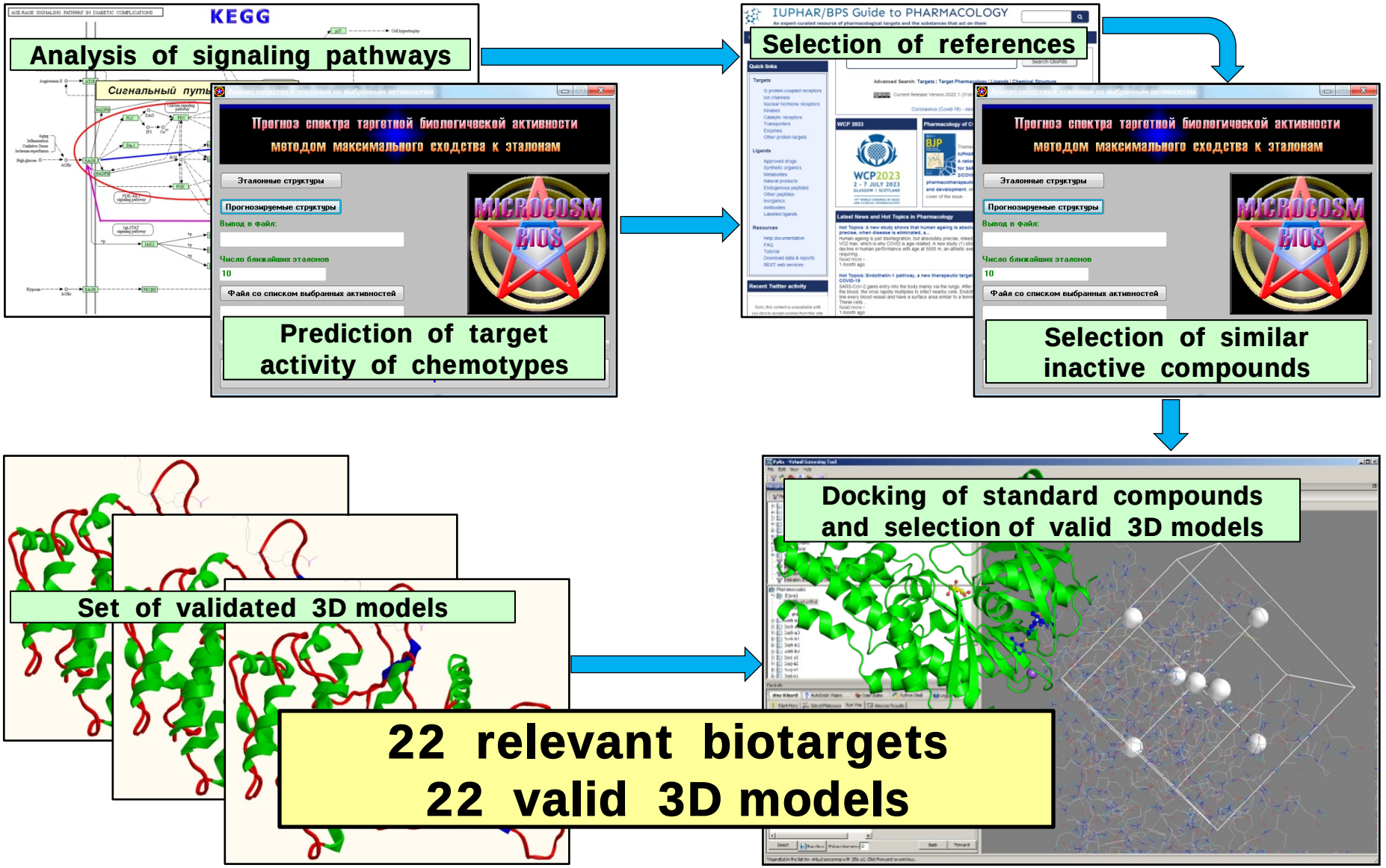


Quantum chemistry PM7



Vassiliev P. M., et al. Biochem. (Mosc.) Suppl. B: Biomed. Chem., 2019; 13(3):256-263.

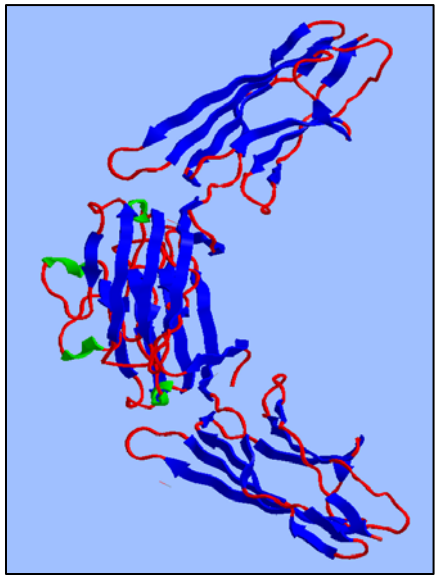
Selection and validation of relevant biotargets



Vassiliev P. M., et al. Pharmaceuticals, 2023; 16(5):731.

Multiple docking

Ligands interact with the protein throughout its entire volume



- Active concentration 10^{-10} M.

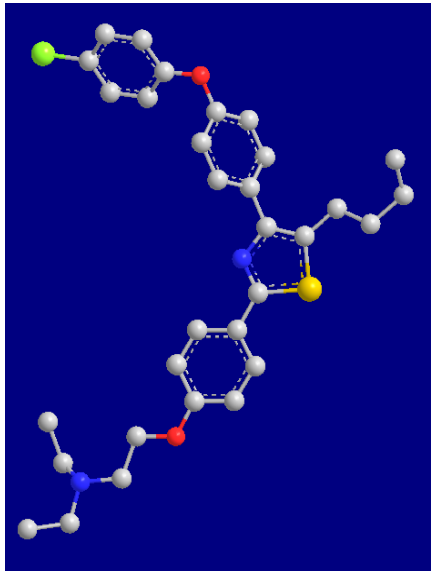
Avogadro's number ~$6 \cdot 10^{23}$.

