

# ВВЕДЕНИЕ В БИОИНФОРМАТИКУ

Лекция №17

Структурная биоинформатика

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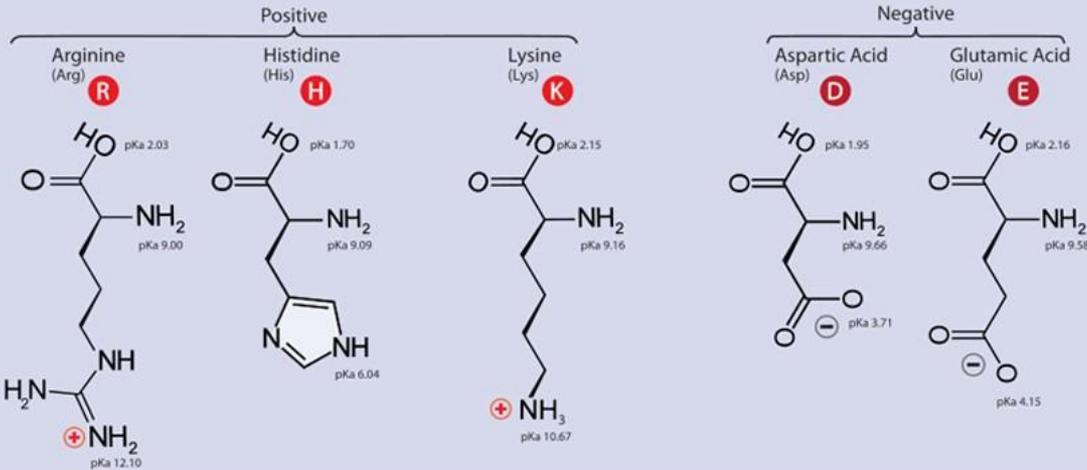
Сайт курса <http://intbio.org/bioinf2019-2020>

# Структура аминокислот

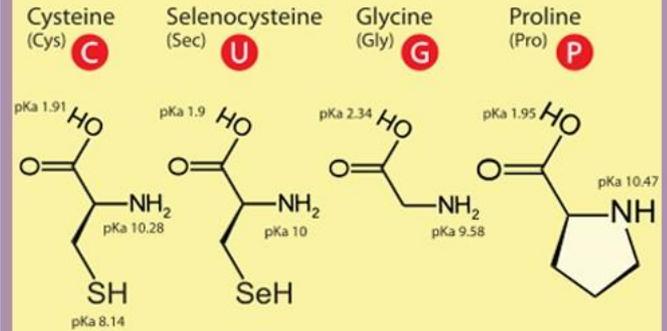
## Twenty-One Amino Acids

⊕ Positive      ⊖ Negative  
 • Side chain charge at physiological pH 7.4

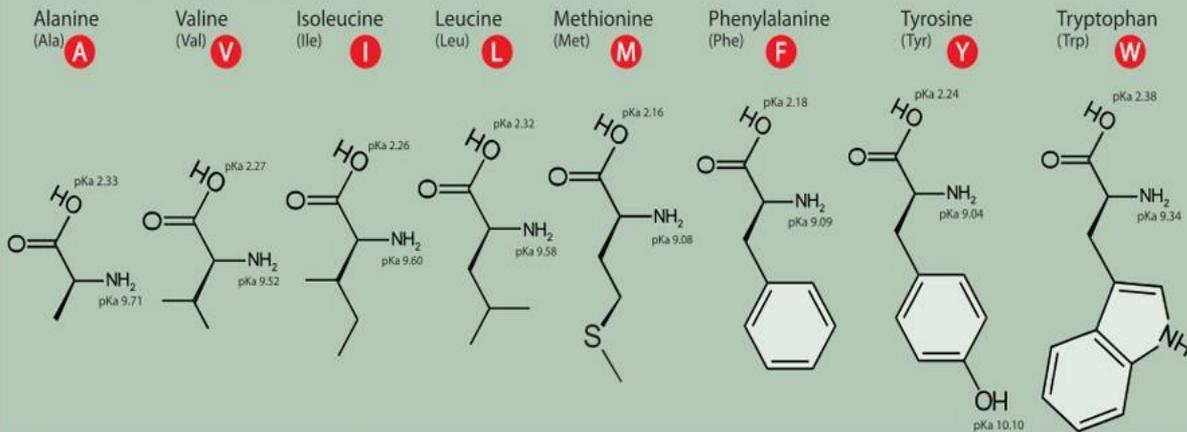
### A. Amino Acids with Electrically Charged Side Chains



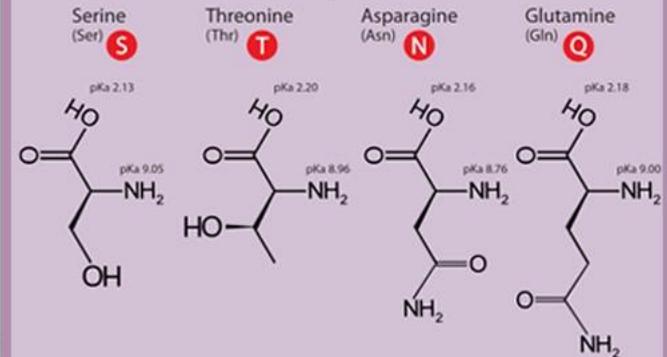
### C. Special Cases



### D. Amino Acids with Hydrophobic Side Chain



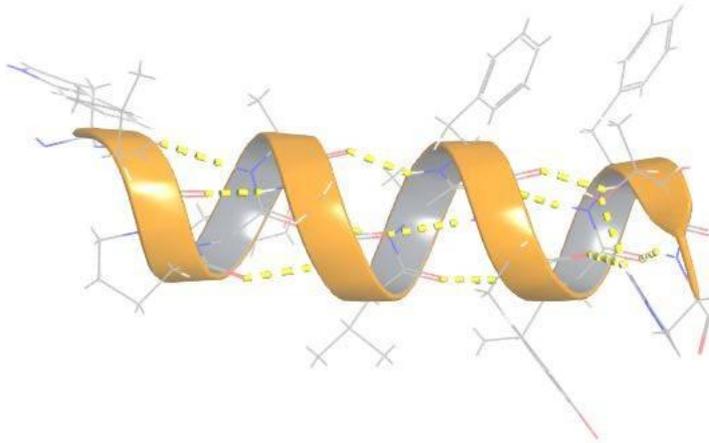
### B. Amino Acids with Polar Uncharged Side Chains



# Структурная организация белков



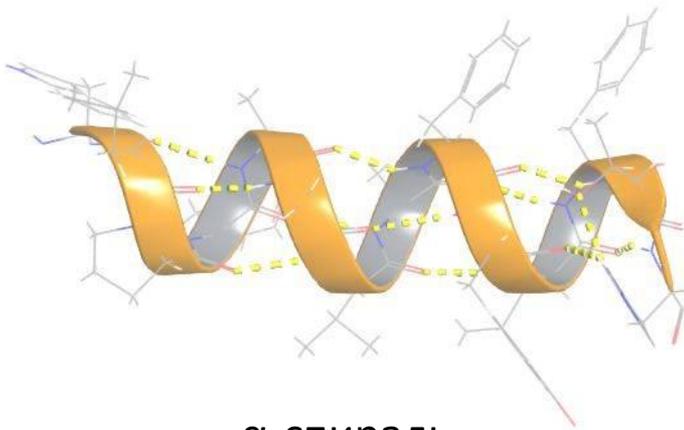
...FYV**PFS**NKT...



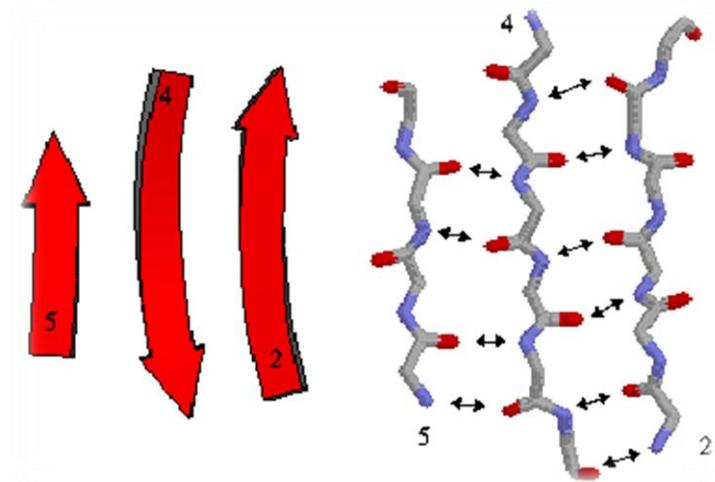
...WLPY**AGVAFYIF**TH...



