

ВВЕДЕНИЕ В БИОИНФОРМАТИКУ

Лекция №22

Хемоинформатика и виртуальный скрининг

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Сайт курса <http://intbio.org/bioinf2019-2020>

Предсказание биологической активности

ИБМХ

PASS online

Better solutions for your research and d

It is easy to use

GO for prediction >



Methods

Multilevel Neighborhoods of Atoms (MNA) structure descriptors of a molecule are generated on the basis of connection table and table of atoms types presented the compound...

» [read more](#)



Applications

PASS predicts simultaneously 3678 kinds of activity with mean accuracy of prediction about 95% (leave-one-out cross validation) on the basis of the compound's structural formula.

» [read more](#)



Publications

Current and past publications, including statistical reports, surveys, press releases, circulars and legislation, are available in electronic format from this section.

» [read more](#)



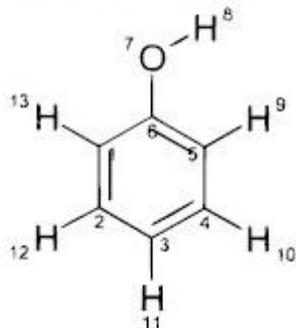
Downloads

You can download and use locally PASS demo version, which predicts 50 biological activities, and test it on your computer. It possible make a batch with several compounds at the same time.

» [click for it](#)

Предсказание биологической активности

Table 2. Representation of Phenol by MNA Descriptors of Zero, First, and Second Levels (MNA/0, MNA/1, MNA/2)^a



MNA – multilevel neighborhoods of atoms

(Filimonov, Poroikov et al., 1999)

atom	MNA/0	MNA/1	MNA/2
1	C	C(CC-H)	C(C(CC-H)C(CC-O)-H(C))
2	C	C(CC-H)	C(C(CC-H)C(CC-H)-H(C))
3	C	C(CC-H)	C(C(CC-H)C(CC-H)-H(C))
4	C	C(CC-H)	C(C(CC-H)C(CC-H)-H(C))
5	C	C(CC-H)	C(C(CC-H)C(CC-O)-H(C))
6	C	C(CC-O)	C(C(CC-H)C(CC-H)-O(C-H))
7	-O	-O(C-H)	-O(C(CC-O)-H(-O))
8	-H	-H(-O)	-H(-O(C-H))
9	-H	-H(C)	-H(C(CC-H))
10	-H	-H(C)	-H(C(CC-H))
11	-H	-H(C)	-H(C(CC-H))
12	-H	-H(C)	-H(C(CC-H))
13	-H	-H(C)	-H(C(CC-H))

^a Hyphen (-) is the chain marker for the atoms in the chains.

PASS

Предсказание биологической активности

Мера сходства – модифицированный коэффициент Танимото:

Calculation of Similarity. We have modified the Tanimoto coefficient to take into account the different frequencies of descriptors. The similarity between two molecules, A and B, is given by

$$\text{sim}(A, B) = \frac{\sum_{i=1}^M \min[A(i), B(i)]}{\sum_{i=1}^M A(i) + \sum_{i=1}^M B(i) - \sum_{i=1}^M \min[A(i), B(i)]} \quad (1)$$

where $A(i)$ and $B(i)$ are the counts of descriptor i in the molecules A and B, respectively; M is the total number of various descriptors in the dictionary.

PASS

Предсказание биологической активности

Ограничения предсказательной способности

PASS cannot predict the activity spectrum for essentially new compound if all its descriptors are new and so they don't occur in the training set. If a compound has more than 2 new descriptors it is rather new and prediction results may be considered as pilot.

In some cases PASS predicts both agonist's and antagonist's (blocker and stimulator) actions simultaneously. Thus, only experiments can clarify the biological activity of a compound, but it has an affinity to appropriate receptor (enzyme).

PASS does not predict if the compound will become a drug, but helps to select the most prospective leads.

The logo for PASS, consisting of the letters P, A, S, and S in a stylized, blue, serif font with a slight shadow effect.

Предсказание биологической активности



Swiss Institute of
Bioinformatics

SwissTargetPrediction

Home FAQ Help Download Contact Disclaimer

This website allows you to predict the targets of a small molecule. Using a combination of 2D and 3D similarity measures, it compares the query molecule to a library of 280'000 compounds active on more than 2000 targets of 5 different organisms.

The webserver is described in detail in our article: [SwissTargetPrediction: a webserver for target prediction of bioactive small molecules, Nucl. Acids Res. \(2014\)](#). For technical information about the prediction algorithm, you can refer to this article: [Shaping the interaction landscape of bioactive molecules, Bioinformatics \(2013\) 29:3073-3079](#).

Choose an organism

- Homo sapiens
- Mus musculus
- Rattus norvegicus
- Bos taurus
- Equus caballus

Paste a SMILES in this box, or draw a molecule

Examples: ▼

Clear

=

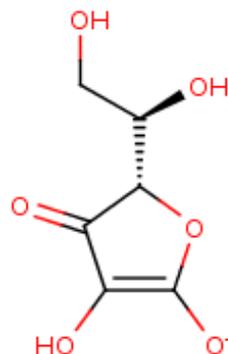
Предсказание биологической активности

List of predicted targets

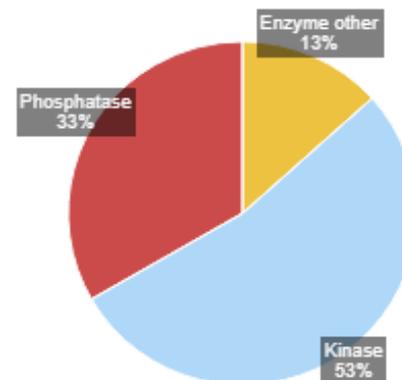
These targets have been predicted using the method described in:

Gfeller D., Michielin O. & Zoete V.
 Shaping the interaction landscape of bioactive molecules, *Bioinformatics* (2013) 29:3073-3079.

Query Molecule



General Target Classes



Retrieve data:



Target	Common name	Uniprot ID	ChEMBL ID	Probability*	# sim. cmpds (3D / 2D)	Target Class
Tyrosyl-DNA phosphodiesterase 1	TDP1	Q9NUW8	CHEMBL1075138	<div style="width: 10%; height: 10px; background-color: green;"></div>	0 / 2	Enzyme
Tubulin-tyrosine ligase	TTL	Q8NG68	CHEMBL5549	<div style="width: 5%; height: 10px; background-color: green;"></div>	0 / 12	Enzyme
Protein kinase C alpha type	PRKCA	P17252	CHEMBL299	<div style="width: 5%; height: 10px; background-color: green;"></div>	0 / 141	Ser_Thr Kinase
Protein kinase C delta type regulatory subunit (by homology)	PRKCD	Q05655	CHEMBL2996	<div style="width: 5%; height: 10px; background-color: green;"></div>	0 / 143	Ser_Thr Kinase
Protein kinase C theta type (by homology)	PRKCQ	Q04759	CHEMBL3920	<div style="width: 5%; height: 10px; background-color: green;"></div>	0 / 143	Ser_Thr Kinase

Базы данных химических соединений




Search PubChem Compound for Go Clear

[Advanced Search](#)
[Preview/Index](#)
[History](#)
[Clipboard](#)
[Details](#)

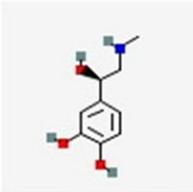
Display Summary Show 20 Sort By Send to

Tools:
 Links: [Related Structures](#), [BioAssays](#), [BioSystems](#), [Literature](#), [Other Links](#)

All: 120 Rule of 5: 62

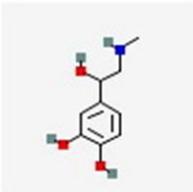
Items 1 - 20 of 120 Page of 6 Next

1: CID: 5816 [Related Structures](#), [BioAssays](#), [BioSystems](#), [Literature](#), [Other Links](#)



epinephrine; Adrenalin; adrenaline ...
 IUPAC: 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol
 MW: 183.204420 g/mol | MF: C₉H₁₃NO₃
 Tested in BioAssays: All: 274, Active: 22; [BioActivity Analysis](#)
 Vasoconstrictor Agents... [more](#)

2: CID: 838 [Related Structures](#), [BioAssays](#), [Literature](#), [Other Links](#)



epinephrine; DL-Adrenaline; Racepinefrine ...
 IUPAC: 4-[1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol
 MW: 183.204420 g/mol | MF: C₉H₁₃NO₃
 Tested in BioAssays: All: 17, Active: 1; [BioActivity Analysis](#)
 Vasoconstrictor Agents... [more](#)

3: CID: 247704 [Related Structures](#), [BioAssays](#), [Literature](#), [Other Links](#)

Selected Compounds ? Compound Count

- BioActivity Experiments**
- BioAssays, Active 39
- BioAssays, Tested 60
- Protein 3D Structures 6
- Crystal Structure Of Dipeptide... 1
- BioMedical Annotation**
- Pharmacological Actions 69
- Sympathomimetics 37
- BioSystems 16
- Depositor Category**
- Biological Properties 120
- Chemical Vendors 55
- Journal Publishers 47
- NIH Molecular Libraries 52

Recent activity Turn Off Clear

Compounds: 95,276,293
 Substances: 249,470,154
 BioAssays: 1,252,883
 Tested Compounds: 2,570,179
 Tested Substances: 4,157,676
 RNAi BioAssays: 170
 BioActivities: 235,470,936
 Protein Targets: 10,857
 Gene Targets: 22,106

Базы данных химических соединений

Ascorbic acid

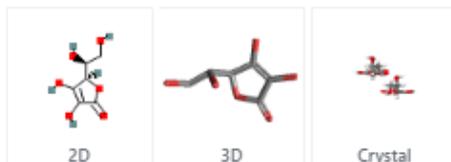
Share Tweet Email

Cite

Download

PubChem CID: 54670067

Structure:



Chemical Safety: DATASHEET AVAILABLE: [Laboratory Chemical Safety Summary \(LCSS\)](#)

InChI Key: CIWBSHSKHKDKBQ-JLAZNSOCSA-N

Molecular Formula: $C_6H_8O_6$ or $HC_6H_7O_6$

UNII: PQ6CK8PD0R

Depositor-Supplied
Synonyms: l-ascorbic acid
ascorbic acid
vitamin C
50-81-7
L(+)-Ascorbic acid

[More...](#)

Molecular Weight: 176.124 g/mol

Dates: Modify: 2019-03-30 Create: 2011-12-26

CONTENTS

Title and Summary

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11 Use and Manufacturing

12 Identification

13 Safety and Hazards

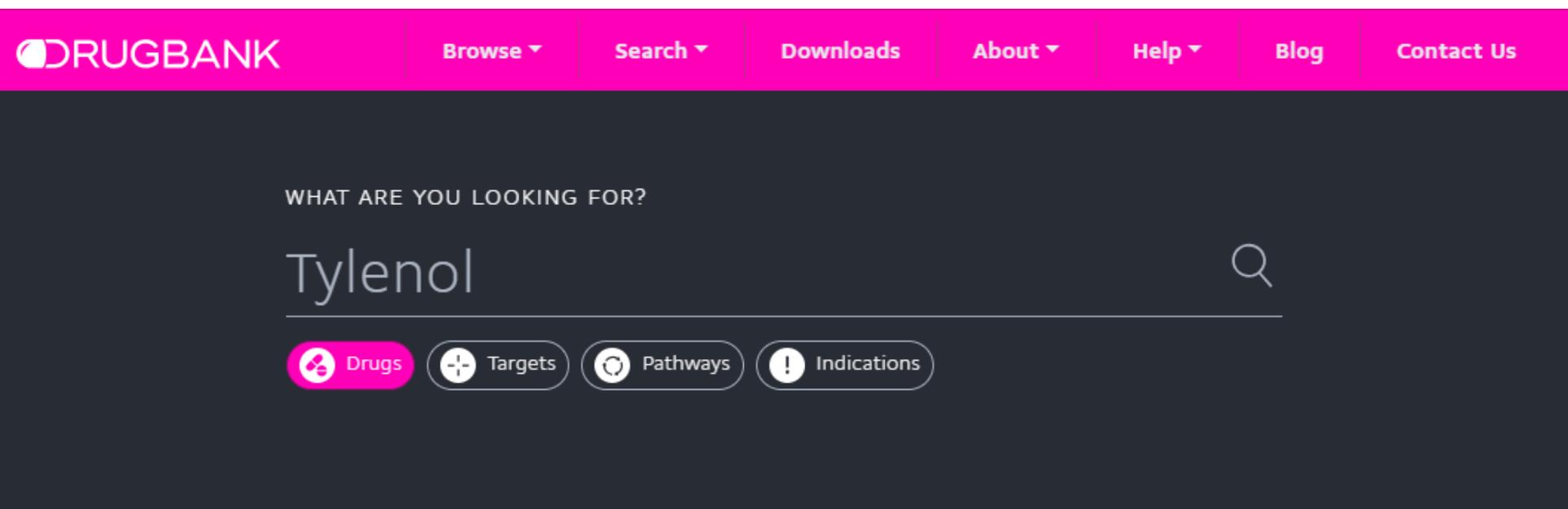
14 Toxicity

15 Literature

16 Patents

17 Biomolecular Interactions and Pathways

Базы данных химических соединений



The screenshot shows the top navigation bar of the DrugBank website, which is pink. It contains the DrugBank logo and several menu items: Browse, Search, Downloads, About, Help, Blog, and Contact Us. Below the navigation bar is a dark grey search area. It features the text "WHAT ARE YOU LOOKING FOR?" followed by a search input field containing the word "Tylenol" and a magnifying glass icon. Below the search field are four filter buttons: "Drugs" (highlighted in pink), "Targets", "Pathways", and "Indications".



The DrugBank database is a unique bioinformatics and cheminformatics resource that combines detailed drug data with comprehensive drug target information.

Базы данных химических соединений

ZINC¹²

Not Authenticated – sign in

Active cart: Temporary Cart (0 items)

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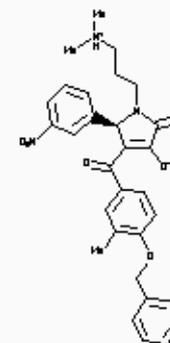
Quick Search Bar...

Go

Please consider switching to [ZINC15](#), which is superior to ZINC12 in most ways. If you prefer ZINC12 after trying ZINC15, we would like to know why @chem4biology so that we can get you to make the switch.