~$6 \cdot 10^{13}$ ligand molecules interact with the target protein!

- RAGE volume 34 902 Å^3.

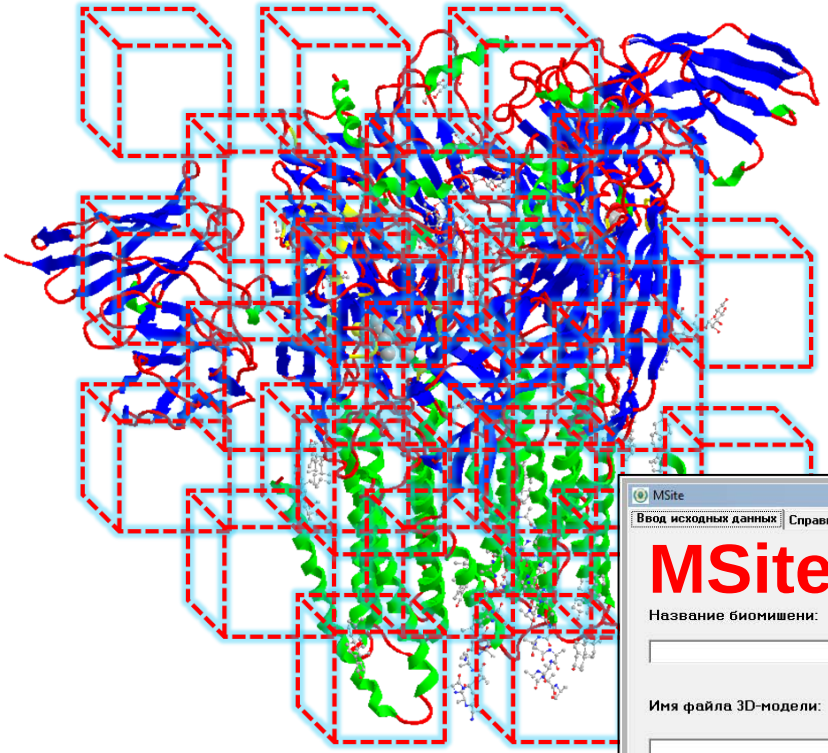
Ligand volume 1 578 Å^3.

The ligand fits into the receptor space at least 22 times!

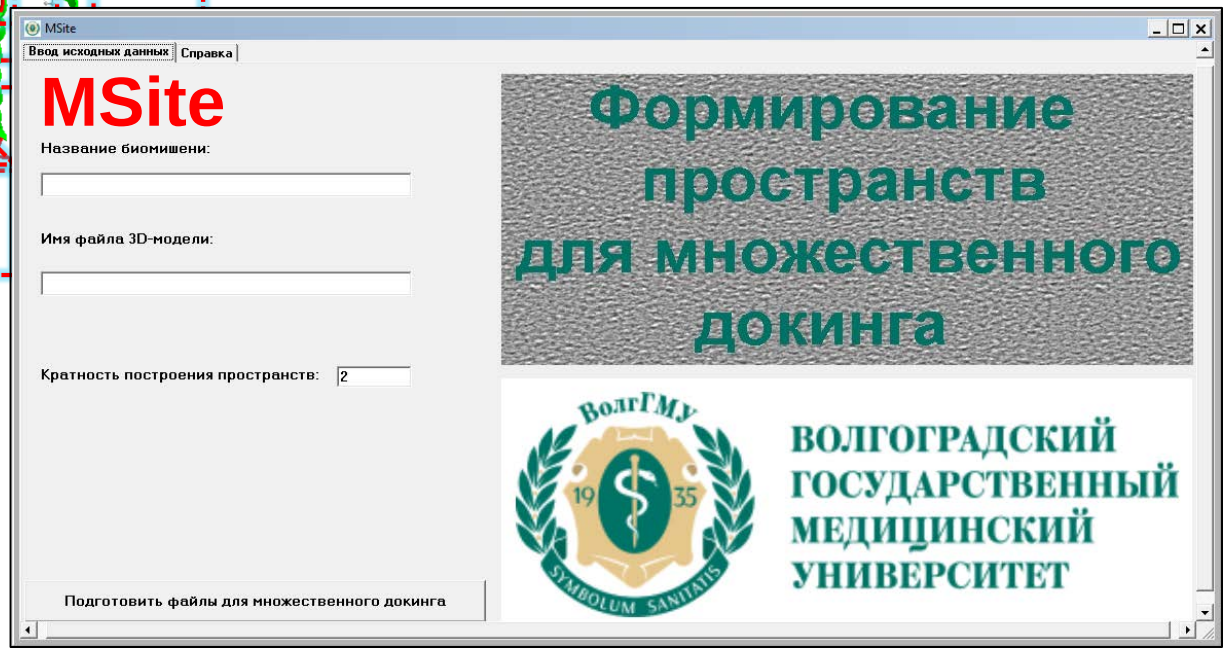


Vassiliev P. M., et al. Volgograd Scientific Medical Journal, 2021; 3:57-61.