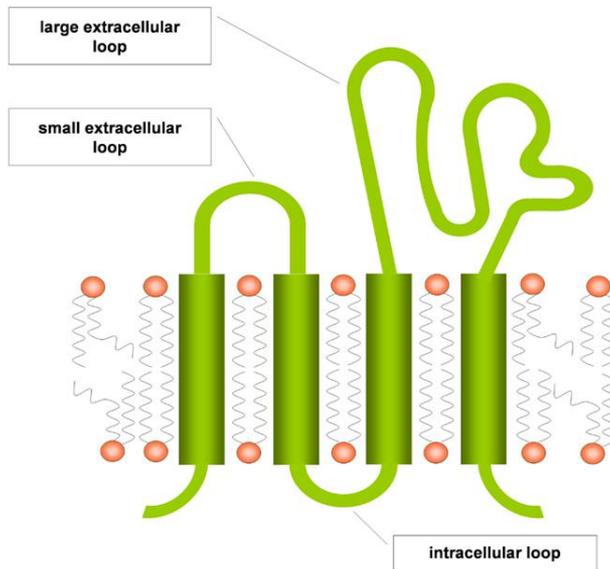
# Типы вторичной структуры белков



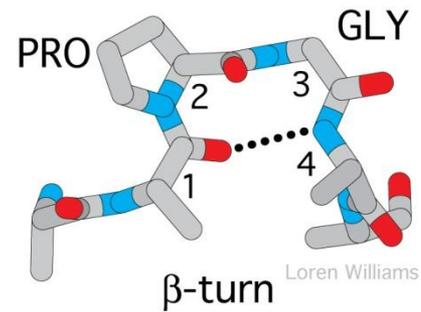
α-спираль



β-лист, состоящий из β-тяжей



петли



поворот

# Define Secondary Structure of Proteins (DSSP)

```

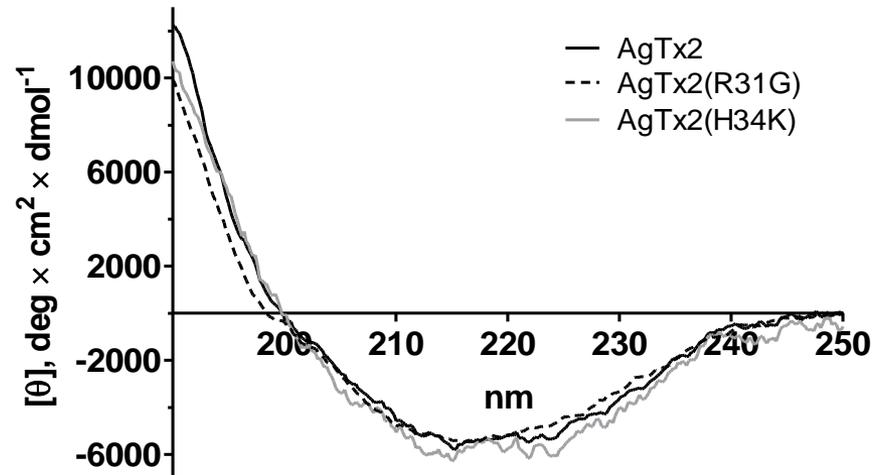
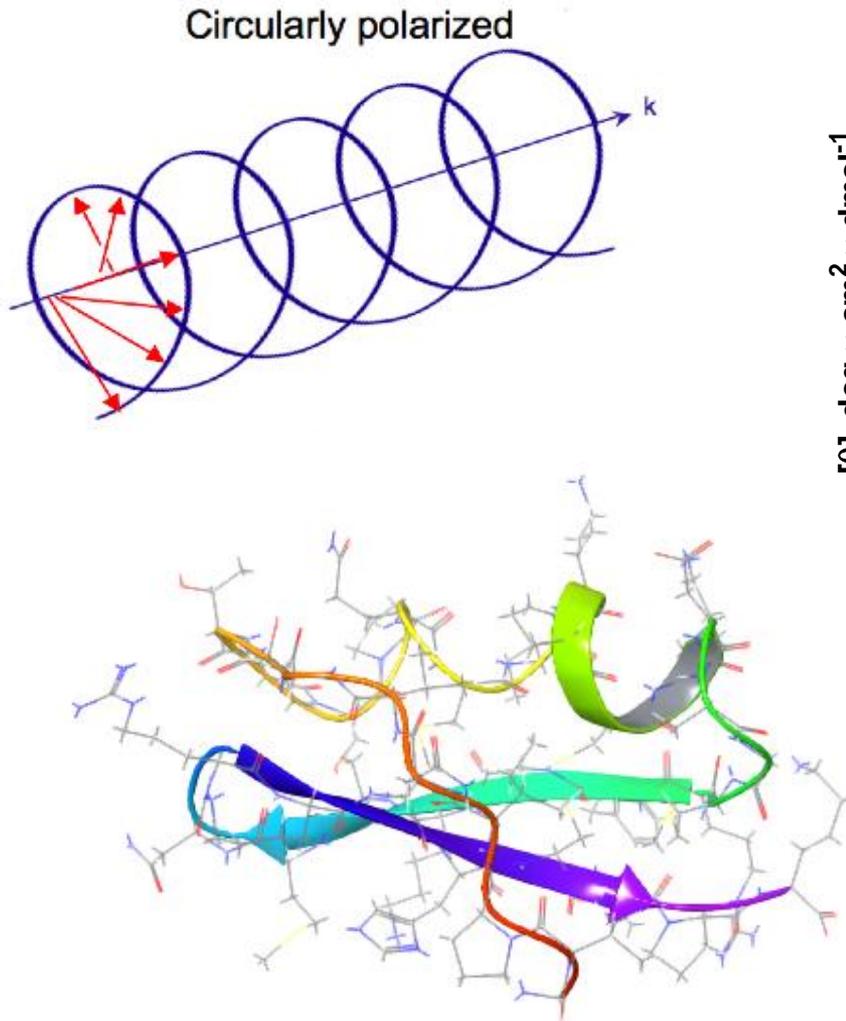
HEADER      HYDROLASE      (SERINE PROTEINASE)          17-MAY-76      1EST
...
 240  1  4  4  0 TOTAL NUMBER OF RESIDUES, NUMBER OF CHAINS,
          NUMBER OF SS-BRIDGES (TOTAL, INTRACHAIN, INTERCHAIN)
10891.0  ACCESSIBLE SURFACE OF PROTEIN (ANGSTROM**2)
 162 67.5  TOTAL NUMBER OF HYDROGEN BONDS OF TYPE O(I)-->H-N(J) ; PER 100 RESIDUES
  84 35.0  TOTAL NUMBER OF HYDROGEN BONDS IN ANTIPARALLEL BRIDGES; PER 100 RESIDUES
...
#  RESIDUE AA STRUCTURE BP1 BP2  ACC   N-H-->O  O-->H-N  N-H-->O  O-->H-N
  2   17   V  B 3   +A 182   0A   8  180,-2.5 180,-1.9   1,-0.2 134,-0.1
...;.....1.....;.....2.....;.....3.....;.....4.....;.....5.....;.....6.....;.....7..
.-- sequential resnumber, including chain breaks as extra residues
|   .-- original PDB resname, not nec. sequential, may contain letters
|   |   .-- amino acid sequence in one letter codeS
|   |   |   .-- secondary structure summary based on columns 19-38
|   |   |   |   xxxxxxxxxxxxxxxxxxxxxxxx recommend columns for secstruc details
|   |   |   |   .-- 3-turns/helix
|   |   |   |   |.-- 4-turns/helix
|   |   |   |   ||.-- 5-turns/helix
|   |   |   |   |||.-- geometrical bend
|   |   |   |   ||||.-- chiralityS
|   |   |   |   |||||.-- beta bridge label
|   |   |   |   |||||.-- beta bridge label
|   |   |   |   |||||.-- beta bridge partner resnum
|   |   |   |   |||||.-- beta bridge partner resnum
|   |   |   |   |||||.-- beta sheet label
|   |   |   |   |||||.-- solvent accessibility
|   |   |   |   |||||.
#  RESIDUE AA STRUCTURE BP1 BP2  ACC
|   |   |   |   |||||.
|   |   |   |   |||||.
35  47   I  E   +   0  0   2
36  48   R  E > S- K  0 39C 97
37  49   Q  T 3  S+   0  0  86      (example from 1EST)
38  50   N  T 3  S+   0  0  34

