

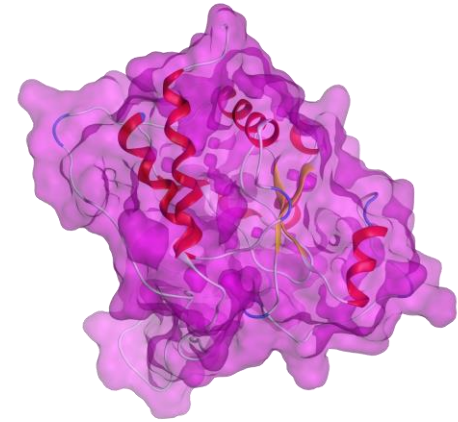
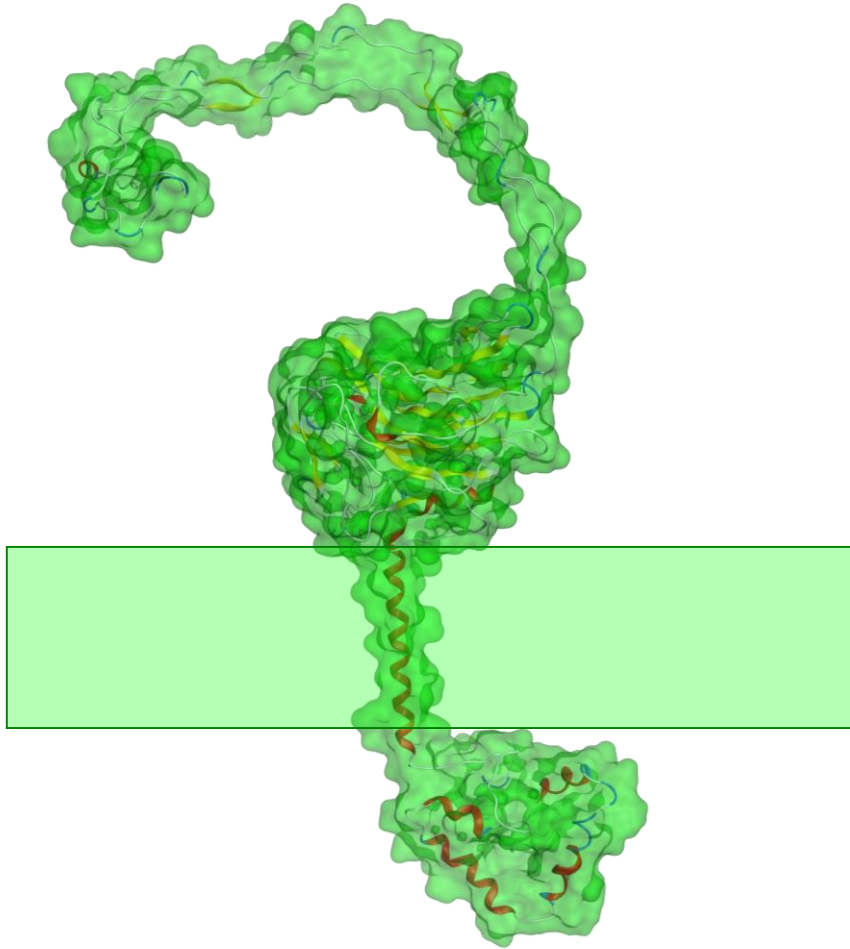
MMRO-2019



Ранжирование и анализ моделей белок-белкового докинга онлайн метасервером QASDOM

*Кузнецов Е.Н., Кравацкий Ю.В., Туманян
В.Г., Аджубей А.А.,
Анашкина Анастасия Андреевна*

Motivation





Protein-Protein Docking Servers

- Hex (Macindoe et al., 2010)
- SwarmDock (Torchala et al., 2013)
- ClusPro (Comeau et al., 2004)
- Gramm-X (Tovchigrechko and Vakser, 2006)
- Zdock (Pierce et al., 2014).

Docking

Test Set

The Qasdom server provides assessment and ranking of docking models created by multiple runs of various docking software.

Help

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Last update 2018.06.05

Online version

Please upload your files using the buttons below.

Select Receptor

Receptor name

Select Ligand

Ligand name

+ Docking files

Distance

Clustering

Submit

Reset

When uploading docking models multiple files can be selected simultaneously. An archive file (zip and other) containing docking results, or single PDB file can be also uploaded. All files except *.pdb and archives (*.zip, *.gz, etc.) will be ignored.

Help on Qasdom

Receptor and ligand structures must be uploaded as PDB formatted files. The docking results are accepted in the original output format as they are produced by the docking programs/servers. Alternatively docking results can be uploaded as PDB formatted structures of the complex. Models can be uploaded to the server as multiple PDB files or archives, with the file(s) containing single or multiple models. For the PDB format description please see [PDB web site](#). All files except archives and *.pdb will be ignored. If an archive is uploaded, all *.pdb files in the archive will be processed. Single quotes " ' " are not allowed as part of file names.

Qasdom server is intended to work by processing the models produced by a range of docking programs / servers, and computing all intermolecular receptor-ligand interactions. Since the resulting aggregate interactions data represent predictions by a range of different methods and computational techniques it is more accurate compared to results of a single docking run. Graphical output shows clusters of interactions indicating putative binding sites.