Welcome to ZINC, a free database of commercially-available compounds for virtual screening. ZINC contains over 35 million purchasable compounds in ready-to-dock, 3D formats. ZINC is provided by the [Irwin](#) and [Shoichet](#) Laboratories in the Department of Pharmaceutical Chemistry at the University of California, San Francisco (UCSF). To cite ZINC, please reference: Irwin, Sterling, Mysinger, Bolstad and Coleman, *J. Chem. Inf. Model.* 2012 DOI: [10.1021/ci3001277](#). The original publication is Irwin and Shoichet, *J. Chem. Inf. Model.* 2005;45(1):177-82 [PDF](#), [DOI](#). We thank [NIGMS](#) for financial support (GM71896).

Molecule of the Minute [8817205](#)

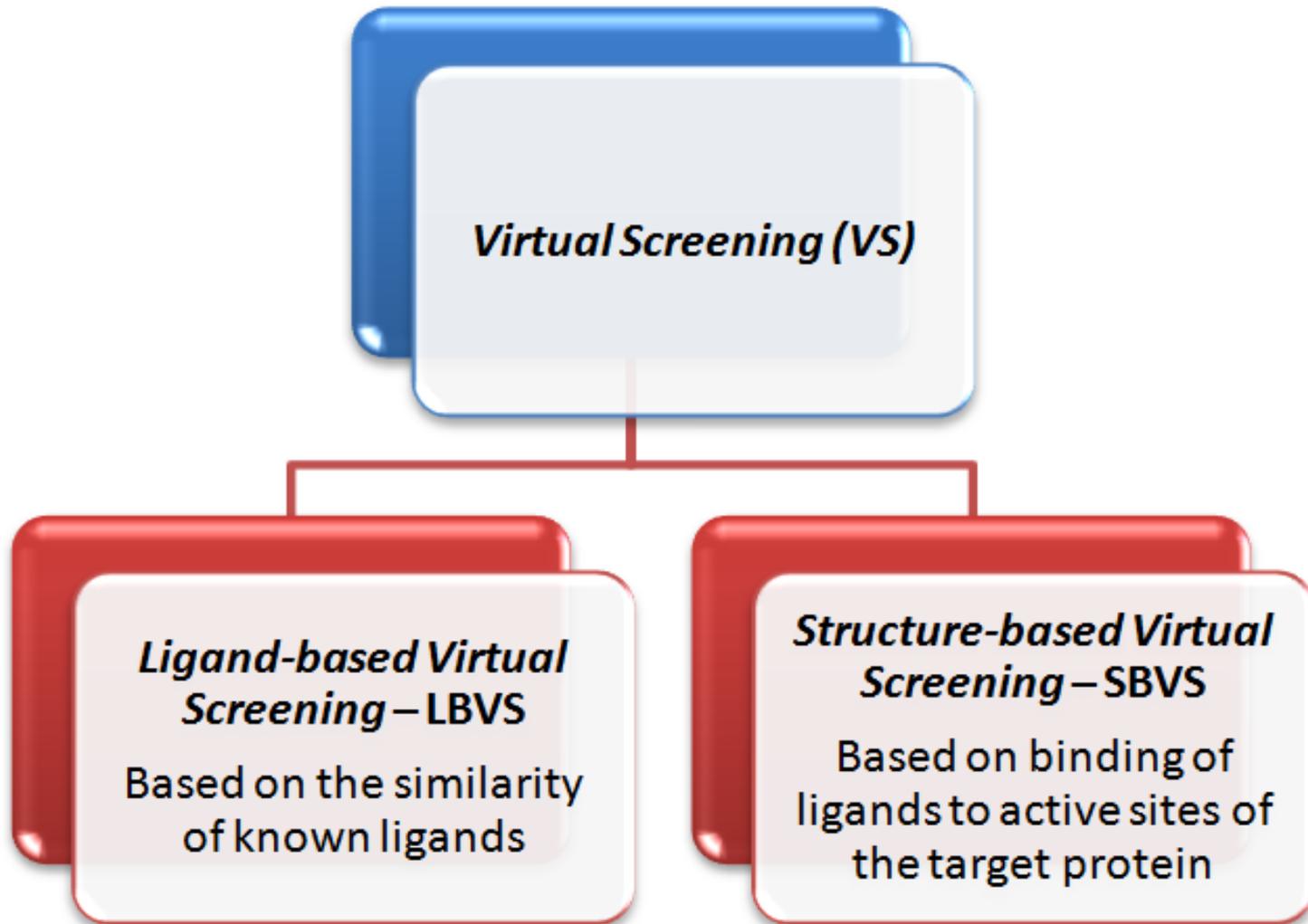


ZINC ID, Drug Name, SMILES, Catalog, Vendor Code, Target & r

Go

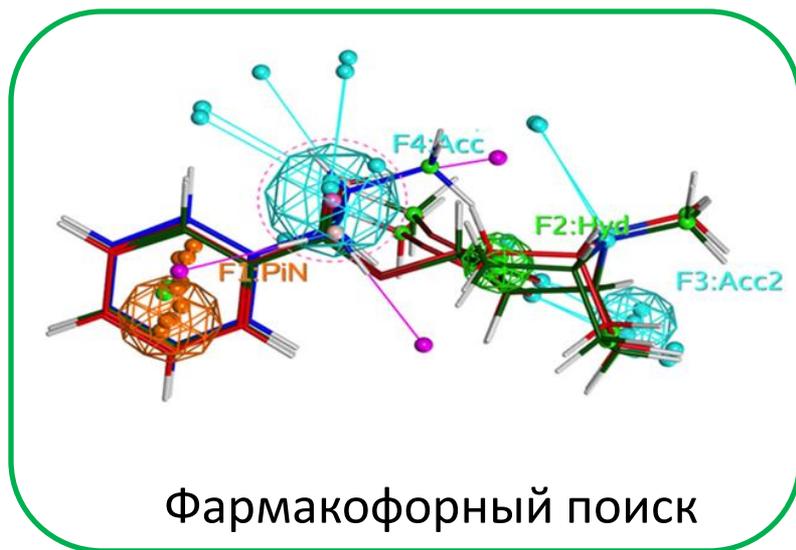
Structure/Draw Physical Properties Catalogs & Vendors ZINC IDS Targets Rings Combination

Виртуальный скрининг



Виртуальный скрининг

L
B
V
S



S
B
V
S

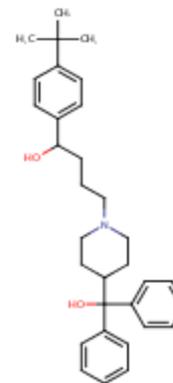
Отбор по формальным признакам. SwissSimilarity

Run parameters

Library screened ZincDrugLike
Screening method Combined
Date Fri Nov 10 11:13:52 2017

If you publish these results, please, cite the following paper: Zoete, V., Daina, A., Bovigny, C., & Michielin, O. SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening., *J. Chem. Inf. Model.*, 2016, 56(8), 1399-1404.

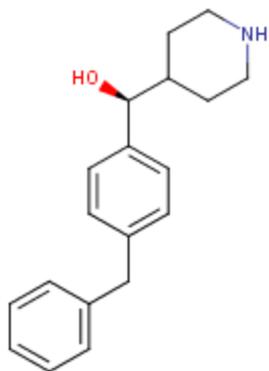
Query Molecule



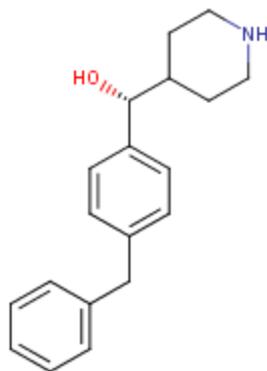
Results

Retrieve data:     

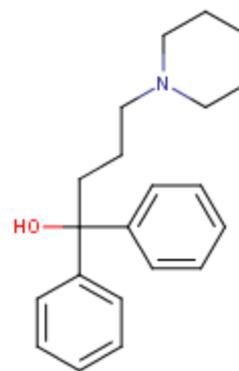
ZINC80181216
Score : 0.983



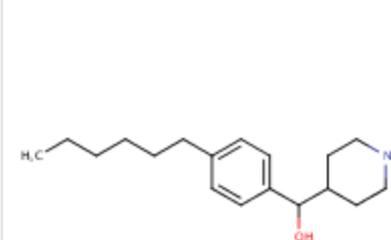
ZINC80181212
Score : 0.983



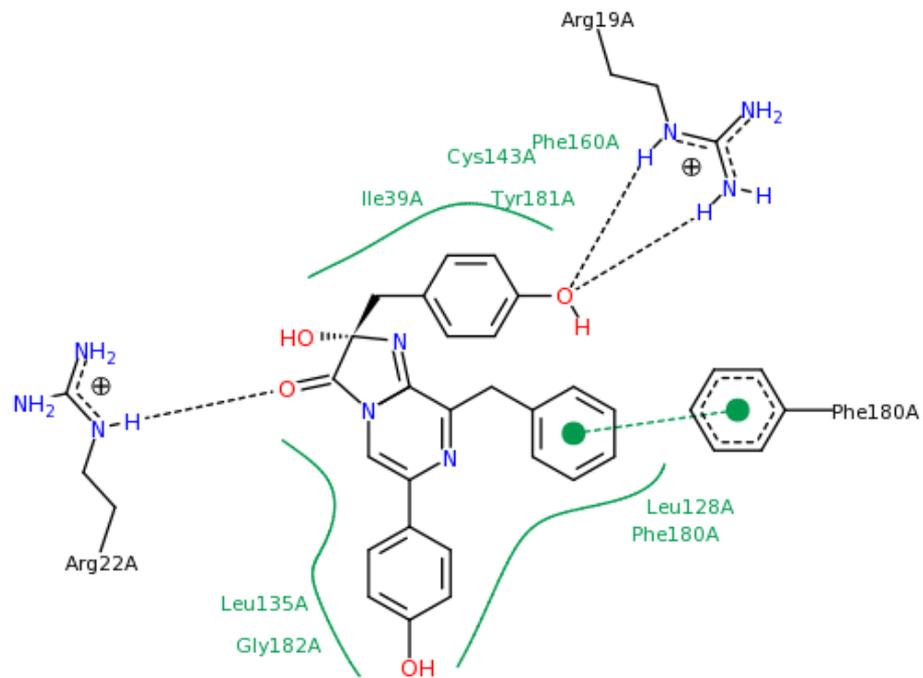
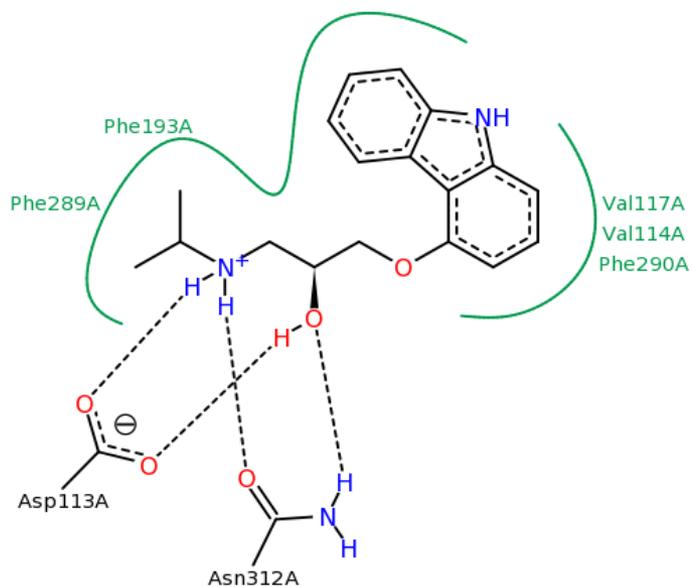
ZINC00968266
Score : 0.972



ZINC74369400
Score : 0.969



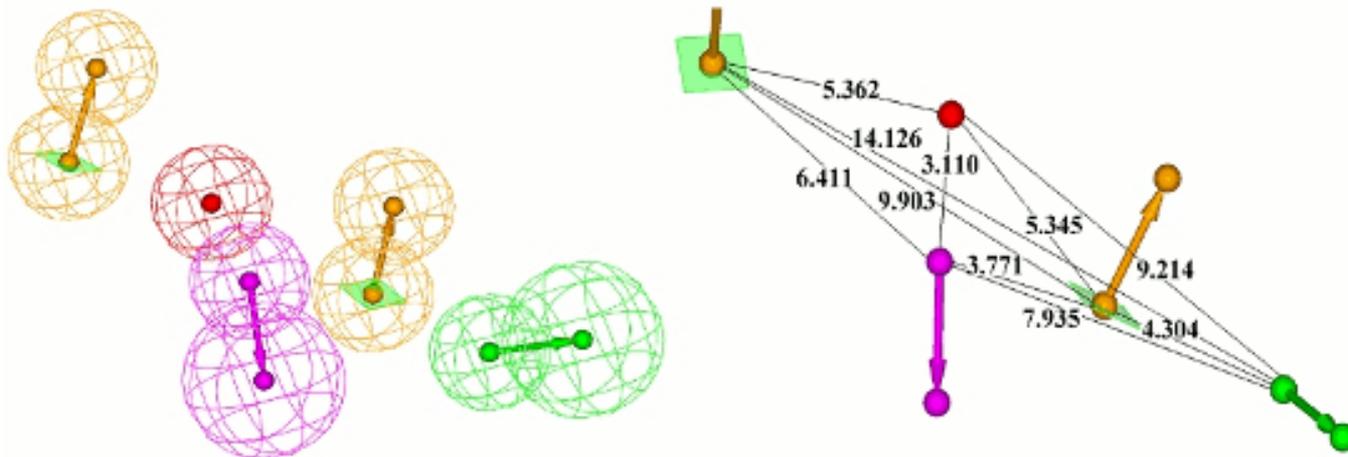
Межмолекулярные взаимодействия



Фармакофорный поиск

Pharmacophore – “proposed receptor pattern” (Kier, 1971)

Фармакофор — набор пространственных и электронных признаков, необходимых для обеспечения оптимальных супрамолекулярных взаимодействий со специфической биологической мишенью, которые могут вызывать (или блокировать) ее биологический ответ (ИЮПАК).

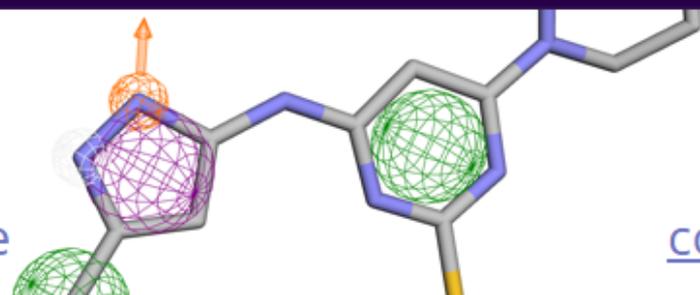


Pharmacophore model for β 2-adrenoreceptor agonists generated by HipHop. Features are portrayed as mashed spheres, color-coded as follows: **green, hydrogen-bond acceptor**, **magenta, hydrogen-bond donor**, **orange, aromatic ring**, **red, positive ionizable feature**.

