



Лекция № 3

Структурная биоинформатика

3D-структура белков

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Для студентов, обучающихся по направлению 06.03.01 «Биология»
профили Биохимия, Генетика
при изучении дисциплины «Биоинформатика»

П л а н л е к ц и и

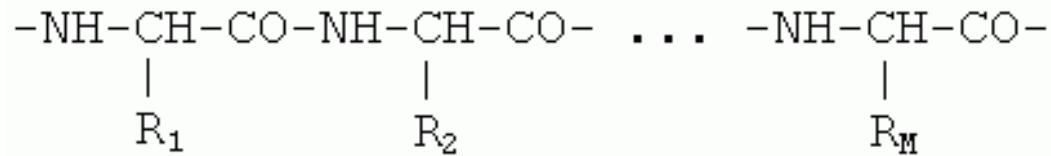
- Третичная структура белка.
- Фолдинг.
- Моделирование третичной структуры белка по гомологии.
- База данных ModBase.
- Методы экспериментального определения пространственной структуры белков.
- Банк PDB.
- Анализ белковых структур.

Структурная биоинформатика

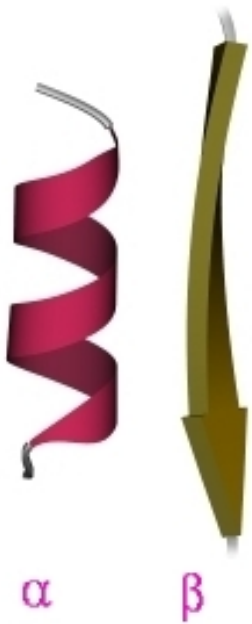
- Предсказание функциональных участков белковой молекулы
- Сравнительный анализ структур родственных белков
- Классификация белков на основе их 3D-структуры
- Анализ структур комплексов двух или нескольких молекул белка
- Анализ комплексов молекул белка с другими молекулами
- Предсказание воздействия молекул химических веществ (например, потенциальных лекарств) на молекулы белков
- Предсказание структуры белка по структуре белка с похожей последовательностью

Пространственные структуры белков и их предсказание

Структуры белков



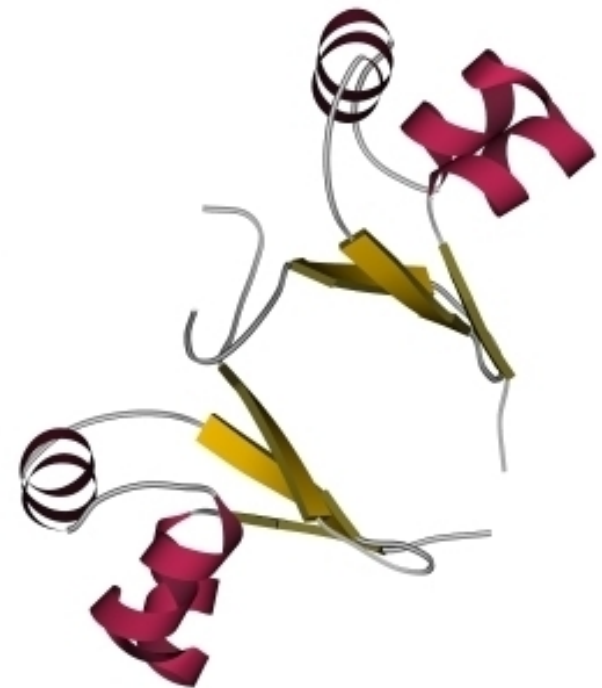
Первичная ... – *Gly* – *Val* – *Tyr* – *Gln* – *Ser* – *Ala* – *Ile* – *Asn* – *Lys* – *Ala* – ...



Вторичная



Третичная



Четвертичная

**«Структурирующие»
аминокислоты**

Trp Phe Ile Tyr Val Leu

**«Неструктурирующие»
аминокислоты**

Gly Ser Pro

Вторичные структуры

Регулярные (структурированные)

α -Спирали

β -Листы

Нерегулярные (неструктурированные)

Повороты

Петли

Концевые домены

Третичные структуры

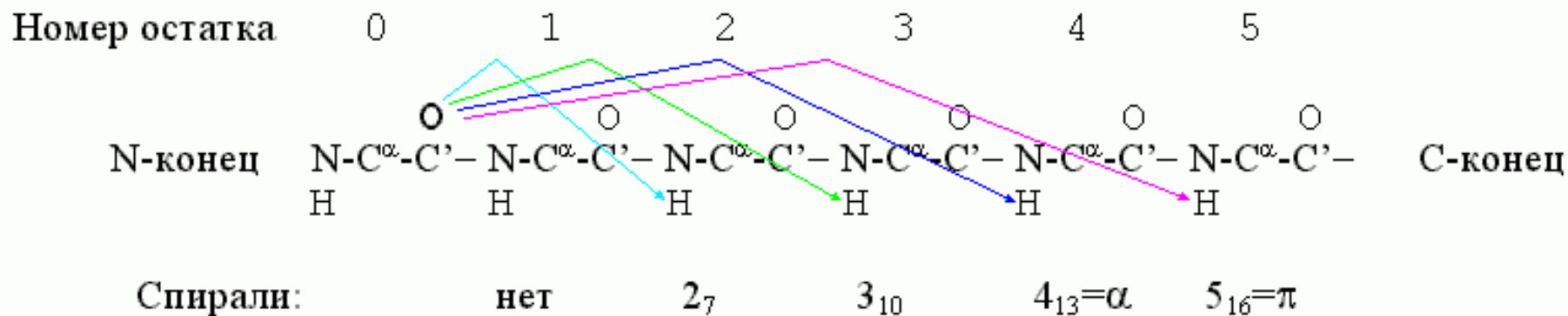
α -

β -

$(\alpha+\beta)$ -

α/β -

Спирали



2_7

3_{10}

4_{13} (α)

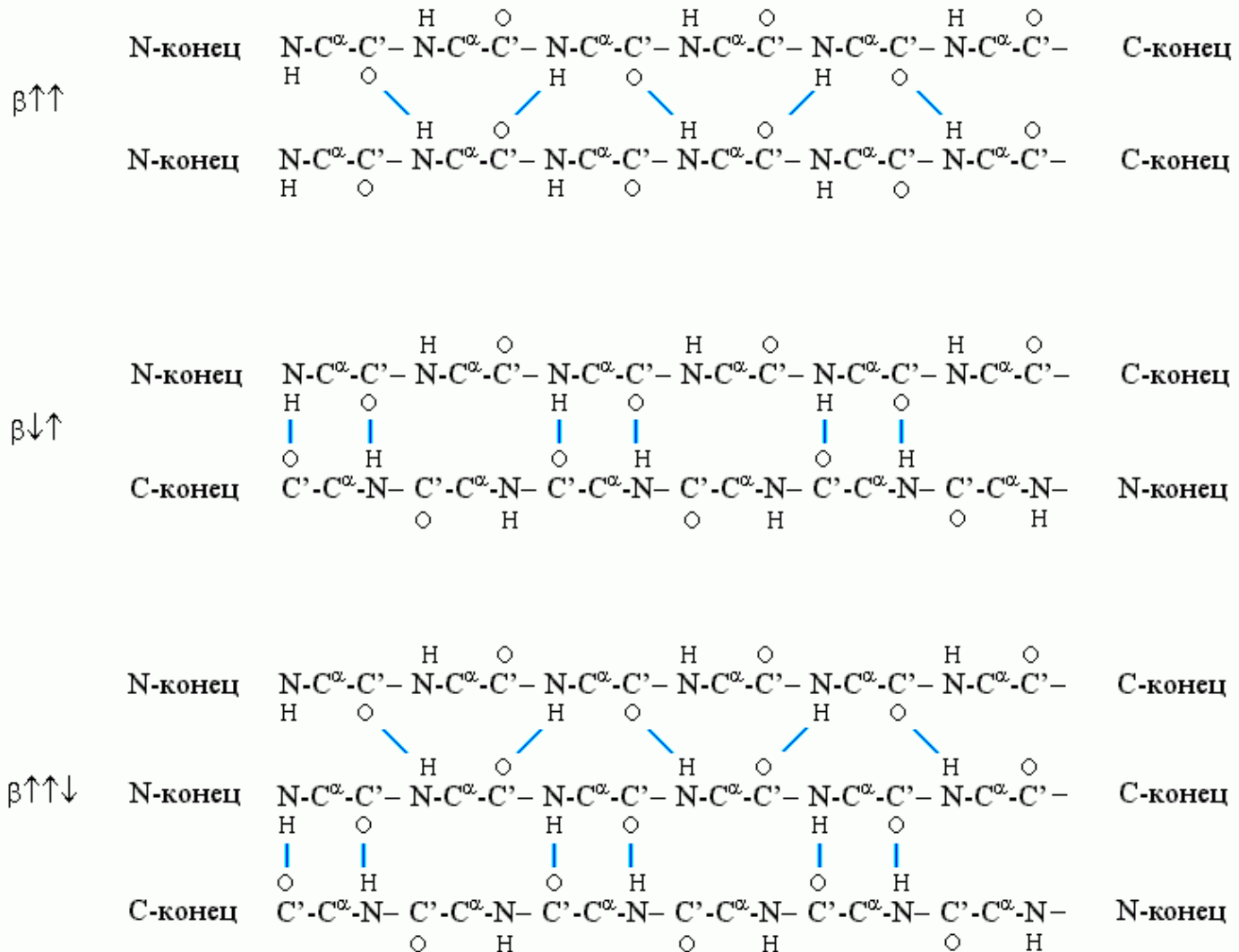
5_{16} (π)

R

L

α_R – самая устойчивая

Листы



Последовательность определяет структуру белка

Белки, похожие по последовательности, имеют похожую структуру

Структуру можно предсказать, сравнивая анализируемую последовательность с последовательностями белков, для которых экспериментально установлена структура

МОТИВЫ

**Специфический фрагмент
последовательности**

**Различают структурированные и
неструктурированные мотивы и
повторы**

Неструктурированные мотивы

30% белков частично или полностью неструктурированы

Повторы

Pro — Pro — Pro — Pro — Pro — Pro

Gln — Gln — Gln — Gln — Gln — Gln

His — His — His — His — His — His

Домены

**Независимая глобулярная единица
в белке**

**Часть белка, обладающая
некоторой активностью или
свойствами**

**Каждый домен играет свою роль
в функции белка**

Домены

Только небольшая часть известных доменов была изучена экспериментально, остальные описаны как сходные части гомологичных белков

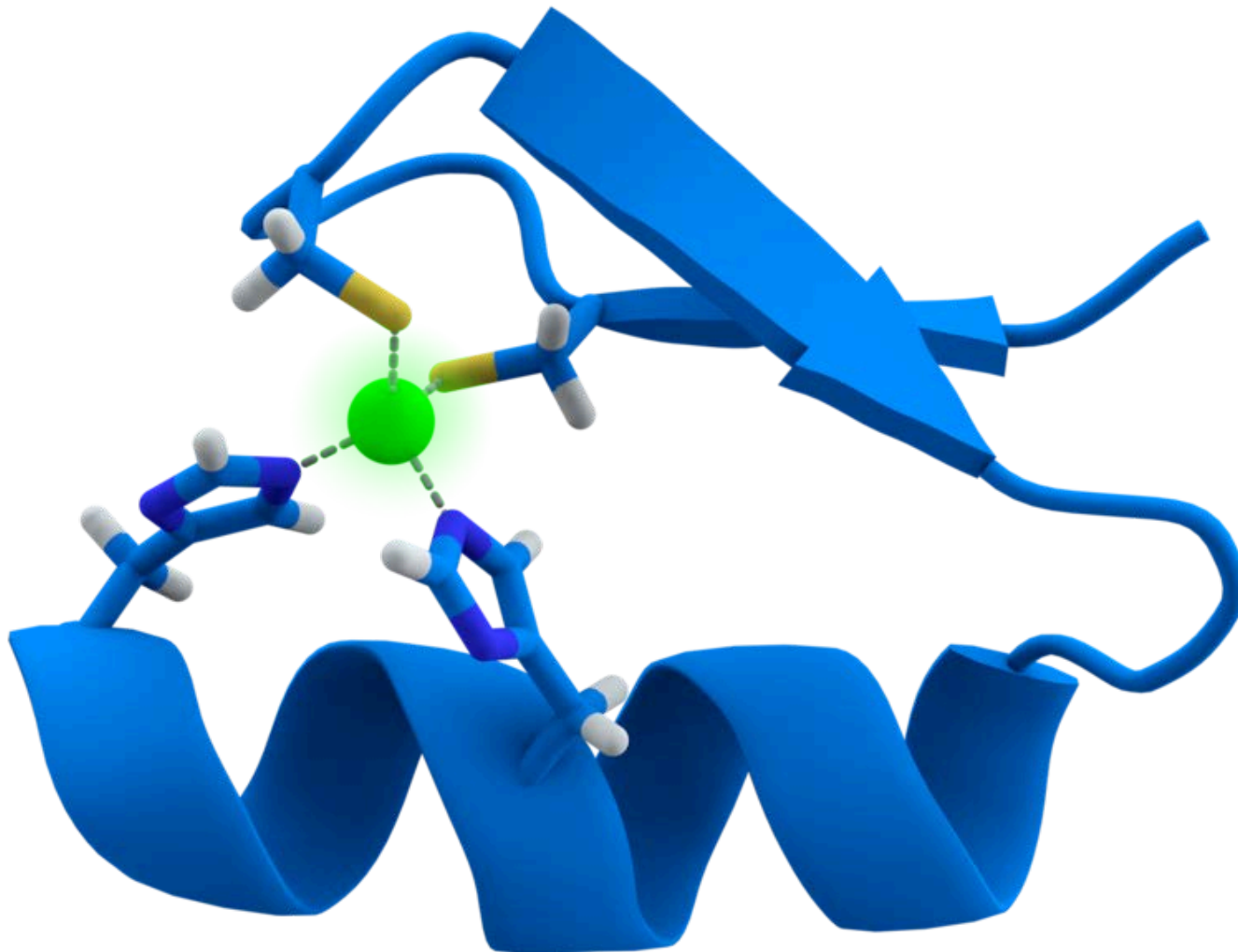
Точно определить домен и его границы очень сложно