Formation of spaces for multiple docking

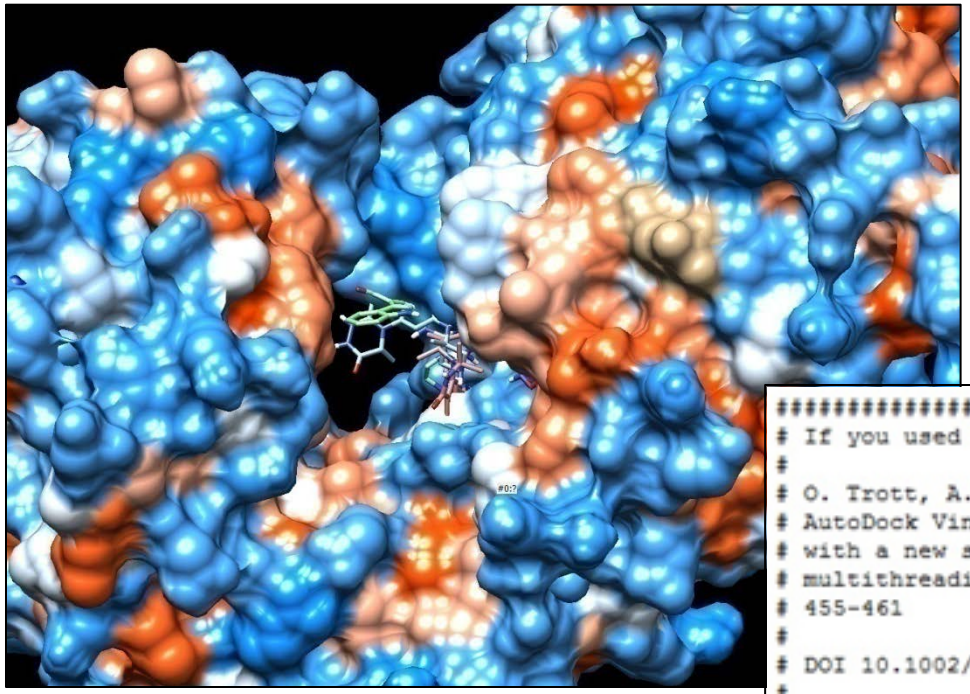


3·3·3 = 27 spaces



Vassiliev P. M., et al. Journal of Volgograd State Medical University, 2022; 19(4):88-93.

Multiple ensemble docking to relevant biotargets



Each of 537 ligands
to each of 22 3D models
to each of 27 spaces
5 times in 10 conformations

$$\Delta E_{ijkl} = \min(\Delta E_{ijklm})$$

AutoDock Vina

```
##############################################################################
# If you used AutoDock Vina in your work, please cite:                       #
#                                                                            #
# O. Trott, A. J. Olson,                                                     #
# AutoDock Vina: improving the speed and accuracy of docking                 #
# with a new scoring function, efficient optimization and                    #
# multithreading, Journal of Computational Chemistry 31 (2010)               #
# 455-461                                                                    #
#                                                                            #
# DOI 10.1002/jcc.21334                                                      #
#                                                                            #
# Please see http://vina.scripps.edu for more information.                   #
##############################################################################

Output will be ..\..\Ligands\Flavopiridol-PM7_out.pdbqt
Detected 12 CPUs
WARNING: at low exhaustiveness, it may be impossible to utilize all CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 58910256
Performing search ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**********
```

Total processed
537 · 22 · 27 · 5 · 10
~ 16 000 000
docking energies

Perfilev M. A., Vassiliev P. M., et al. Russian Chemical Bulletin, 2023; 72(4):1075–1082.

Correlation convolution

$$R_{ijkl} = \frac{Cov_{ijkl}}{S_{ikl} \cdot S_{jkl}}, \quad i, j = 1 \ldots M, \; k = 1 \ldots K, \; l = 1 \ldots L, \; i \neq j$$

$$W_{kn} = \frac{1}{2} \sum_{\substack{l=1 \\ i,j \\ i \neq j}}^{L} \sum^{M} R_{ijkl} \cdot X_{ilkn} \cdot X_{jlkn}, \quad k = 1 \ldots K, \; n = 1 \ldots N$$