Фармакофорный поиск. PharmIt

pharmit

interactive exploration of chemical space



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virtual screening in your browser

[enter pharmit search](#)

start from PDB: ligand ▼

binding site waters: ▼

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submit your own chemical libraries

[log in to manage libraries](#)

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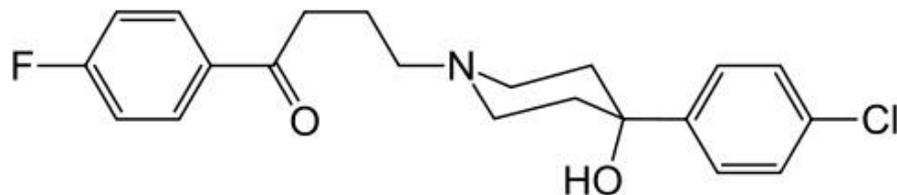
password:

[log in](#)

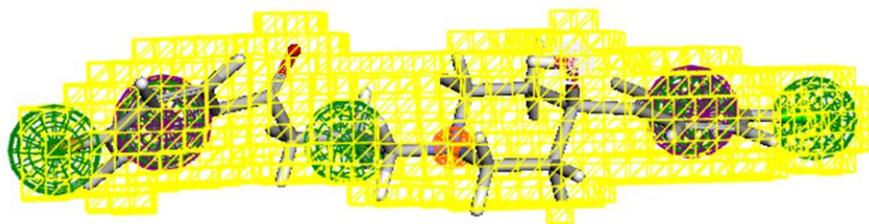
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Фармакофорный поиск. PharmIt



Галоперидол



Search PubChem

Pharmacophore Search -> Shape Filter

Load Receptor... Load Features...

Pharmacophore

- Aromatic**
(6.08,0.16,-0.02) Radius 1.1
- Aromatic**
(-6.31,0.28,-0.05) Radius 1.1
- HydrogenDonor**
(2.94,1.31,-1.29) Radius 0.5
- HydrogenAcceptor**
(0.47,-0.38,0.73) Radius 0.5
- HydrogenAcceptor**
(2.94,1.31,-1.29) Radius 0.5
- HydrogenAcceptor**
(-3.19,-0.63,-1.63) Radius 0.5
- Hydrophobic**
(6.08,0.16,-0.02) Radius 1.0
- Hydrophobic**
(-6.31,0.28,-0.05) Radius 1.0
- Hydrophobic**
(9.18,-0.06,0.22) Radius 1.0
- Hydrophobic**
(-8.77,1.37,0.43) Radius 1.0
- Hydrophobic**
(-1.89,-1.26,0.6) Radius 1.0

Load Session... Save Session...

Pharmacophore Results

Name	RMSD	Mass	RBnds
PubChem-118753530	0.390	377	6
PubChem-8957387	0.486	396	9
PubChem-7773328	0.492	379	9
PubChem-7773305	0.519	397	9
PubChem-122716498	0.556	381	9
PubChem-119265	0.581	378	6
PubChem-8957383	0.606	373	10
PubChem-10200496	0.624	392	6
PubChem-11257780	0.645	390	6
PubChem-2795977	0.779	389	10

Showing 1 to 10 of 10 hits
Previous 1 Next

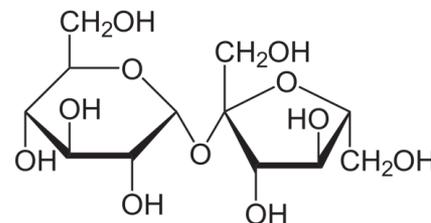
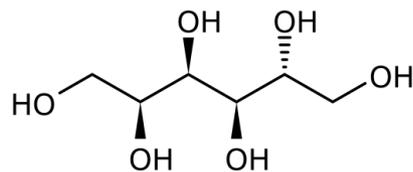
Minimize Save..31

Восприятие вкуса

Сапофор – структурный мотив, обуславливающий вкус вещества (Cohn, 1914)

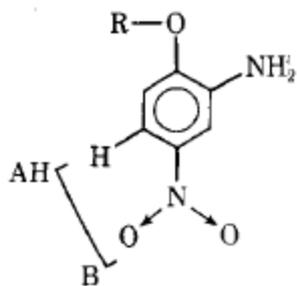
В частности, **несколько гидроксильных групп обуславливают сладкий вкус**.

Сорбит (0,6)

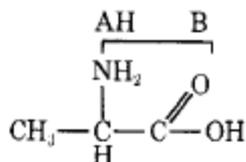


Сахароза (1,0)

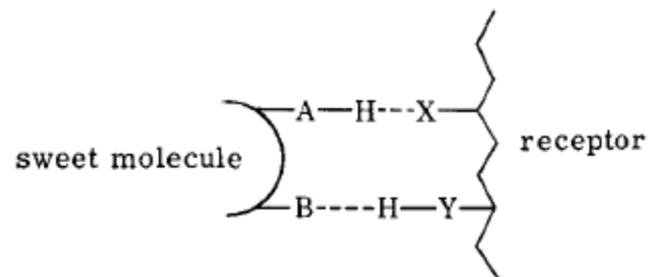
AH-B theory of sweetness proposed that to be sweet, a compound must contain a hydrogen bond donor (AH) and a Lewis base (B) separated by about 3 Å (1963)



2-amino-4-nitrobenzenes



alanine

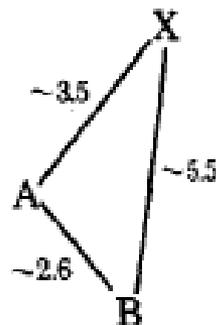


Scheme II—Postulated interaction of molecular sweet feature and receptor, according to Shallenberger and Acree (5)

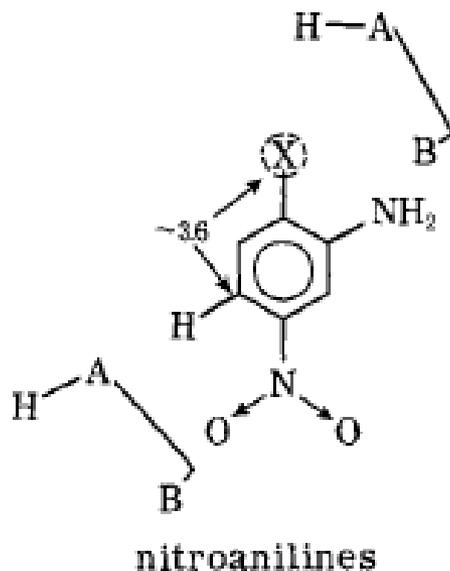
Scheme I—Various sweet molecules showing the A—H and B structural features involved cited by Shallenberger and Acree (5)

Восприятие вкуса

B-X theory: существует третий сайт (X), образующий гидрофобный контакт с рецептором (Kier, 1972)



Scheme V—Pattern of atoms imparting a sweet taste (glucophore), postulated from this study

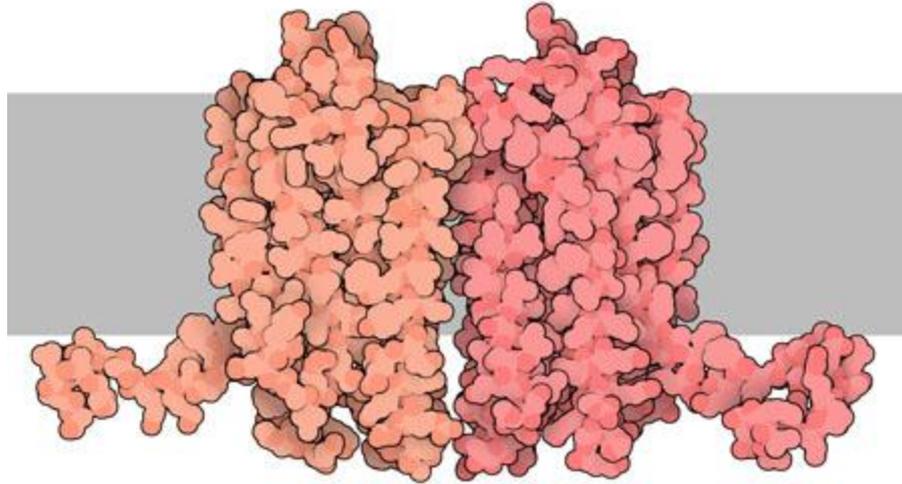


Multipoint attachment theory (MPA): существует 8 сайтов взаимодействия между «сладкими молекулами» и рецепторами сладкого, хотя не все они должны быть задействованы (1991).

Scheme VI—Identity of third structural feature comprising the postulated glucophore (Scheme V) in several sweet molecules

Восприятие вкуса

Сладкий вкус, горький вкус и вкус умами воспринимаются рецепторами GPCR.

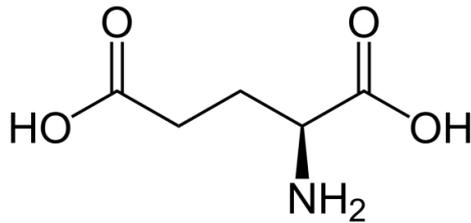


Димер GPCR: two receptors are better than one

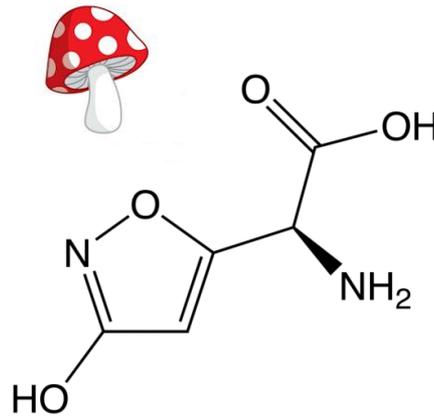
The breakthrough for the present understanding of sweetness occurred in 2001, when experiments with laboratory mice showed that mice possessing different versions of the gene **T1R3** prefer sweet foods to different extents. Subsequent research has shown that the **T1R3** protein forms a complex with a related protein, called **T1R2**, to form a G-protein coupled receptor that is the sweetness receptor in mammals.[25]

Восприятие вкуса

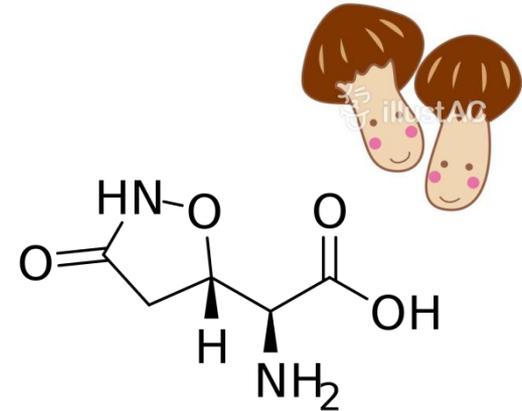
Сладкий вкус, горький вкус и **вкус умами** воспринимаются рецепторами GPCR.



L-глутамат



Иботеновая кислота

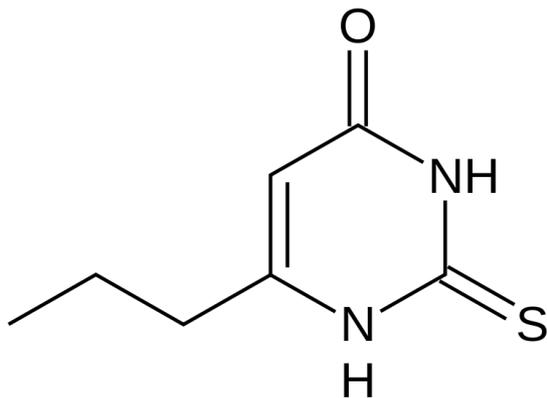


Tricholomic acid

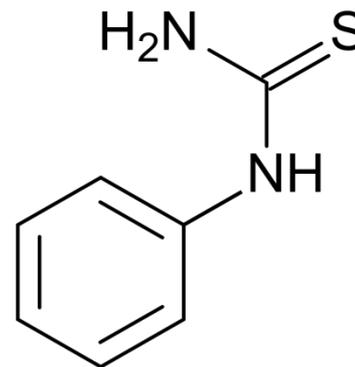
Recent molecular biological studies have now identified **strong candidates for umami receptors**, including the heterodimer **T1R1/T1R3**, and truncated type 1 and 4 **metabotropic glutamate receptors** missing most of the N-terminal extracellular domain (taste-mGluR4 and truncated-mGluR1) and **brain-mGluR4**." [15] Receptors **mGluR1** and **mGluR4** are specific to glutamate whereas T1R1 + T1R3 are responsible for the synergism... However, the specific role of each type of receptor in taste bud cells remains unclear.

Восприятие вкуса

Сладкий вкус, **горький вкус** и вкус умами воспринимаются рецепторами GPCR.



пропилтиоурацил



фенилтиокарбамид

Research has shown that **TAS2Rs** (taste receptors, type 2, also known as T2Rs) such as TAS2R38 coupled to the G protein gustducin are responsible for the human ability to taste bitter substances.[38] The TAS2R family in humans is thought to comprise about 25 different taste receptors, some of which can recognize a wide variety of bitter-tasting compounds.[39]

BitterDB



BitterDB

Institute of Biochemistry, Food Science and Nutrition, Faculty of Agriculture,
The Hebrew University of Jerusalem האוניברסיטה העברית ירושלים

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Welcome to BitterDB!

Bitter taste is one of the basic taste modalities. It is innately aversive for various species, and can be elicited by numerous, chemically different compounds. The aim of this database is to gather information about bitter-tasting natural and synthetic compounds, and their cognate bitter taste receptors (T2Rs or TAS2Rs).

How to Cite BitterDB:

Ayana Dagan Wiener, Antonella Di Pizio, Ido Nissim, Malkeet Singh Bahia; Nitzan Dubovski, Eitan Margulis, Masha Y. Niv. BitterDB: Taste ligands and receptors database in 2019. *Nucleic Acids Res* 2019; gky974.

Click here to view the paper: [BitterDB 2019 paper](#)

Ayana Wiener; Marina Shudler; Anat Levit; Masha Y. Niv. BitterDB: a database of bitter compounds. *Nucleic Acids Res* 2012, 40(Database issue):D413-419.