Существует много подходов и различных доменных коллекций

Глобулярные домены α -Кристаллин



Цинковый палец



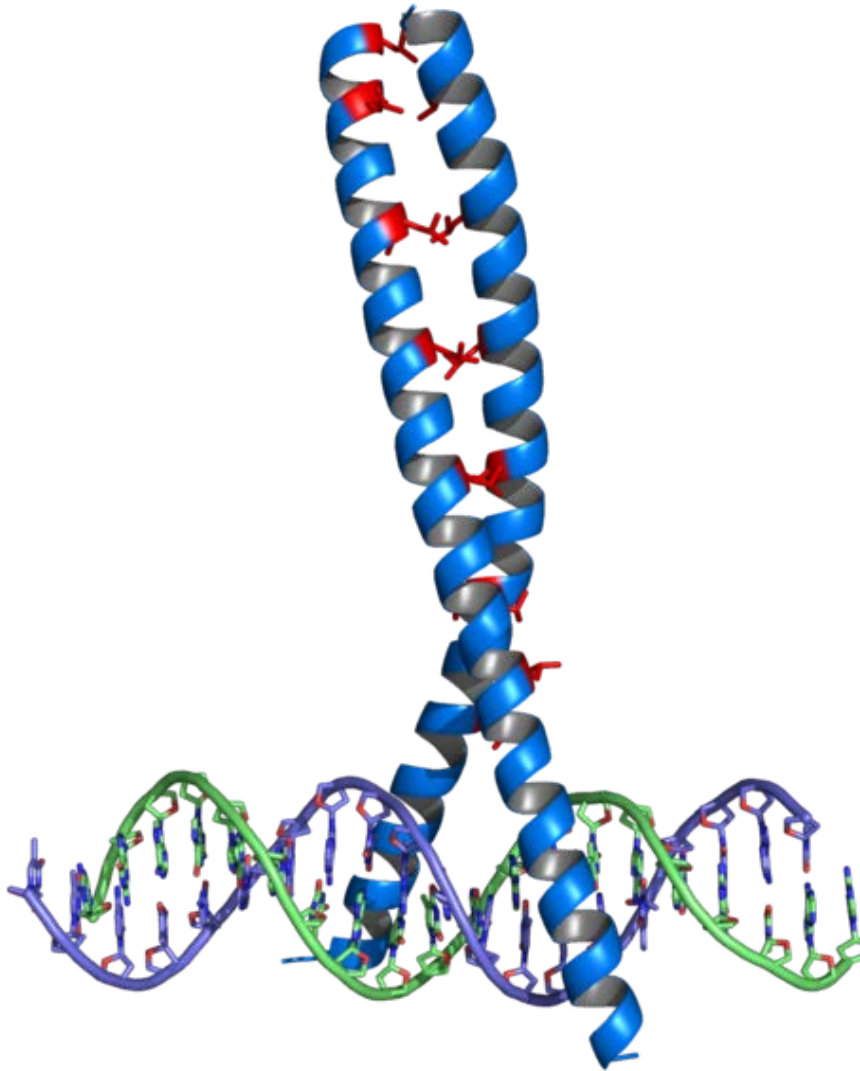
~20 AA

Zn²⁺

2 Cys

2 His

Лейциновая застёжка-молния



Leu

каждая

ВОСЬМАЯ

ПОЗИЦИЯ

Серверы для поиска доменов

InterPro

<http://www.ebi.ac.uk/interpro/>

CD (Conserved Domain) server (NCBI)