If you use **Qasdom**, please cite:

A.Anashkina, Y.Kravatsky, E.Kuznetsov, A.Makarov, A.Adzhubei. Meta-server for automatic analysis, scoring and ranking of docking models.

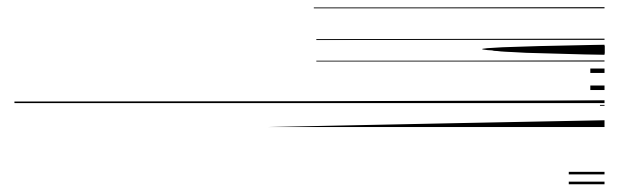
Bioinformatics, DOI: [10.1093/bioinformatics/btx591](https://doi.org/10.1093/bioinformatics/btx591), PMID: [28968724](https://pubmed.ncbi.nlm.nih.gov/28968724/)



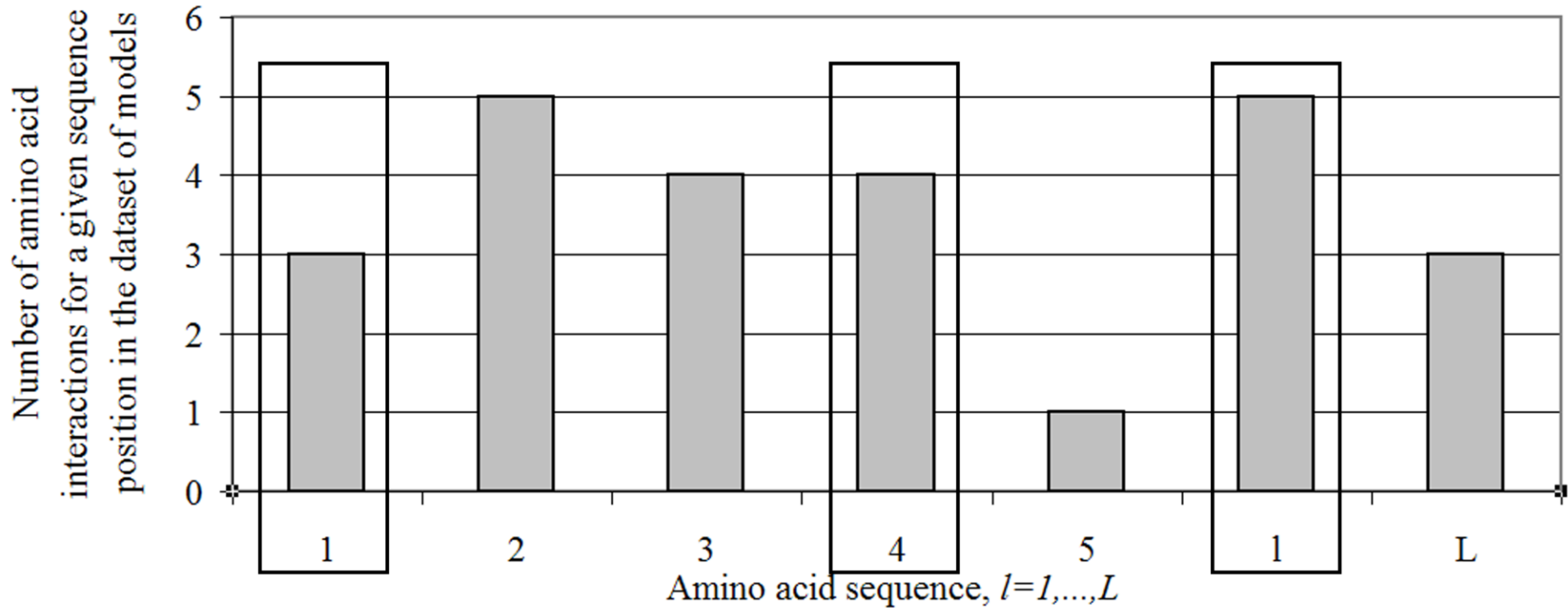
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Bioinformatics, 2018

Ranking scores

		Amino acid sequence $l=1,\dots,L$							
		1	2	3	4	5	l	L	Σ
Dataset of models $m=1,\dots,M$	1		•	•	•			•	RC_1^{mod}
	2	•		•		•	•		RC_2^{mod}
	3		•	•			•	•	RC_3^{mod}
	4		•		•		•		RC_4^{mod}
	5	•	•		•			•	RC_5^{mod}
	m	•			•		•		RC_m^{mod}
	M		•	•			•		RC_M^{mod}
	Σ	RC_1^{aa}	RC_2^{aa}	RC_3^{aa}	RC_4^{aa}	RC_5^{aa}	RC_l^{aa}	RC_L^{aa}	



