

Молекулярный докинг пептидов YDPEYRNFWGCG и EGLNRPSGGCG в отношении CTLA-4

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- Mus musculus (5)
- Camelidae (2)
- Camelus bactrianus (2)
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TAXONOMY Clear

- Eukaryota (33)

EXPERIMENTAL METHOD Clear

- X-RAY DIFFRACTION (36)
- SOLUTION NMR (1)

POLYMER ENTITY TYPE Clear

- Protein (37)

RESOLUTION Clear

- 1.5 - 2.0 (11)
- 2.0 - 2.5 (9)
- 2.5 - 3.0 (6)
- 3.0 - 3.5 (9)
- 3.5 - 4.0 (1)

RELEASE DATE Clear

- 1995 - 1999 (1)
- 2000 - 2004 (7)
- 2005 - 2009 (5)
- 2010 - 2014 (5)



1DQT

THE CRYSTAL STRUCTURE OF MURINE CTLA4 (CD152)

Ostrov, D.A., Shi, W., Schwartz, J.C., Almo, S.C., Nathenson, S.G.

(2000) Science 290: 816-819

Released 2000-10-27

Method X-RAY DIFFRACTION 2 Å

Organisms Mus musculus

Macromolecule CYTOTOXIC T LYMPHOCYTE ASSOCIATED ANTIGEN 4 (protein)

Unique Ligands CL, EDO

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3OSK

Crystal structure of human CTLA-4 apo homodimer

Yu, C., Sonnen, A.F.-P., Ikemizu, S., Stuart, D.I., Gilbert, R.J.C., Davis, S.J.

(2011) J Biol Chem 286: 6685-6696

Released 2010-12-08

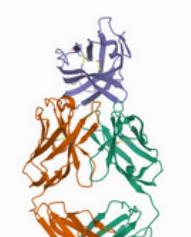
Method X-RAY DIFFRACTION 1.8 Å

Organisms Homo sapiens

Macromolecule Cytotoxic T-lymphocyte protein 4 (protein)

Unique Ligands GOL, NAG

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5TRU

Structure of the first-in-class checkpoint inhibitor Ipilimumab bound to human CTLA-4

Ramagopal, U.A., Liu, W., Garrett-Thomson, S.C., Yan, Q., Srinivasan, M., Wong, S.C., Bell, A., Mankikar, S., Rangan, V.S., Deshpande, S., Bonanno, J.B., Korman, A.J., Almo, S.C.

(2017) Proc Natl Acad Sci U S A 114: E4223-E4232

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QUERY: Full Text = ""CTLA-4"" AND (Scientific Name of Source Organism = "Homo sapiens" AND Experimental Method = "SOLUTION NMR") Open In Query Builder MyPDB Login

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SCIENTIFIC NAME OF SOURCE ORGANISM Homo sapiens (1) Clear