Click here to view the paper: [BitterDB paper](#)

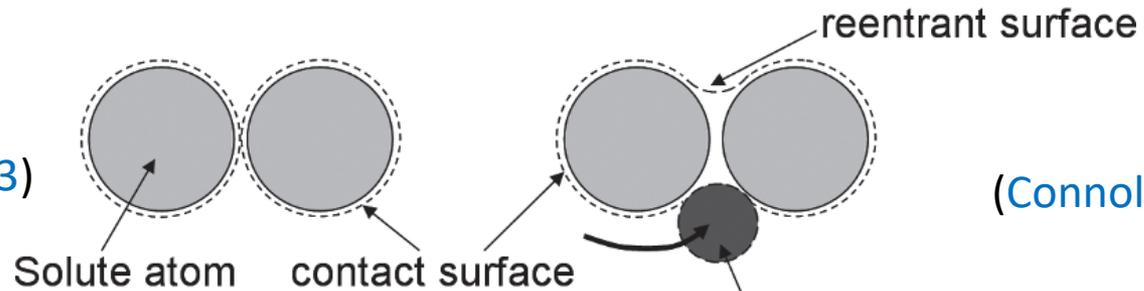


Молекулярные поверхности

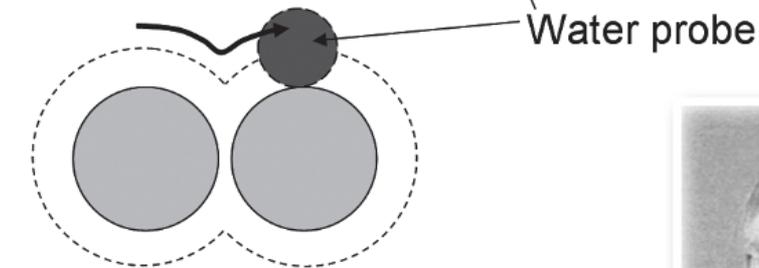
Van der Waals surface

Molecular surface

(Corey & Pauling, 1953)

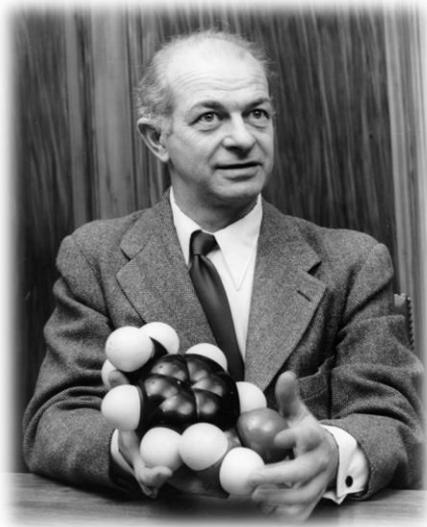


(Connolly, 1983)

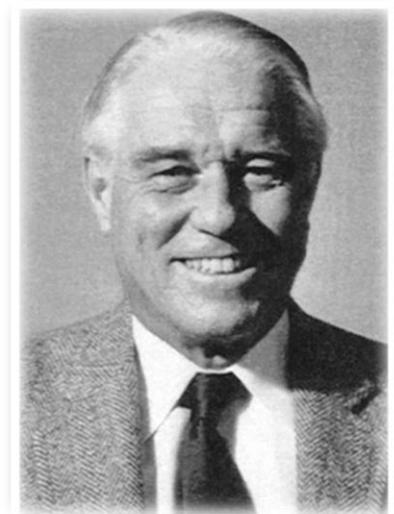


Solvent accessible surface

(Richards, 1977)

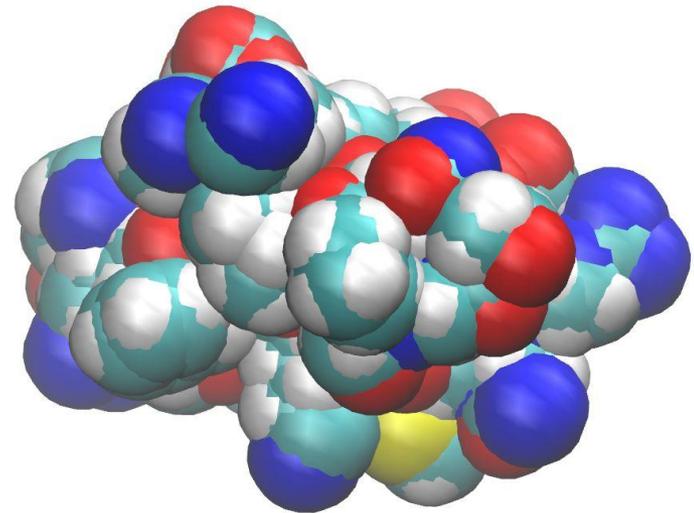
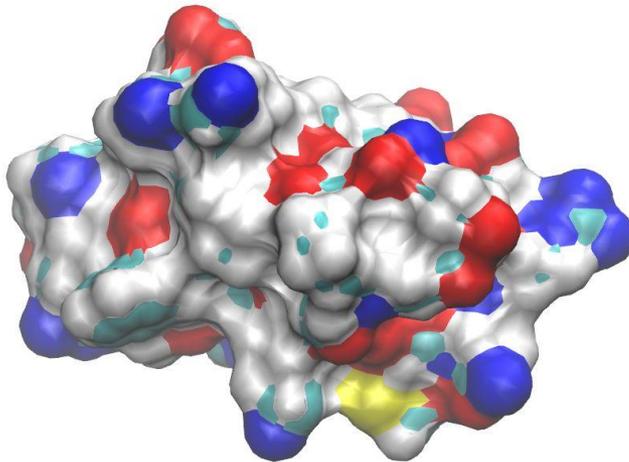
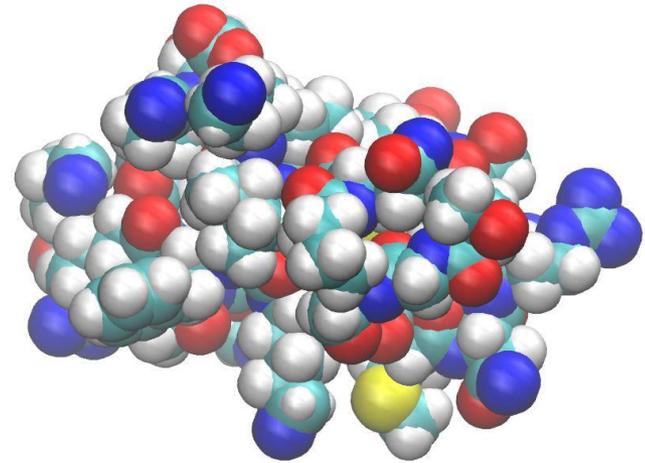
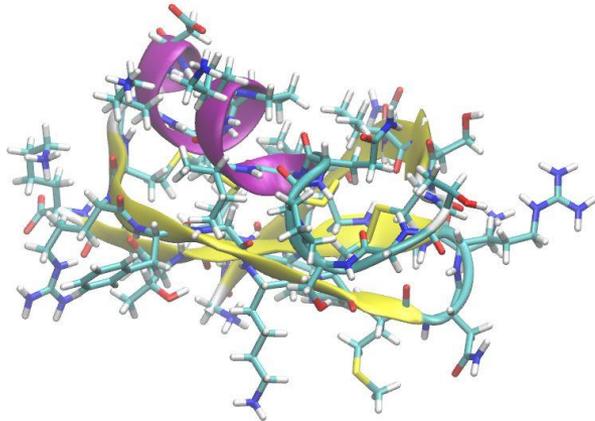


Linus Pauling
(1901 - 1994)



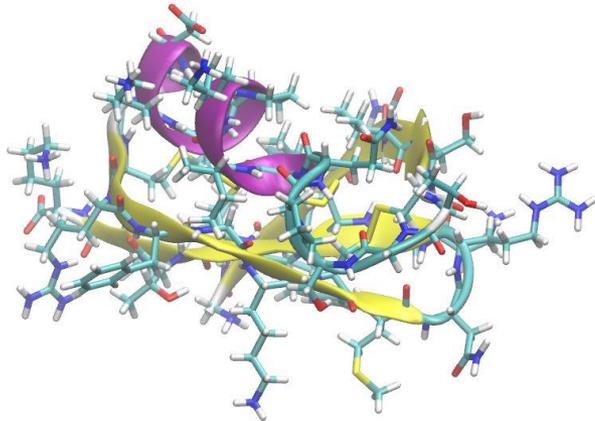
Frederic Richards
(1925 - 2009)

Молекулярные поверхности

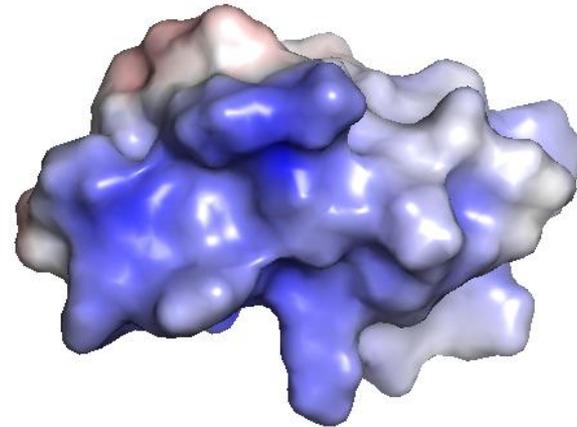
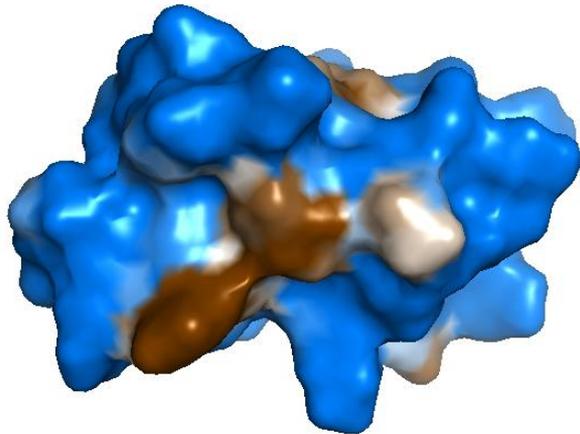
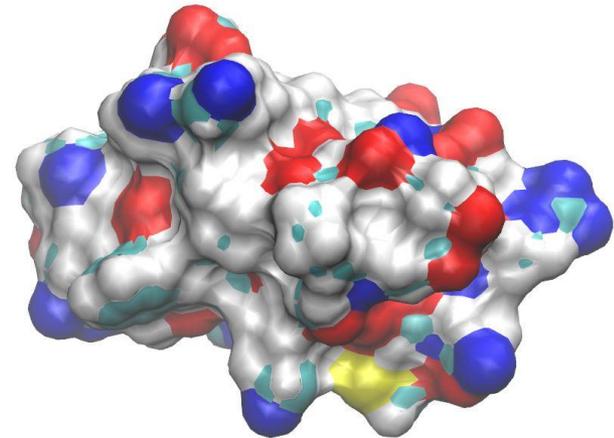


Структура аджитоксина-2 (pdb 1agt) в ленточном и стержневом представлении, в виде сфер ван-дер-Ваальса, а также ее молекулярная поверхность и поверхность, доступная растворителю (SAS)

Молекулярные поверхности

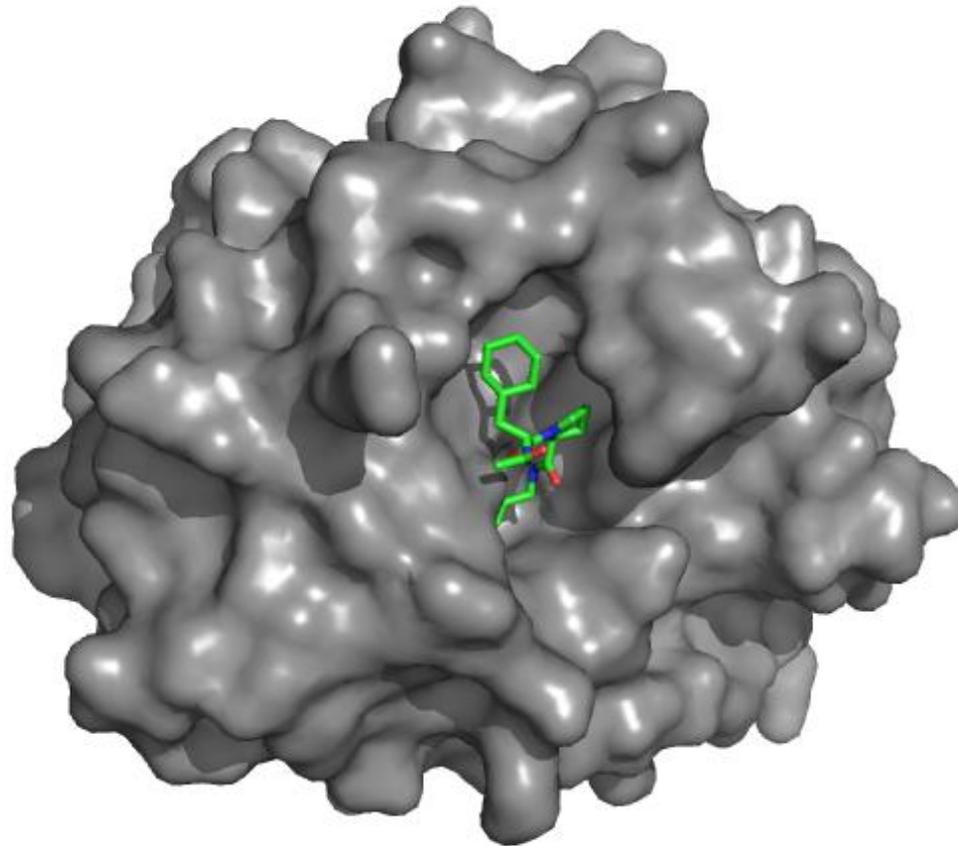


:ion Only (30

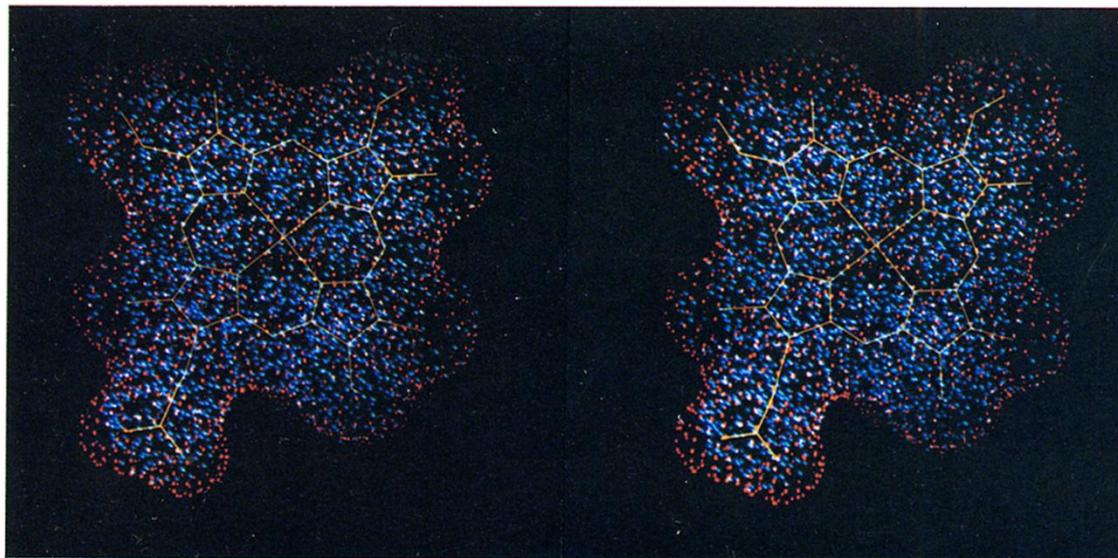


Структура аджитоксина-2 и её молекулярная поверхность, раскрашенная по химическому элементу, гидрофобности и электростатическому потенциалу (синий цвет соответствует положительным значениям, красный отрицательным)