```

Программа для расчёта  
водородных связей и  
определения типов  
вторичной структуры  
остатков в белках  
(Kabsch & Sander, 1983)

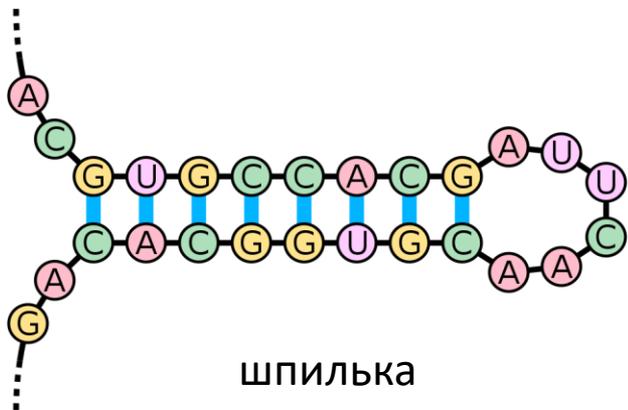
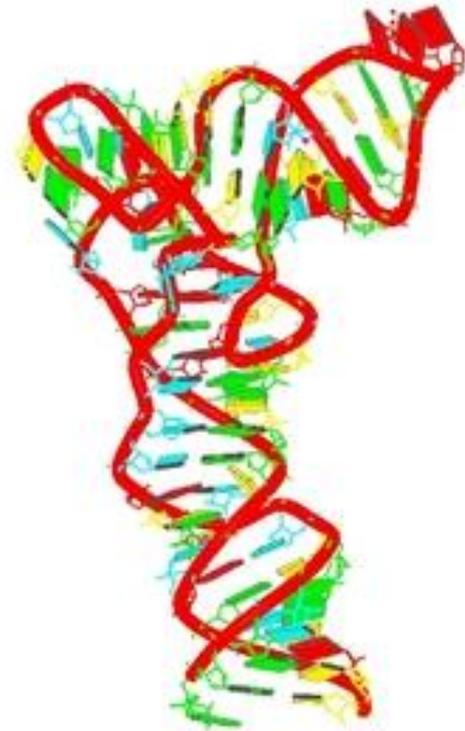
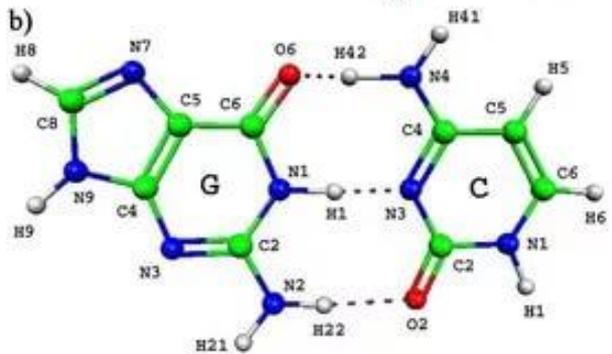
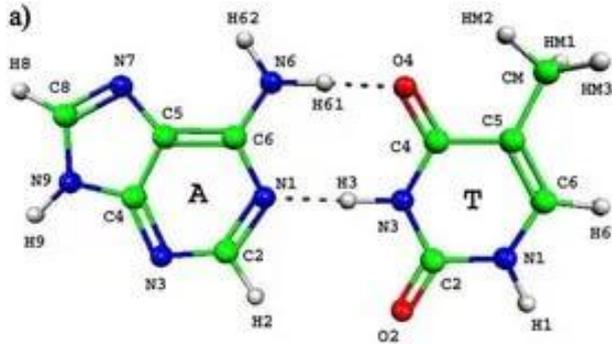
# Спектроскопия кругового дихроизма

## Экспериментальный метод изучения вторичной структуры белков

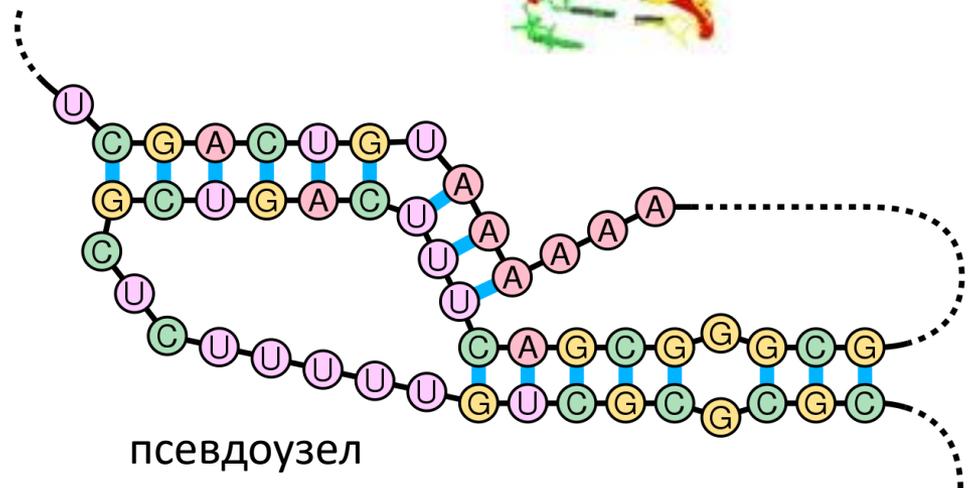


Спектр кругового дихроизма природного аджитоксина и двух его мутантных форм

# Структурная организация нуклеиновых кислот



шпилька



псевдоузел

# Предсказание вторичной структуры РНК



**Sparks Lab**

Laboratory of Structural  
Bioinformatics

## SPOT-RNA: RNA Secondary Structure Prediction using an Ensemble of Two-dimensional Deep Neural Networks and Transfer Learning.

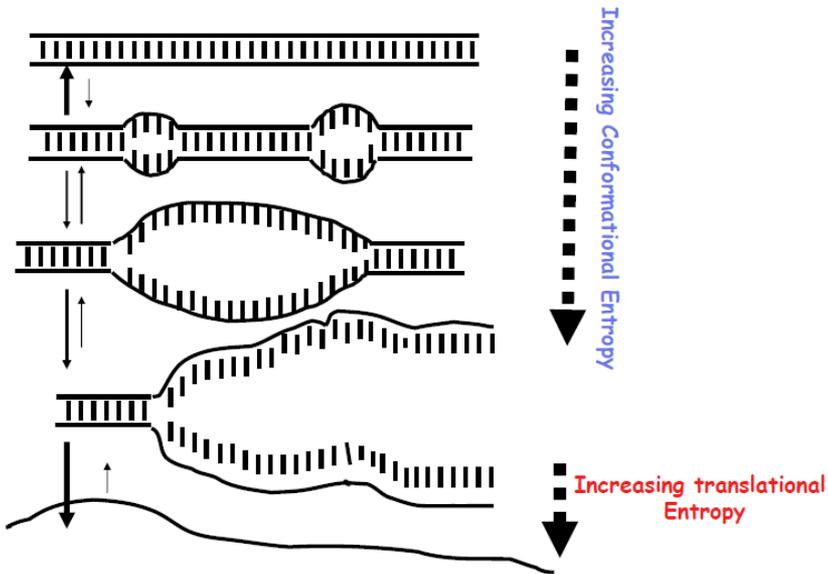
📅 2020-01-29 👤 [Jaswinder Singh](#)

### Submit

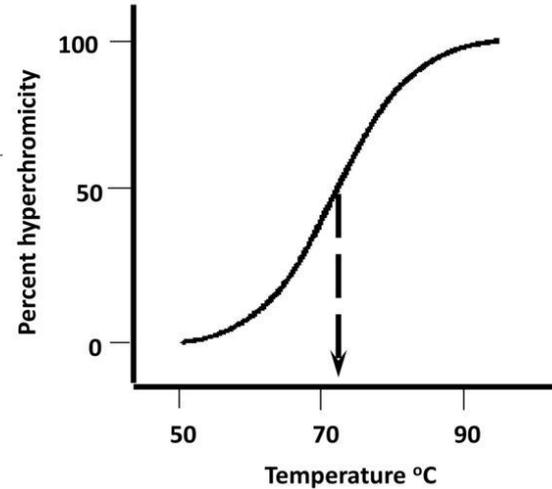
E-mail address (optional):	<input type="text"/>
Target (optional):	<input type="text"/>
Input your RNA Sequences: <input type="button" value="CLEAR"/>	<b>Maximum: 2000 nts, Only one RNA sequence at a time</b>
<pre>&gt; Example sequence 4wj4_B UCCGCGAUAGCUCAGUCGGUAGAGCAAUGACUGUUAUCAUUGGGUCCUGGUU CGAGU CCAGGUCGCGGAGCCA</pre>	