Ranking scores



$$S_m = \frac{1}{C_{k,h}^L} \sum_{i=1}^L C_{i,h}^k R_i$$

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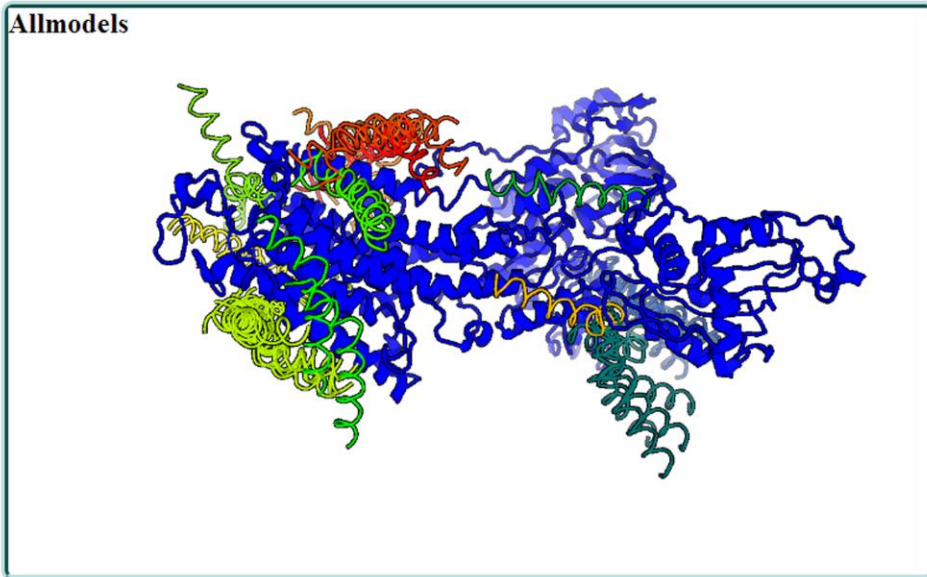
Show log

Go back

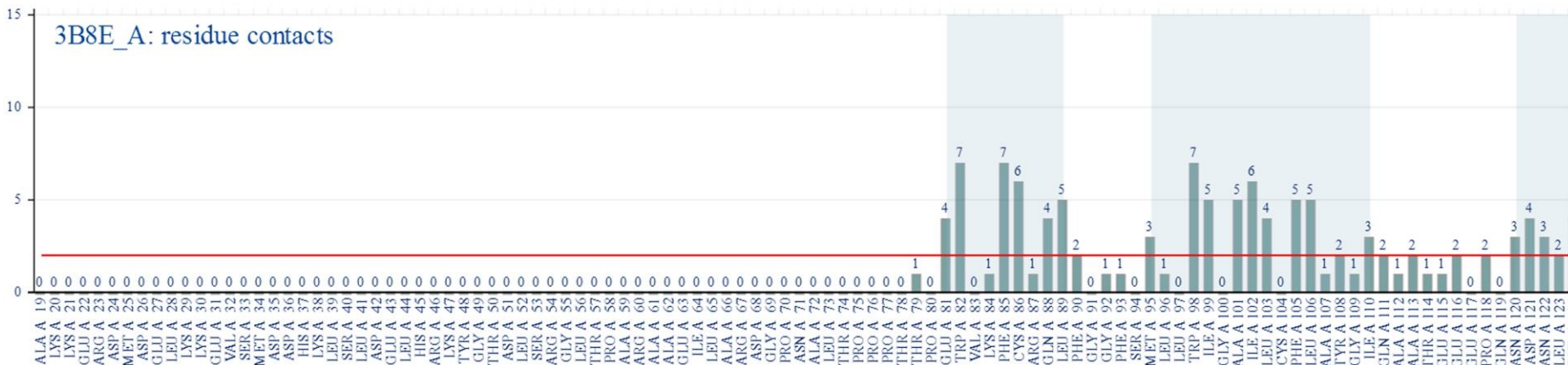
Model	S	S Atomic	RC	RC Atomic	Cluster		
complex.10	0.2114	0.3800	26	519	7	R	>
complex.8	0.2040	0.3781	24	469	7	R	>
complex.7	0.2040	0.3075	23	388	7	R	>
cluspro_model3	0.1928	0.1074	28	173	7	R	>
complex.2	0.1842	0.3091	23	423	7	R	>
complex.1	0.1718	0.2688	26	455	7	R	>
gramm_x_model5	0.1693	0.1770	20	258	7	R	>
gramm_x_model2	0.1656	0.2028	16	263	7	R	>
cluspro_model4	0.1619	0.0922	16	125	7	R	>
complex.3	0.1397	0.3067	27	616	12	W	>
complex.9	0.1286	0.2312	14	296	7	R	>
gramm_x_model10	0.1248	0.1493	40	541	9	T	>
complex.5	0.1224	0.2331	25	475	12	W	>
complex.6	0.1187	0.2430	22	527	12	W	>
cluspro_model7	0.1100	0.0735	20	170	11	V	>
cluspro_model1	0.1088	0.0560	19	125	11	V	>
cluspro_model0	0.1051	0.1270	18	262	11	V	>
gramm_x_model1	0.1051	0.1080	24	284	2	M	>
gramm_x_model7	0.1026	0.1483	31	485	5	P	>
cluspro_model8	0.1014	0.0761	25	274	5	P	>
hex_model8	0.1001	0.0810	18	173	2	M	>
gramm_x_model8	0.0964	0.1056	22	338	4	O	>
cluspro_model2	0.0964	0.0774	22	227	8	S	>
cluspro_model5	0.0927	0.0762	14	148	10	U	>