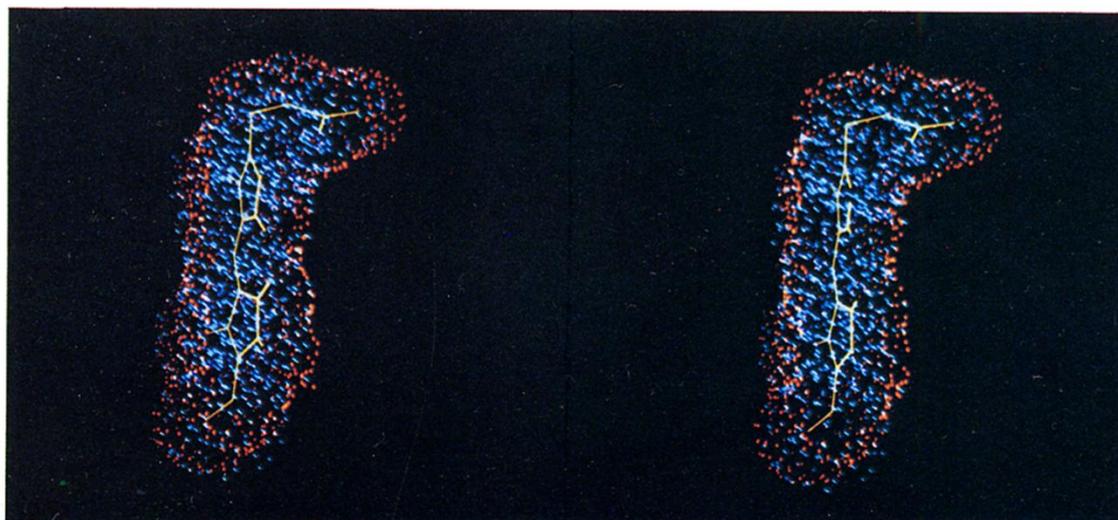
Молекулярный докинг



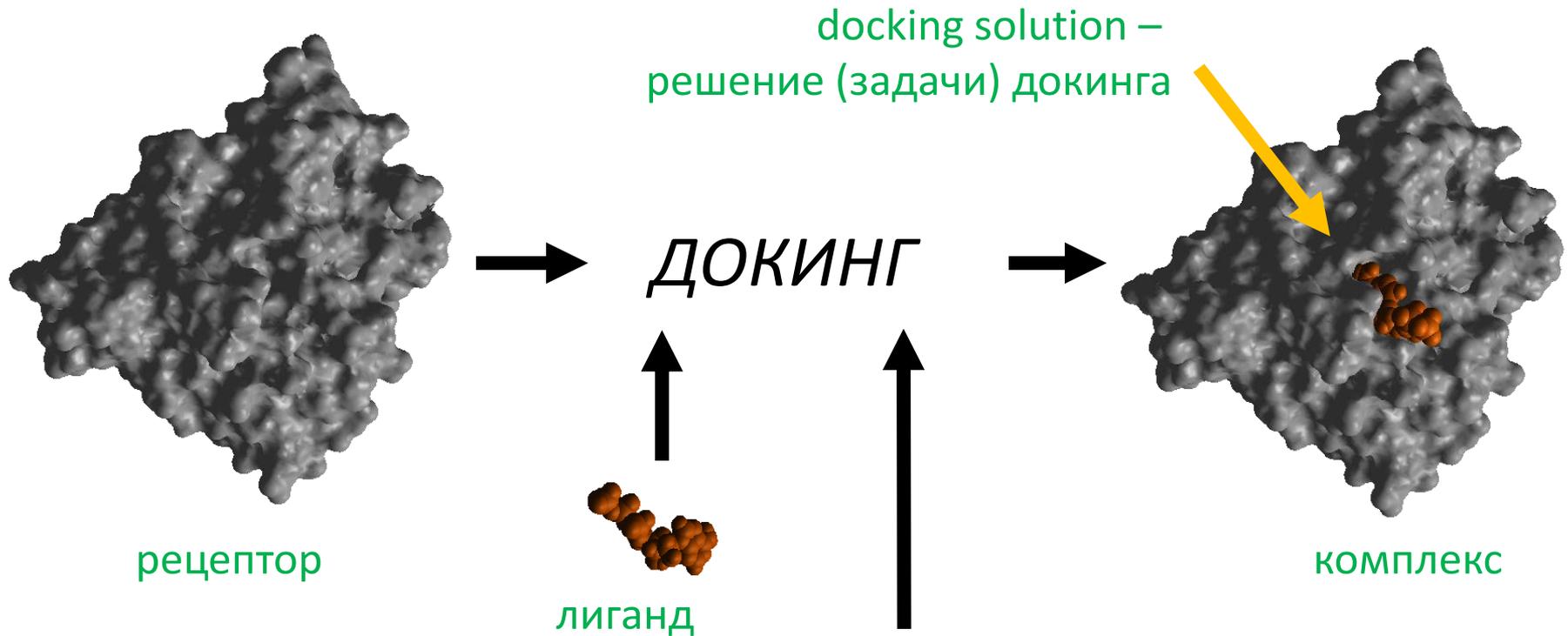
A Geometric Approach to Macromolecule-Ligand Interactions (1982)



(a)



Молекулярный докинг. Общая постановка задачи

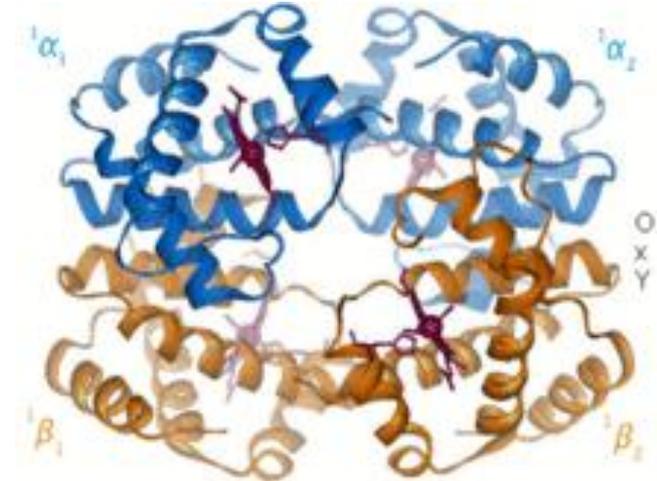


оценочная функция:
водородные связи, гидрофобные контакты, стэкинг-
взаимодействия, ...

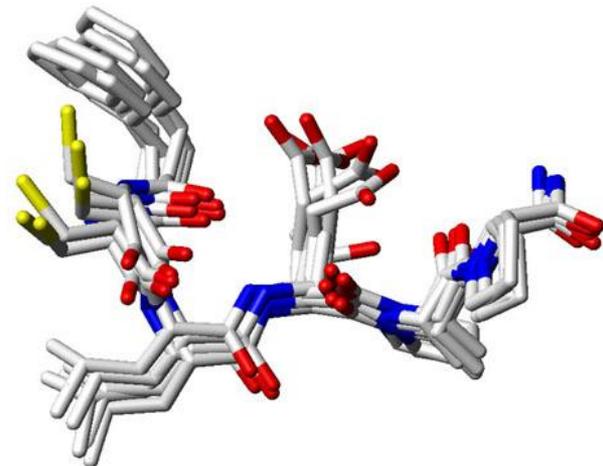
Представление белков и лигандов

Гибкость белка:

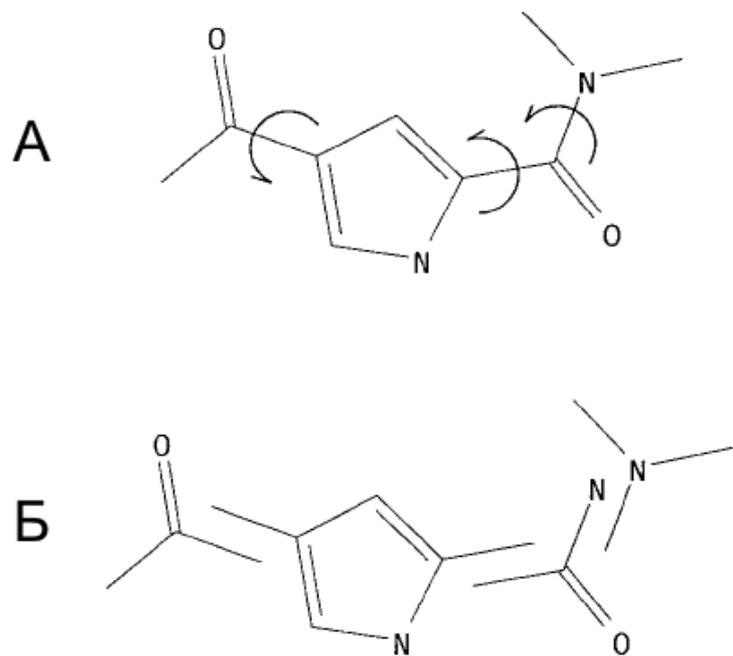
- быстрые движения малого масштаба – движение боковых цепей и петель
- медленные движения крупного масштаба – движение доменов
- ренатурация частично развернутых белков



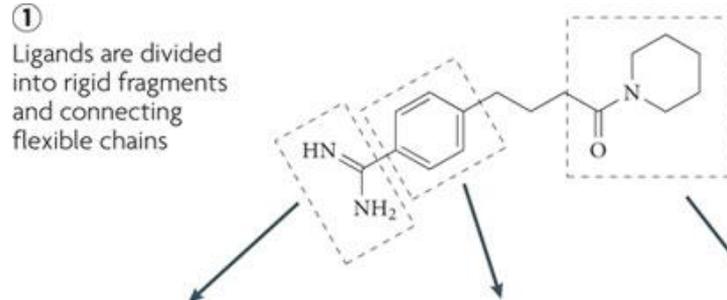
Гибкость лиганда



Молекулярный докинг. Последовательная сборка и сборка из фрагментов



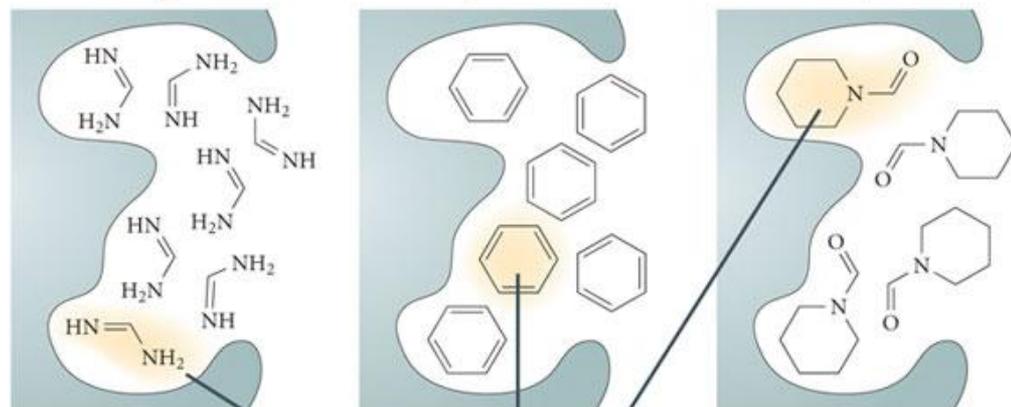
① Ligands are divided into rigid fragments and connecting flexible chains



②

Rigid dock:

Each fragment is docked independently everywhere in the receptor

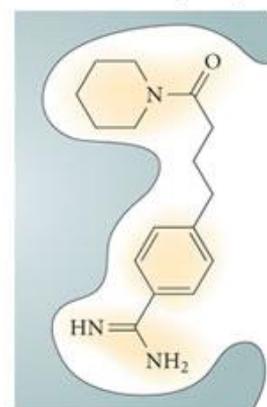


③

Pose match:

A fast graph-matching algorithm finds all matching solutions to reconstruct the original molecules

Reconnected-ligand pose



④

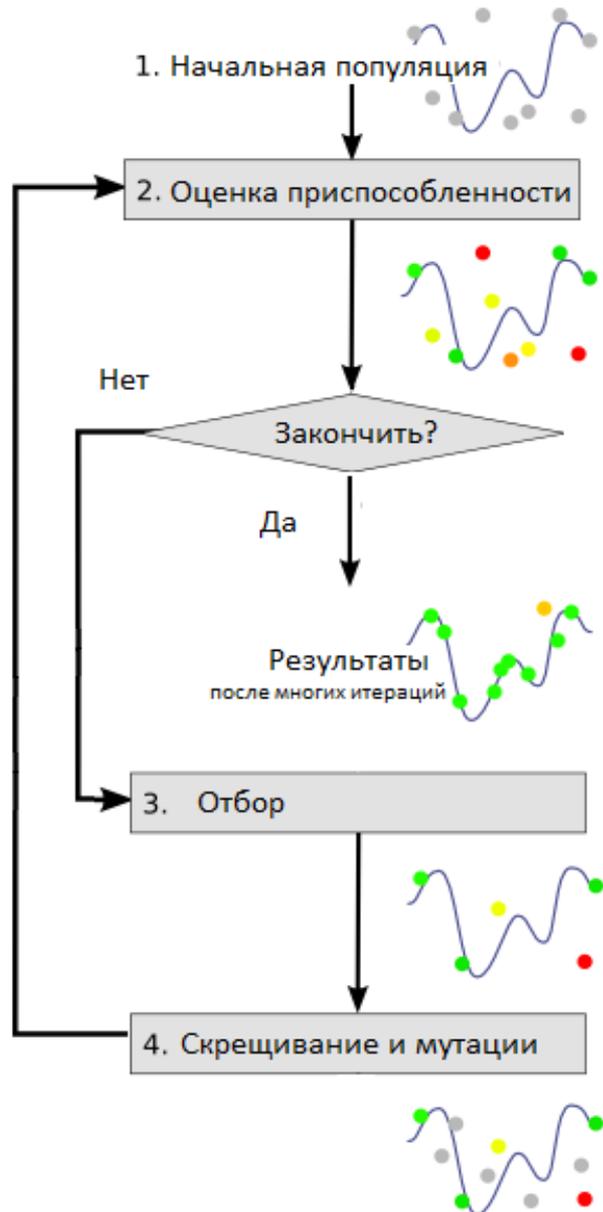
Local energy optimization:

The structure is optimized in the receptor

⑤ **Ranking:**

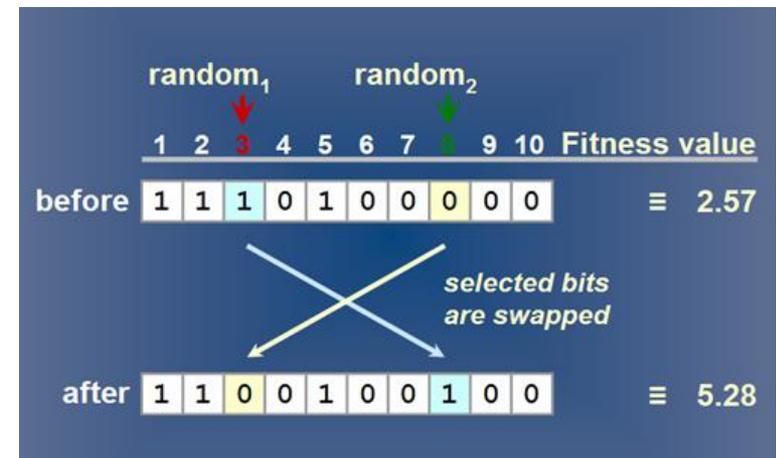
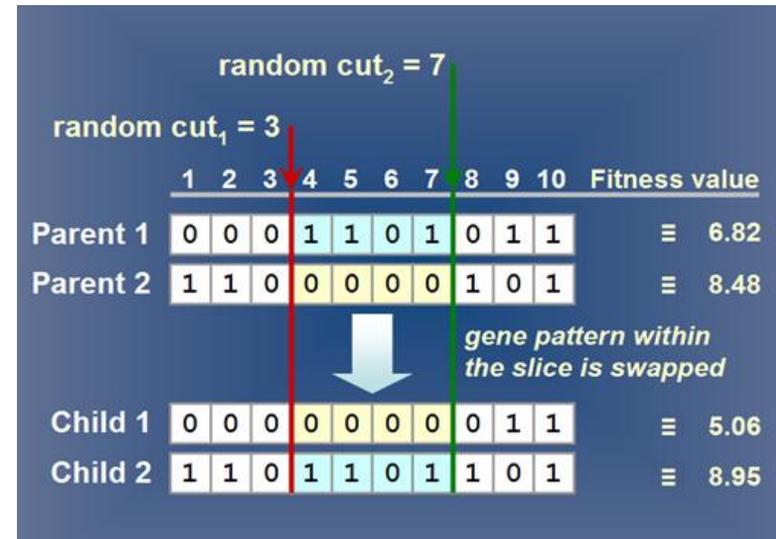
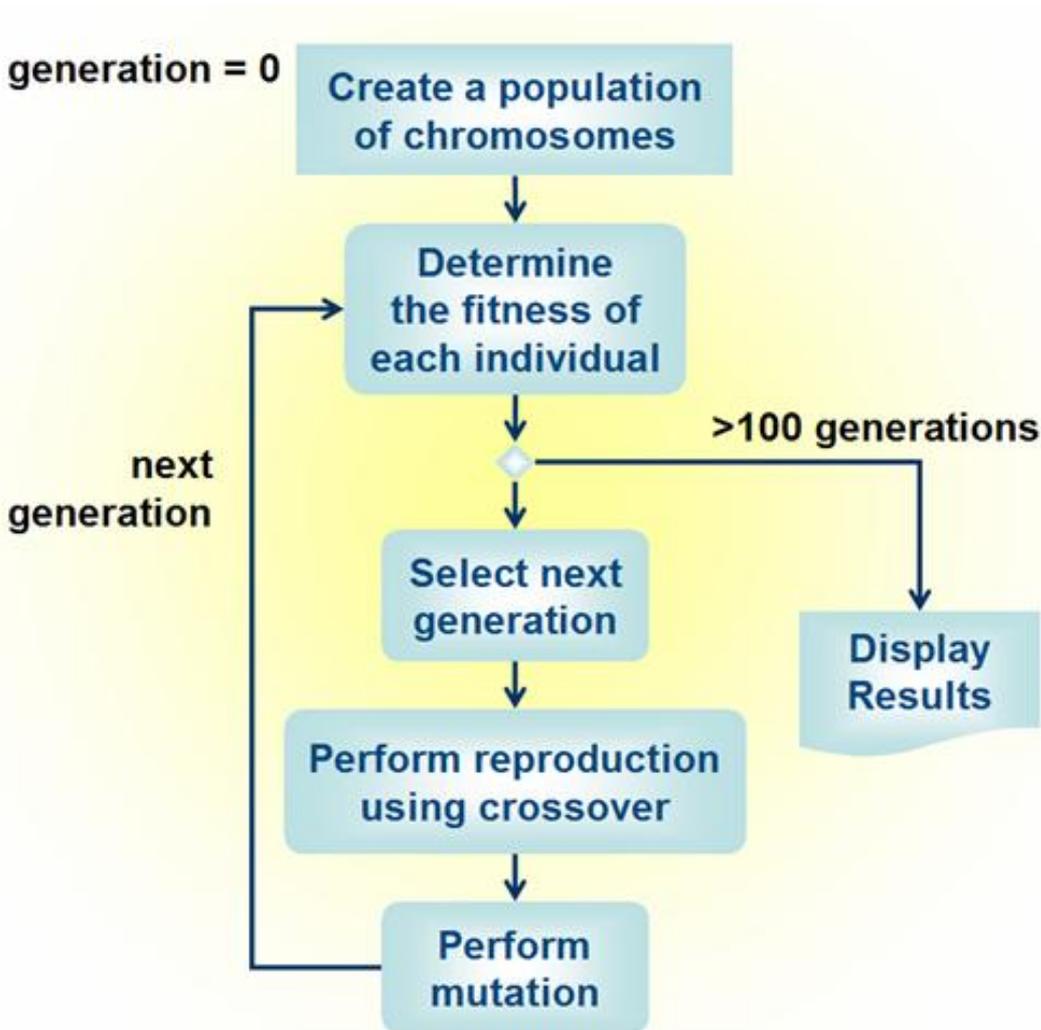
Structures are ranked based on scoring functions

Молекулярный докинг. Генетический алгоритм

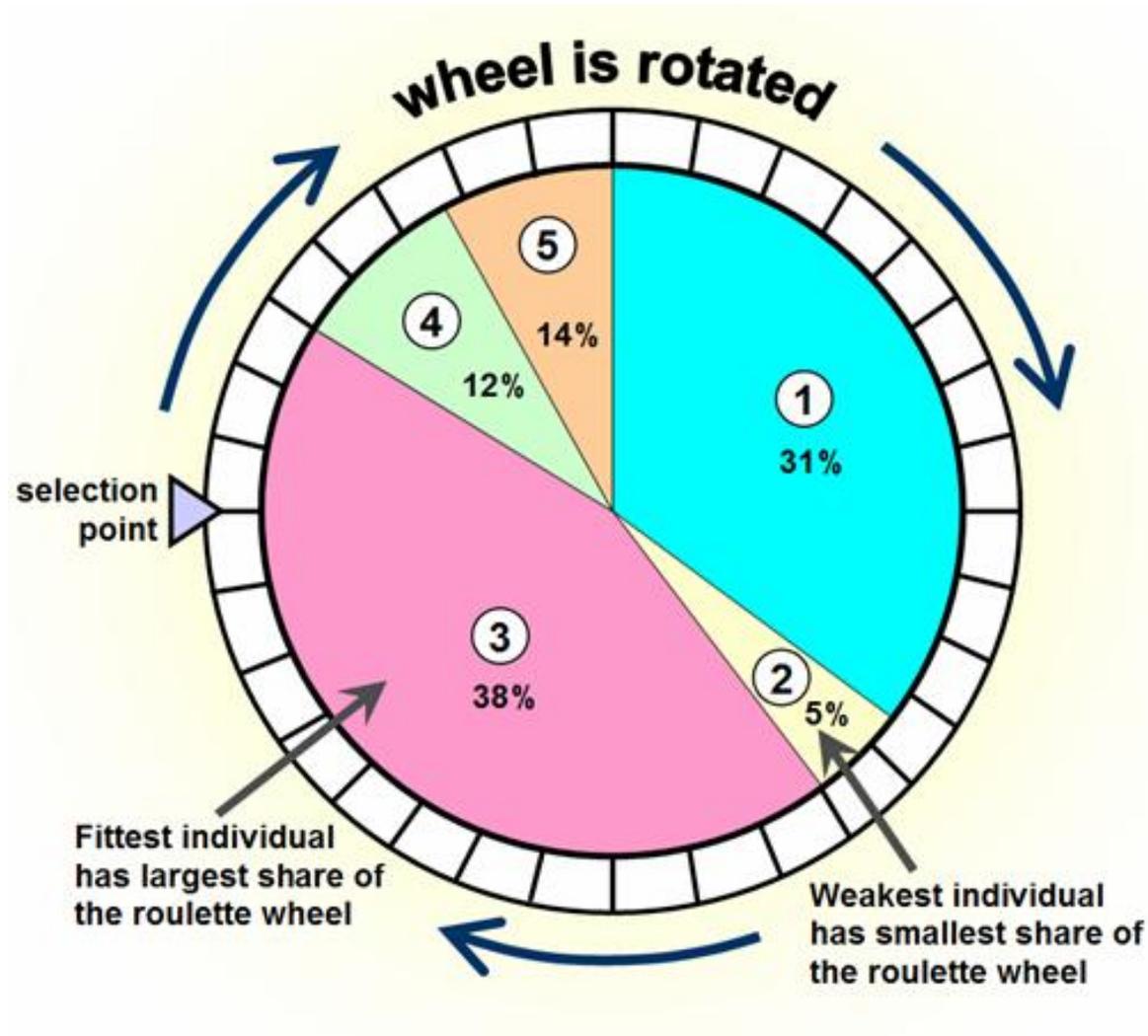


The 2006 NASA ST5 spacecraft antenna. This complicated shape was found by an evolutionary computer design program to create the best radiation pattern.

Молекулярный докинг. Генетический алгоритм



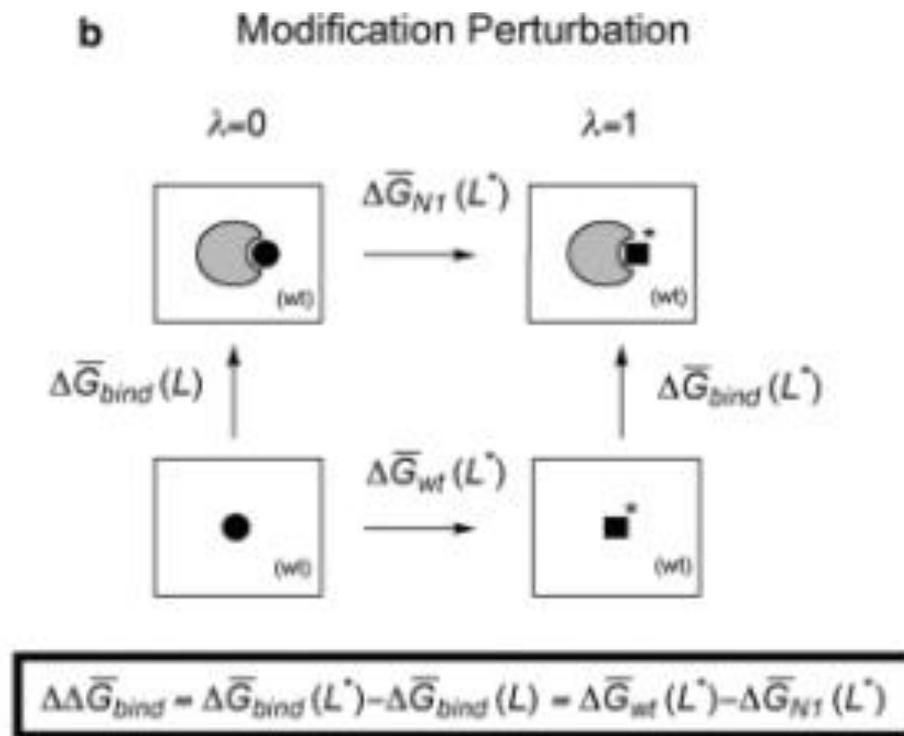
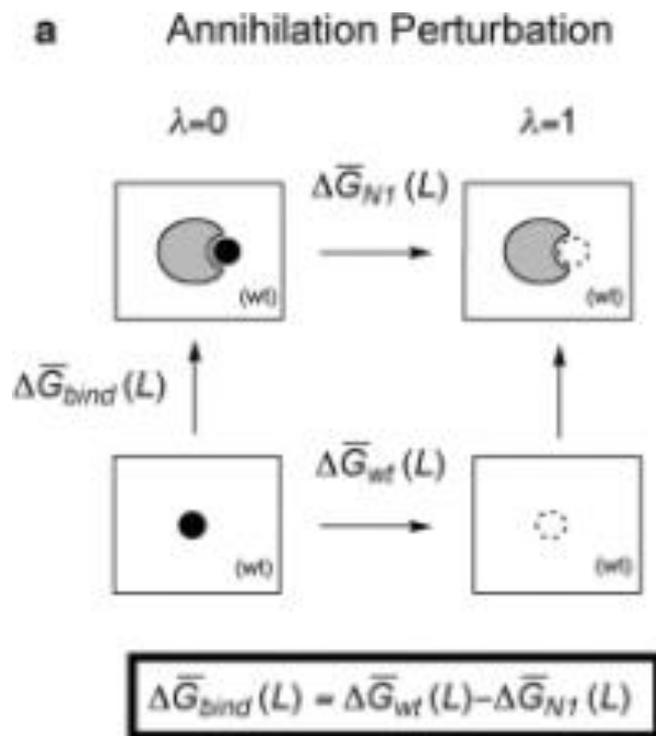
Молекулярный докинг. Генетический алгоритм