TAXONOMY Eukaryota (1) Clear

EXPERIMENTAL METHOD SOLUTION NMR (1) Clear

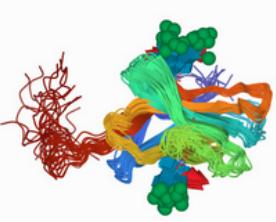
POLYMER ENTITY TYPE Protein (1) Clear

RESOLUTION Clear

RELEASE DATE 1995 - 1999 (1) Clear

ENZYME CLASSIFICATION NAME Clear

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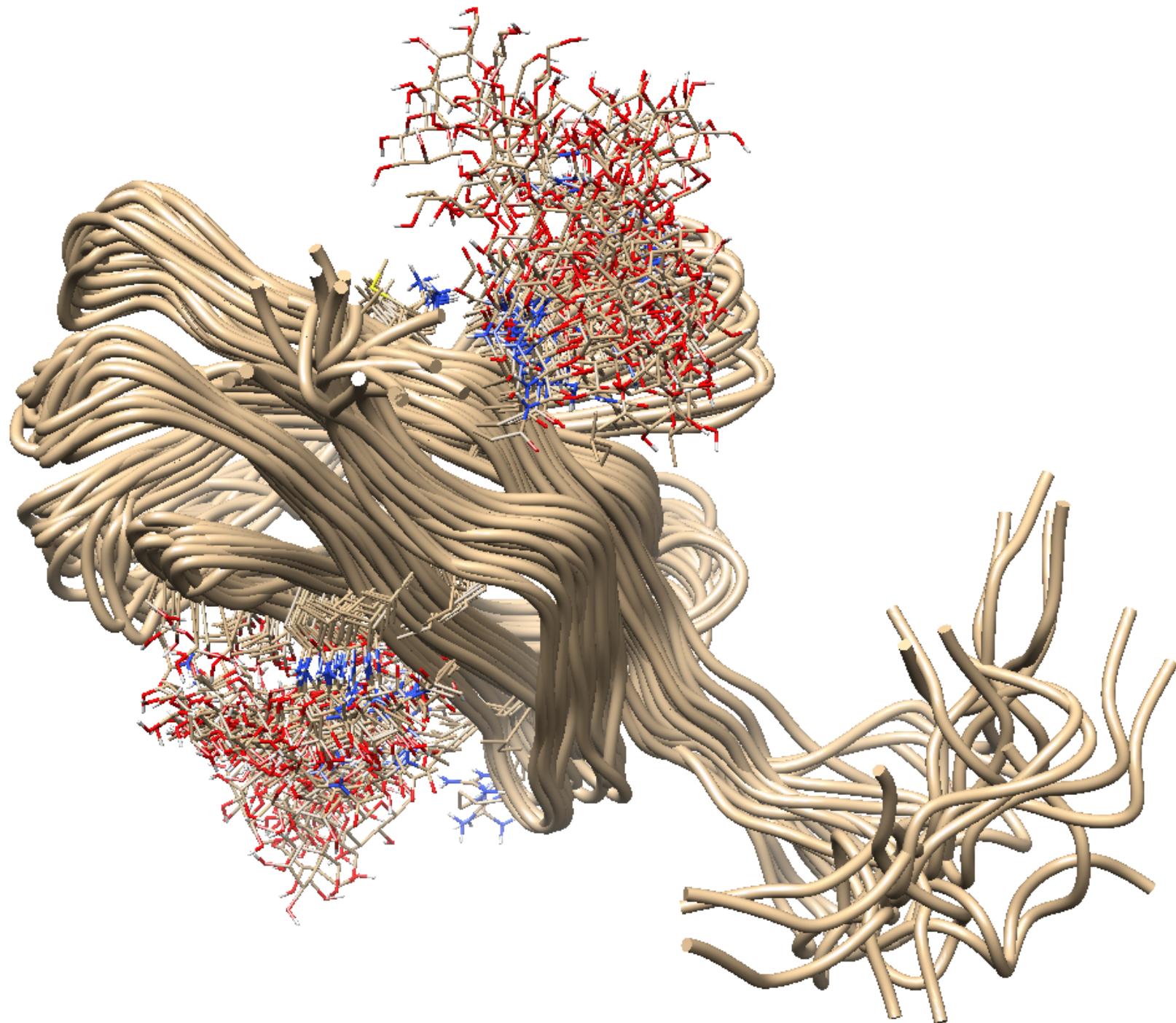

[3D View](#)

1AH1
CTLA-4, NMR, 20 STRUCTURES
Metzler, W.J., Bajorath, J., Fenderson, W., Shaw, S.-Y., Peach, R., Constantine, K.L., Naemura, J., Leytze, G., Lavoie, T.B., Mueller, L., Linsley, P.S.
(1997) Nat Struct Biol 4: 527-531
Released 1998-04-15
Method SOLUTION NMR
Organisms Homo sapiens
Macromolecule CTLA-4 (protein)
Unique Ligands BMA, FUC, FUL, NAG