Permalink: <http://qasdom.eimb.ru/results/eIO5jrUdAXgkogze/results.html>

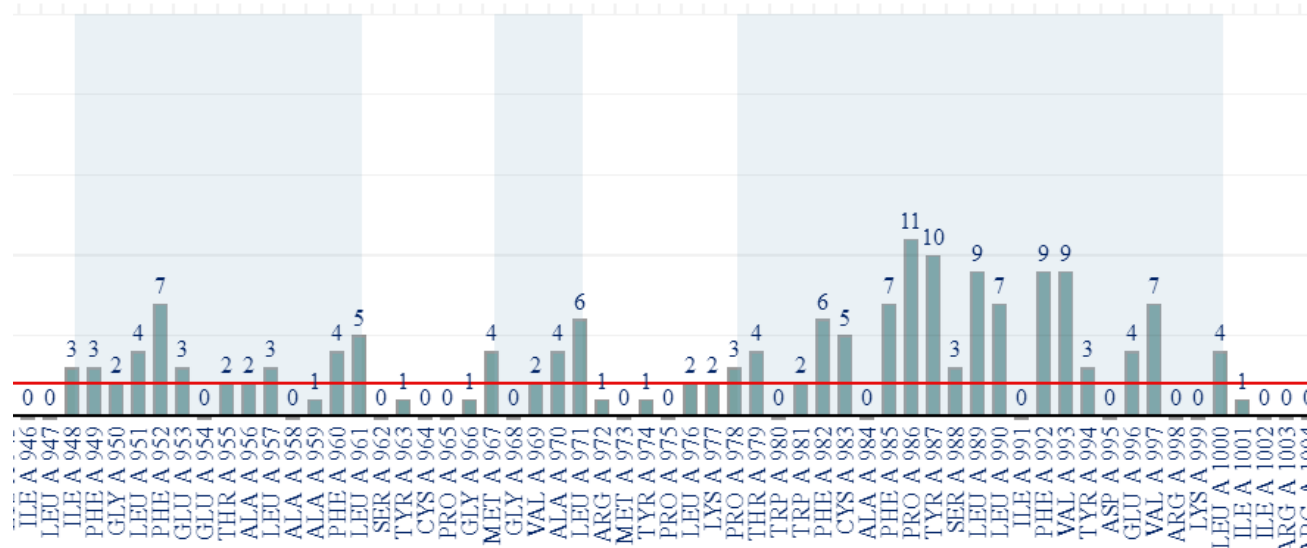
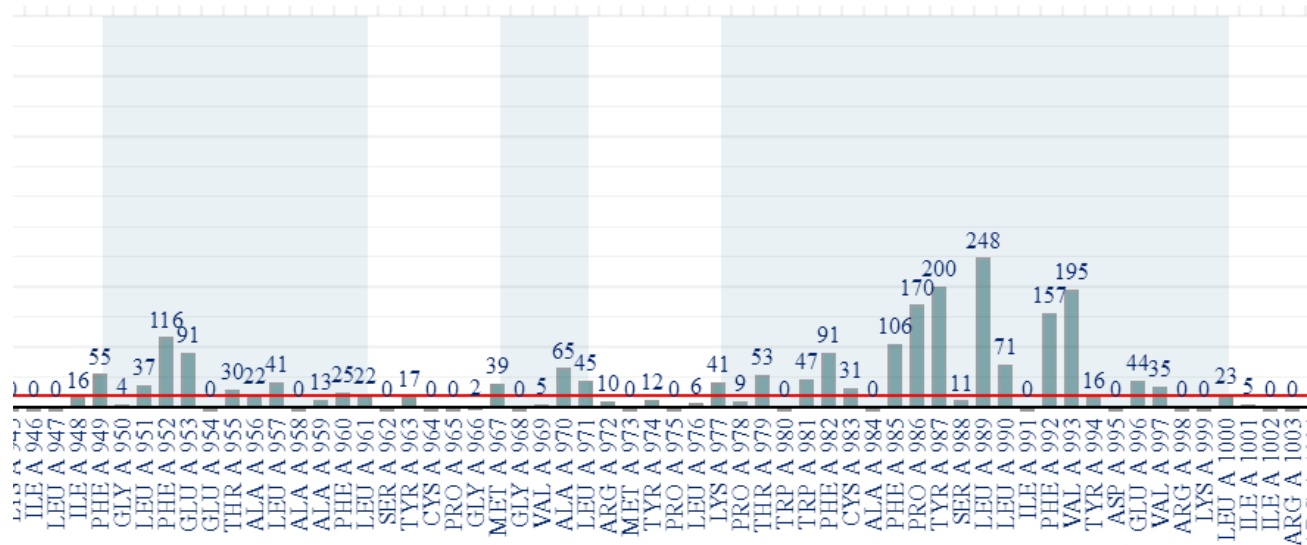
Ligand	2mlt_A.pdb
Receptor	3B8E_A.pdb
All Models	All models