<https://www.ncbi.nlm.nih.gov/Structure/cdd/wrpsb.cgi>

Motif Scan

<https://myhits.isb-sib.ch/cgi-bin/PFSCAN>

Группы белков

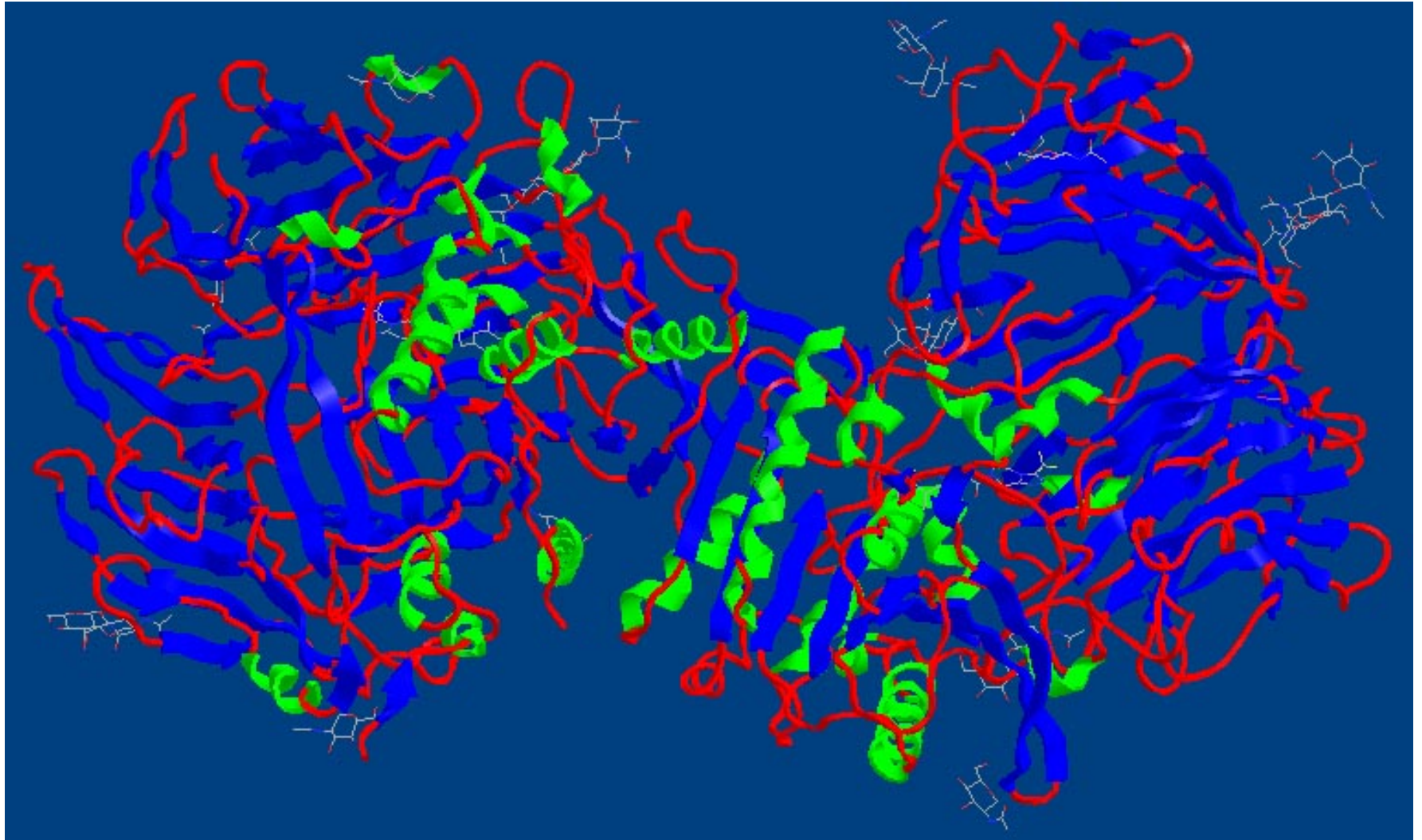
Глобулярные

Мембранные

Фибриллярные

Неупорядоченные

Глобулярный белок Дипептидилпептидаза-4



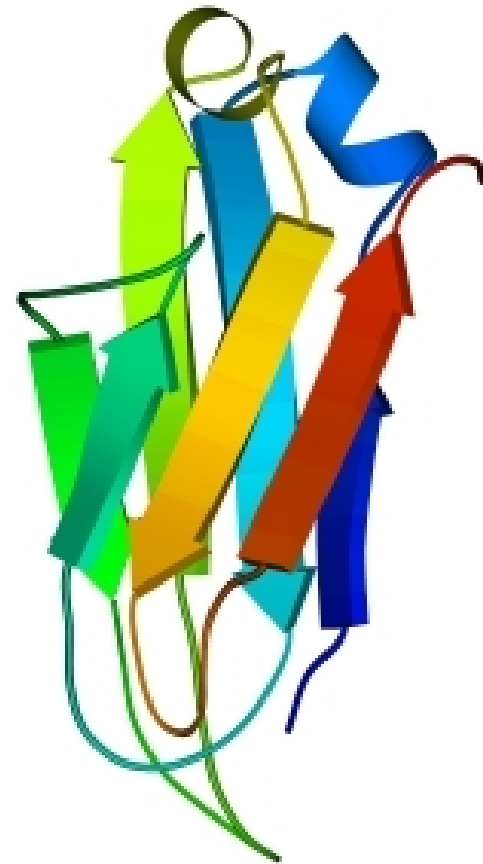
Упаковка листов

Ортогональная



Ретинол-связывающий
белок

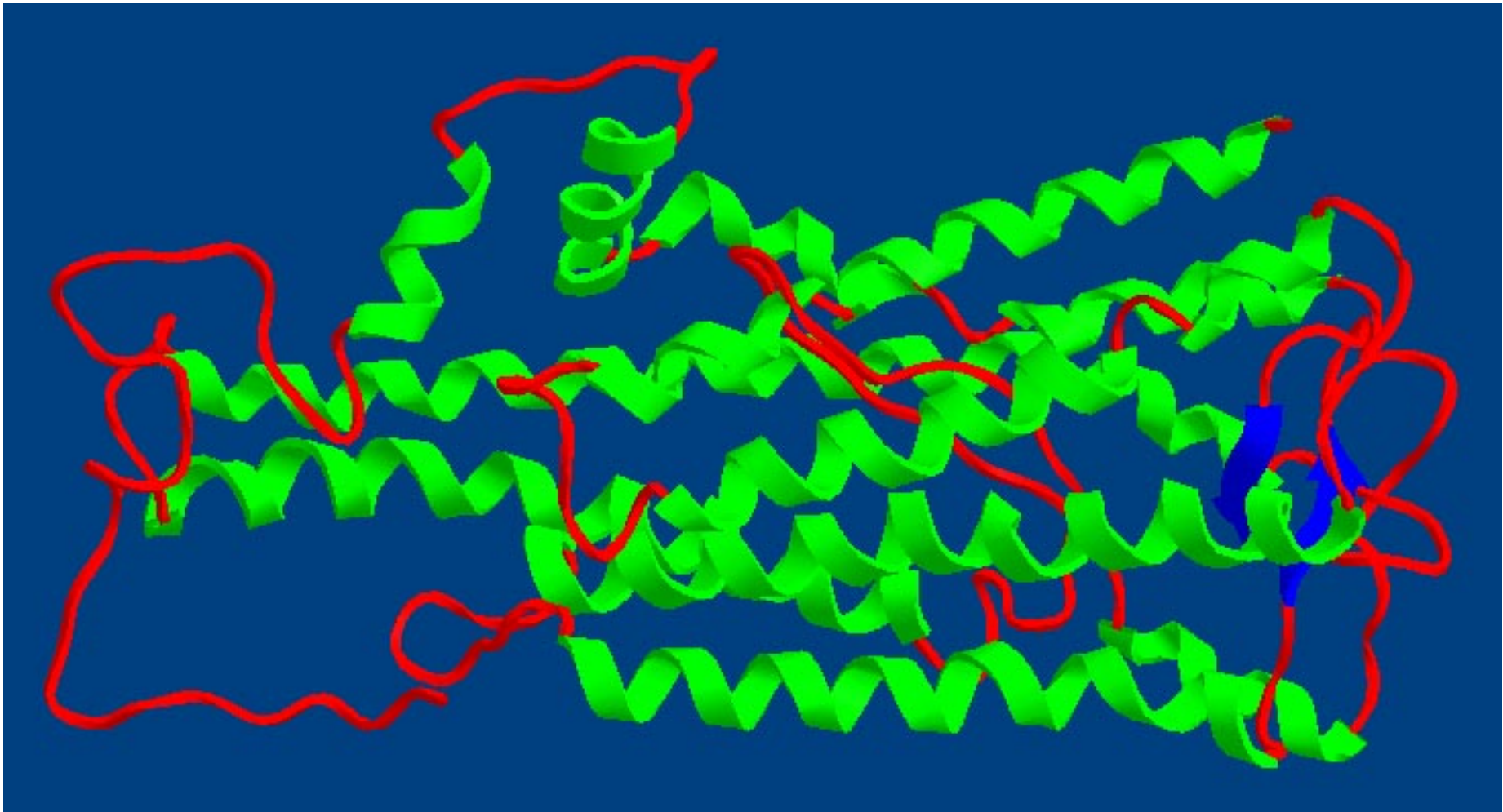
Продольная



Константный домен
гемоглобина

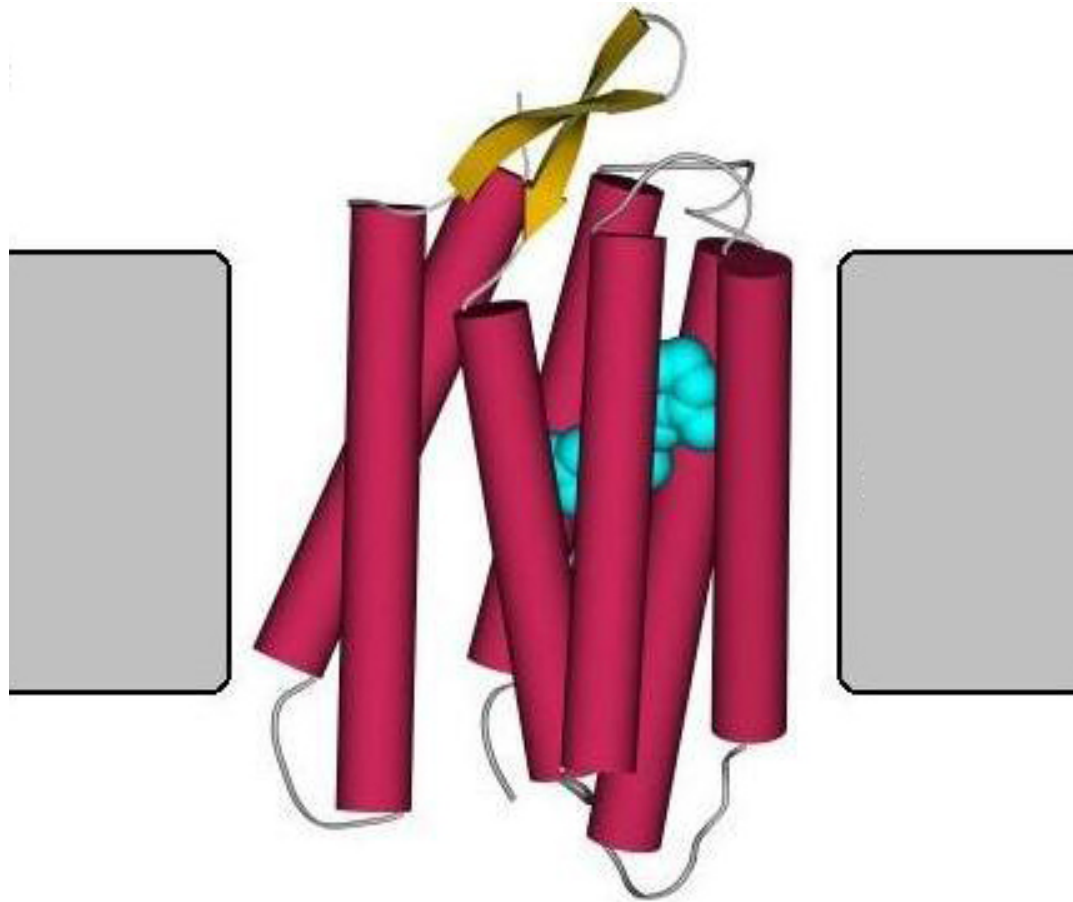
Мембранный белок

5-HT_{2a}-рецептор



Упаковка α -спиралей

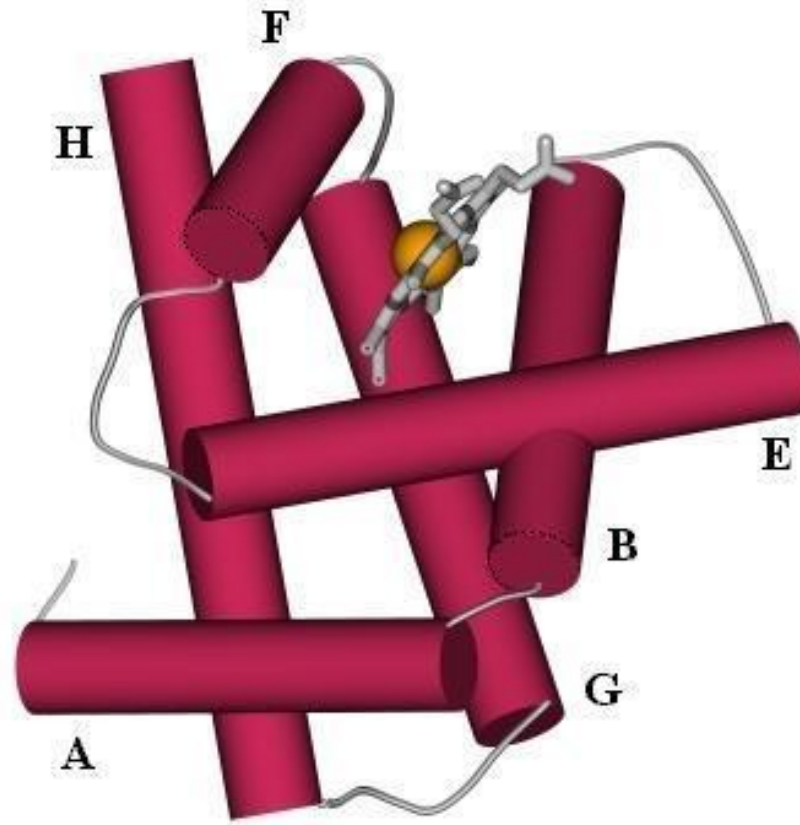
Пучок



Бактериородопсин

Упаковка α -спиралей

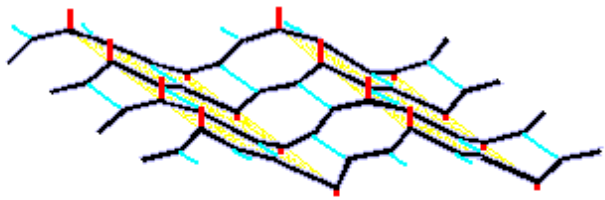
Перпендикулярные слои



Глобин

Фибриллярные белки

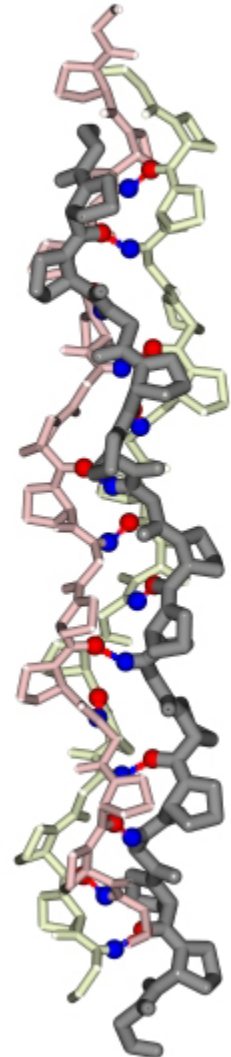
От листов к суперспиралям



Фиброин



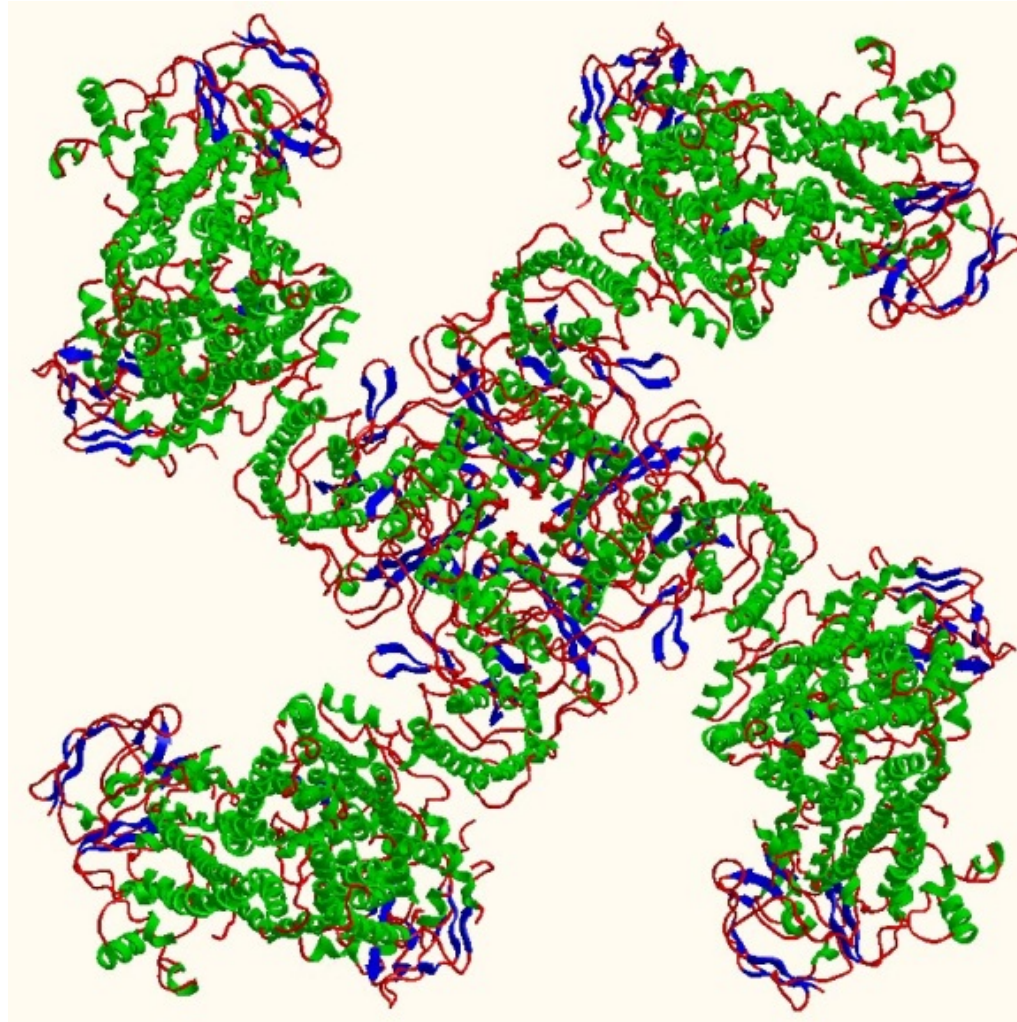
α -Кератин



Коллаген

Четвертичная структура АТФ-зависимый калиевый ионный канал

**IKATP
Kir6.2**



UniProtKB – ProtScale

Предказание трансмембранных сегментов

The screenshot displays the UniProtKB ProtScale tool interface. The browser address bar shows the URL `https://www.uniprot.org/uniprot/P28223#sequences`. The page title is "Sequences (2+)".

Display sidebar (left):

- Entry (selected)
- Publications
- Feature viewer
- Feature table

Sequences (2+) main content:

Sequence status: Complete.
This entry describes 2 isoforms produced by **alternative splicing**. [Align](#) [Add to basket](#)

This entry has 2 described isoforms and 1 potential isoform that is computationally mapped. [Show all](#) [Align All](#)

Isoform 1 (identifier: **P28223-1**) [[UniParc](#)] [FASTA](#) [Add to basket](#)

This isoform has been chosen as the canonical sequence. All positional information in this entry refers to it. This is also the sequence that appears in the downloadable versions of the entry.

« Hide

10	20	30	40	50
MDILCEENTS	LSSTTNSLMQ	LNDDTRLYSN	DFNSGEANTS	DAFNWTVDSE
60	70	80	90	100
NRTNLSCEGC	LSPSCLSLH	LQEKNSALL	TAVVIILTA	GNILVIMAVS
110	120	130	140	150
LEKRLQNTN	YFLMSLAID	MLLGFLMPV	SMLTILYGYR	WPLPSKLCV
160	170	180	190	200
WIYLDVLFST	ASIMHLCAIS	LDRYVAIQNP	IHHSRFSRST	KAPLKIIAVW
210	220	230	240	250
TISVGISMPI	PVFGQLQDDSK	VFKEGSCLLA	DDNFVLIGSF	VSFFIPLTIM
260	270	280	290	300
VITYFLTIKS	LQKEATLCVS	DLGTRAKLAS	FSFLPQSSLS	SEKLPQRSIH
310	320	330	340	350
REPGSYTRRR	TMQISISNEQK	ACKVLGIVFF	LFVVMWCPFF	ITNIMAVICK
360	370	380	390	400
ESCNEVDIGA	LLNVFVWIGY	LSSAVNPLVY	TLFNKTYRSA	FSRYIQCCYK
410	420	430	440	450
ENKRPQLLIL	VNTIPALAYK	SSQLQMGQKK	NSKQDARTD	NDCSMVALGK
460	470			
QHSEEASKDN	SDGVNEKVC	V		

Length: 471
Mass (Da): 52,603
Last modified: June 1, 1994 - v2
Checksum: EF8AAC69C5379DA2

ProtScale

Isoform 2 (identifier: **P28223-2**) [[UniParc](#)] [FASTA](#) [Add to basket](#)

The sequence of this isoform differs from the canonical sequence as follows:

1-138: MDILCEENTS...PVSMLTILYG → MQFLKSAKQK...ISCVDPEDKW

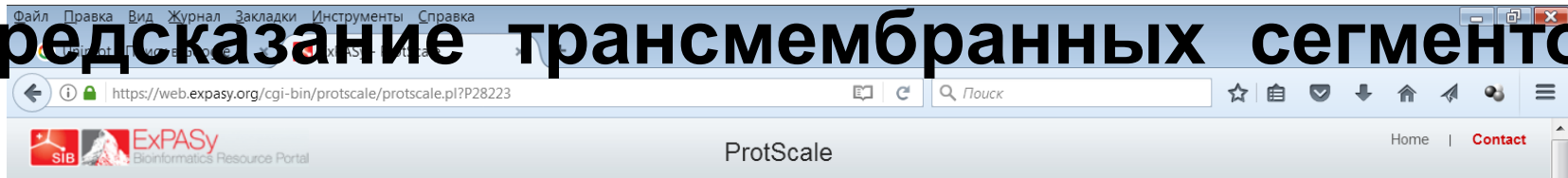
[Show >](#)

Length: 387
Mass (Da): 43,940
Checksum: DA98167A87C1AAB7

BLAST

UniProtKB – ProtScale

Предказание трансмембранных сегментов



ProtScale

ProtScale [\[Reference / Documentation\]](#) allows you to compute and represent the profile produced by any amino acid scale on a selected protein.

An **amino acid scale** is defined by a numerical value assigned to each type of amino acid. The most frequently used scales are the hydrophobicity or hydrophilicity scales and the secondary structure conformational parameters scales, but many other scales exist which are based on different chemical and physical properties of the amino acids. This program provides 57 predefined scales entered from the literature.

Enter a [UniProtKB/Swiss-Prot](#) or [UniProtKB/TrEMBL](#) accession number (AC) (e.g. P05130) or a sequence identifier (ID) (e.g. KPC1_DROME):

Or you can paste your own sequence in the box below:

```
>sp|P28223|5HT2A_HUMAN 5-hydroxytryptamine
receptor 2A OS=Homo sapiens OX=9606 GN=HTR2A PE=1
SV=2
MDILCEENTSLSSSTTNSLMQLNDDTRLYNSDFNSGEANTSDAFNWTVDSE
NRTNLSCEGC
LSPSCISLILHLOEKNSALLTAVVILITLTIAGNLIIVIMAVSLEKKIQATN
YFLMSLAIAAD
MLLGLVMPVSMILITILYGYRWLPSKLCVAWVYLDVLFSTASIMHLCAIS
LDRYVAIQNP
```

Вводим fasta белка
5-HT_{2a} Human

Please choose an amino acid scale from the following list. To display information about a scale (author, reference, amino acid scale values) you can click on its name.

- | | |
|--|---|
| <input type="radio"/> Molecular weight | <input type="radio"/> Number of codon(s) |
| <input type="radio"/> Bulkiness | <input type="radio"/> Polarity / Zimmerman |
| <input type="radio"/> Polarity / Grantham | <input type="radio"/> Refractivity |
| <input type="radio"/> Recognition factors | <input type="radio"/> Hphob. / Eisenberg et al. |
| <input type="radio"/> Hphob. OMH / Sweet et al. | <input type="radio"/> Hphob. / Hopp & Woods |
| <input checked="" type="radio"/> Hphob. / Kyte & Doolittle | <input type="radio"/> Hphob. / Manavalan et al. |
| <input type="radio"/> Hphob. / Abraham & Leo | <input type="radio"/> Hphob. / Black |
| <input type="radio"/> Hphob. / Bull & Breese | <input type="radio"/> Hphob. / Fauchere et al. |
| <input type="radio"/> Hphob. / Guy | <input type="radio"/> Hphob. / Janin |
| <input type="radio"/> Hphob. / Miyazawa et al. | <input type="radio"/> Hphob. / Rao & Argos |
| <input type="radio"/> Hphob. / Roseman | <input type="radio"/> Hphob. / Tanford |
| <input type="radio"/> Hphob. / Wolfenden et al. | <input type="radio"/> Hphob. / Welling & al |
| <input type="radio"/> Hphob. HPLC / Wilson & al | <input type="radio"/> Hphob. HPLC / Parker & al |
| <input type="radio"/> Hphob. HPLC pH3.4 / Cowan | <input type="radio"/> Hphob. HPLC pH7.5 / Cowan |
| <input type="radio"/> Hphob. / Rf mobility | <input type="radio"/> HPLC / HFBA retention |
| <input type="radio"/> HPLC / TFA retention | <input type="radio"/> Transmembrane tendency |
| <input type="radio"/> HPLC / retention pH 2.1 | <input type="radio"/> HPLC / retention pH 7.4 |
| <input type="radio"/> % buried residues | <input type="radio"/> % accessible residues |
| <input type="radio"/> Hphob. / Chothia | <input type="radio"/> Hphob. / Rose & al |

UniProtKB – ProtScale

Предказание трансмембранных сегментов

Файл Правка Вид Журнал Закладки Инструменты Справка

https://web.expasy.org/cgi-bin/protscale/protscale.pl?1

Using the scale [Hphob. / Kyte & Doolittle](#), the individual values for the 20 amino acids are:

Ala:	1.800	Arg:	-4.500	Asn:	-3.500	Asp:	-3.500	Cys:	2.500	Gln:	-3.500
Glu:	-3.500	Gly:	-0.400	His:	-3.200	Ile:	4.500	Leu:	3.800	Lys:	-3.900
Met:	1.900	Phe:	2.800	Pro:	-1.600	Ser:	-0.800	Thr:	-0.700	Trp:	-0.900
Tyr:	-1.300	Val:	4.200	:	-3.500	:	-3.500	:	-0.490		

Weights for window positions 1,...,9, using **linear weight variation model**:

1	2	3	4	5	6	7	8	9
1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
edge			center					edge

ProtScale output for user_sequence

Score

Position

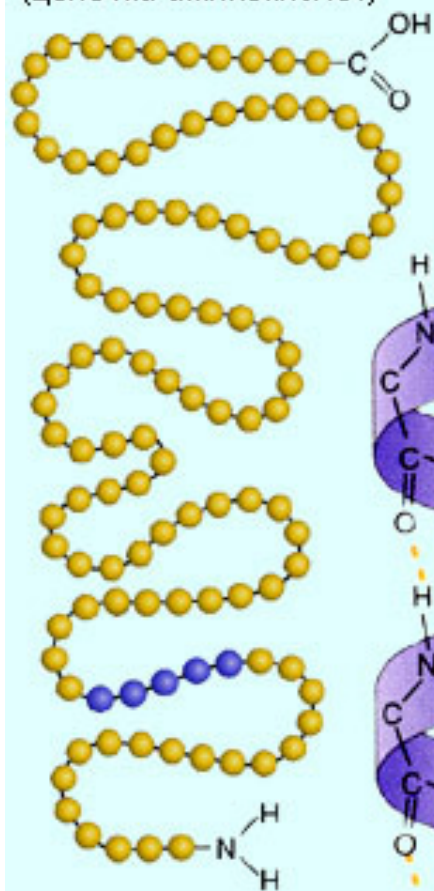
Hphob. / Kyte & Doolittle

The results of your ProtScale query are available in the following formats:

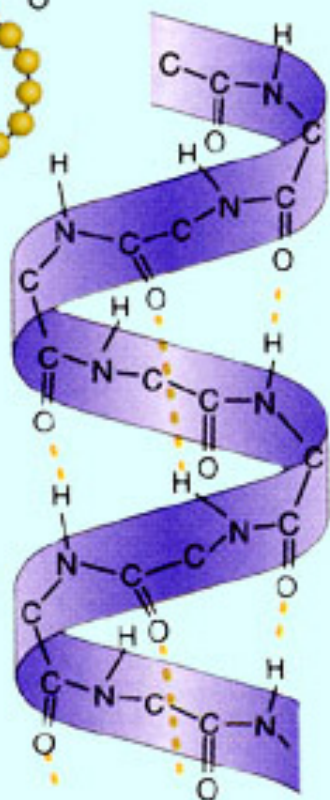
- [Image in GIF-format](#)
- [Image in Postscript-format](#)
- [Numerical format \(verbose\)](#)
- [Numerical format \(minimal, to be exported into an external application\)](#)

Фолдинг

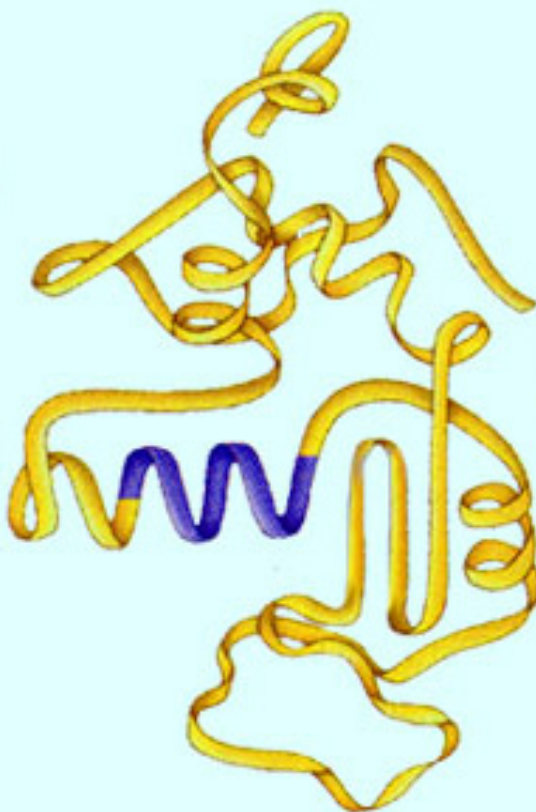
Первичная структура
(цепочка аминокислот)



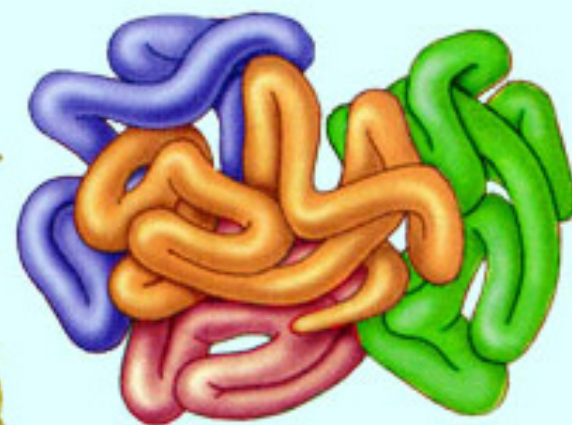
Вторичная структура
(α -спираль)



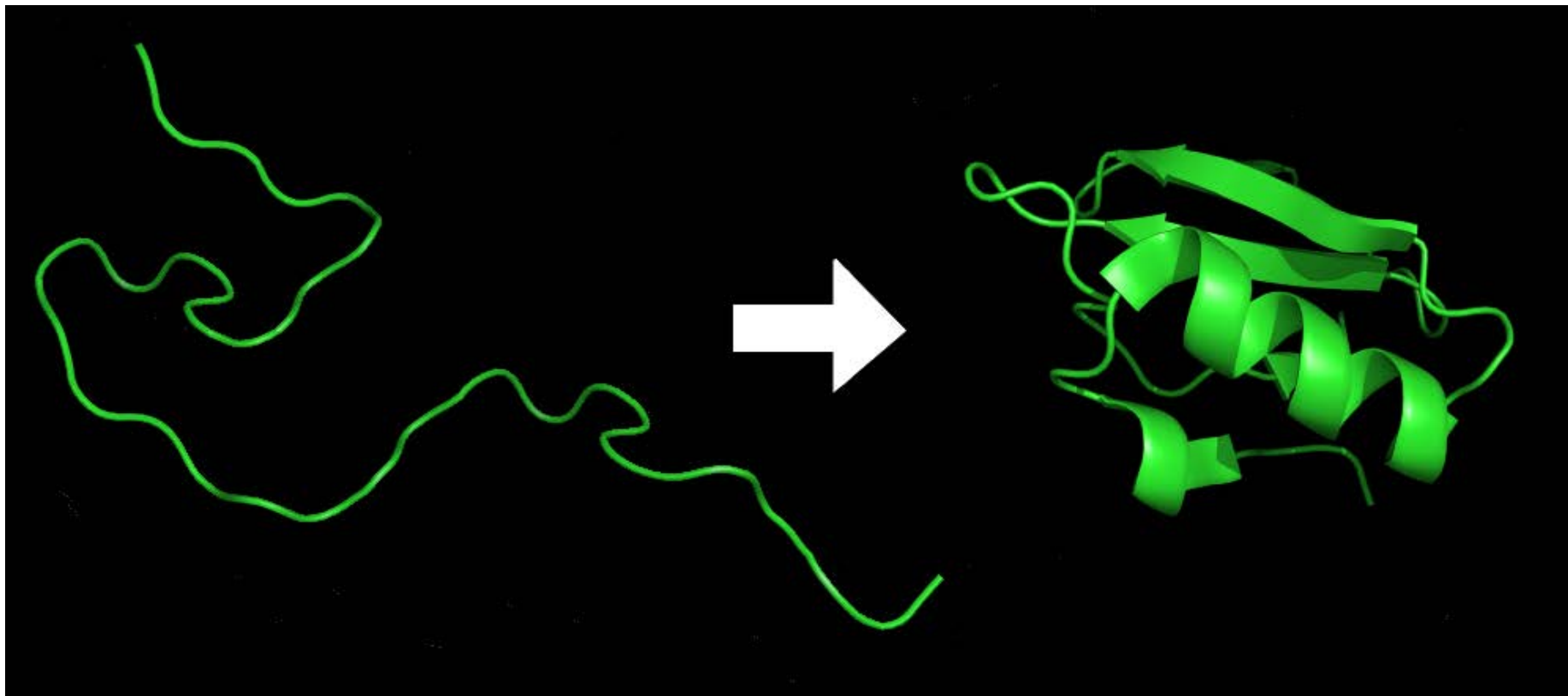
Третичная структура



Четвертичная структура
(клубок белков)

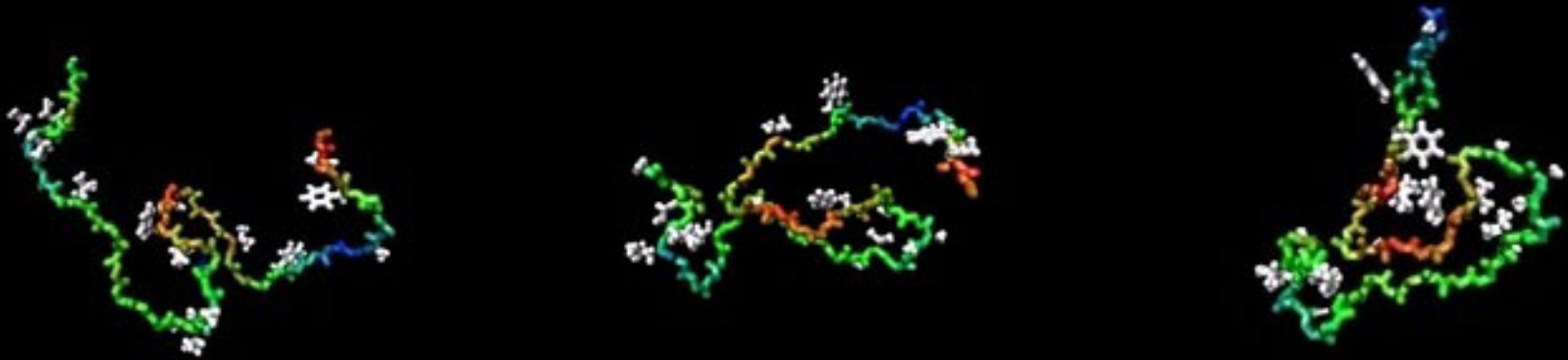


Фолдинг



Молекулярная динамика

Фолдинг



Молекулярная динамика

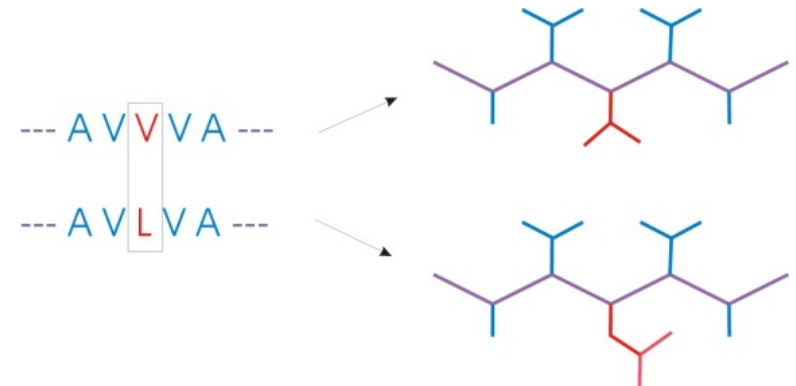
Моделирование по гомологии

Выравнивание:

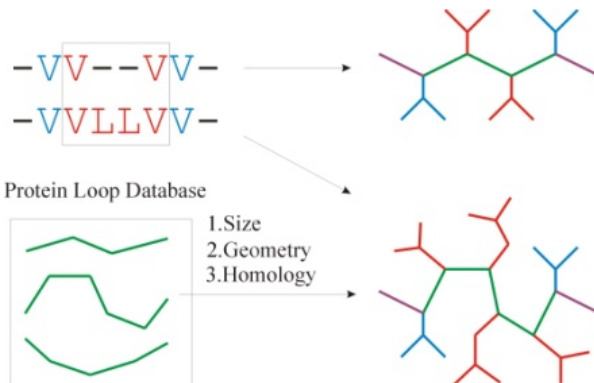
```

AMPA 392 NK--TVVVTTILESPYVMMK-----KNHEMLE-----GNER---
NR2B 403 DD---HLSIVTLEEAPFVIVESVDPL--SGTCMRNTVPCQ-KRIV---TENKTDEEPGYI
NR1 392 YQMSTRLKIVTIHQEPFVYVKPTLSDGTCKEEFTVNGDPVKKVICTGPNDTSPGSPR-HTV
AMPA 420 ---YEGYCVDLAAEIAKHCGFKYKLTIVGDGKYGARDADT---KIWNGMVGELVYGKADI
NR2B 454 KKCKGFGCIDILKKISKSVKFTYDLYLVNKGKHGKING-----TWNGMIGEVVMKRAYM
NR1 451 PQCCYGFCDILLIKLARTMNFYEVHLVADGKFGTQERVNNSNKKEWNGMMGELLGQADM
AMPA 473 AIAPLTITLVREEVIDFSKPFMSLGISIMIKG--[-]T-PIESAEDLSKQT-----EIA
NR2B 508 AVGSLTINEERSEVDFSVPFIEI GISVMVSRNSG[-]VDQVSGLSDKKFORPNDFSPPFR
NR1 511 IVAPLTINNERAQYIEFSKPFKYQGLTILVKKEIP[-]EERITGINDPRLRNPSD---KFI
AMPA 631 YGTLD SGSTKEFFRRSKIAVFDKMWTYMRSAPSVFVRTTAEGVARVRKSKGKYALLEST
NR2B 660 FGTVPNGSTERNIRNN---YAEMHAYMGKFNQ---RGVDDALLSLKTGK-LDAFIYDAA
NR1 661 YATVKQSSVDIYFRRQ--VELSTMYRHMEKHNY---ESAAEAIQAVRDNK-LHAFIWDSA
AMPA 692 MNEYIEQRKP-CDTMKVG-G-NLDSKGYGIATPKGSSLGNVNLAVLKLNEQGLLDKLKNK
NR2B 712 VLNYMAGRDEGCKLVIGSGKVFASTGYGIAIQKDSGWKRQVDLAILQLFGDGEMEELEAL
NR1 713 VLEFEASQK--CDLVTTG--ELFFRSFGFGRKDSPWKQNVLSILKSHENGFMEDLDKT
    
```

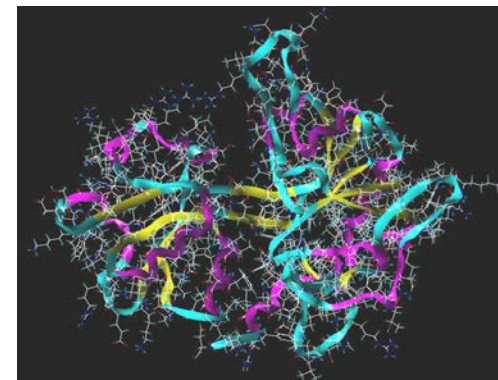
Мутации



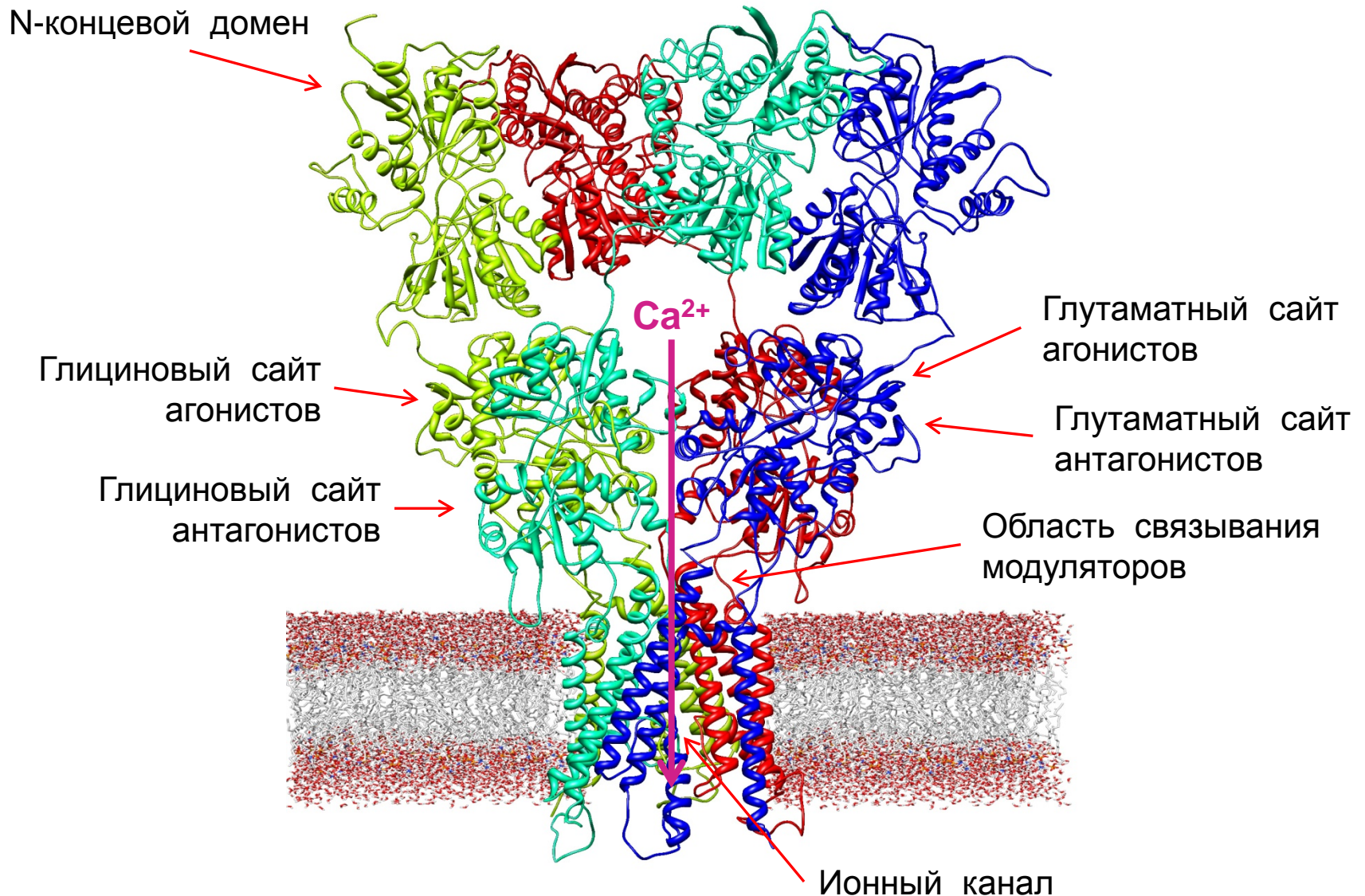
Добавление петель



Оптимизация



Модель NMDA-рецептора



Теоретические 3D-модели белков

ModBase

<https://modbase.compbio.ucsf.edu/>

База данных ModBase



Файл Правка Вид Журнал Закладки Инструменты Справка

Modbase - Google Search x ModBase Search Page x +

https://modbase.compbio.ucsf.edu/modbase-cgi/index.cgi 90% Поиск

Часто посещаемые

University of California San Francisco | About UCSF | UCSF Benioff Children's Hospital San Francisco

**ModBase: Database of Comparative Protein Structure Models**

[Sali Lab Home](#) [ModWeb](#) [ModLoop](#) [ModBase](#) [ModEval](#) [PCSS](#) [FoXS](#) [IMP](#) [ModPipe](#)

[ModBase Home](#) [ModBase Datasets for User/Anonymous](#) [User Login](#) [Help](#) [News](#) [Contact](#) [Current Datasets](#)

- [General Information](#)
- [Statistics and Genome Datasets](#)
- [News](#)
- [Project Pages](#)
- [Authors and Acknowledgements](#)
- [Publications](#)
- [Downloads](#)
- [Related Resources](#)

Please address inquiries to: modbase@sallab.org

MODBASE contains theoretically calculated models, not experimentally determined structures. The models may contain **significant** errors.