K = 22, number of biotargets

M = 27, number of docking spaces

L = 5, number of docking energies for space i

N = 537, number of substances

2970 docking energies ⟶ 22 convolution variables

Formation of training set

Mol_ID	Code	LevHM	ADRA1A	ADRA1B	ADRA2A	ADRA2B	AGTR1	CA2	CA4	CNR1	GABAR	HTR1A	HTR1B	HTR1D	HTR2A	HTR2B	HTR2C	HTR4	HTR7	MTNR1A	MTNR1B	NMDA	SCN11A	SLC18A2	Samp1	Samp2	Samp3
1	CHEMBL99259	hm	16278	18509	17455	18446	18109	14903	12669	14127	20663	21214	16198	17404	19442	13662	19454	19865	15295	10879	18473	31531	22906	16151	train	val	test
2	CHEMBL513136	hm	14868	17099	14794	16137	15451	12078	10294	11251	16248	17422	12848	16467	18570	11539	16997	18216	11970	9607	15880	27271	20472	14342	train	train	val
3	CHEMBL3410223	hm	11852	13939	12749	14939	13927	11120	9701	9533	15033	15999	12326	13836	15856	10189	15055	16350	11869	8939	14991	27412	17231	13713	train	train	train
4	CHEMBL323519	hm	10932	11218	10318	12985	11799	10191	8659	8351	12785	15856	10832	13169	13155	8758	12770	13362	10077	7212	13512	21909	14430	11048	train	train	train
5	CHEMBL204240	hm	10088	11098	9952	11353	10717	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	8943	7737	11629	19264	13112	10969	train	train	train
6	CHEMBL314608	hm	10056	11154	9986	11380	[illegible]	[illegible]	[illegible]	7854	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	8753	7276	11685	21543	14357	10778	test	train	train
7	CHEMBL319178	hm	15755	17820	16585	17774	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	14662	10543	17765	30412	21758	15589	val	test	train
8	CHEMBL101045	hm	10159	11086	9850	12585	11113	10085	8762	8396	12079	15169	10256	11146	12901	8242	11878	11981	9819	7311	13254	20097	13973	11041	train	val	test
9	CHEMBL543621	hm	10644	10914	10052	12555	11158	9763	8392	8134	11871	14655	10046	10965	12494	8124	12326	12538	9293	7226	12988	19797	13608	10626	train	train	val
10	CHEMBL545731	hm	10239	10862	9665	12236	11070	9481	8237	8191	11803	14189	10021	11317	12112	7838	11833	12787	9229	7184	12139	19905	13106	10489	train	train	train
11	CHEMBL3409256	hm	[illegible]	[illegible]	15835	18932	[illegible]	[illegible]	13122	12425	20048	20790	15207	17841	19084	12438	19261	[illegible]	14037	10866	[illegible]	[illegible]	[illegible]	17211	train	train	train
12	CHEMBL153823	hm	[illegible]	[illegible]	11147	[illegible]	[illegible]	[illegible]	9547	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	8960	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	12414	train	train	train
13	CHEMBL466847	hm	[illegible]	16420	14651	[illegible]	[illegible]	[illegible]	10774	[illegible]	14609	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	14420	test	train	train
14	CHEMBL3084529	hm	13034	14415	13602	14811	15314	11688	9927	9810	15329	17164	11916	14686	16647	10625	14668	15677	11395	9014	14695	27452	20032	13602	val	test	train
15	CHEMBL3410224	hm	11747	14147	12607	15214	13653	11026	9401	9638	14955	16242	12059	13196	15475	9764	14485	16342	12004	8434	14444	25397	16959	12735	train	val	test
16	CHEMBL13662	hm	15243	15965	14150	15769	14374	12930	12157	11423	18667	17019	13803	15380	16634	11023	16270	17534	12992	11708	15470	26886	17962	15776	train	train	val
17	CHEMBL3246317	hm	13229	15026	[illegible]	[illegible]	[illegible]	12142	[illegible]	[illegible]	[illegible]	14471	[illegible]	14655	15052	10221	14263	[illegible]	10954	[illegible]	14236	23029	17118	12373	train	train	train
18	CHEMBL3808873	hm	9778	11786	10670	[illegible]	[illegible]	8466	[illegible]	[illegible]	[illegible]	11727	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	20562	14043	9865	train	train	train
19	CHEMBL67100	hm	12898	14435	12203	[illegible]	13452	10616	[illegible]	[illegible]	[illegible]	15552	[illegible]	14316	14250	[illegible]	[illegible]	[illegible]	11253	[illegible]	13684	24600	17597	14736	train	train	train