3B8E_A: residue contacts



Clustering: *Linear clusters*



Clustering: *Structural clusters*

QASDOM: Assessment of Docking Models

Show log

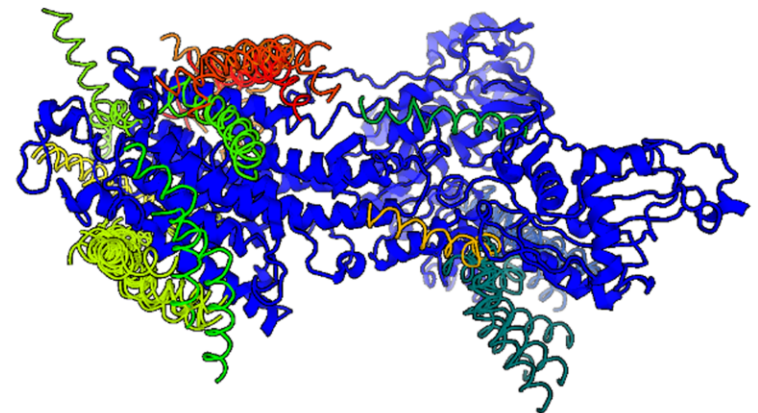
Go back

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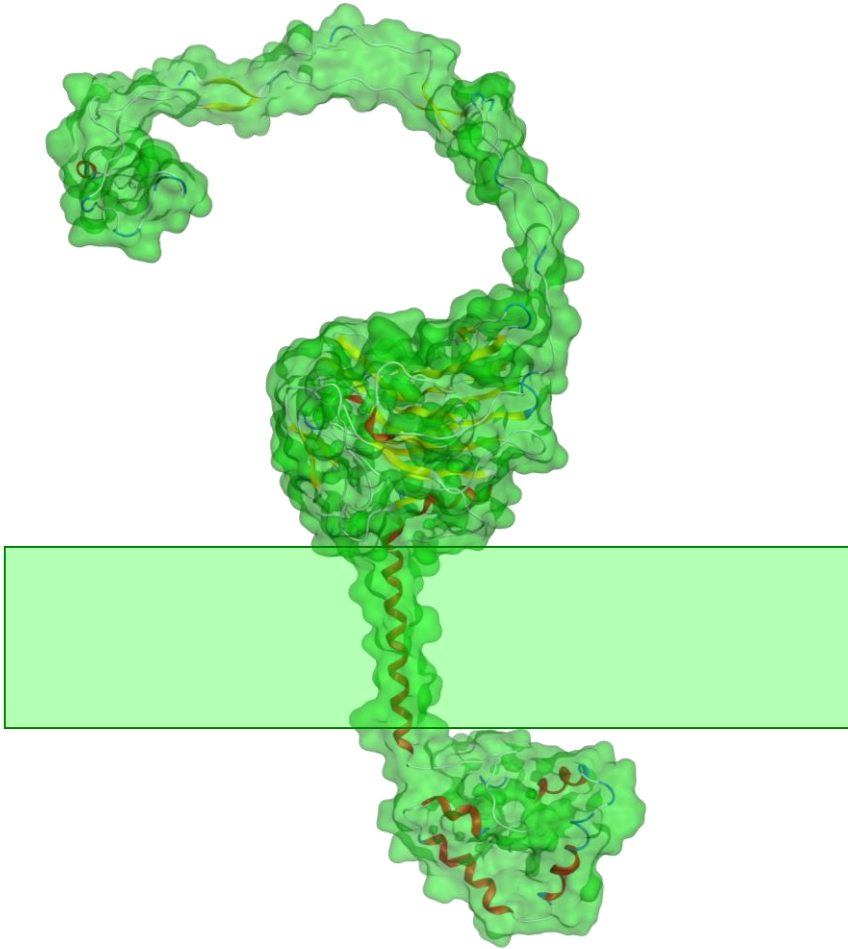
Permalink: <http://qasdom.eimb.ru/results/eIO5jrUdAXgkogze/results.html>