ModBase Search

ModBase is a database of comparative protein structure models, calculated by our modeling pipeline [ModPipe](#).

Search type Display type

All available datasets are selected

Search by properties

Property

Organism or

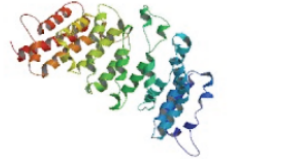
[Advanced search](#)

Model Details Example

Database ID: Q12321
This page makes all models and model details for one sequence available.

Sequence Model Coverage Summary for all Models of this Sequence

All Models



- The current model is shown prominently
- Additional models are accessible through their thumbnails.
- Use the **Perform action** pull-down menu for

Overview Example

[Denque Virus](#)
Models for several sequences are displayed on the **Sequence Overview** page.

<input type="checkbox"/>	1S9024817	nonstructural protein ns4a [denque virus 2]
<input type="checkbox"/>	1S9024814	nonstructural protein ns2a [denque virus 2]
<input type="checkbox"/>	1S9024816	nonstructural protein ns3 [denque virus 2]
<input type="checkbox"/>		ns4b
<input type="checkbox"/>	1S9024810	membrane glycoprotein precursor [denque virus 2]
<input type="checkbox"/>	1S9024815	nonstructural protein ns2b [denque virus 2]
<input type="checkbox"/>	Q04040	subname: full=nonstructural protein 1;flag: fragment;
<input type="checkbox"/>	1S9024811	membrane glycoprotein [denque virus 2]
<input type="checkbox"/>	1S9024820	nonstructural protein ns5 [denque virus 2]
<input type="checkbox"/>	1S9024808	anchored capsid protein [denque virus 2]
<input type="checkbox"/>		ns2b/3
<input type="checkbox"/>	1S9024812	envelope protein [denque virus 2]

- A coverage sketch illustrates sequence section(s) covered by a model
- The sketch also links to the **Model Details** page.

UniProtKB

UniProtKB - P28223 (5HT2A_HUMAN)

Display | BLAST | Align | Format | Add to basket | History | Feedback | Help video | Other tutorials and videos

Entry | Publications | Feature viewer | Feature table

Protein | 5-hydroxytryptamine receptor 2A
Gene | HTR2A
Organism | *Homo sapiens (Human)*
Status | Reviewed - Annotation score: ●●●●● - Experimental evidence at protein levelⁱ

Functionⁱ

G-protein coupled receptor for 5-hydroxytryptamine (serotonin) (PubMed:1330647, PubMed:18703043, PubMed:19057895). Also functions as a receptor for various drugs and psychoactive substances, including mescaline, psilocybin, 1-(2,5-dimethoxy-4-iodophenyl)-2-aminopropane (DOI) and lysergic acid diethylamide (LSD) (PubMed:28129538). Ligand binding causes a conformation change that triggers signaling via guanine nucleotide-binding proteins (G proteins) and modulates the activity of down-stream effectors (PubMed:28129538). Beta-arrestin family members inhibit signaling via G proteins and mediate activation of alternative signaling pathways (PubMed:28129538). Signaling activates phospholipase C and a phosphatidylinositol-calcium second messenger system that modulates the activity of phosphatidylinositol 3-kinase and promotes the release of Ca²⁺ ions from intracellular stores (PubMed:18703043, PubMed:28129538). Affects neural activity, perception, cognition and mood (PubMed:18297054). Plays a role in the regulation of behavior, including responses to anxiogenic situations and psychoactive substances. Plays a role in intestinal smooth muscle contraction, and may play a role in arterial vasoconstriction. [7 Publications](#)

(Microbial infection) Acts as a receptor for human JC polyomavirus/JCPyV. [1 Publication](#)

Miscellaneous

Binds lysergic acid diethylamine (LSD) in the orthosteric pocket (Probable). Binds LSD and associates extremely slowly, with a residence time of about 221 minutes at 37 degrees Celsius. [1 Publication](#)

Sites

Feature key	Position(s)	Description	Actions	Graphical view	Length
Site ⁱ	229	Hydrophobic barrier that decreases the speed of ligand binding and dissociation 1 Publication			1

Structure

5-HT2a Human

UniProtKB

Файл Правка Вид Журнал Закладки Инструменты Справка

uniport - Поиск в Google x HTR2A - 5-hydroxytryptam... x ModBase Search Page x +

https://www.uniprot.org/uniprot/P28223#structure

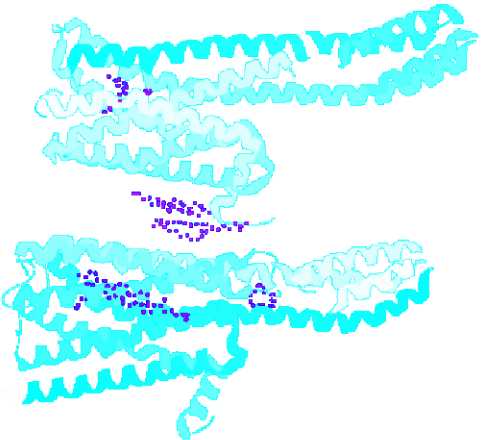
Display

- Entry
- Publications
- Feature viewer
- Feature table

None

- Function
- Names & Taxonomy
- Subcellular location
- Pathology & Biotech
- PTM / Processing
- Expression
- Interaction
- Structure
- Family & Domains
- Sequences (2+)
- Similar proteins
- Cross-references
- Entry information
- Miscellaneous

Structure



PDB Entry	Method	Resolution	Chain	Positions	Links
6A93	X-ray	3.00 Å	A/B A/B	70-265 313-403	PDBe RCSB PDB PDBj PDBsum
6A94	X-ray	2.90 Å	A/B A/B	70-265 313-403	PDBe RCSB PDB PDBj PDBsum

Secondary structure

1

Legend: ■ Helix ■ Turn ■ Beta strand ■ PDB Structure known for this area

[Show more details](#)

3D structure databases

EMBL	P28223
ModBase	Search...
PDBe-KB	Search...

Family & Domains

Region

Feature key	Position(s)	Description	Accession	Initial view	Length
Region	155 - 160	Agonist binding By similarity			6
Region	336 - 340	Agonist binding By similarity			5

5-HT2a Human

ModBase

5-HT2a Human

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ModBase: Database of Comparative Protein Structure Models

Sali Lab Home ModWeb ModLoop ModBase ModEval PCSS FoXS IMP ModPipe

ModBase Home ModBase Datasets for User Anonymous User Login Help News Contact Current Datasets

Model Details Page

Sequence Information

- Primary Database Link [P28223.2](#)
- Original Database ID sp P28223
- Organism [Gorilla gorilla gorilla, Homo sapiens](#)
- Annotation 5ht2a_human recname: full=5-hydroxytryptamine receptor 2a; short=5-ht-2; short=5-ht-2a; alname: full=serotonin receptor 2a
- Sequence Length 471

Model Information

Perform action on this model
select option

Quality criteria indicate whether the model is considered reliable (green) or unreliable (red).

<input checked="" type="checkbox"/> Target Region	72-400
<input checked="" type="checkbox"/> Protein Length	471
<input checked="" type="checkbox"/> Template PDB Code	4ib4A
<input checked="" type="checkbox"/> Template Region	52-400
<input checked="" type="checkbox"/> Sequence Identity	52.00%
<input checked="" type="checkbox"/> E-Value	0
<input checked="" type="checkbox"/> GA341	1.00
<input checked="" type="checkbox"/> MPQS	1.22211
<input checked="" type="checkbox"/> z-DOPE	-0.4
<input checked="" type="checkbox"/> TSVM Method	MSALL
<input checked="" type="checkbox"/> TSVM RMSD	11.043
<input checked="" type="checkbox"/> TSVM NO35	0.197
<input checked="" type="checkbox"/> Dataset	MW-ModWeb20170312_D8
<input checked="" type="checkbox"/> ModPipe Version	SVN.r1602
<input checked="" type="checkbox"/> Model Date	2017-03-15

Dataset Information:


The newest dataset for this sequence was created on 2017-03-15. If you think that a better template has been added to the template database since, you can [start a new calculation](#).


The calculation typically takes 1-2 days, and the results will be added to this page. Registered users will receive an email notification.

Information for additional models of this sequences are available by clicking on the model [thumbnails](#) below.


Mouse over the images for more information

Sequence Model Coverage Summary for all Models of this Sequence

 All Models Current



Filtered models for current sequence [Show all models](#)



Cross-references

ModBase

5-HT2a Human

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ModBase: Database of Comparative Protein Structure Models

Sali Lab Home ModWeb ModLoop ModBase ModEval PCSS FoXS IMP ModPipe

ModBase Home ModBase Datasets for User Anonymous User Login Help News Contact Current Datasets

Model Details Page

Sequence Information

- Primary Database Link [P28223.2](#)
- Original Database ID [sp P28223](#)
- Organism [Gorilla gorilla gorilla, Homo sapiens](#)
- Annotation 5ht2a_human recname: full=5-hydroxytryptamine receptor 2a; short=5-ht-2; short=5-ht-2a; alname: full=serotonin receptor 2a
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Model Information


Perform action on this model


Quality criteria indicate whether the model is considered **reliable (green)** or **unreliable (red)**.

<input checked="" type="checkbox"/> Target Region	72-400
<input checked="" type="checkbox"/> Protein Length	471
<input checked="" type="checkbox"/> Template PDB Code	4ib4A
<input checked="" type="checkbox"/> Template Region	52-400
<input checked="" type="checkbox"/> Sequence Identity	52.00%
<input checked="" type="checkbox"/> E-Value	0
<input checked="" type="checkbox"/> GA341	1.00
<input checked="" type="checkbox"/> MPQS	1.22211
<input checked="" type="checkbox"/> z-DOPE	-0.4
<input checked="" type="checkbox"/> TSVM Method	MSALL
<input checked="" type="checkbox"/> TSVM RMSD	11.043
<input checked="" type="checkbox"/> TSVM NO35	0.197
<input checked="" type="checkbox"/> Dataset	MW-ModWeb20170312_D8
<input checked="" type="checkbox"/> ModPipe Version	SVN.r1602
<input checked="" type="checkbox"/> Model Date	2017-03-15


Mouse over the images for more information

Sequence Model Coverage Summary for all Models of this Sequence

 All Models Current



Filtered models for current sequence [Show all models](#)



Cross-references

ModBase

5-HT2a Human

Файл Правка Вид Журнал Закладки Инструменты Справка

Modbase: Google... ModBase: Search Results x +

https://modbase.com/comp/ucsf/modbase.cgi/models/details.cgi?query=5... 120% Поиск

Часто посещаемые

Model Information


Perform action on this model :
Select option

Quality criteria indicate whether the model is considered **reliable (green)** or **unreliable (red)**.

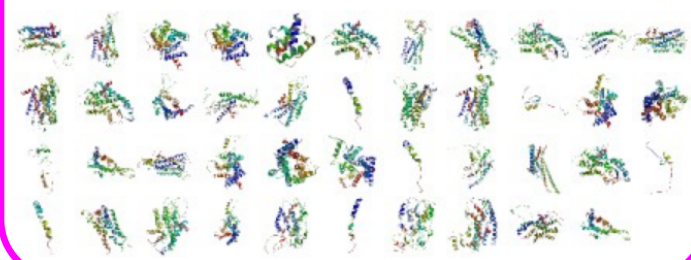
Target Region	72-400
Protein Length	471
Template PDB Code	4ib4A
Template Region	52-400
Sequence Identity	52.00%
E-Value	0
GA341	1.00
MPQS	1.22211
z-DOPE	-0.4
TSVMOD Method	MSALL
TSVMOD RMSD	11.043
TSVMOD NO35	0.197
Dataset	MW-ModWeb20170312_D8
ModPipe Version	SVN.r1602
Model Date	2017-03-15

Mouse over the images for more information

Sequence Model Coverage Summary for all Models of this Sequence .