20	CHEMBL157522	hm	14875	15179	13821	15268	13823	12489	11467	11140	19337	16193	13134	14992	15574	10707	15799	16502	12868	10911	14782	26470	17931	14736	test	train	train
21	CHEMBL540812	hm	10418	11050	9974	12446	11001	9614	8231	8011	12255	14812	10343	11392	12327	8338	12007	12520	9604	6964	12904	20891	14109	10443	val	test	train
22	CHEMBL98258	hm	15543	18148	17201	18217	18314	14526	12590	13336	20207	20255	16127	17094	19634	13950	18494	19099	14831	10679	18614	31388	22355	16279	train	val	test
23	CHEMBL155270	hm	12207	12152	10890	12752	11726	10204	9411	9194	16741	13263	10848	12896	12850	8975	12968	13210	10370	9190	12525	21024	15422	12080	train	train	val
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27	CHEMBL44515	hm	13115	15980	14560	14938	14428	12015	10593	10639	15365	17236	13396	16130	16277	10324	16437	19481	11785	9385	14946	27084	18447	13196	test	train	train
28	CHEMBL378298	hm	13736	14746	13252	15864	14743	12150	10803	11017	16776	18649	13469	15770	16682	11151	16054	16636	12515	9686	16004	27446	18379	14476	val	test	train
29	CHEMBL562219	hm	10807	12231	10826	11644	11287	9476	9009	8556	12461	13105	10539	[illegible]	[illegible]	8955	12724	13639	9546	8246	11916	21203	14752	11753	train	val	test
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31	CHEMBL87790	hm	8778	9286	8355	9454	9233	8059	[illegible]	7357	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	11351	7764	6528	10139	16602	11650	9368	train	train	train
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33	CHEMBL431298	hm	12756	15059	14106	15543	14609	12406	10098	10429	16614	18177	12861	13703	16421	10492	15973	17116	12296	8615	16389	28327	18777	13971	train	train	train
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36	CHEMBL41	hm	11803	13027	11635	12743	12449	9943	9154	9423	14441	13549	10609	12520	13443	9602	13234	13866	10005	9400	11920	22693	15355	11640	train	val	test
37	CHEMBL40906	hm	13625	16599	13508	14176	14077	12267	10561	10253	14907	16017	13311	15028	16724	10310	14670	18695	11431	10325	15014	24632	17792	13498	train	train	val
38	CHEMBL465161	hm	13384	14197	10658	14399	13165	13360	10355	9366	14232	16762	11595	14843	16323	10218	14080	13511	11278	8549	15991	25592	19747	12489	train	train	train
39	CHEMBL88106	hm	9256	10248	9442	10774	10380	8757	7842	7792	12106	11711	9318	10561	11011	8012	11212	12535	8663	6888	10887	18117	12618	10224	train	train	train
40	CHEMBL86557	hm	9941	11026	10154	11463	10714	9409	8235	8262	12016	12569	9724	10956	11653	8050	12106	13468	9160	7486	11480	19973	13184	10885	train	train	train
41	CHEMBL70418	hm	12224	14630	11327	11652	11920	10445	9220	8870	13129	12974	10889	12727	14353	9722	13603	15299	10070	8867	12759	21937	15306	11389	test	train	train
42	CHEMBL2263293	hm	12840	13703	12143	15298	13616	12201	11071	10624	16386	17167	12739	14183	15288	10895	14828	15345	12110	8730	15122	24634	18509	13511	val	test	train
43	CHEMBL190772	hm	12598	14141	12959	15600	14644	11760	10286	10687	17909	17352	12803	14546	16289	10470	16731	15714	11558	9252	16395	25860	18291	13749	train	val	test
44	CHEMBL20042	hm	13304	15150	13958	15757	14863	12837	11193	11143	18038	16625	12530	15427	16978	11420	16073	17947	12366	10293	15369	26131	18160	15789	train	train	val
45	CHEMBL556089	hm	9519	11178	9937	10650	10283	9138	8041	7811	11399	12913	9369	10430	11810	8004	11703	12711	8422	7154	11591	19674	13785	10955	train	train	train
46	CHEMBL371631	hm	6886	7357	6544	7895	6947	6665	5506	5608	7841	9091	6530	7066	7812	5296	7668	7672	6138	4803	7934	12007	9237	7134	train	train	train
47	CHEMBL187827	hm	12896	14861	12081	15262	13637	10747	9478	10236	18442	15800	12107	14164	14939	10449	14726	16024	11186	9076	14924	24102	17766	13776	train	train	train