Ligand	2mlt_A.pdb
Receptor	3B8E_A.pdb
All Models	All models

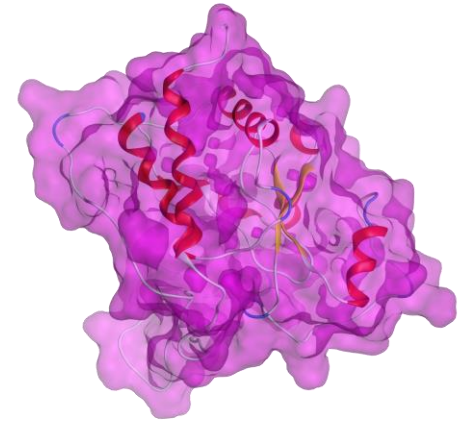
Allmodels



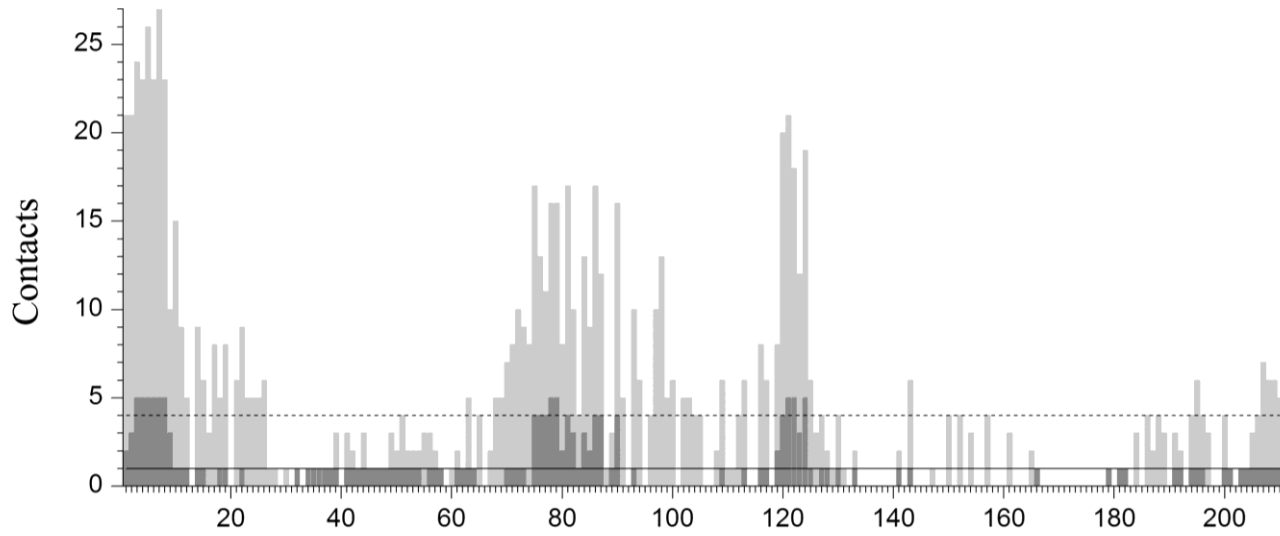
Nef-Calnexin interaction



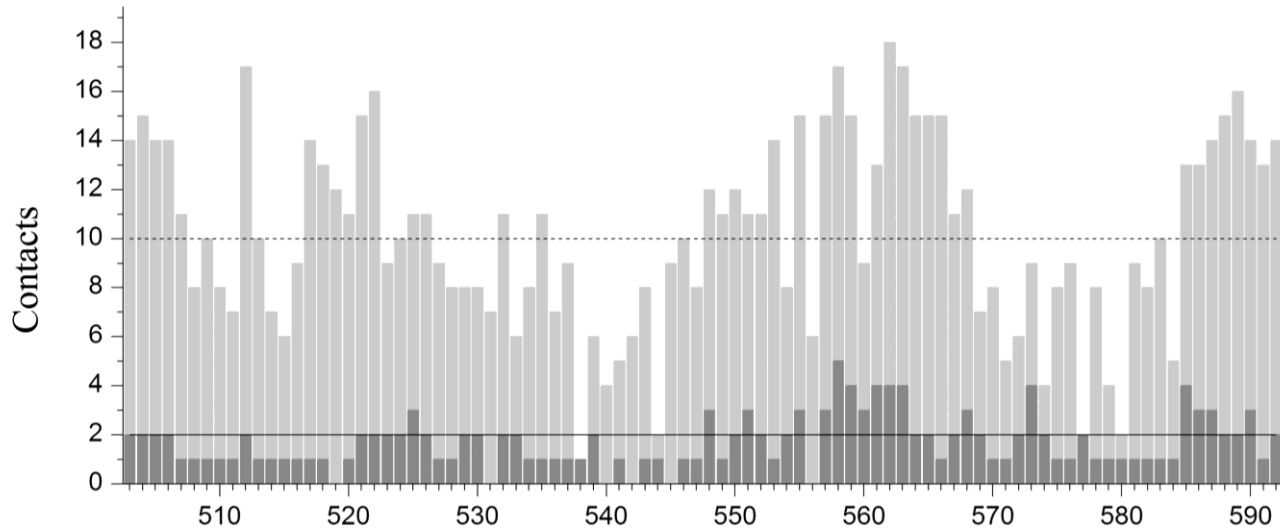
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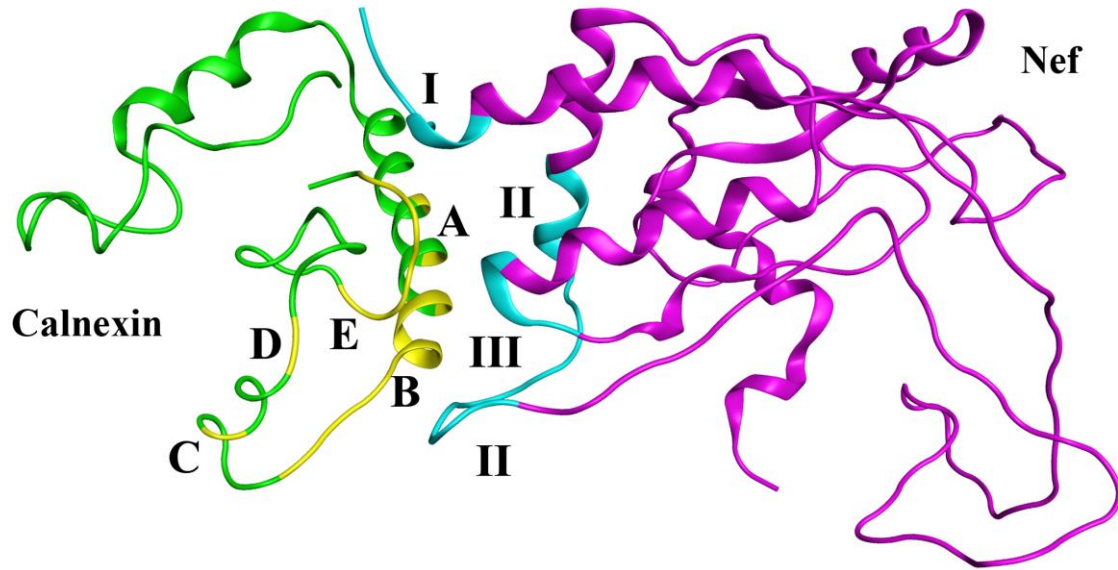