Расчет энергии связывания

Термодинамическое интегрирование

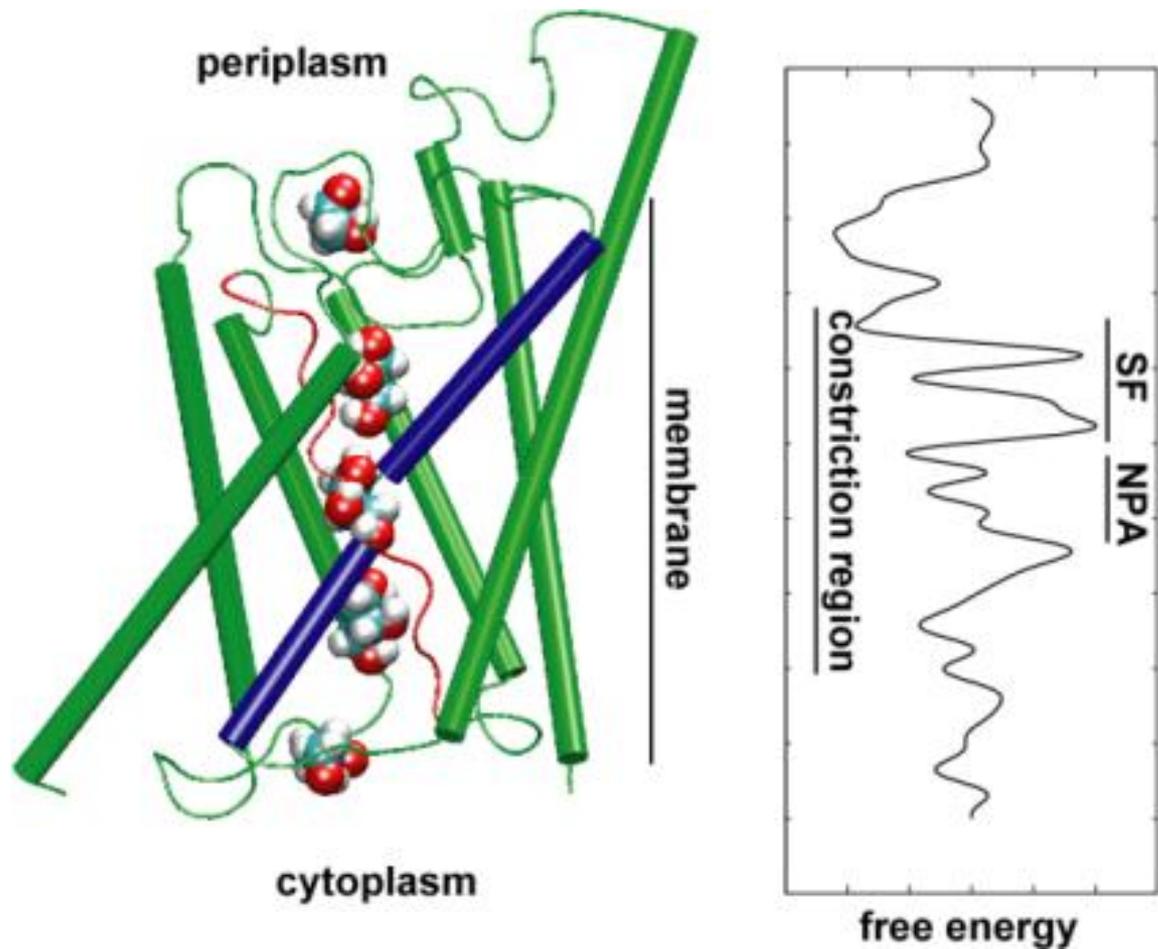
$$\Delta G_{TI}^0 = \int_0^1 \left\langle \frac{\partial V(\lambda)}{\partial \lambda} \right\rangle_{\lambda} d\lambda$$



Не используется в методах молекулярного докинга

Расчет энергии связывания

Потенциал средней силы



Не используется в методах молекулярного докинга

Молекулярный докинг. Оценочные функции

– Forcefield-based

- Based on terms from molecular mechanics forcefields
- GoldScore, DOCK, AutoDock

– Empirical

- Parameterised against experimental binding affinities
- ChemScore, PLP, Glide SP/XP

– Knowledge-based potentials

- Based on statistical analysis of observed pairwise distributions
- PMF, DrugScore, ASP

Молекулярный докинг. Обучающие наборы

Положение лигандов и константы связывания уже известны

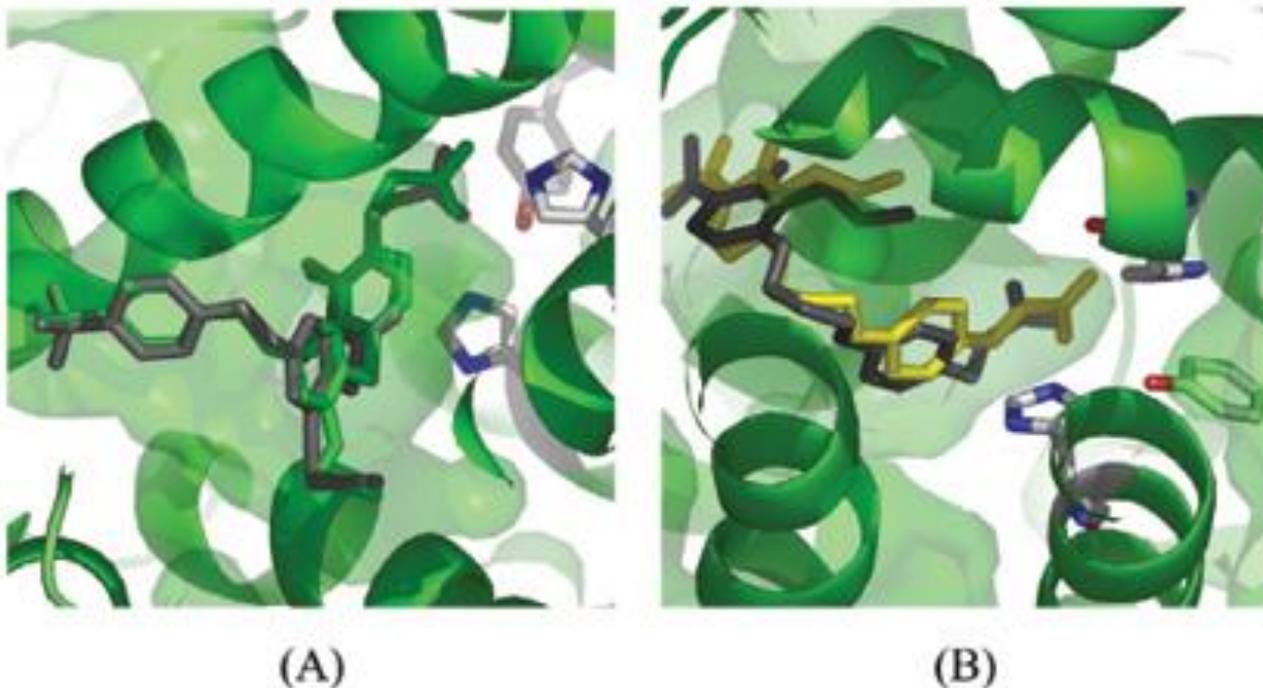
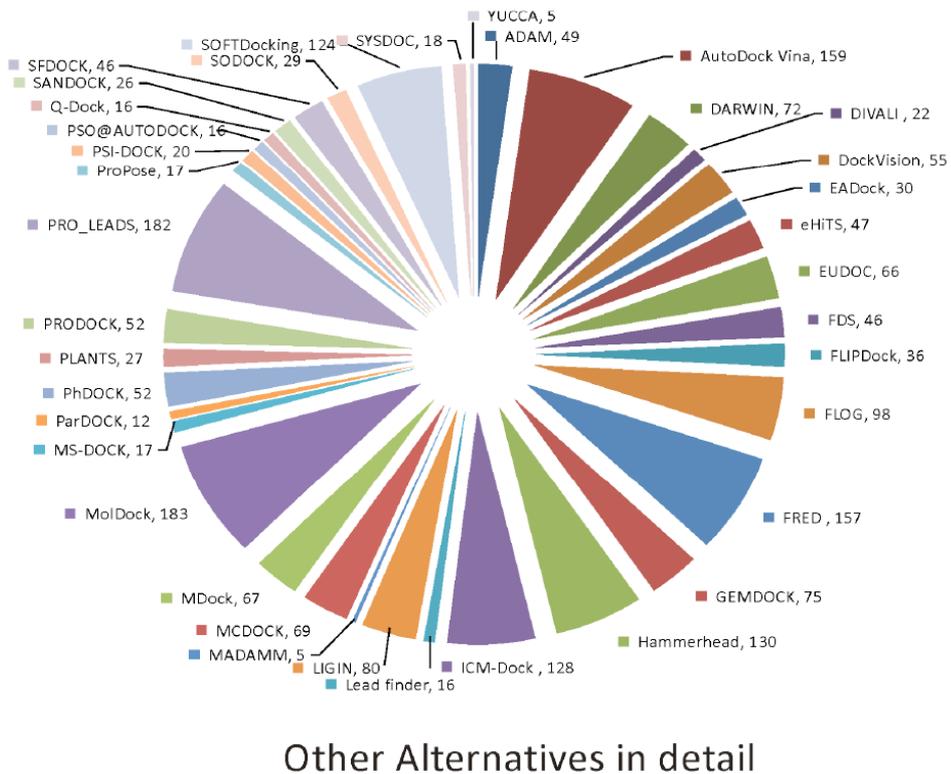
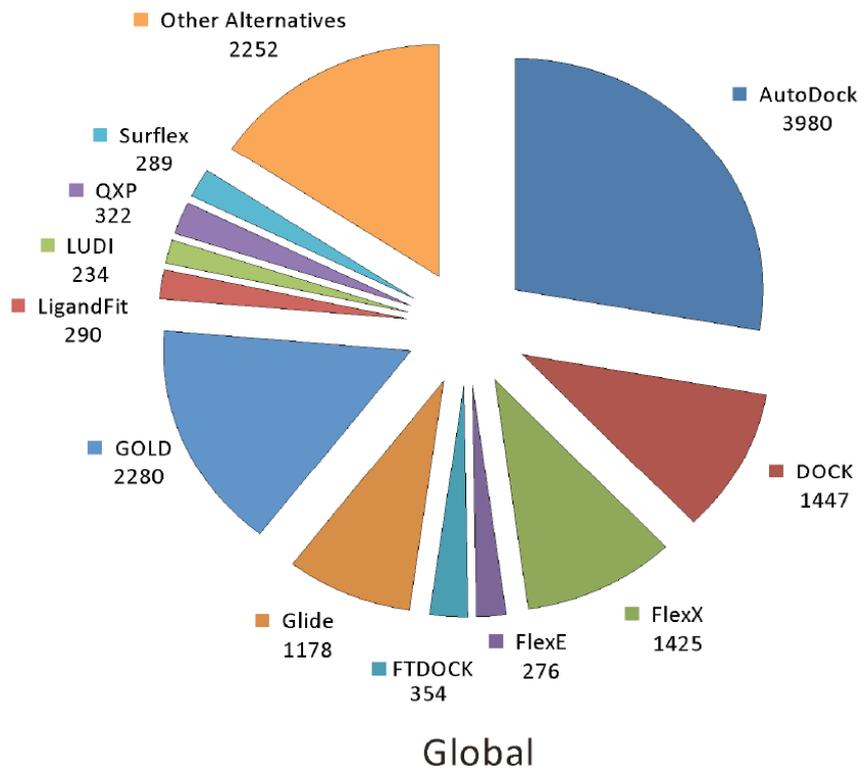


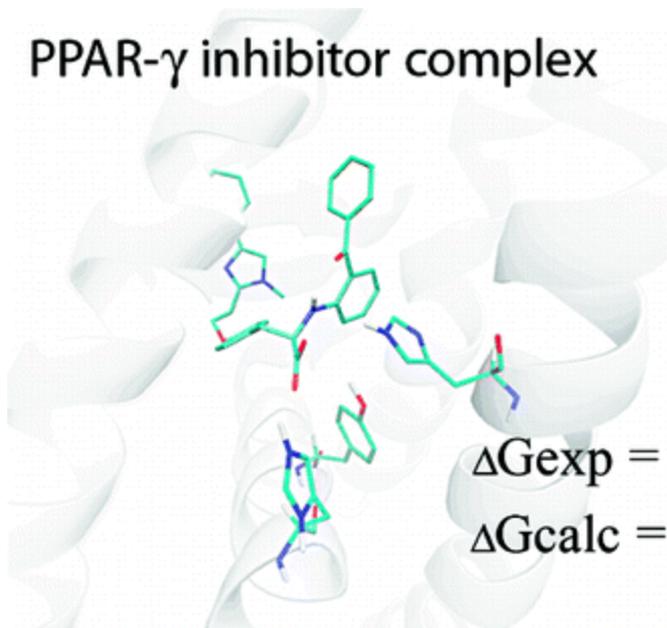
Figure 4. (A) Redocking and (B) crossdocking results. Both crystallographic ligands are shown in gray and the docked ligands are in green (D32) and yellow (L41), respectively. See online for color image.