All models for current sequence (Show filtered models only)



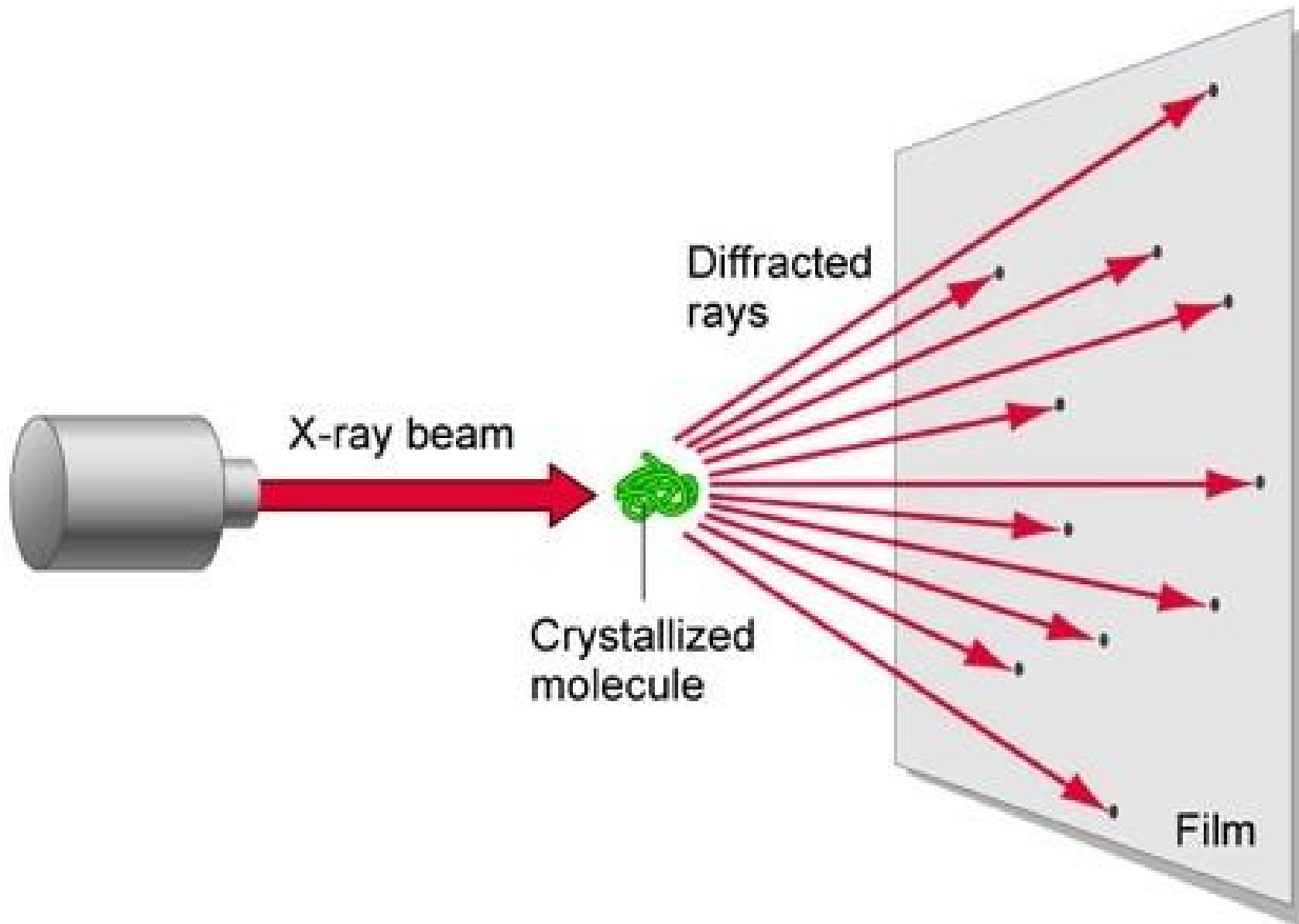
Cross-references

Mutation Data
PharmGKB

PharmGKB data available for 5HT2A

**Методы
экспериментального
определения
пространственной
структуры белков**

Рентгеноструктурный анализ



Рентгеноструктурный анализ



получение кристалла



получение дифракционной картины



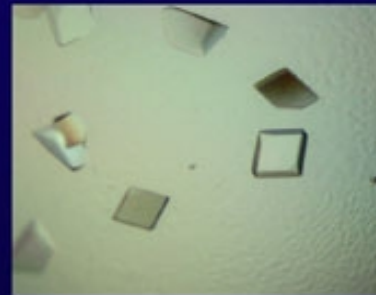
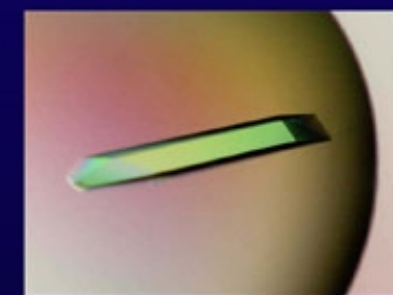
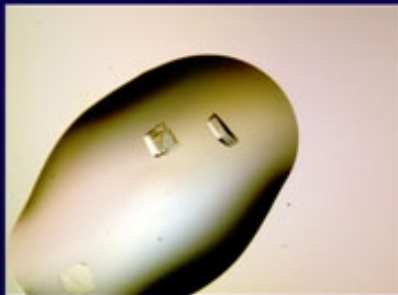
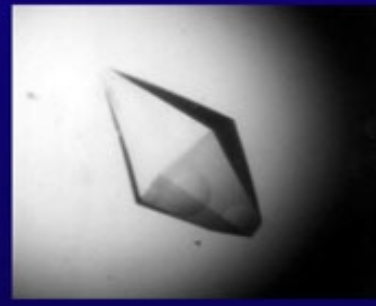
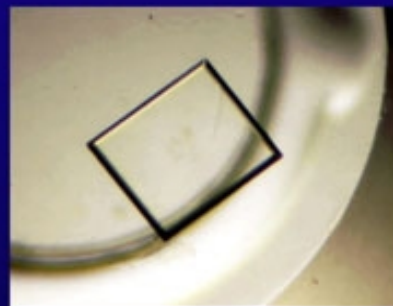
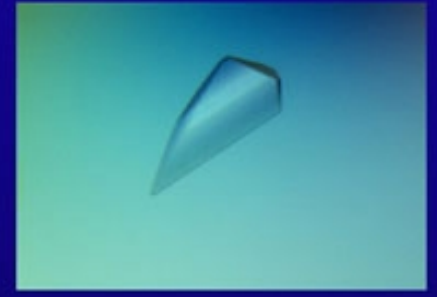
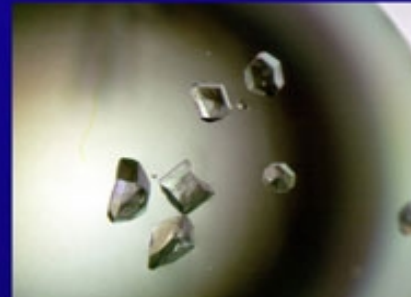
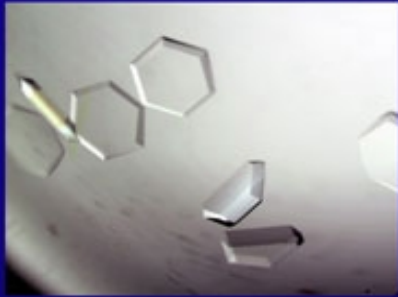
расчет распределения
электронной плотности



определение атомарной
модели

Рентгеноструктурный анализ

Кристаллы белков



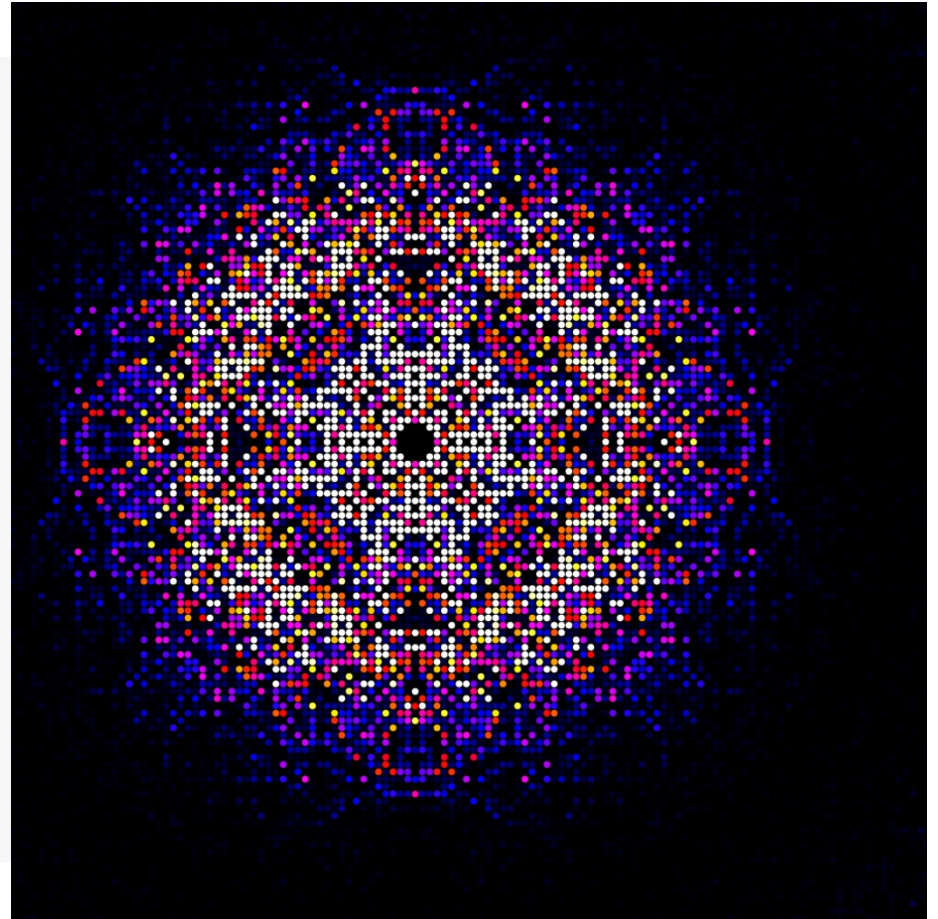
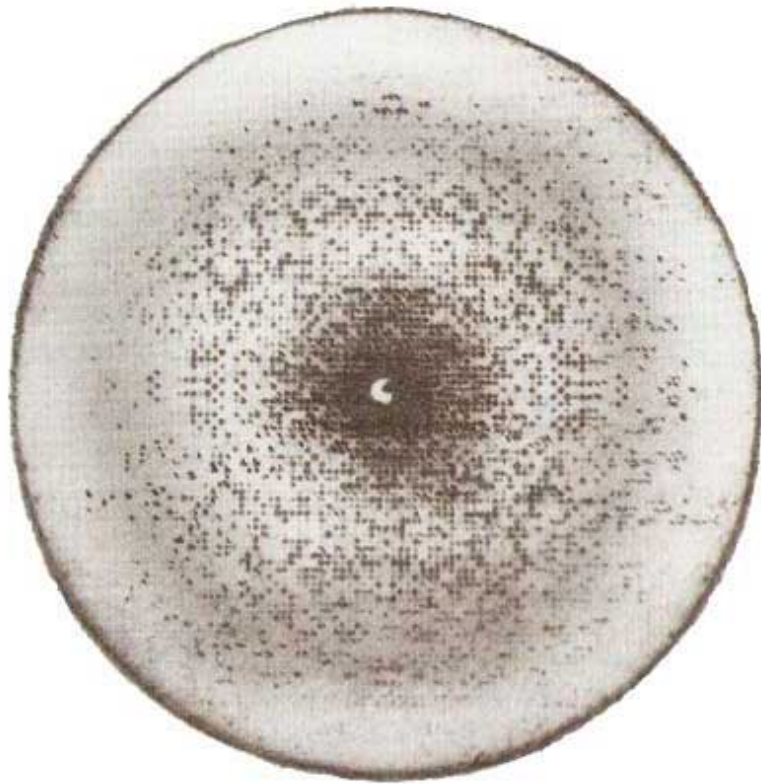
Рентгеноструктурный анализ

Диффракция и интерференция

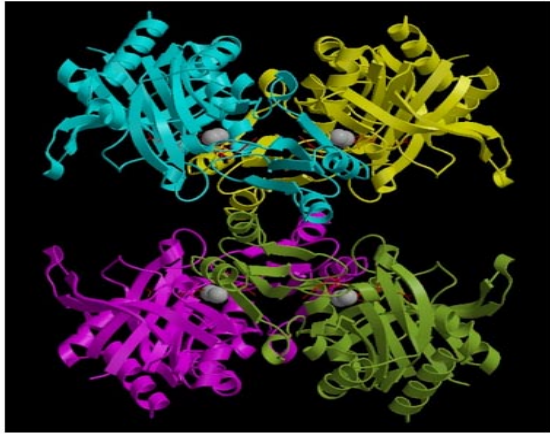


Рентгеноструктурный анализ

Диффракционная картина



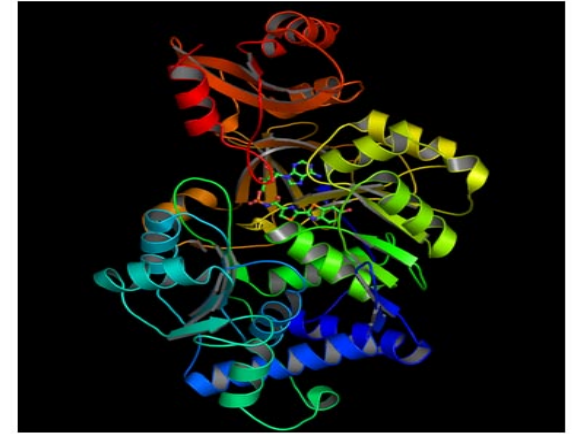
Рентгеноструктурный анализ 3D-модели белков