# Плавление нуклеиновых кислот

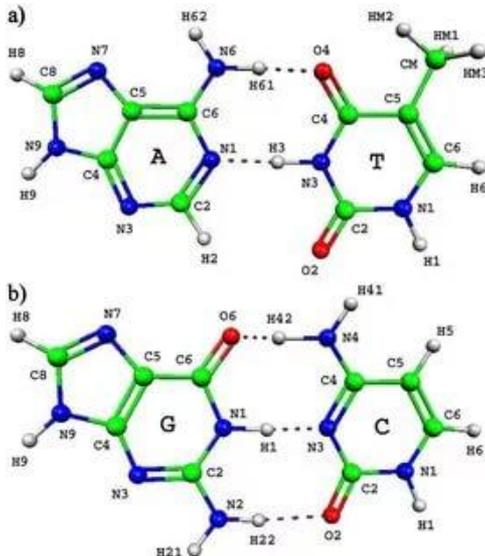
DNA melting is a cooperative process



DNA melting curve



$T_m$  is the temperature at the midpoint of the transition •



(Wetmur and Sninsky, 1995)

$$T_m = 41p(G + C) + 16.6 \lg \left( \frac{[SALT]}{1.0 + 0.7[SALT]} \right) - \frac{500}{L} + 81.5$$

$$[SALT] = [K^+] + 4[Mg^{2+}]^{0.5}$$

# Плавление нуклеиновых кислот

## Oligo Calc: Oligonucleotide Properties Calculator

Enter Oligonucleotide Sequence Below  
*OD calculations are for single-stranded DNA or RNA*

[Nucleotide base codes](#)

ATC GGT AAC GAT TAC ATT C

Reverse Complement Strand(5' to 3') is:

GAA TGT AAT CGT TAC CGA T

[5' modification](#) (if any)

[3' modification](#) (if any)

Select molecule

nM Primer

Measured Absorbance at 260 nanometers

mM Salt (Na<sup>+</sup>)

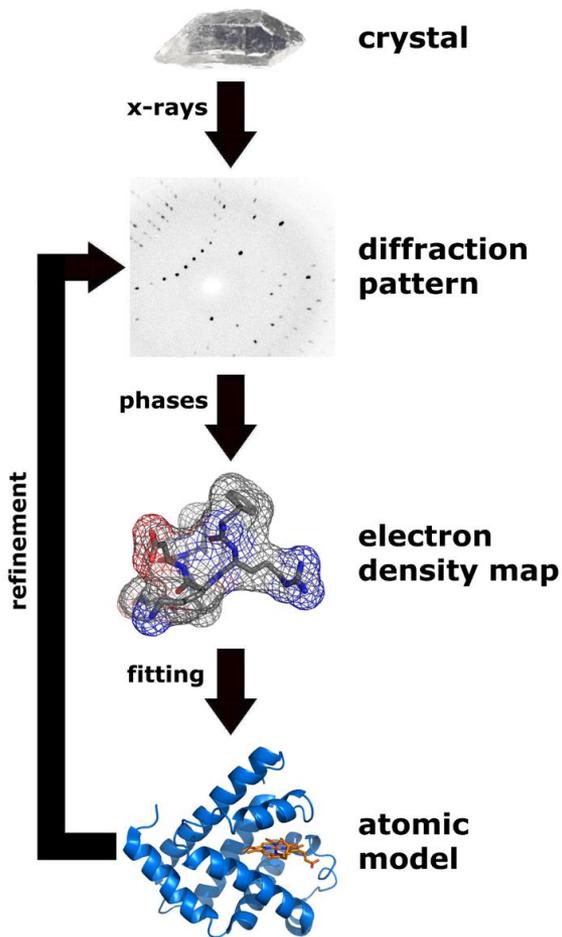
Calculate

Swap Strands

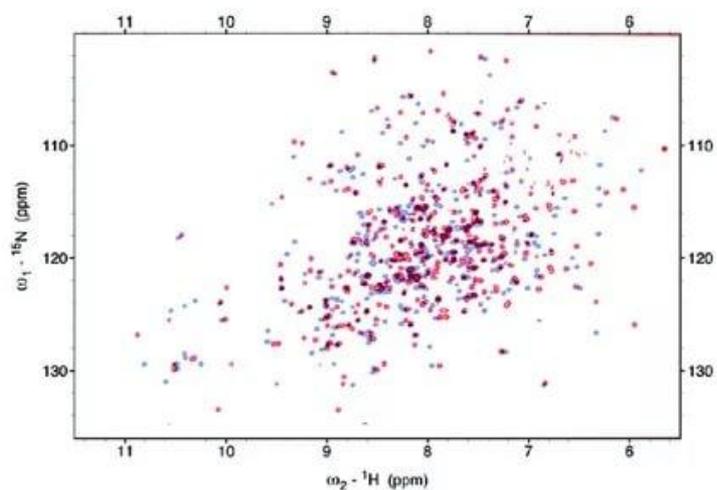
BLAST

mfold

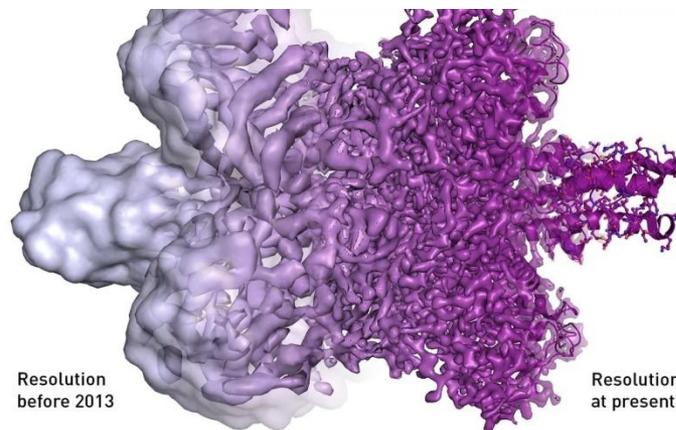
# Методы определения структуры макромолекул