Displaying 1 to 1 of 1 Structure Page 1 of 1 Display 25 per page

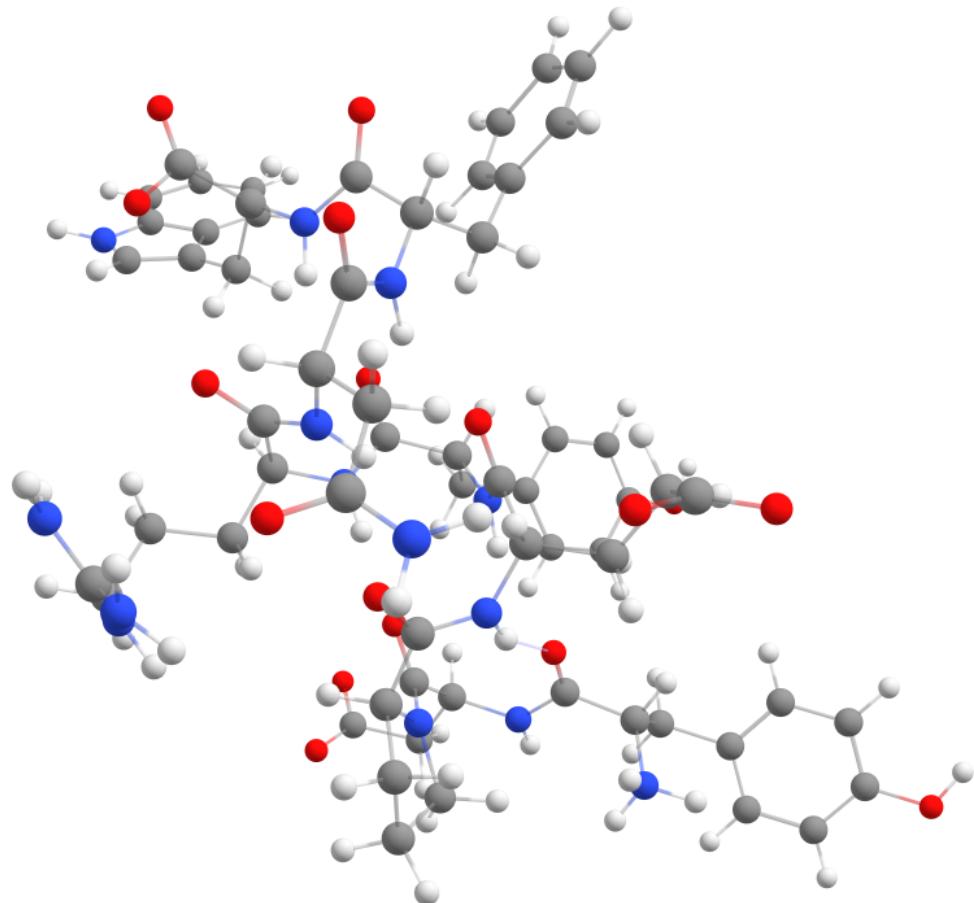
[displaying] - отображение (en->ru)
[показывать] show, indicate, display; [демонстрировать] demonstrate, show, display; [выставлять] expo up

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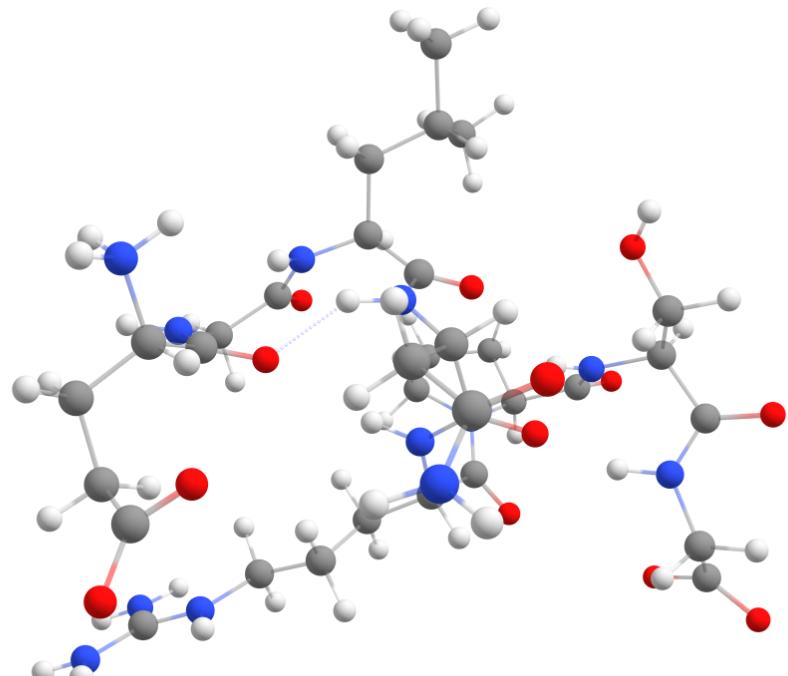