Nef sequence



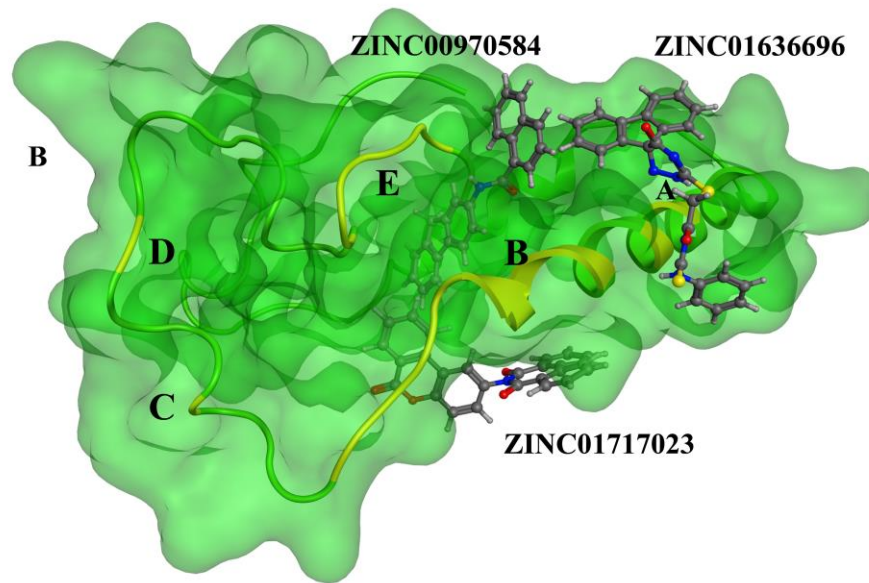
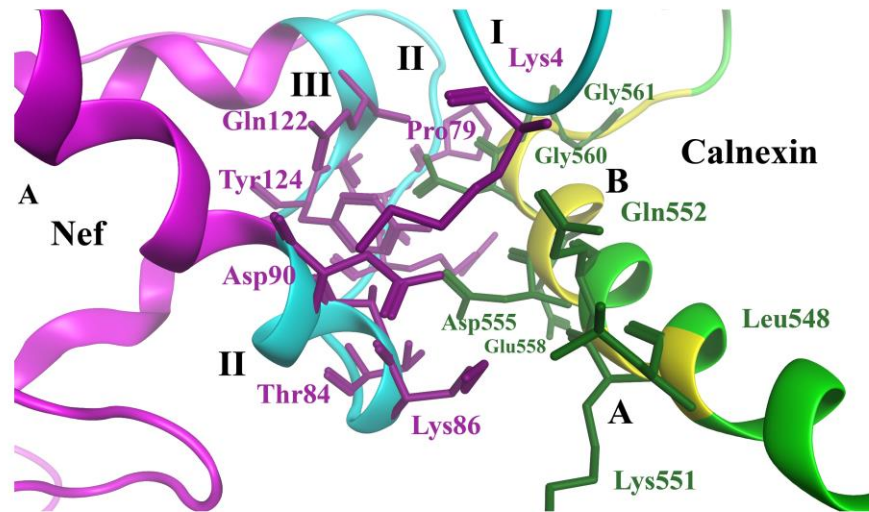
Nef sequence