Этапы определения структуры с помощью рентгеновской кристаллографии

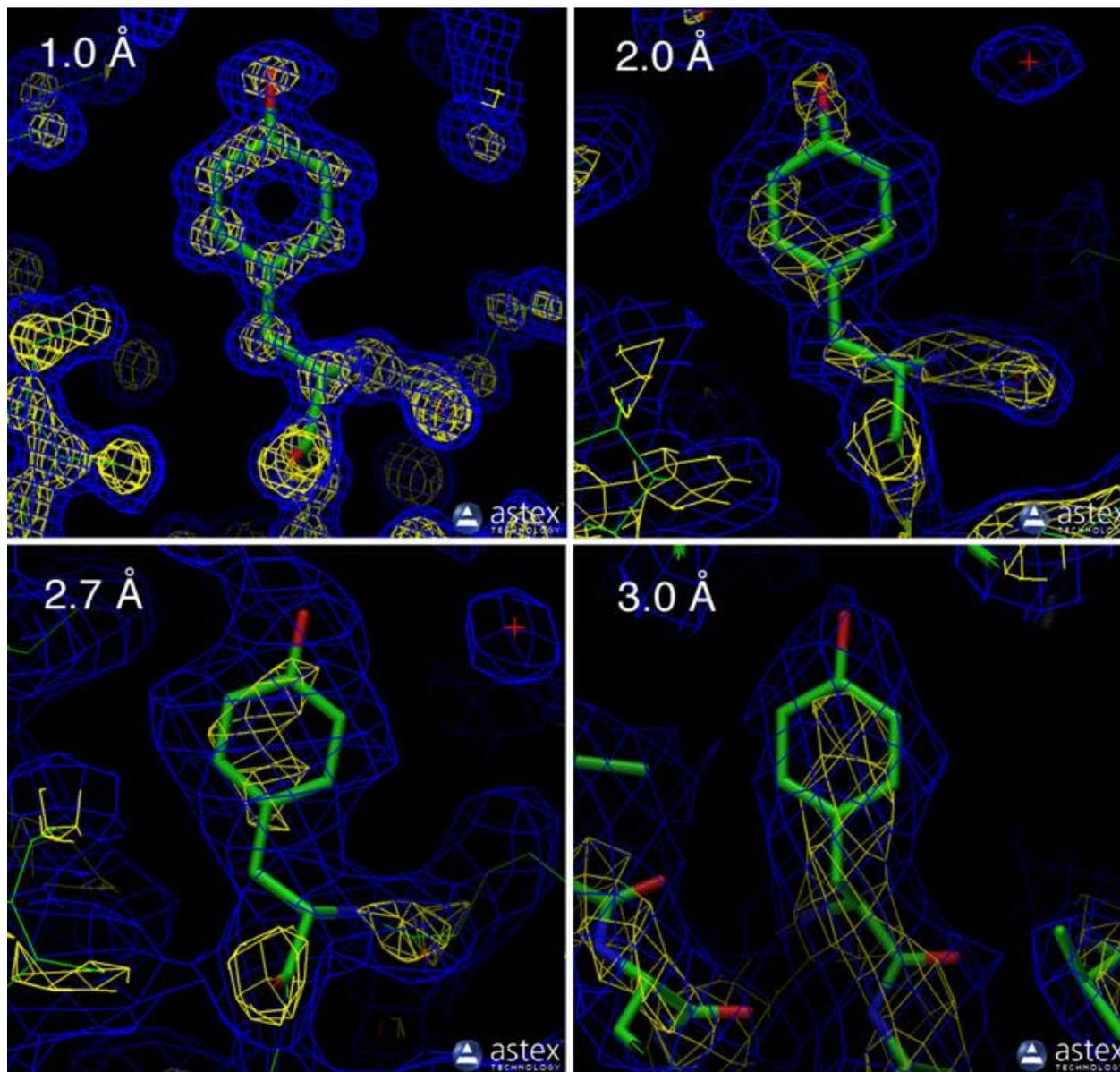


Спектроскопия ядерного магнитного резонанса (ЯМР)



(Крио) электронная микроскопия

# Разрешение в рентгеноструктурном анализе (РСА)



# Структурные базы данных. PDB

**RCSB PDB**  
PROTEIN DATA BANK

A MEMBER OF THE **PDB**

An Information Portal to Biological Macromolecular Structures

As of Tuesday Oct 12, 2010 at 5 PM PDT there are 68562 Structures | PDB Statistics

Contact Us | Print | PDB ID or Text | Search | Advanced Search

## A Resource for Studying Biological Macromolecules

The PDB archive contains information about experimentally-determined structures of proteins, nucleic acids, and complex assemblies. As a member of the **wwPDB**, the RCSB PDB curates and annotates PDB data according to agreed upon standards.

The RCSB PDB also provides a variety of tools and resources. Users can perform simple and advanced searches based on annotations relating to sequence, structure and function. These molecules are visualized, downloaded, and analyzed by users who range from students to specialized scientists.

**Hide Welcome Message**

### Featured Molecules (MoM Category View / Previous) Hide

Features: MoM | PSI

**Structural View of Biology**

**Protein Synthesis**

**Molecule of the Month: Riboswitches**  
Why use two or more molecules when one

### Customize This Page

#### New Features Hide

**Improved Domain Display on Sequence Tab**

Latest features released:

Website Release Archive: [Dropdown]

#### RCSB PDB News Hide

Weekly | Quarterly | Yearly

2010-10-12

**Categorized View of Molecule of the Month**

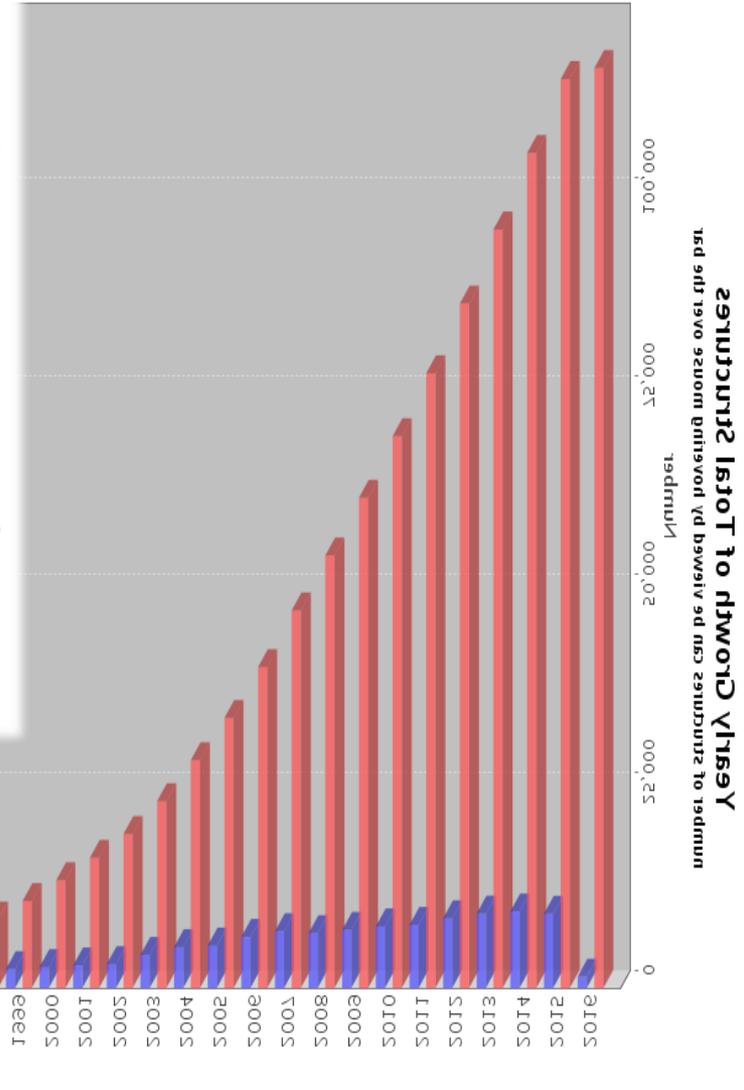
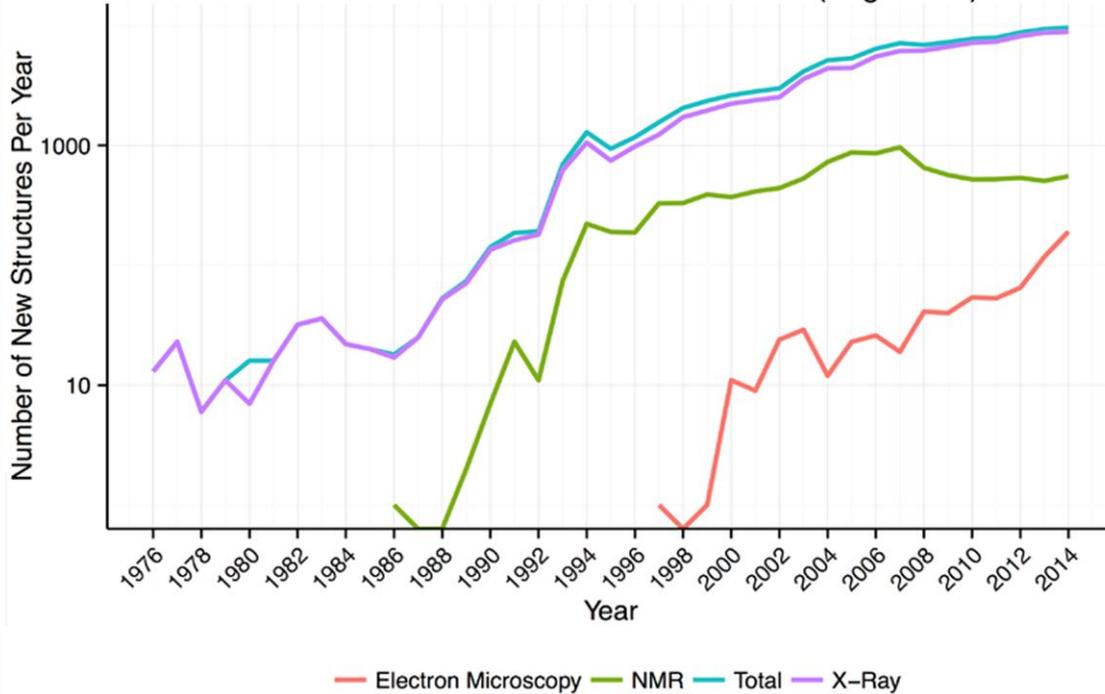
Explore new Molecule of the Month feature categories.