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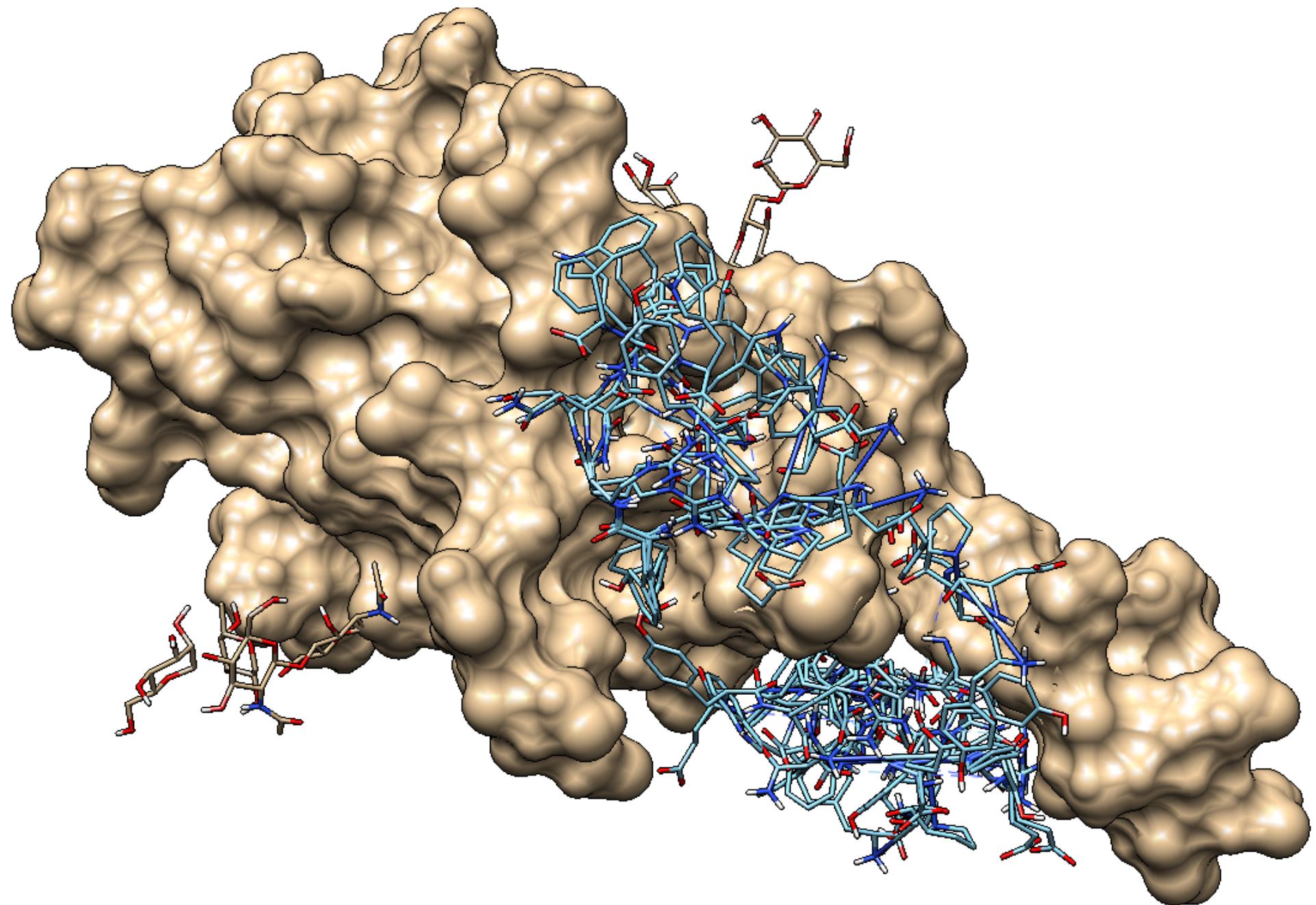
YDPEYRNFW (+)