Молекулярный докинг. Программы



Молекулярный докинг. LeadFinder

PPAR- γ inhibitor complex



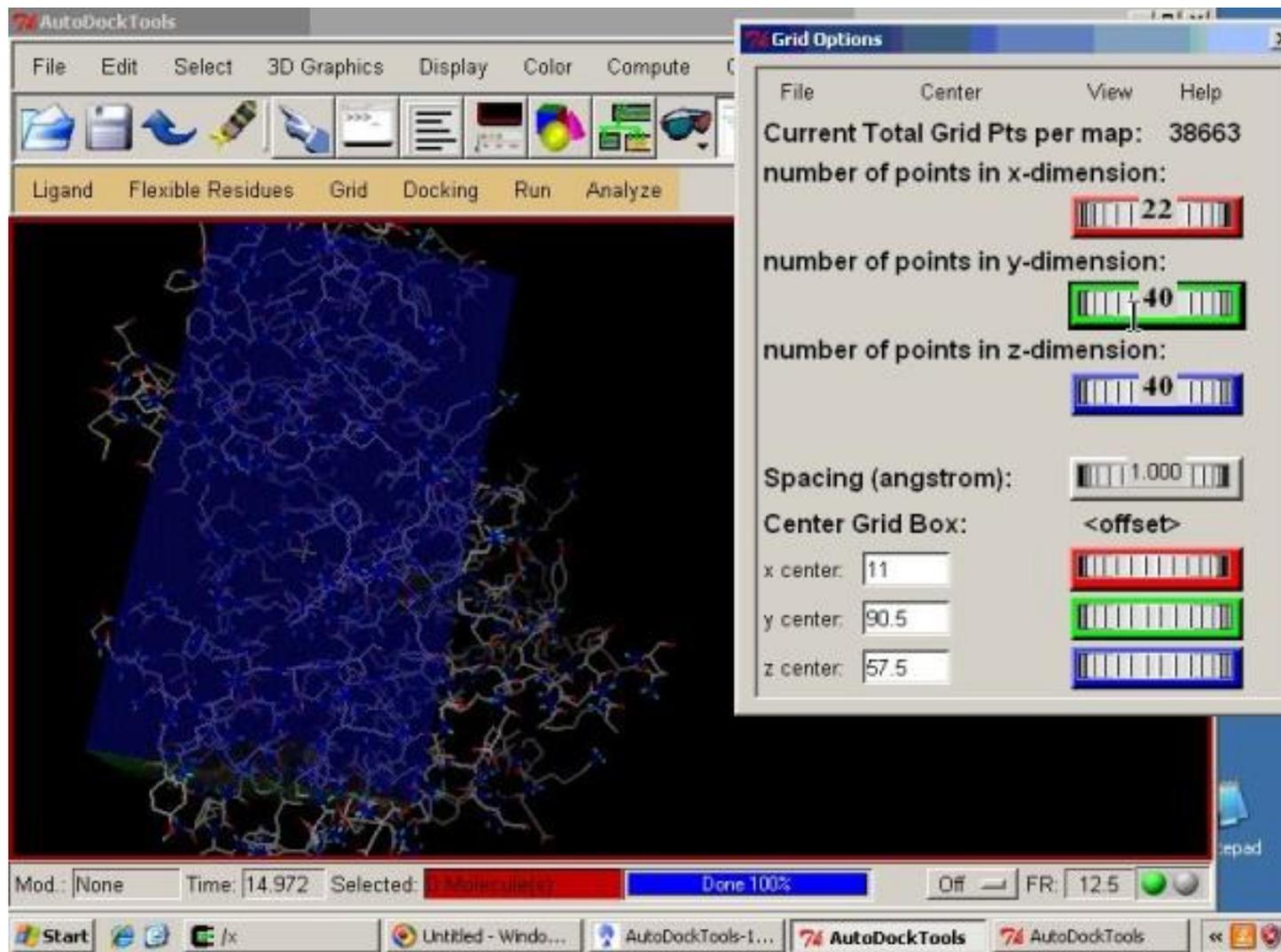
(Stroganov, Chilov et al., 2008)

$\Delta G_{\text{exp}} = -12.65 \text{ kcal/mol}$

$\Delta G_{\text{calc}} = -12.71 \text{ kcal/mol}$

Молекулярный докинг. AutoDock (->AutoDock Vina)

(Goodsell & Olson, 1990; Trott & Olson, 2010)



Молекулярный докинг. SwissDock



Swiss Institute of
Bioinformatics



Molecular
Modelling Group

SwissDock

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Target selection

Search for targets:

ie. **PDB code**, **protein name**, **sequence**, or **URL**
or **upload file (max 5MB)**

Ligand selection

Search for ligands:

ie. **ZINC AC**, **ligand name** or category (like **scaffolds** or **sidechains**), or **URL**
or **upload file (max 5MB)**

Description

Job name (required):

Help

Search for a ligand

A success rate >80% can be achieved with drug-like ligand with less than 15 free dihedral angles.

You can search for ligands using a ZINC accession number (AC), its name, or its category.

ZINC AC and names will be looked for in the ZINC database.

Names and categories (scaffolds or sidechains) will be searched for in our database of 58 compounds consisting of 27 scaffolds and 31 sidechains. See [here](#) and [here](#) for further details.

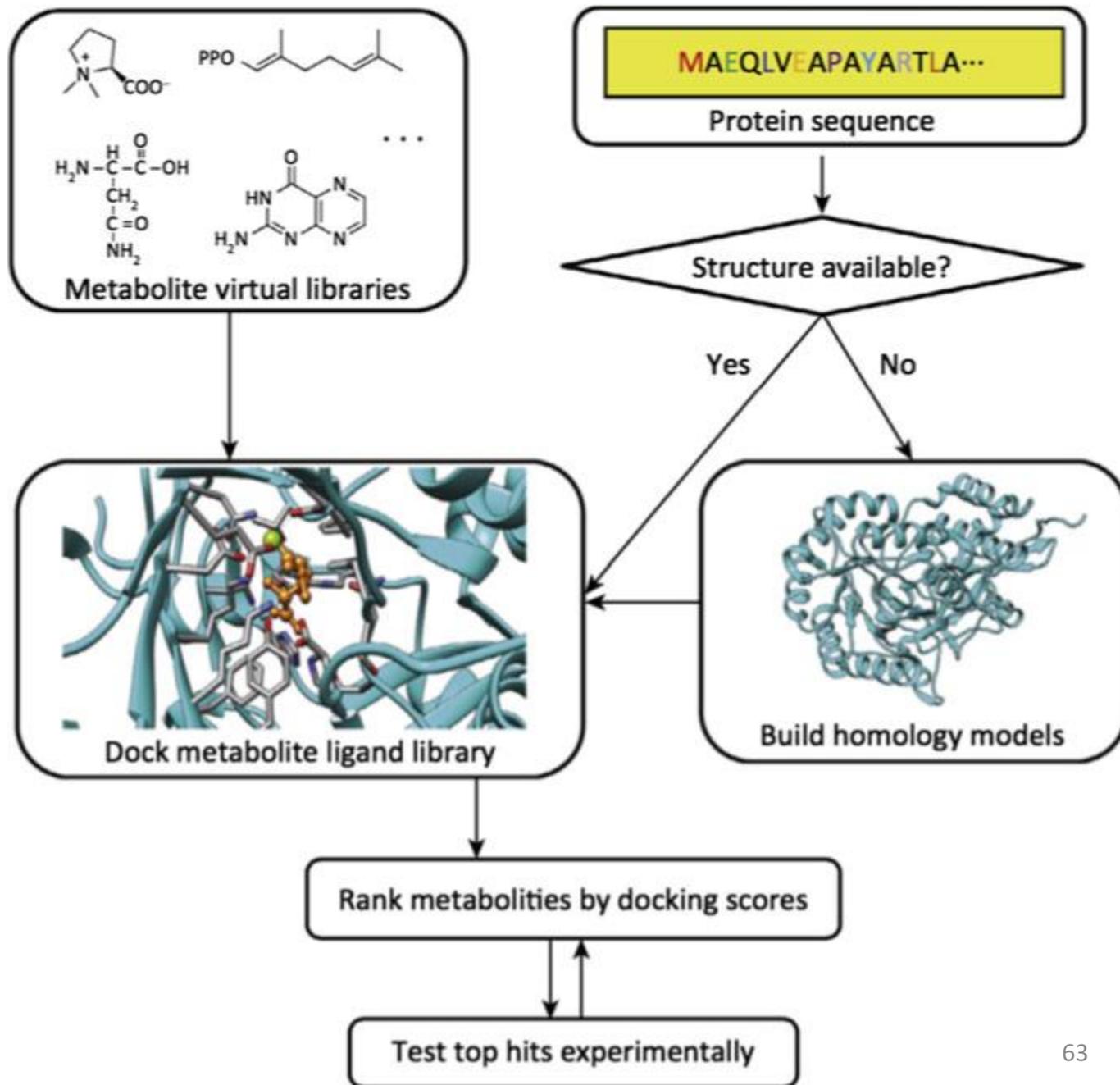
Load a ligand from a URL

You can also load a file from a URL, provided that it is either:

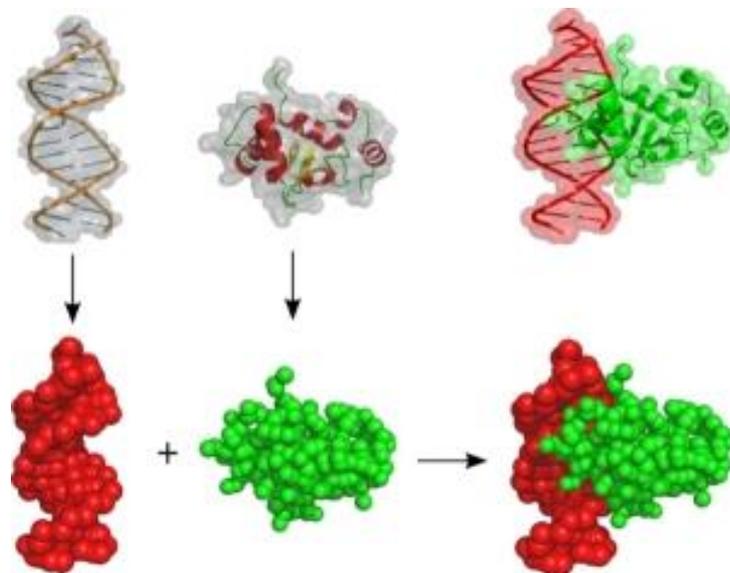
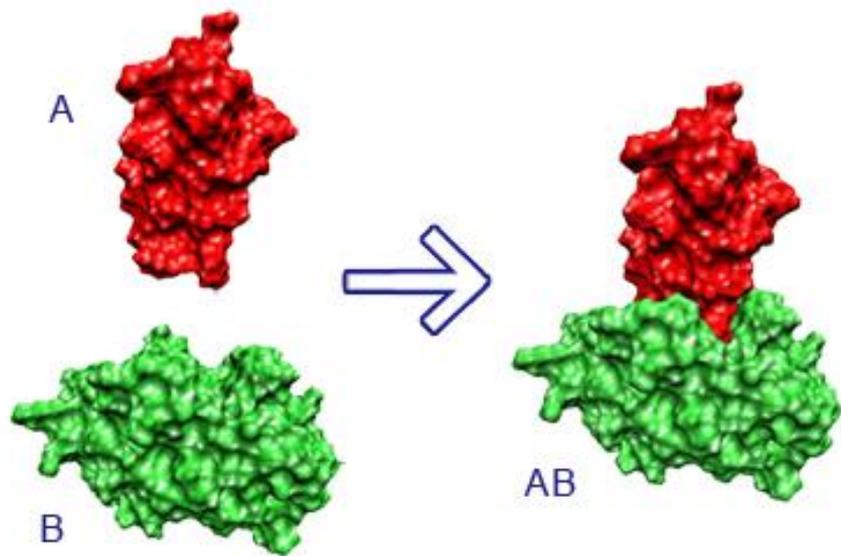
- a MOL2 file with all hydrogens and 3D coordinates. Check atom **chirality**, and adjust protonation states according to your needs (e.g. carboxylate groups are usually deprotonated at physiological pH), and make sure that it has a correct topology (we recommend **UCSF Chimera**, **OpenBabel**, **MarvinSketch**, **XDrawChem**, **ChemDraw**).
- a ZIP file containing files in the **CHARMM format** (PDB/RTF/PAR).

Before moving on, make sure that the protonation states are reasonable, since they have a big impact on the docking outcome.

Аннотация функции



Докинг макромолекул



Докинг макромолекул

ZDOCK SERVER

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[Input Protein 1](#)

PDB ID ▼

[Input Protein 2](#)

PDB ID ▼

[Enter your email:](#)

Optional:

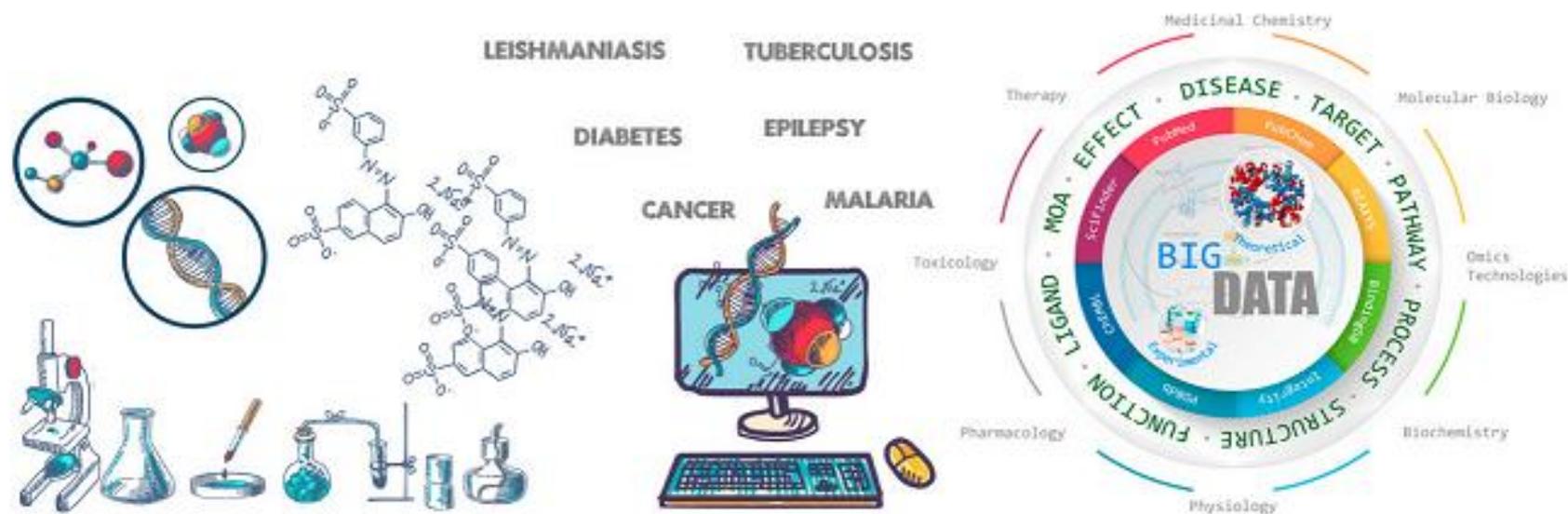
[Select ZDOCK version](#)

ZDOCK 3.0.2 ▼

[Skip residue selection](#)

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XXVI Симпозиум «Биоинформатика и компьютерное конструирование лекарств» в рамках XXVII Российского национального конгресса «Человек и лекарство»



Проводится онлайн с 6 по 25 апреля 2020 года.