- Latest Website Release
- Poster Prize Awarded at ECM
- Analyze small molecule interactions in the PDB with

PDB (с 1971 по н.в.) – содержит информацию об экспериментально определенных структурах белков, нуклеиновых кислот и различных комплексов.

# Структурные базы данных. PDB

Rate of Protein Structure Determination (Log Scale)



На февраль 2020: около 160 тыс. структур

# Структурные базы данных. PDB

## POTASSIUM CHANNEL KCSA IN COMPLEX WITH TETRABUTYLAMMONIUM IN HIGH K

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Usage/Reference Policies  
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Electron Microscopy  
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Latest Release  
New Structure Papers  
Sequence Search  
Chemical Components  
Unreleased Entries  
Browse Database

Summary Sequence Derived Data Seq. Similarity 3D Similarity Literature Biol. & Chem. Methods Geometry Links

### POTASSIUM CHANNEL KCSA IN COMPLEX WITH TETRABUTYLAMMONIUM IN HIGH K

2JK5

Display Files ▾  
Download Files ▾  
Print this Page  
Share this Page ▾

DOI: 10.2210/pdb2jk5/pdb

Primary Citation

**Structure of a Potassium Channel in Complex with Symmetrical Quaternary Ammonium Compounds Reveals a Novel Hydrophobic Binding Site**

Lenaus, M.J., Focia, P.J., Wagner, T., Gross, A.

Journal: To be Published

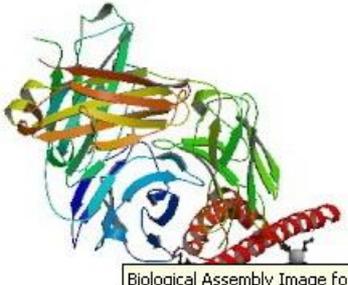
Not in PubMed

Molecular Description Hide

Classification: Immune System/metal Transport  
Structure Weight: 61280.07

Molecule:	ANTIBODY FAB FRAGMENT LIGHT CHAIN	Length:	219
Polymer:	1 Type: polypeptide(L)		
Chains:	A		
Molecule:	ANTIBODY FAB FRAGMENT HEAVY CHAIN	Length:	212
Polymer:	2 Type: polypeptide(L)		
Chains:	B		
Molecule:	VOLTAGE-GATED POTASSIUM CHANNEL	Length:	124
Polymer:	3 Type: polypeptide(L)		
Chains:	C		

Biological Assembly ?



Biological Assembly Image for 2JK5

More Images...

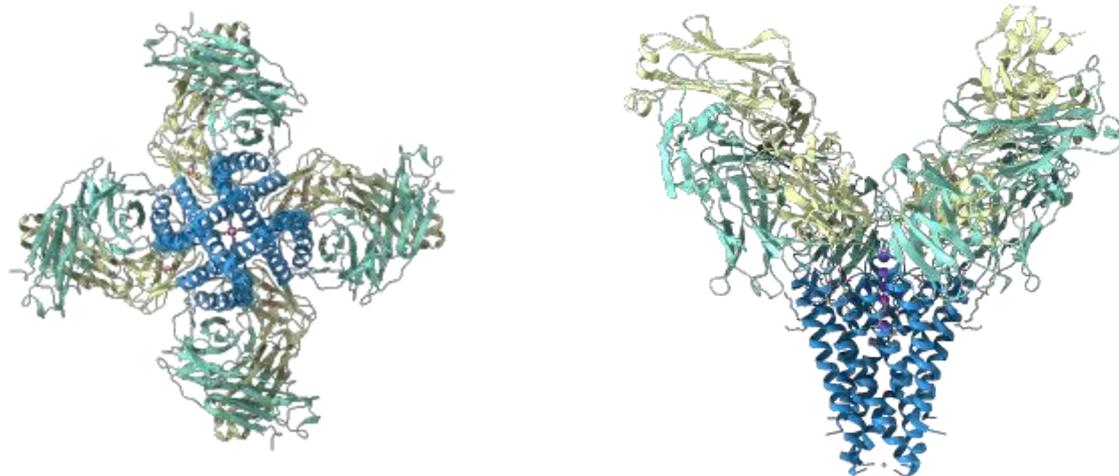
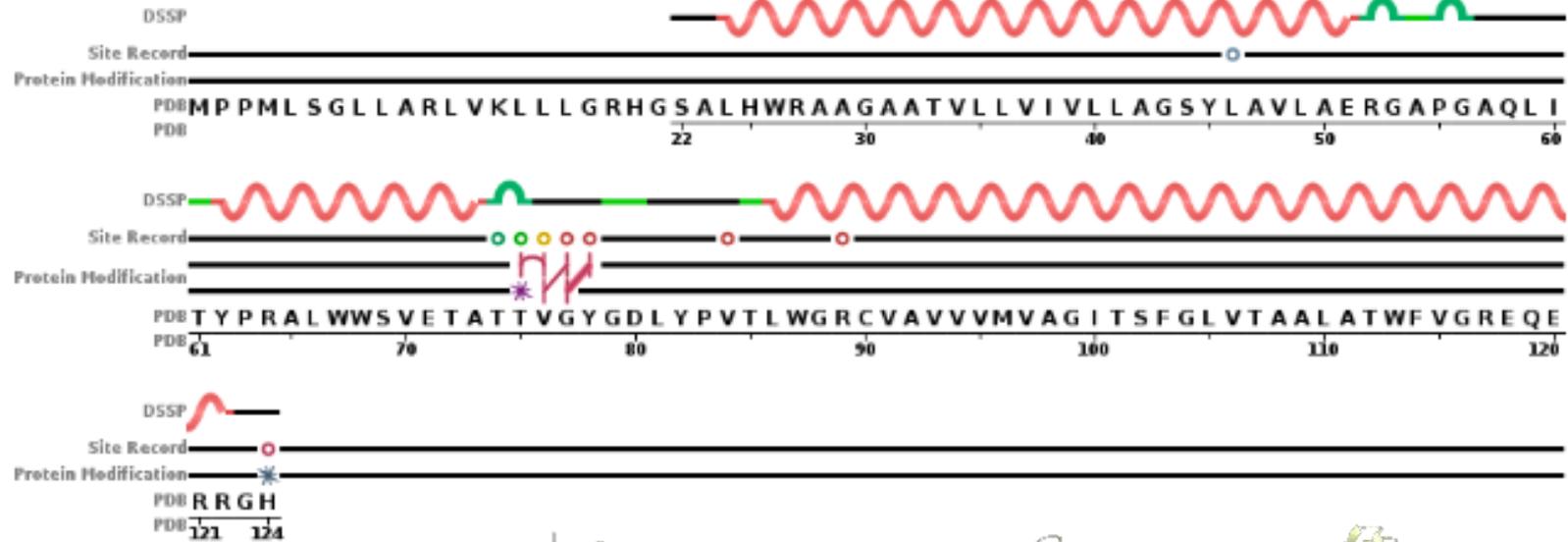
View in Jmol SimpleViewer  
Other Viewers ▾ Protein Workshop

Biological assembly generated by PISA (software)