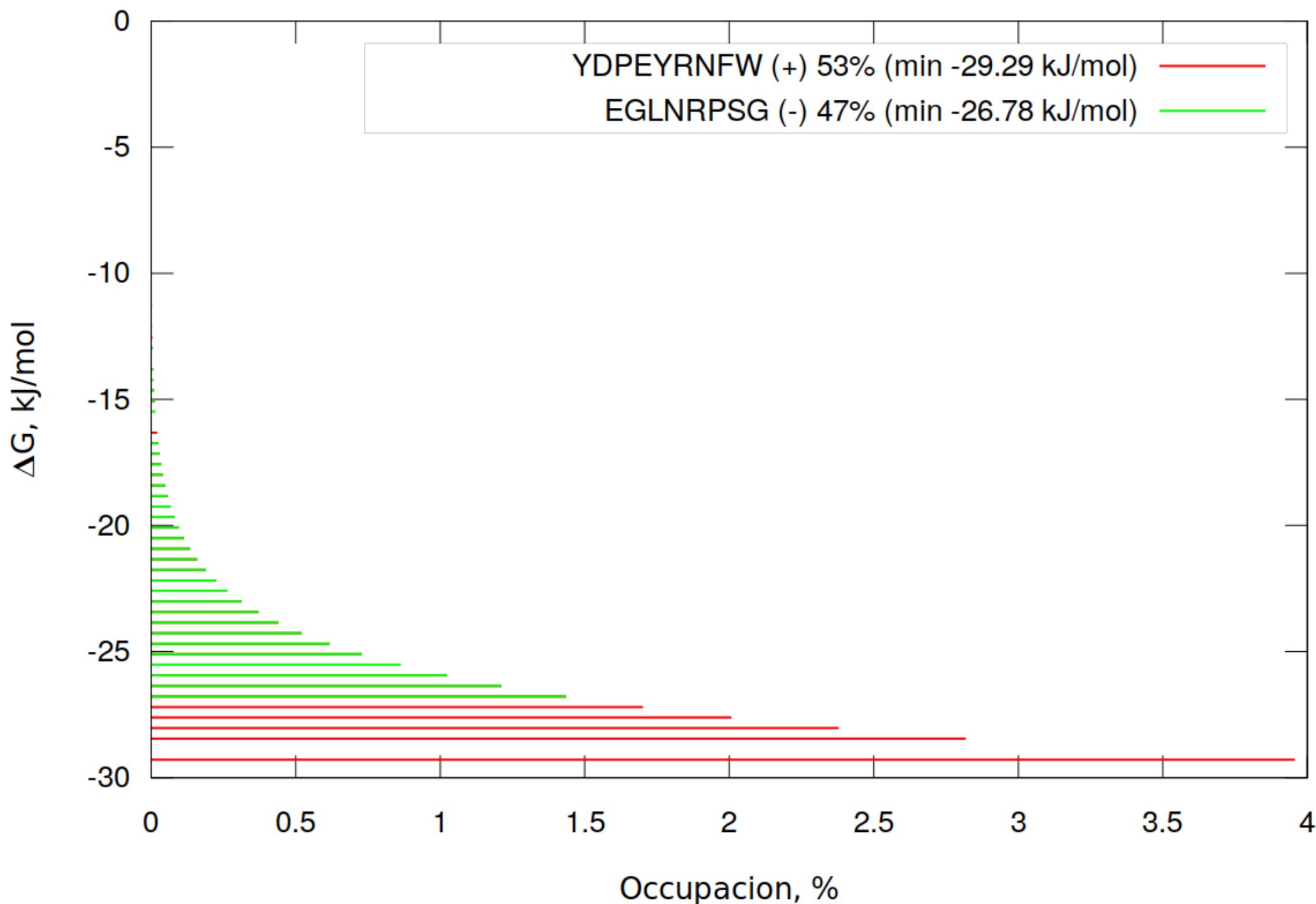
EGLNRPSG (-)