537 Anxiolytics

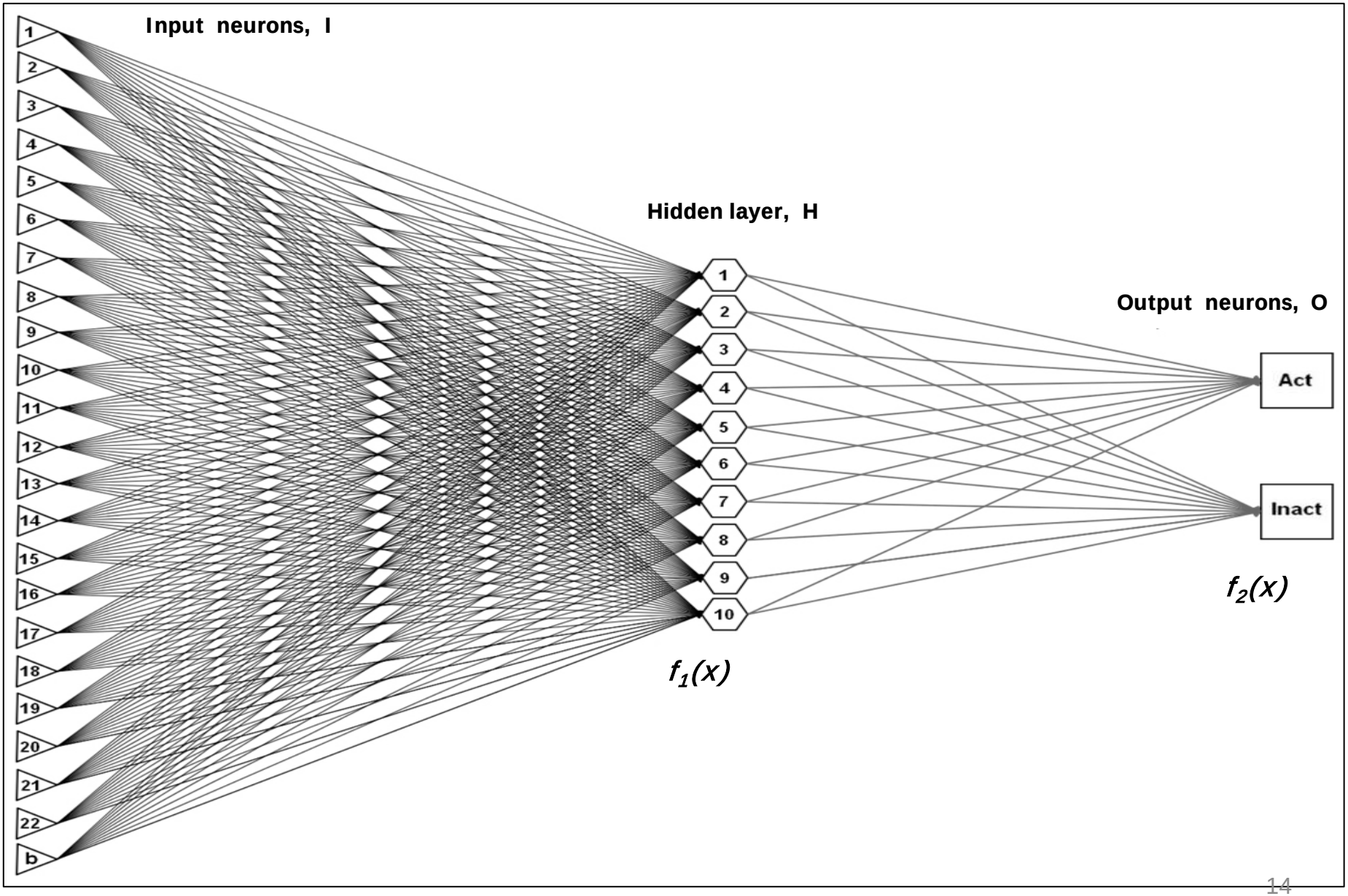
273 with pronounced activity

264 with low activity

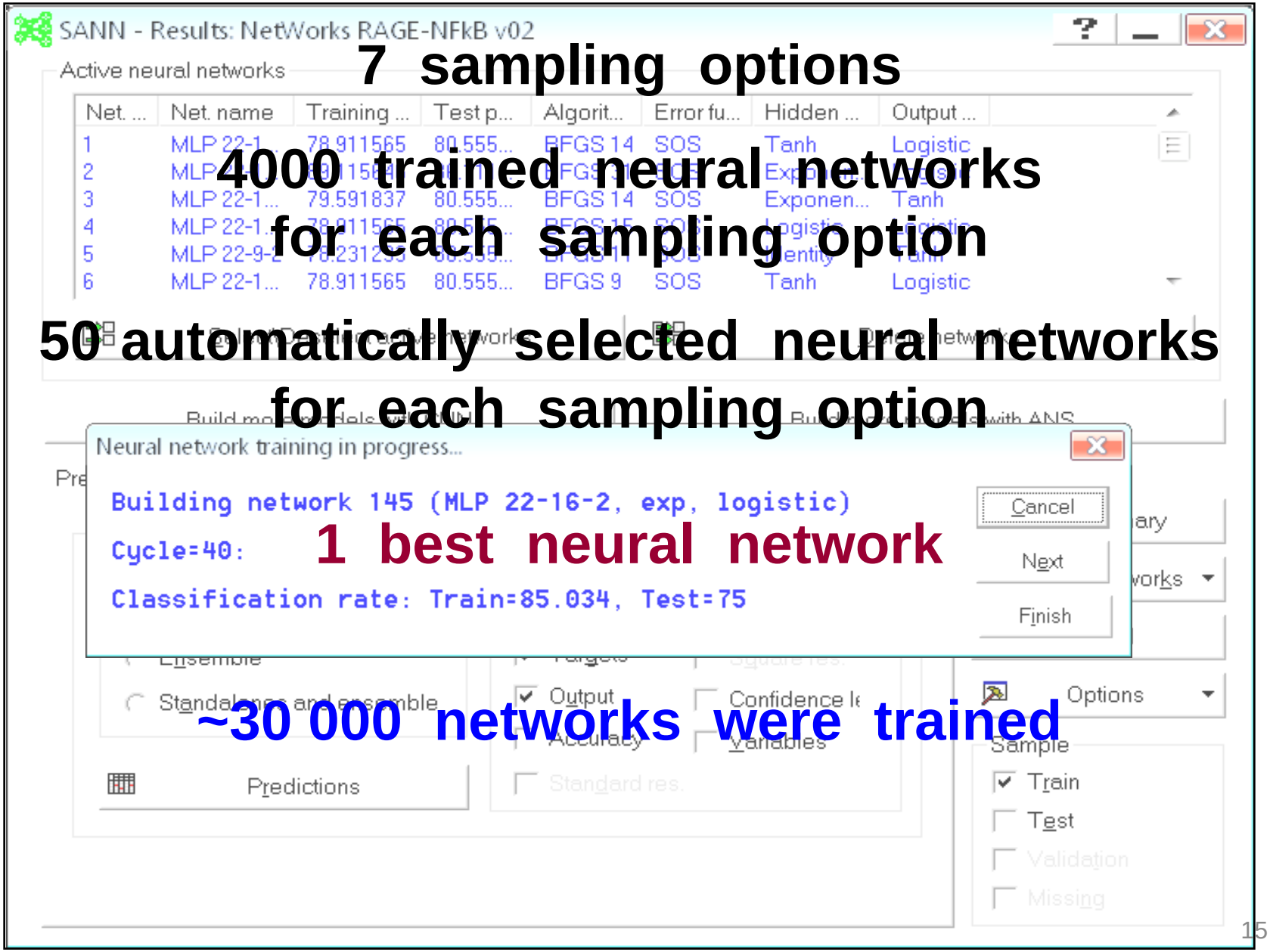
22 neurons

7 samplings

Neural network with bottle-neck



Training of neural networks



7 sampling options

4000 trained neural networks for each sampling option

50 automatically selected neural networks for each sampling option

1 best neural network

~30 000 networks were trained

Accuracy of the best neural network

MLP 22-14-2 (tanh, softmax)