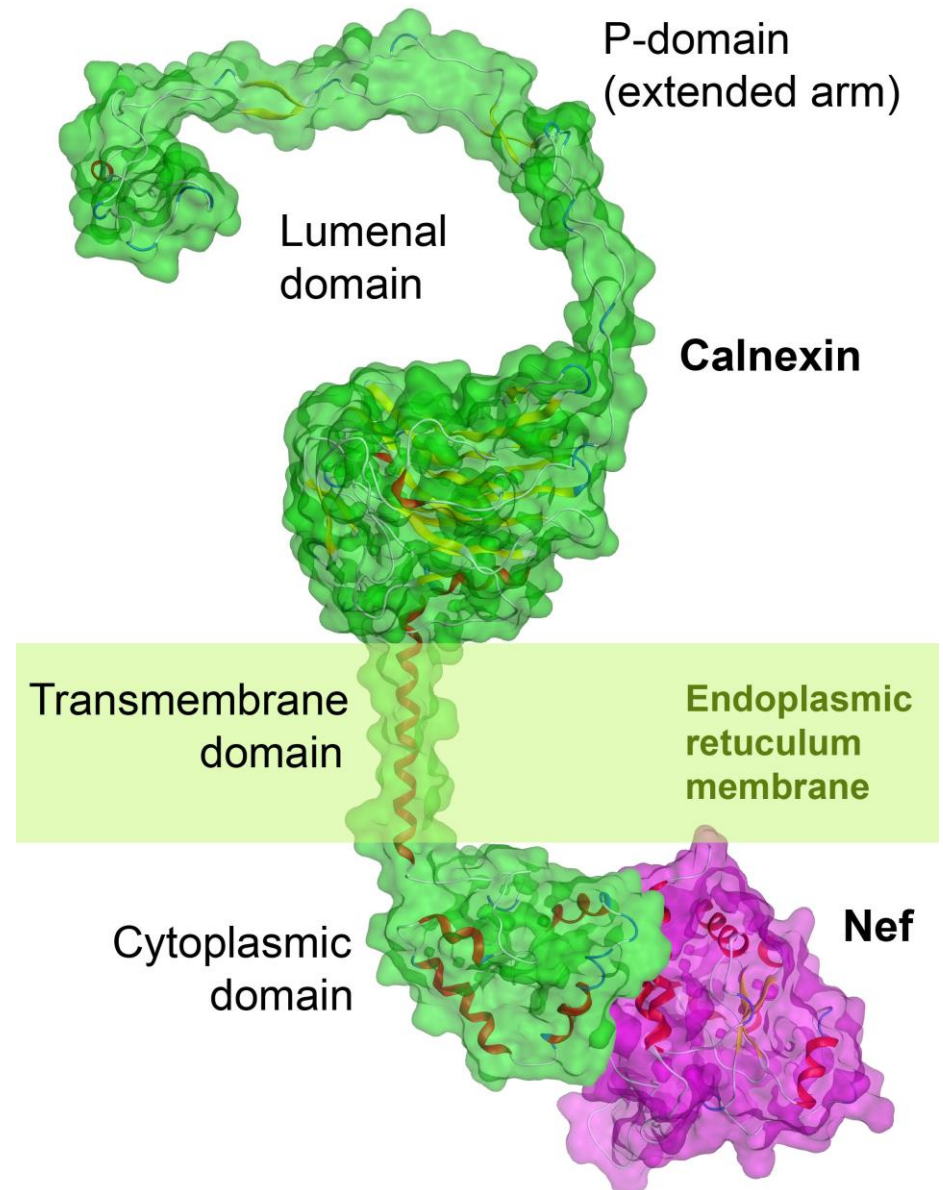


Nef interaction sites		
I	II	III
1-MGGKWSKRS-9	75-RPQVPLRPMTYKAALD-90	121-TQGY-124

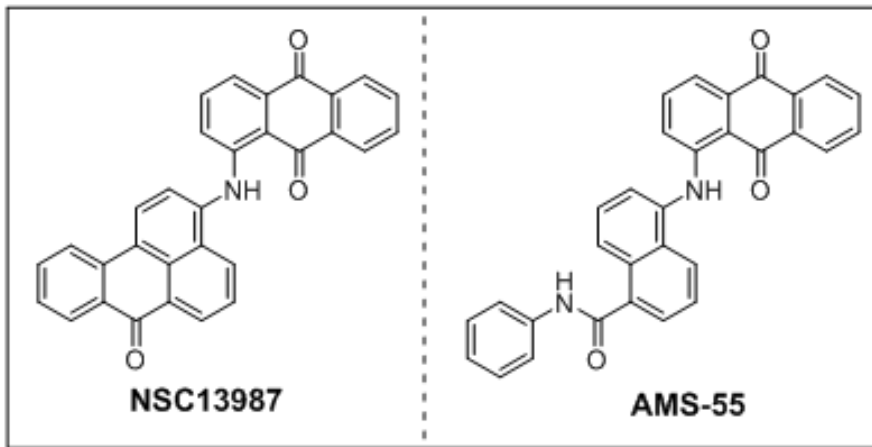
Calnexin interaction sites	Nef interaction sites		
	I	II	III
A 548L, 551K	75	7	10
B 555-DAEEDGGTV-563	90	314	131
C 568E	0	14	0
D 573K	13	12	0
E 585-RNRKPR-590	113	60	47



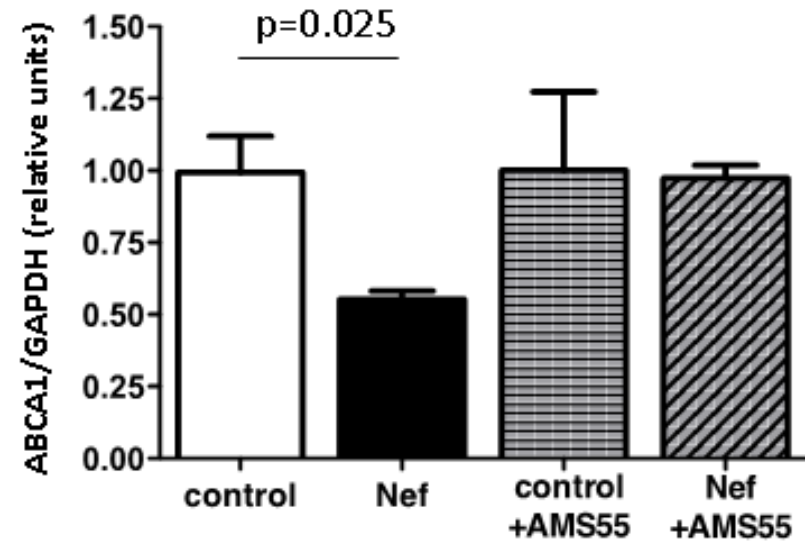
Hunegnaw, R., Vassilyeva, M., Dubrovsky, L., Pushkarsky, T., Sviridov, D., Anashkina, A.A., Üren, A., Brichacek, B., Vassilyev, D.G., Adzhubei, A.A. and Bukrinsky, M., 2016. Interaction between HIV-1 Nef and calnexin: From modeling to small molecule inhibitors reversing HIV-induced lipid accumulation. *Arteriosclerosis, thrombosis, and vascular biology*, 36(9), pp.1758-1771.



A



B



Adzhubei AA, Anashkina AA, Tkachev YV, Kravatsky YV, Pushkarsky T, Kulkarni A, Makarov AA, Bukrinsky MI. *Modelling interaction between HIV-1 Nef and calnexin*. **AIDS**. 2018.



Thank you for attention!

- This work was supported by Russian Science Foundation grant 14-24-00100 and Russian Foundation for Basic Research 17-54-30021 grant.