Молекулярный докинг пептидов YDPEYRNFWGCG и EGLNRPSGGCG в отношении CTLA-4

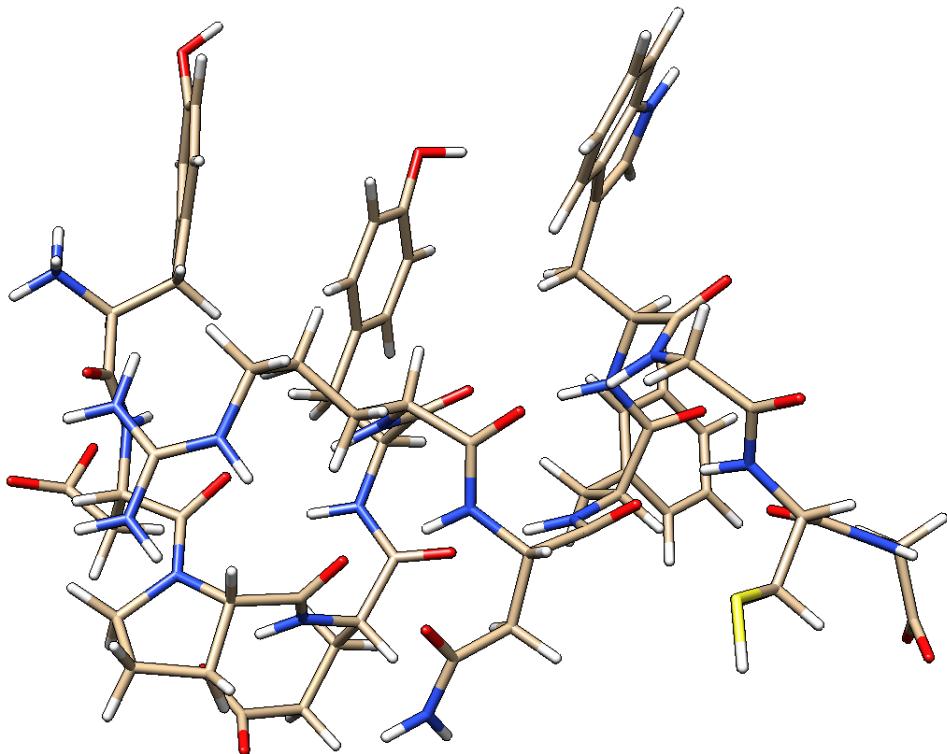


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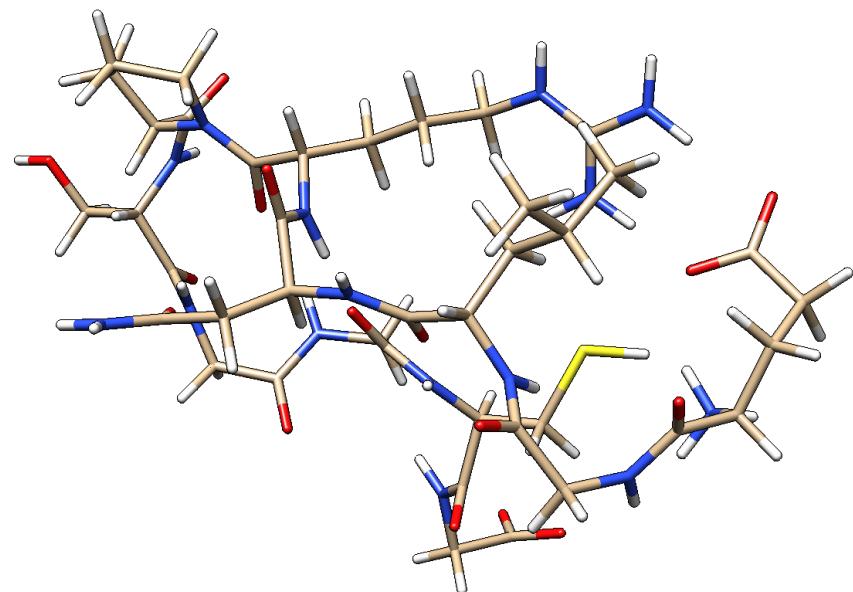