Accuracy F_0 = 90.7%

Sensitivity F_a = 90.9%

Specificity F_n = 90.5%

AUC_{ROC} = 91.5%

Mol_ID	Code	Sampl1	F	F(h)	Sampl2	F	F(h)	Sampl3	F	F(h)	Sampl4	F	F(h)	Sampl5	F	F(h)	Sampl6	F	F(h)	Sampl7	F
1	CHEMBL99259	hm	0.985	0.985	hm	1.000	1.000	hm	0.808	0.808	hm	0.725	0.725	hm	0.596	0.596	hm	1.000	1.000	hm	1.000
2	CHEMBL513136	nhm	0.605	0.395	hm	0.504	0.504	hm	0.844	0.844	nhm	0.984	0.016	hm	0.938	0.938	hm	0.868	0.868	hm	1.000
3	CHEMBL3410223	hm	0.889	0.889	hm	0.808	0.808	hm	1.000	1.000	hm	1.000	1.000	hm	0.975	0.975	hm	1.000	1.000	hm	0.954
4	CHEMBL323519	hm	0.968	0.968	hm	0.816	0.816	hm	1.000	1.000	hm	1.000	1.000	hm	0.857	0.857	hm	0.878	0.878	hm	1.000
5	CHEMBL204240	nhm	0.[illegible]	0.[illegible]	nhm	0.[illegible]	0.[illegible]	nhm	0.859	0.[illegible]	hm	0.857	0.857	hm	[illegible]	[illegible]	nhm	0.938	0.062	nhm	1.000
6	CHEMBL314608	hm	[illegible]	[illegible]	hm	[illegible]	[illegible]	hm	1.000	1.000	hm	1.000	1.000	hm	[illegible]	[illegible]	hm	0.949	0.949	hm	0.954
7	CHEMBL319178	nhm	1.000	0.000	hm	1.000	1.000	hm	0.842	0.842	hm	0.780	0.780	hm	0.630	0.630	hm	1.000	1.000	hm	1.000
8	CHEMBL101045	hm	0.[illegible]	0.[illegible]	hm	0.572	0.572	hm	1.000	1.000	hm	1.000	1.000	hm	0.702	0.702	hm	0.588	0.588	hm	1.000
9	CHEMBL543621	hm	0.990	0.990	hm	0.649	0.649	hm	0.707	0.707	hm	1.000	1.000	hm	0.609	0.609	hm	0.699	0.699	hm	1.000
10	CHEMBL545731	hm	0.998	0.998	hm	0.721	0.721	hm	1.000	1.000	nhm	1.000	0.000	hm	0.783	0.783	hm	0.664	0.664	hm	1.000
11	CHEMBL3409256	hm	1.000	1.000	hm	1.000	1.000	hm	1.000	1.000	hm	1.000	1.000	hm	0.535	0.535	hm	1.000	1.000	hm	0.954
12	CHEMBL153823	hm	1.000	1.000	hm	0.510	0.510	hm	1.000	1.000	hm	1.000	1.000	hm	0.617	0.617	hm	0.823	0.823	hm	0.954
13	CHEMBL466847	nhm	1.000	0.000	hm	0.564	0.564	hm	1.000	1.000	hm	1.000	1.000	hm	0.633	0.633	hm	0.860	0.860	hm	1.000
14	CHEMBL3084529	hm	0.742	0.742	hm	0.765	0.765	hm	1.000	1.000	hm	0.991	0.991	hm	0.664	0.664	hm	1.000	1.000	hm	1.000
15	CHEMBL3410224	hm	0.734	0.734	hm	0.930	0.930	hm	1.000	1.000	hm	1.000	1.000	nhm	0.596	0.404	hm	0.901	0.901	hm	0.954
16	CHEMBL13662	hm	0.850	0.850	nhm	0.602	0.398	hm	0.656	0.656	nhm	0.908	0.092	nhm	0.739	0.261	hm	1.000	1.000	hm	0.954
17	CHEMBL3246317	hm	0.978	0.978	hm	0.961	0.961	hm	1.000	1.000	nhm	1.000	0.000	hm	0.937	0.937	hm	0.912	0.912	hm	0.954
18	CHEMBL3808873	hm	0.957	0.957	hm	1.000	1.000	hm	0.997	0.997	hm	1.000	1.000	hm	0.911	0.911	hm	0.974	0.974	hm	1.000
19	CHEMBL67100	hm	0.884	0.884	hm	[illegible]	[illegible]	hm	[illegible]	0.[illegible]	hm	1.000	1.000	hm	0.945	0.945	nhm	1.000	0.000	hm	0.954
20	CHEMBL157522	hm	0.836	0.836	nhm	0.634	0.366	hm	0.695	0.695	hm	0.967	0.967	nhm	0.714	0.286	hm	1.000	1.000	nhm	1.000
21	CHEMBL540812	hm	1.000	1.000	hm	0.603	0.603	hm	1.000	1.000	hm	0.961	0.961	hm	0.771	0.771	nhm	0.516	0.484	hm	0.954
22	CHEMBL98258	hm	1.000	1.000	hm	1.000	1.000	hm	0.845	0.845	hm	0.897	0.897	hm	0.862	0.862	hm	1.000	1.000	hm	1.000
23	CHEMBL155270	hm	1.000	1.000	nhm	0.651	0.349	hm	1.000	0.000	hm	1.000	1.000	hm	0.515	0.515	hm	0.656	0.656	hm	0.940
24	CHEMBL68606	nhm	0.680	0.320	hm	[illegible]	[illegible]	hm	[illegible]	[illegible]	nhm	0.[illegible]	[illegible]	hm	0.936	0.936	hm	0.837	0.837	hm	1.000
27	CHEMBL86611	hm	0.999	0.999	hm	0.959	0.959	hm	1.000	1.000	hm	1.000	1.000	hm	0.993	0.993	hm	1.000	1.000	hm	1.000
28	CHEMBL357362	hm	1.000	1.000	hm	0.761	0.761	hm	0.879	0.879	hm	0.655	0.655	hm	0.895	0.895	hm	0.600	0.600	hm	0.954
25	CHEMBL44515	hm	0.751	0.751	hm	0.874	0.874	hm	1.000	1.000	hm	0.998	0.998	hm	0.899	0.899	hm	0.898	0.898	hm	0.929
26	CHEMBL378298	hm	0.888	0.888	hm	0.[illegible]	0.[illegible]	hm	[illegible]	0.65[illegible]	hm	0.[illegible]	[illegible]	hm	0.880	0.880	hm	1.000	1.000	hm	0.954
30	CHEMBL562219	hm	1.000	1.000	[illegible]	[illegible]	[illegible]	hm	1.000	1.000	[illegible]	[illegible]	[illegible]	hm	0.984	0.984	hm	0.998	0.998	hm	0.954
31	CHEMBL260870	hm	0.767	0.767	nhm	0.755	0.245	hm	0.656	0.656	nhm	0.922	0.078	nhm	0.634	0.366	hm	1.000	1.000	hm	0.954
32	CHEMBL87790	nhm	0.649	0.351	hm	0.986	0.986	hm	1.000	1.000	hm	0.690	0.690	hm	0.573	0.573	hm	0.992	0.992	hm	1.000
33	CHEMBL188335	hm	0.892	0.892	hm	1.000	1.000	hm	0.846	0.846	hm	0.963	0.963	hm	0.990	0.990	hm	1.000	1.000	hm	0.954
34	CHEMBL431298	hm	0.691	0.691	hm	1.000	1.000	hm	0.841	0.841	hm	1.000	1.000	nhm	0.561	0.439	hm	1.000	1.000	nhm	1.000
35	CHEMBL559437	hm	1.000	1.000	hm	0.778	0.778	hm	1.000	1.000	hm	1.000	1.000	hm	0.641	0.641	hm	0.985	0.985	nhm	0.879
36	CHEMBL319966	hm	0.849	0.849	hm	0.999	0.999	hm	1.000	1.000	hm	0.986	0.986	hm	0.978	0.978	hm	1.000	1.000	hm	0.954
37	CHEMBL41	hm	1.000	1.000	nhm	0.526	0.474	nhm	0.765	0.235	hm	0.977	0.977	hm	0.835	0.835	hm	0.977	0.977	nhm	0.879
38	CHEMBL40906	hm	0.878	0.878	hm	0.932	0.932	hm	0.656	0.656	hm	0.892	0.892	nhm	0.502	0.498	hm	0.865	0.865	hm	0.954
29	CHEMBL465161	hm	0.654	0.654	hm	0.514	0.514	hm	1.000	1.000	hm	1.000	1.000	hm	0.713	0.713	hm	1.000	1.000	hm	1.000
39	CHEMBL88106	hm	1.000	1.000	hm	0.926	0.926	hm	1.000	1.000	hm	1.000	1.000	hm	0.980	0.980	hm	1.000	1.000	hm	1.000