# Структурные базы данных. PDB

POTASSIUM CHANNEL KCSA IN COMPLEX WITH TETRABUTYLAMMONIUM IN HIGH K

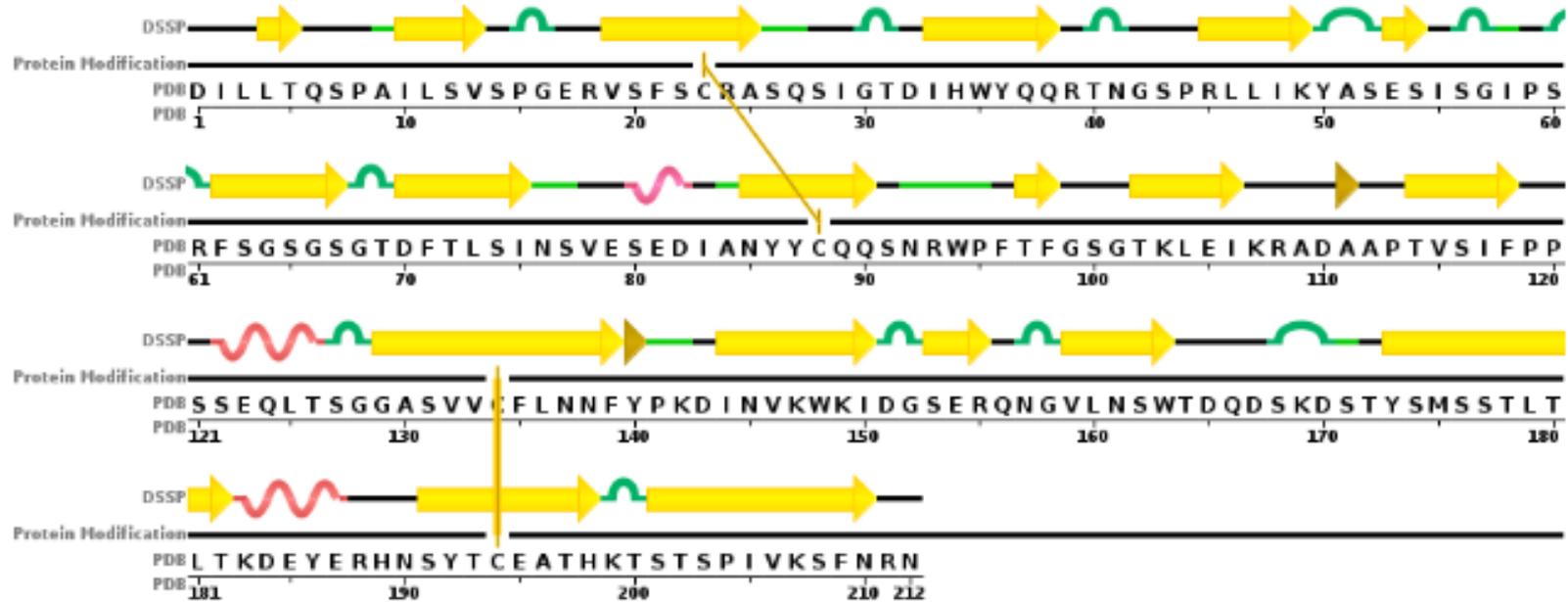
## Sequence Chain View



# Структурные базы данных. PDB

POTASSIUM CHANNEL KCSA IN COMPLEX WITH TETRABUTYLAMMONIUM IN HIGH K

## Sequence Chain View



### Protein Modification Legend

—+— L-cystine

### DSSP Legend

— empty: no secondary structure assigned

➔ B: beta bridge

— S: bend

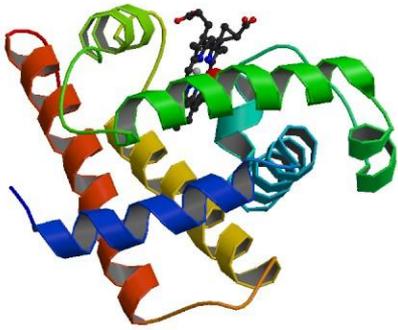
⤿ T: turn

➔ E: beta strand

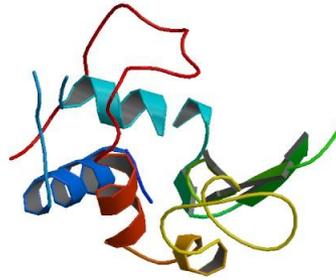
⤿ G: 3/10-helix

⤿ H: alpha helix

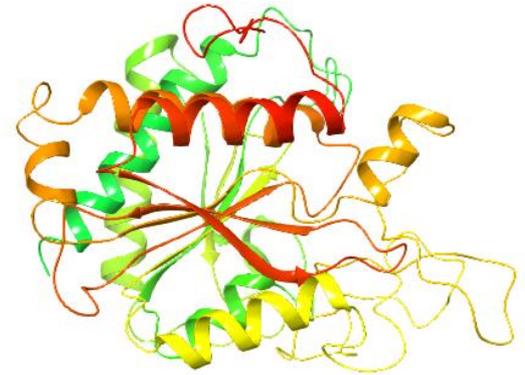
# Разнообразии белковых структур



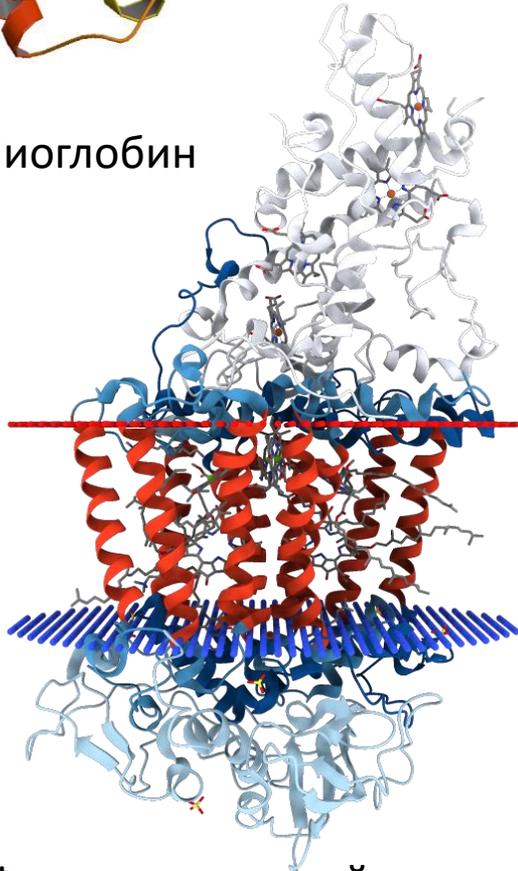
Миоглобин



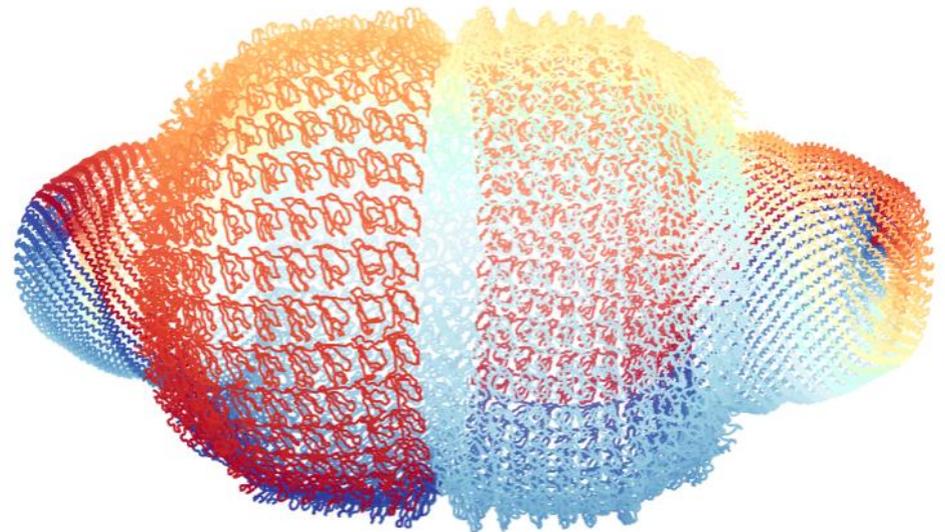
Лизоцим



Карбоксипептидаза



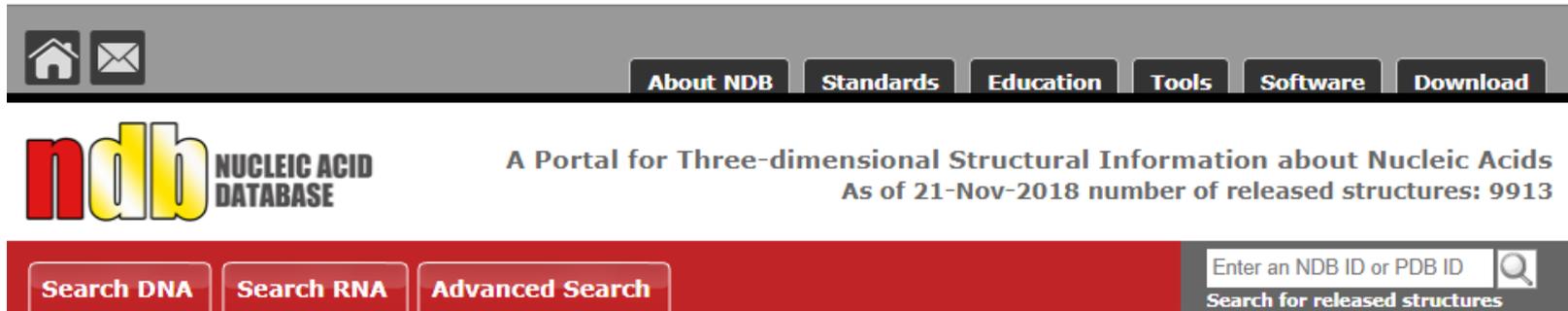
Фотореакционный центр



Структура органеллы vault из печени крысы

# Структурные базы данных. NDB

NDB (с 1992 по н.в.) – сбор и распространение информации о структуре нуклеиновых кислот. Формат хранения данных идентичен PDB.