Молекулярный докинг пептидов YDPEYRNFWWGCG и EGLNRPSGGCG в отношении CTLA-4

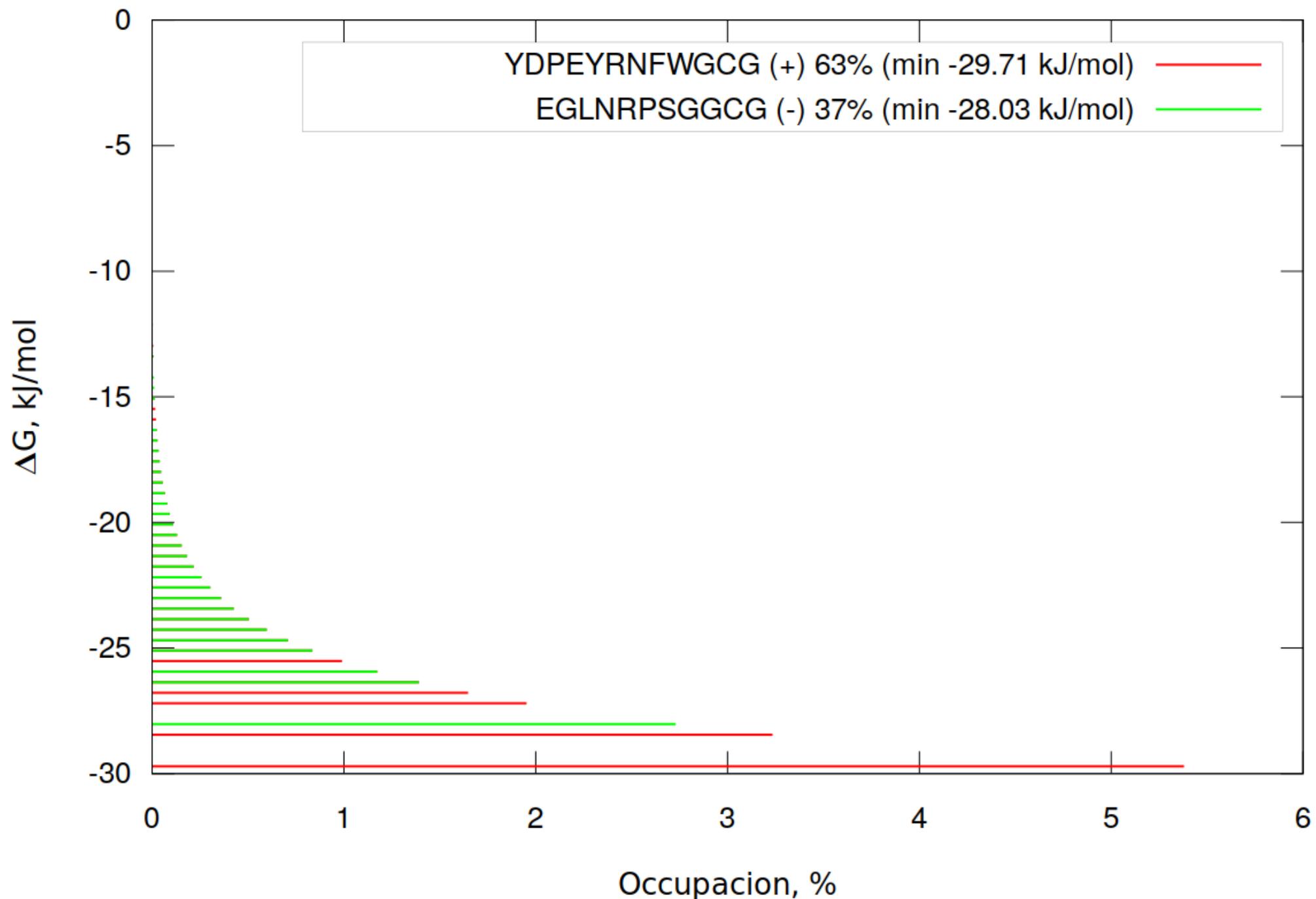
YDPEYRNFWWGCG (+)