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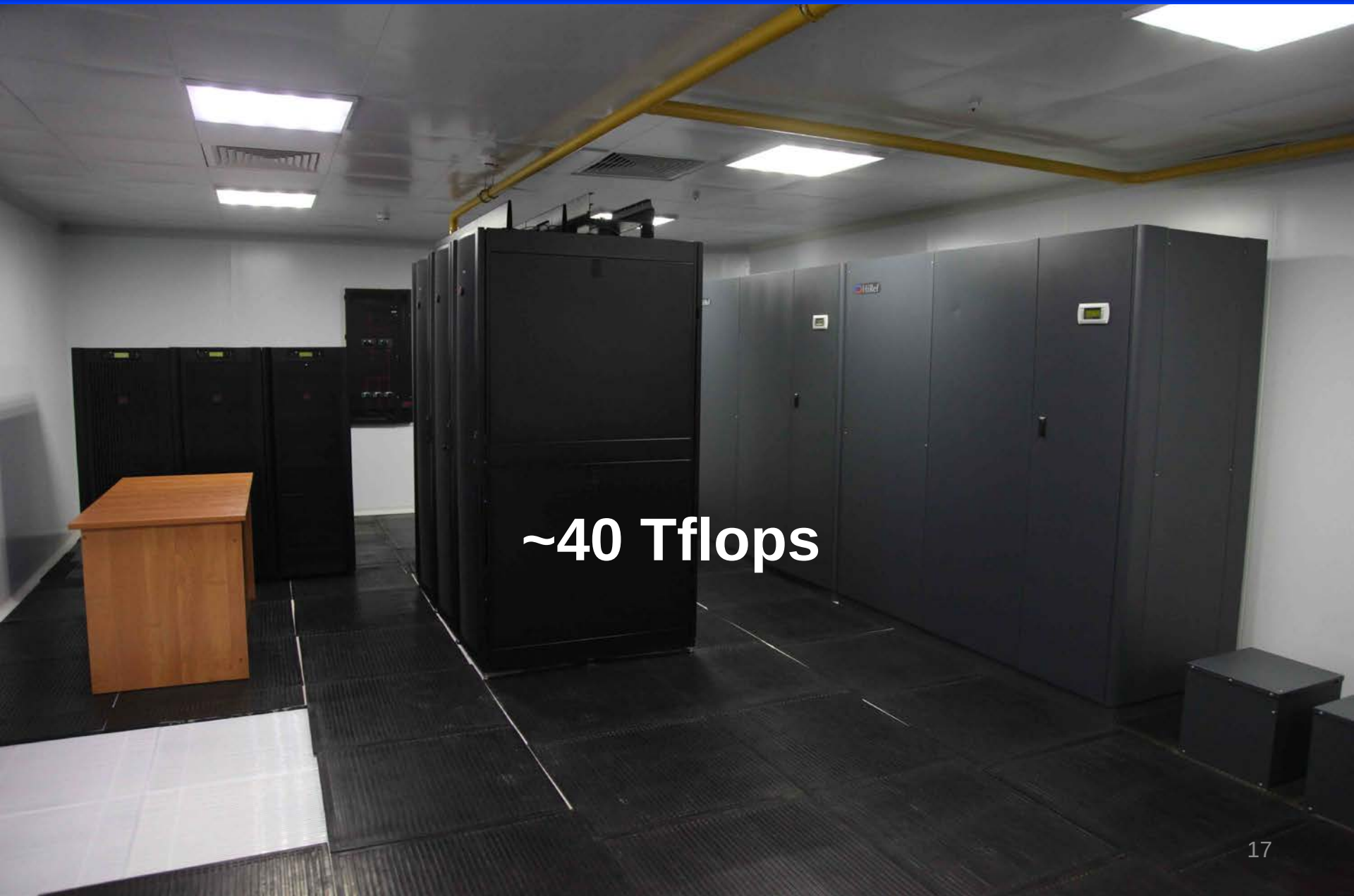

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Thank You for Your attention!