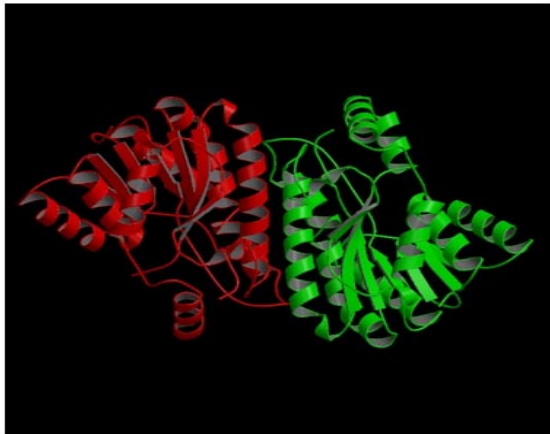
Glutathione Synthetase



Asparagine Synthetase



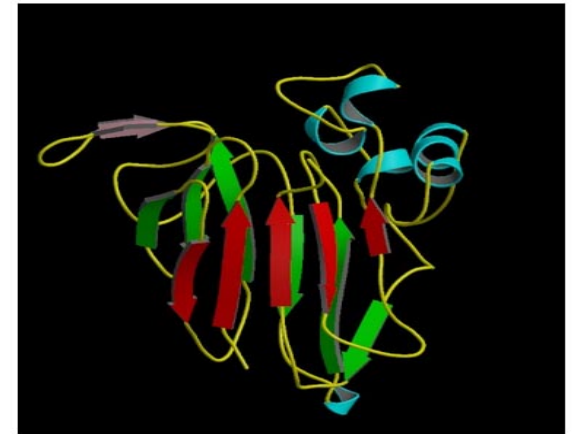
Luciferase



Tropinone Reductase I



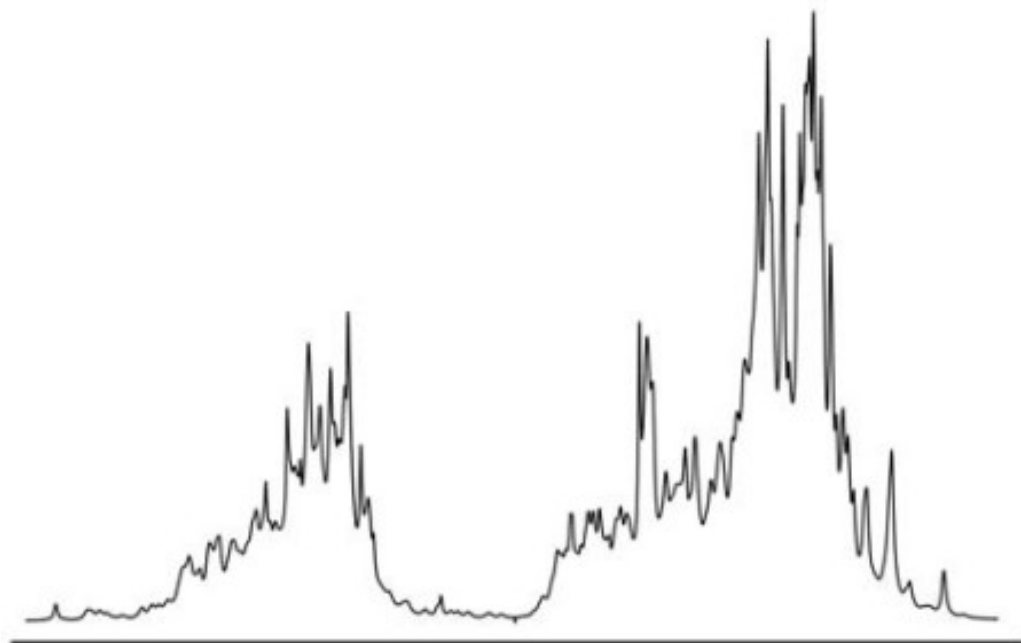
Tropinone Reductase II



PR-5d

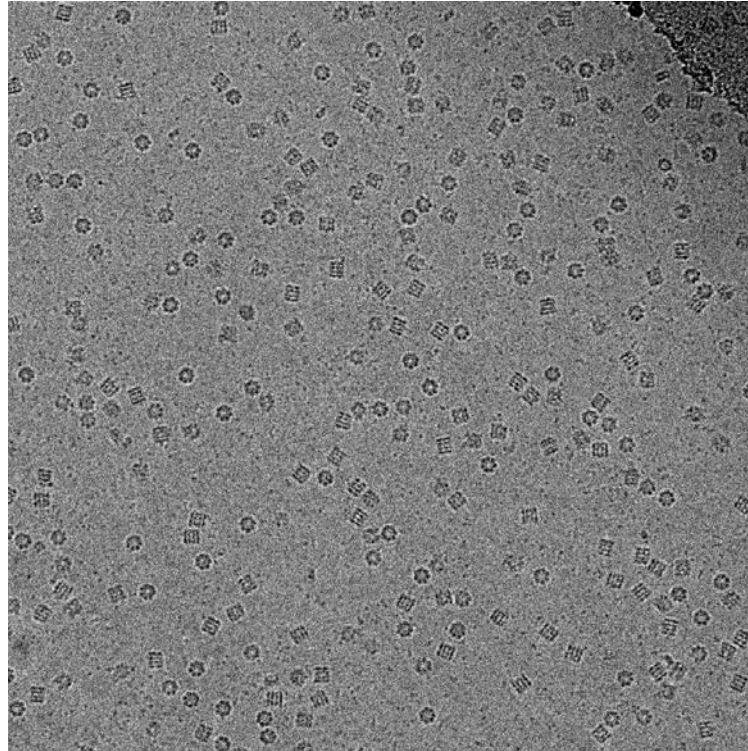
Импульсный 2D-ЯМР

Нобелевская премия по химии 2002



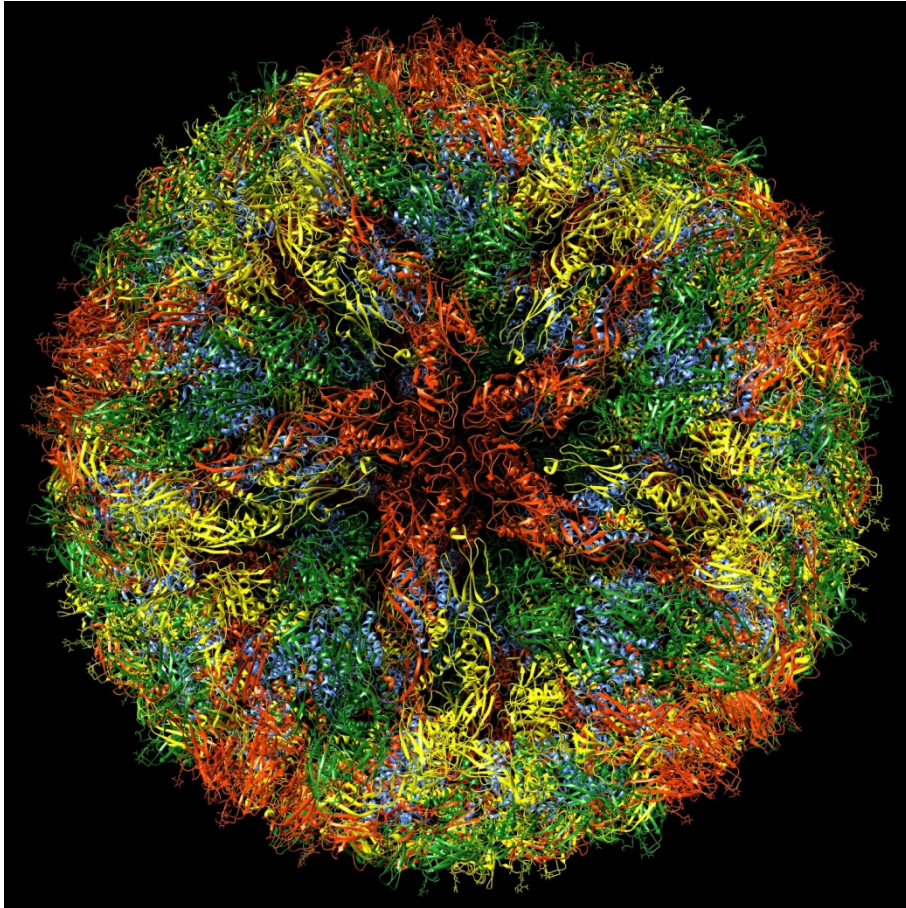
Криоэлектронная микроскопия

Нобелевская премия по химии 2017

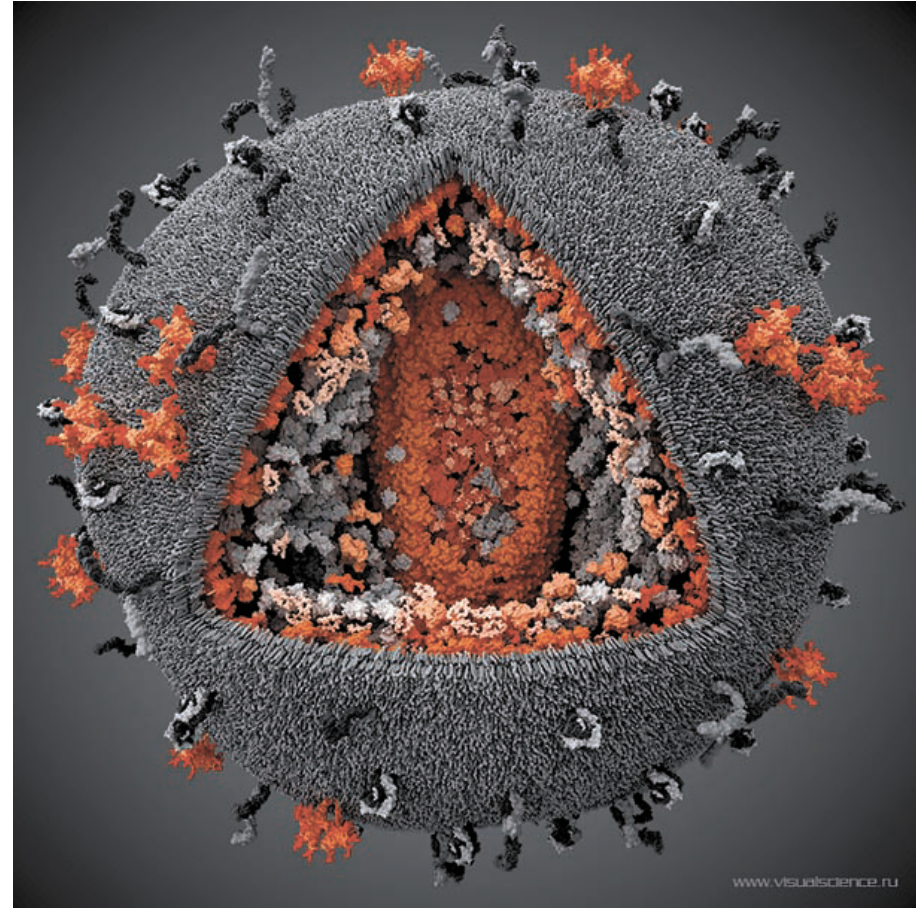


Замороженный раствор белка ~100 нм
Множество электронных фотографий
Компьютерная обработка

Криоэлектронная микроскопия



Зика



ВИЧ

Экспериментальные 3D-модели белков

PDB

Protein Data Bank

<https://www.rcsb.org/>

RCSB PDB

Файл Правка Вид Журнал Закладки Инструменты Справка

RCSB PDB - Поиск в Google x RCSB PDB: Homepage x +

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RCSB PDB 160796 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

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A Structural View of Biology

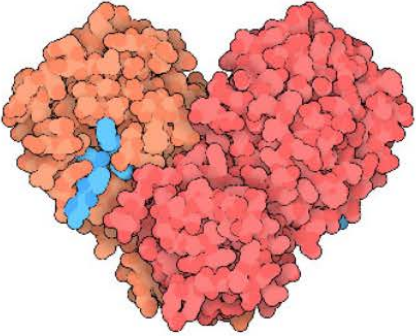
This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.



February Molecule of the Month

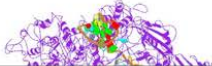


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As of Tuesday Feb 18 2020




Features & Highlights

WORLDWIDE PDB Improve Your Coordinates, Keep Your ID (Phase II)
PDB versioning, which enables

News

Publications ▾



Education Corner: Using PDB in the College Classroom

RCSB PDB

Cav1.1 — Кальциевый ионный канал L-типа



137043 Biological
Macromolecular Structures
Enabling Breakthroughs in
Research and Education

Search by PDB ID, author, macromolecule, sequence, or ligands

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Structure Summary

3D View

Annotations

Sequence

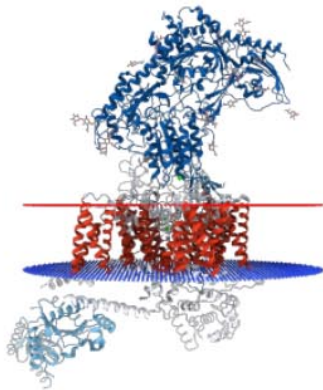
Sequence Similarity

Structure Similarity

Experiment

Transmembrane View

transmembrane regions **OPM**



5GJV

Structure of the mammalian voltage-gated calcium channel Cav1.1 complex at near atomic resolution

DOI: [10.2210/pdb5GJV/pdb](https://doi.org/10.2210/pdb5GJV/pdb) EMDatabank: [EMD-9513](https://www.ebi.ac.uk/emdb/EMD-9513)

Classification: [MEMBRANE PROTEIN](#)

Organism(s): [Oryctolagus cuniculus](#)

Expression System: [Escherichia coli](#)

Mutation(s): 1

Deposited: 2016-07-02 Released: 2016-09-14

Deposition Author(s): [Wu, J.P.](#), [Yan, Z.](#), [Li, Z.Q.](#), [Zhou, Q.](#), [Yan, N.](#)

Funding Organization(s): the Ministry of Science and Technology of China; National Natural Science Foundation of China

Display Files

Download Files

Experimental Data Snapshot

Method: ELECTRON MICROSCOPY

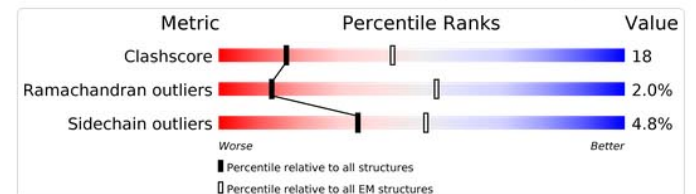
Resolution: 3.6 Å

Aggregation State: PARTICLE

Reconstruction Method: SINGLE PARTICLE

wwPDB Validation

[3D Report](#) [Full Report](#)



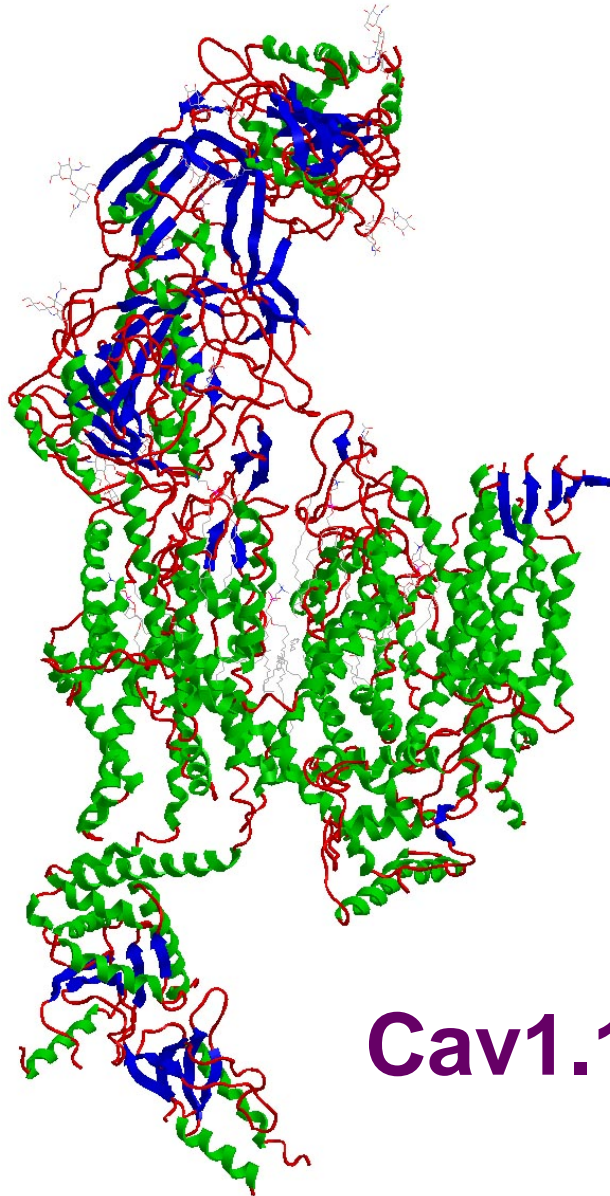
3D View: [Structure](#)

Заголовок PDB-файла

```
HEADER      MEMBRANE PROTEIN                      02-JUL-16  5GJU
TITLE      STRUCTURE OF THE MAMMALIAN VOLTAGE-GATED CALCIUM CHANNEL CAU1.1
TITLE      2 COMPLEX AT NEAR ATOMIC RESOLUTION
COMPND     MOL_ID: 1;
COMPND     2 MOLECULE: VOLTAGE-DEPENDENT L-TYPE CALCIUM CHANNEL SUBUNIT ALPHA-1S;
COMPND     3 CHAIN: A;
COMPND     4 SYNONYM: CALCIUM CHANNEL,L TYPE,ALPHA-1 POLYPEPTIDE,ISOFORM 3,
COMPND     5 SKELETAL MUSCLE,VOLTAGE-GATED CALCIUM CHANNEL SUBUNIT ALPHA CAU1.1;
COMPND     6 MOL_ID: 2;
COMPND     7 MOLECULE: VOLTAGE-DEPENDENT L-TYPE CALCIUM CHANNEL SUBUNIT BETA-1;
COMPND     8 CHAIN: B;
COMPND     9 FRAGMENT: UNP RESIDUES 80-174;
COMPND    10 SYNONYM: CAB1,CALCIUM CHANNEL VOLTAGE-DEPENDENT SUBUNIT BETA 1;
COMPND    11 ENGINEERED: YES;
COMPND    12 OTHER_DETAILS: THIS DOMAIN WAS DOCKED BY A CRYSTAL STRUCTURE (4DEY);
COMPND    13 MOL_ID: 3;
COMPND    14 MOLECULE: VOLTAGE-DEPENDENT L-TYPE CALCIUM CHANNEL SUBUNIT BETA-1;
COMPND    15 CHAIN: C;
COMPND    16 FRAGMENT: UNP RESIDUES 265-463;
COMPND    17 SYNONYM: CAB1,CALCIUM CHANNEL VOLTAGE-DEPENDENT SUBUNIT BETA 1;
COMPND    18 ENGINEERED: YES;
COMPND    19 OTHER_DETAILS: THIS DOMAIN WAS DOCKED BY A CRYSTAL STRUCTURE (4DEY);
COMPND    20 MOL_ID: 4;
COMPND    21 MOLECULE: VOLTAGE-DEPENDENT CALCIUM CHANNEL GAMMA-1 SUBUNIT;
COMPND    22 CHAIN: E;
COMPND    23 SYNONYM: DIHYDROPYRIDINE-SENSITIVE L-TYPE,SKELETAL MUSCLE CALCIUM
COMPND    24 CHANNEL SUBUNIT GAMMA;
COMPND    25 MOL_ID: 5;
COMPND    26 MOLECULE: VOLTAGE-DEPENDENT CALCIUM CHANNEL SUBUNIT ALPHA-2/DELTA-1;
COMPND    27 CHAIN: F;
COMPND    28 SYNONYM: VOLTAGE-GATED CALCIUM CHANNEL SUBUNIT ALPHA-2/DELTA-1
SOURCE     MOL_ID: 1;
SOURCE     2 ORGANISM_SCIENTIFIC: ORYCTOLAGUS CUNICULUS;
SOURCE     3 ORGANISM_COMMON: RABBIT;
SOURCE     4 ORGANISM_TAXID: 9986;
SOURCE     5 MOL_ID: 2;
SOURCE     6 ORGANISM_SCIENTIFIC: ORYCTOLAGUS CUNICULUS;
SOURCE     7 ORGANISM_COMMON: RABBIT;
SOURCE     8 ORGANISM_TAXID: 9986;
SOURCE     9 GENE: CACNB1, CACNLB1;
SOURCE    10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE    11 EXPRESSION_SYSTEM_TAXID: 562;
SOURCE    12 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE    13 EXPRESSION_SYSTEM_PLASMID: PGEX-4T-2;
SOURCE    14 MOL_ID: 3;
SOURCE    15 ORGANISM_SCIENTIFIC: ORYCTOLAGUS CUNICULUS;
SOURCE    16 ORGANISM_COMMON: RABBIT;
SOURCE    17 ORGANISM_TAXID: 9986;
SOURCE    18 GENE: CACNB1, CACNLB1;
SOURCE    19 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
```