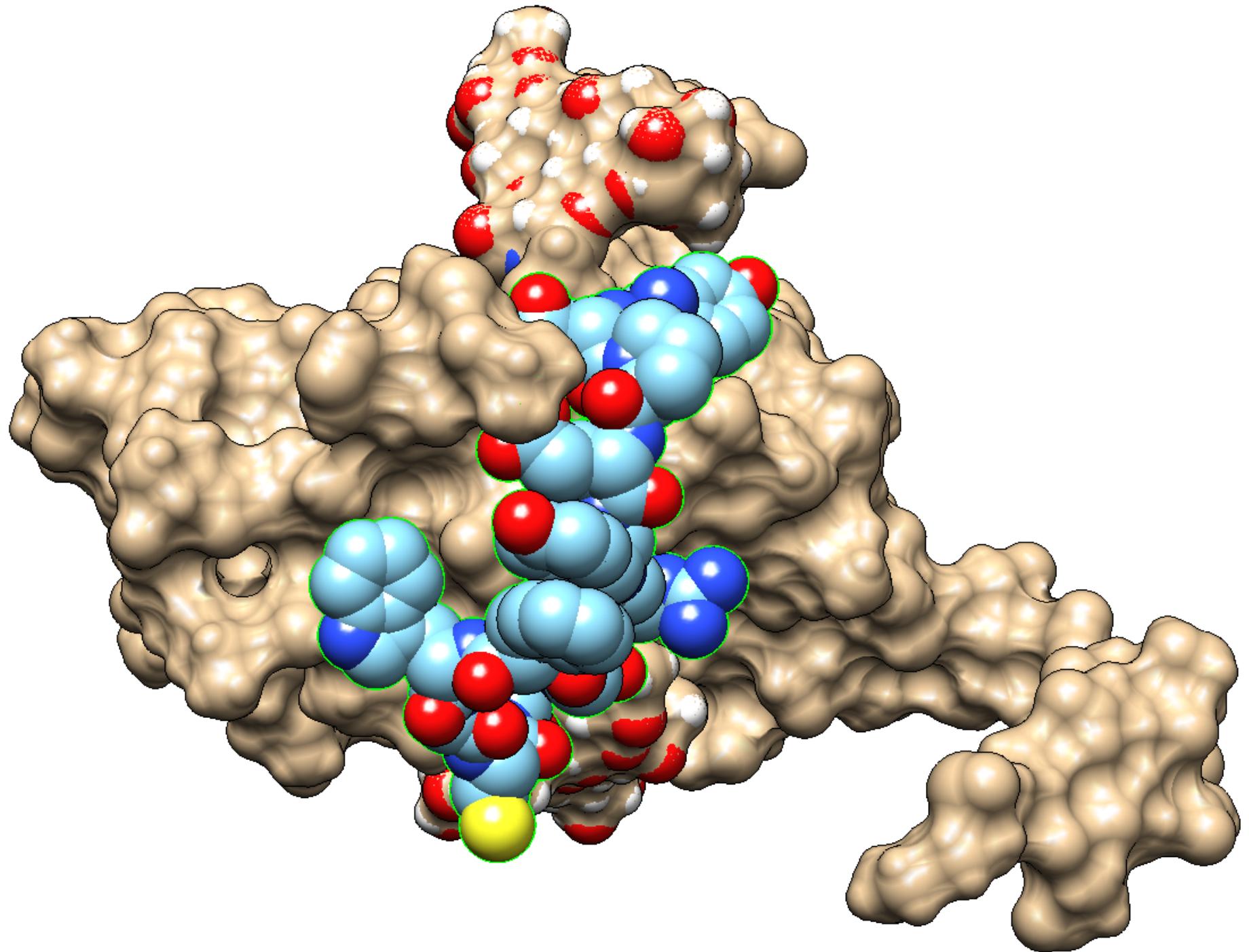
EGLNRPSGGCG (-)

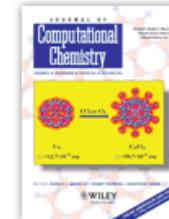


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Review

Can we trust docking results? Evaluation of seven commonly used programs on PDBbind database

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Dariusz Plewczynski [programs] - **программы (en->ru)**

First published: [программа] program, schedule, scheme; [план] plan, outline, schedule; [спектакль] performance, play, show
[программировать] program, programme; [составлять программу] program, programme

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Abstract

Docking is one of the most commonly used techniques in drug design. It is used for both identifying correct poses of a ligand in the binding site of a protein as well as for the estimation of the strength of protein-ligand interaction. Because millions of compounds must be screened, before a suitable target for biological testing can be identified, all calculations should be done in a reasonable time frame. Thus, all programs currently in use exploit empirically based algorithms, avoiding systematic search of the conformational space. Similarly, the scoring is done using simple equations, which makes it possible to speed up the entire process. Therefore, docking results have to be verified by subsequent *in vitro* studies. The purpose of our work was to evaluate seven popular docking programs (Surflex, LigandFit, Glide, GOLD, FlexX, eHiTS, and AutoDock) on the extensive dataset composed of 1300 protein-ligands complexes from PDBbind 2007 database, where experimentally measured binding affinity values were also available. We compared independently the ability of proper



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