Cav1.1 Mammalian

Экспериментальная 3D-модель



Cav1.1 Mammalian

Экспериментальные 3D-модели белков

PDBe

Protein Data Bank in Europe

<https://www.ebi.ac.uk/pdbe/>

UniProtKB

UniProtKB - P53779 (MK10_HUMAN)

From June 20, 2018 all traffic will be automatically redirected to HTTPS. [More information](#) or [view this page using https](#)

Display: [t BLAST](#) [i Align](#) [b Format](#) [b Add to basket](#) [{ History](#) [U Feedback](#) [V Help video](#) [V Other tutorials and videos](#)

Entry
Publications
Feature viewer
Feature table

Function
 Names & Taxonomy
 Subcellular location
 Pathology & Biotech
 PTM / Processing
 Expression
 Interaction
 Structure
 Family & Domains
 Sequences (3)
 Similar proteins
 Cross-references

Protein | Mitogen-activated protein kinase 10
Gene | MAPK10
Organism | *Homo sapiens (Human)*
Status | **S** Reviewed - Annotation score: ●●●●● - Experimental evidence at protein levelⁱ

Functionⁱ

Serine/threonine-protein kinase involved in various processes such as neuronal proliferation, differentiation, migration and programmed cell death. Extracellular stimuli such as proinflammatory cytokines or physical stress stimulate the stress-activated protein kinase/c-Jun N-terminal kinase (SAP/JNK) signaling pathway. In this cascade, two dual specificity kinases MAP2K4/MKK4 and MAP2K7/MKK7 phosphorylate and activate MAPK10/JNK3. In turn, MAPK10/JNK3 phosphorylates a number of transcription factors, primarily components of AP-1 such as JUN and ATF2 and thus regulates AP-1 transcriptional activity. Plays regulatory roles in the signaling pathways during neuronal apoptosis. Phosphorylates the neuronal microtubule regulator STMN2. Acts in the regulation of the amyloid-beta precursor protein/APP signaling during neuronal differentiation by phosphorylating APP. Participates also in neurite growth in spiral ganglion neurons. Phosphorylates the CLOCK-ARNTL/BMAL1 heterodimer and plays a role in the photic regulation of the circadian clock (PubMed:22441692). [2 Publications](#)

Catalytic activityⁱ
ATP + a protein = ADP + a phosphoprotein.

Cofactorⁱ
Mg²⁺ [1 Publication](#)

Enzyme regulationⁱ
Activated by threonine and tyrosine phosphorylation by two dual specificity kinases, MAP2K4 and MAP2K7. MAP2K7 phosphorylates MAPK10 on Thr-221 causing a conformational change and a large increase in Vmax. MAP2K4 then phosphorylates Tyr-223 resulting in a further increase in Vmax. Inhibited

JNK3 MAPK10 Human

UniProtKB

Файл Правка Вид Журнал Закладки Инструменты Справка

uniprot - Поиск в Google x MAPK10 - Mitogen-activat... x +

https://www.uniprot.org/uniprot/P53779#structure

Display

Entry

Publications

Feature viewer

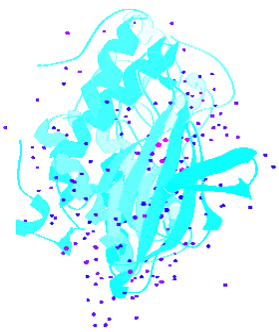
Feature table

None

- Function
- Names & Taxonomy
- Subcellular location
- Pathology & Biotech
- PTM / Processing
- Expression
- Interaction
- Structure
- Family & Domains
- Sequences (3+)
- Similar proteins
- Cross-references
- Entry information
- Miscellaneous

▲ Top

Structureⁱ



PDB Entry	Method	Resolution	Chain	Positions	Links
1JNK	X-ray	2.30 Å	A	1-423	PDBe RCSB PDB PDBj PDBsum
1PMN	X-ray	2.20 Å	A	40-401	PDBe RCSB PDB PDBj PDBsum
1PMU	X-ray	2.70 Å	A	40-401	PDBe RCSB PDB PDBj PDBsum
1PMV	X-ray	2.50 Å	A	40-401	PDBe RCSB PDB PDBj PDBsum
2B1P	X-ray	1.90 Å	A	46-400	PDBe RCSB PDB PDBj PDBsum
2EXC	X-ray	2.75 Å	X	45-400	PDBe

Secondary structure

1 464

Legend: ■ Helix ■ Turn ■ Beta strand ■ PDB Structure known for this area

[Show more details](#)

JNK3 MAPK10 Human

3D structure databases

SMR ⁱ	P53779
ModBase ⁱ	Search...
PDBe-KB ⁱ	Search...

PDBe

Файл Правка Вид Журнал Закладки Инструменты Справка

uniprot - Поиск в Google PDB 1jnk structure summar... +

European Bioinformatics Institute (GB) | <https://www.ebi.ac.uk/pdbe/entry/pdb/1JNK> 90%

Services Research Training About us

EMBL-EBI Protein Data Bank in Europe Bringing Structure to Biology

Search Examples: [hemoglobin](#), [BRCA1_HUMAN](#) Advanced search

Feedback

PDBe > 1jnk

THE C-JUN N-TERMINAL KINASE (JNK3S) COMPLEXED WITH MGAMP-PNP

Source organism: *Homo sapiens*

Primary publication:
[Crystal structure of JNK3: a kinase implicated in neuronal apoptosis.](#)

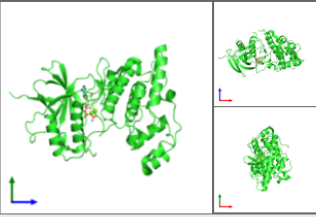
Xie X, Gu Y, Fox T, Coll JT, Fleming MA, Markland W, Caron PR, Wilson KP, Su MS

Structure 6 983-91 (1998)
PMID: 9739089

X-ray diffraction
2.3Å resolution

Released: 08 Jun 1999

Model geometry
Fit model/data █ █
Data not deposited



Quick links

- 1jnk overview
- Citations
- Structure analysis
- Function and Biology
- Ligands and Environments
- Experiments and Validation
- View
- Downloads**
- 3D visualisation

Function and Biology [Details](#)

Reaction catalysed:
ATP + a protein = ADP + a phosphoprotein

Biochemical function:

- transferase activity

Biological process:

- vesicle-mediated transport in synapse

Cellular component:

- glutamatergic synapse

Sequence domains:

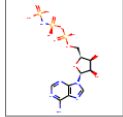
- Mitogen-activated protein (MAP) kinase, JNK
- Protein kinase-like domain superfamily
- Protein kinase domain

Structure domain:

- Protein kinases, catalytic subunit

Ligands and Environments

2 bound ligands:

- Mg+2 [2 x MG](#)
-  [1 x ANP](#)

No modified residues

Experiments and Validation [Details](#)

Metric Percentile Ranks Value
Clashscore █ █ 8

Citations

17 review citations

Computational insights for the discovery of non-ATP competitive inhibitors of MAP kinases.
Schnieders et al. (2012) [16 more](#)

23 mentions without citation

Uses for JNK: the many and varied substrates of the C-Jun N-terminal kinases.
Bogoyevitch et al. (2006) [22 more](#)

JNK3 MAPK10 Human

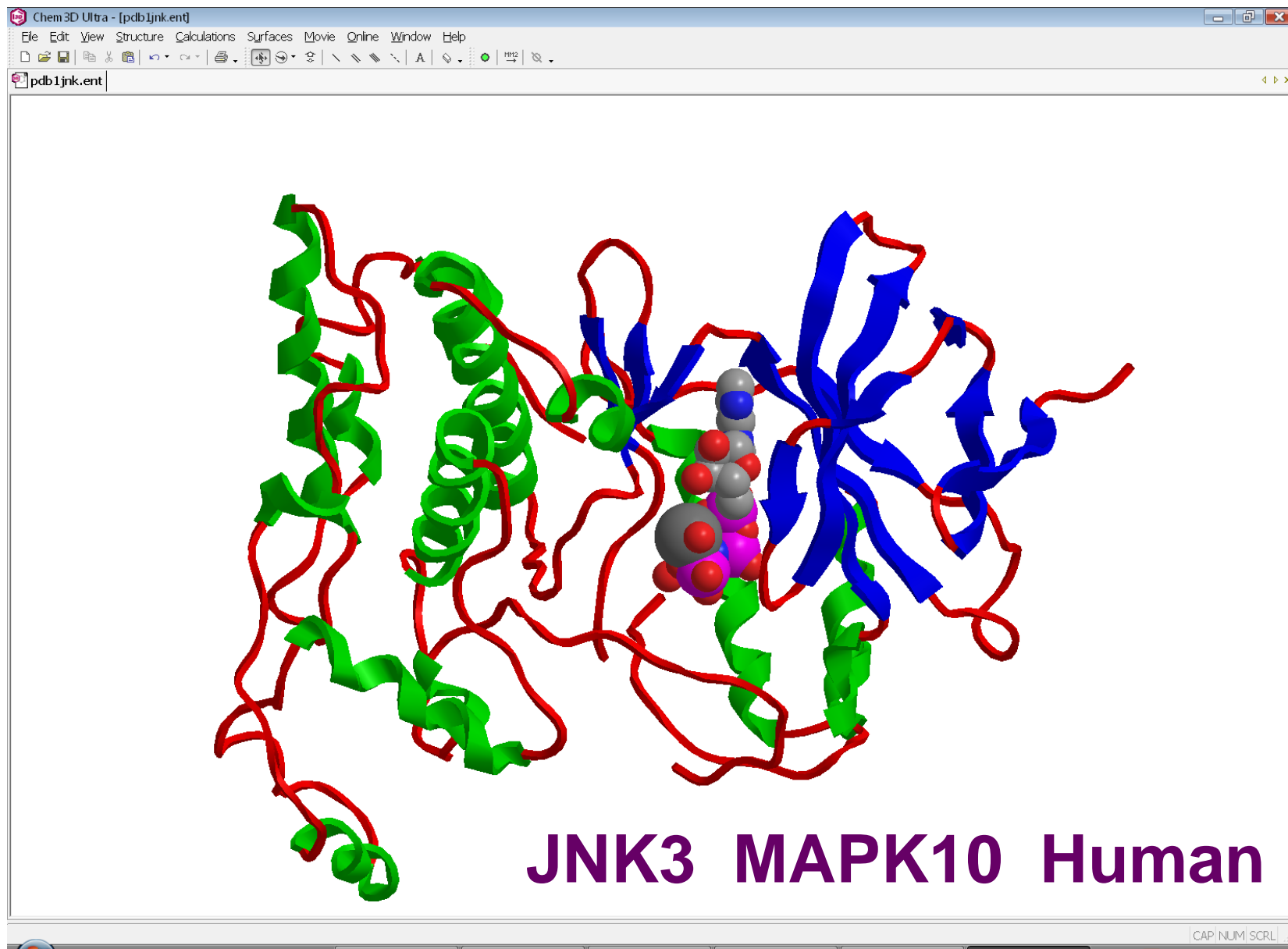
This website requires cookies, and the limited processing of your personal data in order to function. By using the site you are agreeing to this as outlined in our [Privacy Notice](#) and [Terms of Use](#). [I agree, dismiss this banner](#)

Заголовок ENT-файла

```
HEADER      TRANSFERASE                      03-JUN-98  1JNK
TITLE       THE C-JUN N-TERMINAL KINASE (JNK3S) COMPLEXED WITH MGAMP-PNP
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: C-JUN N-TERMINAL KINASE;
COMPND      3 CHAIN: A;
COMPND      4 FRAGMENT: RESIDUES 45 - 400;
COMPND      5 SYNONYM: JNK3;
COMPND      6 EC: 2.7.1.-;
COMPND      7 ENGINEERED: YES
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE      3 ORGANISM_COMMON: HUMAN;
SOURCE      4 ORGANISM_TAXID: 9606;
SOURCE      5 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE      6 EXPRESSION_SYSTEM_TAXID: 562
KEYWDS      TRANSFERASE, JNK3 MAP KINASE, SERINE/THREONINE PROTEIN
KEYWDS      2 KINASE
EXPDTA      X-RAY DIFFRACTION
AUTHOR      X.XIE,M.S.-S.SU
REUDAT      2  24-FEB-09 1JNK  1  UERSN
REUDAT      1  08-JUN-99 1JNK  0
JRNL        AUTH  X.XIE,Y.GU,T.FOX,J.T.COLL,M.A.FLEMING,W.MARKLAND,
JRNL        AUTH 2 P.R.CARON,K.P.WILSON,M.S.SU
JRNL        TITL  CRYSTAL STRUCTURE OF JNK3: A KINASE IMPLICATED IN
JRNL        TITL 2 NEURONAL APOPTOSIS.
JRNL        REF   STRUCTURE                               U.  6  983 1998
JRNL        REFN                               ISSN 0969-2126
JRNL        PMID  9739089
JRNL        DOI   10.1016/S0969-2126(98)00100-2
REMARK      1
REMARK      2
REMARK      2 RESOLUTION.    2.30 ANGSTROMS.
REMARK      3
REMARK      3 REFINEMENT.
REMARK      3 PROGRAM      : X-PLOR 3.843
REMARK      3 AUTHORS      : BRUNGER
REMARK      3
REMARK      3 DATA USED IN REFINEMENT.
REMARK      3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.30
REMARK      3 RESOLUTION RANGE LOW  (ANGSTROMS) : 30.00
REMARK      3 DATA CUTOFF              (SIGMA(F)) : 2.000
REMARK      3 DATA CUTOFF HIGH          (ABS(F)) : NULL
REMARK      3 DATA CUTOFF LOW           (ABS(F)) : NULL
REMARK      3 COMPLETENESS (WORKING+TEST) (%) : 88.3
REMARK      3 NUMBER OF REFLECTIONS      : 16068
REMARK      3
REMARK      3 FIT TO DATA USED IN REFINEMENT.
REMARK      3 CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK      3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK      3 R VALUE              (WORKING SET) : 0.222
```

JNK3 MAPK10 Human

Экспериментальная 3D-модель



To be continued ...