The screenshot shows the top navigation bar of the NDB website. It includes a home icon and an email icon on the left. The main navigation menu contains links for 'About NDB', 'Standards', 'Education', 'Tools', 'Software', and 'Download'. Below the navigation bar is the NDB logo, which consists of the letters 'ndb' in a stylized font with a yellow-to-red gradient, followed by the text 'NUCLEIC ACID DATABASE'. To the right of the logo is the text 'A Portal for Three-dimensional Structural Information about Nucleic Acids' and 'As of 21-Nov-2018 number of released structures: 9913'. At the bottom of the header is a search bar with the text 'Enter an NDB ID or PDB ID' and a magnifying glass icon, with the label 'Search for released structures' below it. To the left of the search bar are three buttons: 'Search DNA', 'Search RNA', and 'Advanced Search'.

## Welcome to the NDB

The NDB contains information about experimentally-determined nucleic acids and complex assemblies. Use the NDB to perform searches based on annotations relating to sequence, structure and function, and to download, analyze, and learn about nucleic acids.

### Search Structures

[Search DNA](#)  
Search DNA and its complexes

[Search RNA](#)  
Search for RNA structures in the NDB archive or in the Non-Redundant list

[Advanced Search](#)  
Search for structures based on structural features, chemical features, binding modes, citation and experimental information



### Featured Tools

[RNA 3D Motif Atlas](#), a representative collection of RNA 3D internal and hairpin loop motifs

[Non-redundant Lists of RNA-containing 3D structures](#)

[RNA Base Triple Atlas](#), a collection of motifs consisting of two RNA basepairs

[WebFR3D](#), a webserver for symbolic and geometric searching of RNA 3D structures

[R3D Align](#), an application for detailed nucleotide to nucleotide alignments of RNA 3D structures



# Структурные базы данных. NDB

## COMPLEX BETWEEN NUCLEOSOME CORE PARTICLE (H3,H4,H2A,H2B) AND 146 BP LONG DNA FRAGMENT

**NDB ID:** PD0001 **PDB ID:** [1AOI](#) 

### Title:

COMPLEX BETWEEN NUCLEOSOME CORE PARTICLE (H3,H4,H2A,H2B) AND 146 BP LONG DNA FRAGMENT

### Molecular Description:

COMPLEX BETWEEN NUCLEOSOME CORE PARTICLE (H3  
H4  
H2A  
H2B) AND 146 BP LONG DNA FRAGMENT

### Structural Keywords:

B DOUBLE HELIX

### Nucleic Acid Sequence:

[Click to show/hide 1 nucleic acid sequences](#)

### Protein Sequence:

[Click to show/hide 4 protein sequences](#)

### Primary Citation:

Luger, K., Mader, A.W., Richmond, R.K., Sargent, D.F., Richmond, T.J.  
[Crystal structure of the nucleosome core particle at 2.8 Å resolution.](#)   
*Nature*, **389**, pp. 251 - 260, 1997.

### Experimental Information:

X-RAY DIFFRACTION

### Space Group:

P 21 21 21

### Cell Constants:

a = 106.04 b = 181.78 c = 110.12 (Ångstroms)

$\alpha = 90.0$   $\beta = 90.0$   $\gamma = 90.0$  (degrees)

### Refinement:

The structure was refined using the X-PLOR program. The R value is 0.0 for 51237 reflections in the resolution range 25.0 to 2.8 Ångstroms with Fobs > 0.0 sigma(Fobs) and with I > 0.0 sigma(I)

### Structural Features

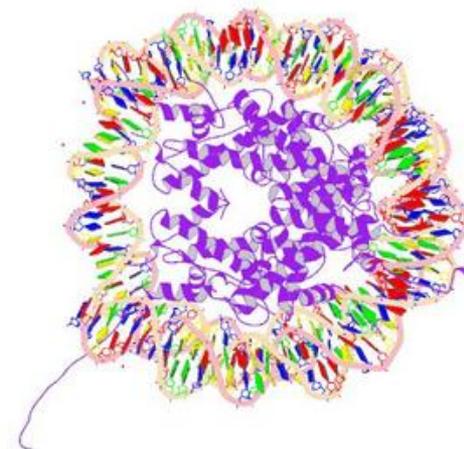
[Base Pair Hydrogen Bonding Classification](#)

[Nucleic Acid Backbone Torsions](#)

[Base Pair Morphology Parameters](#)

[Base Pair Morphology Step Parameters](#)

### Biological Assembly 1



[More Images...](#)

# Структурные базы данных. EMDB

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**Title:** Three-dimensional structure of a voltage-gated potassium channel at 2.5 nm resolution.

**Authors:** Olga Sokolova, Ludmila Kolmakova-Partensky and Nikolaus Grigorieff

**Sample:** Shaker B channel

**Aggregation state:** Single particle (25 angstroms resolution)

**Latest update:** 2011-05-26

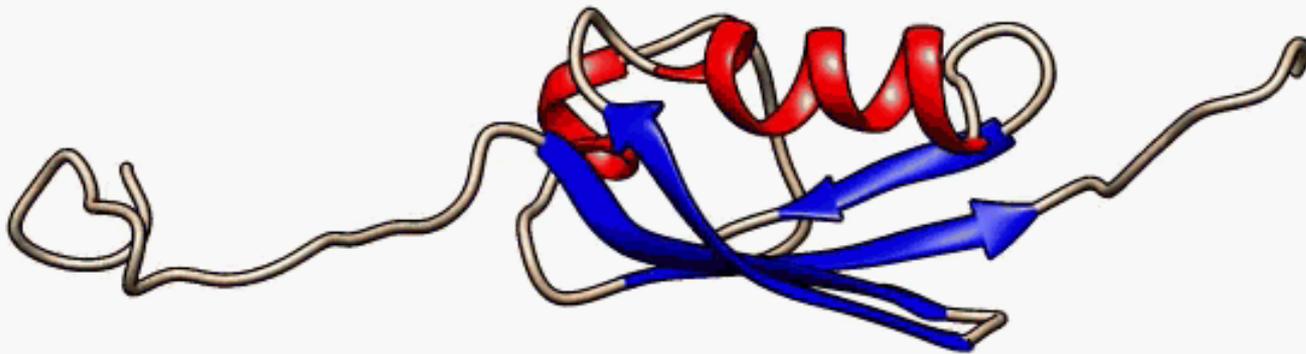
- Summary
- Experimental details
- Visualization
- Map information
- Downloads

**Summary**

<b>Status:</b>	Released												
<b>Deposition date:</b>	2007-05-24												
<b>Header release date:</b>	2007-05-30												
<b>Map release date:</b>	2007-05-30												
<b>Primary citation:</b>	Sokolova O, Kolmakova-Partensky L, Grigorieff N: Three-dimensional structure of a voltage-gated potassium channel at 2.5 nm resolution. <i>STRUCTURE</i> (2001) <b>9</b> , pp. 215-220 [PubMed 11286888]												
<b>Sample:</b>	Shaker B channel												
<b>Resolution:</b>	25 Å (determined by FSC at 0.5 cut-off)												
<b>Fitted PDB:</b>	<table style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;">PDB</th> <th style="text-align: left;">Authors</th> <th style="text-align: left;">PubMed</th> <th style="text-align: left;">Status</th> </tr> </thead> <tbody> <tr> <td>1bl8</td> <td>Doyle, D.A., Cabral, J.M., Pfuetzner, R.A., Kuo, A., Gulbis, J.M., Cohen, S.L., Chait, B.T., Mackinnon, R.</td> <td>9525859</td> <td>Released</td> </tr> <tr> <td>1a68</td> <td>Kreusch, A., Pfaffinger, P.J., Stevens, C.F., Choe, S.</td> <td>9582078</td> <td>Released</td> </tr> </tbody> </table>	PDB	Authors	PubMed	Status	1bl8	Doyle, D.A., Cabral, J.M., Pfuetzner, R.A., Kuo, A., Gulbis, J.M., Cohen, S.L., Chait, B.T., Mackinnon, R.	9525859	Released	1a68	Kreusch, A., Pfaffinger, P.J., Stevens, C.F., Choe, S.	9582078	Released
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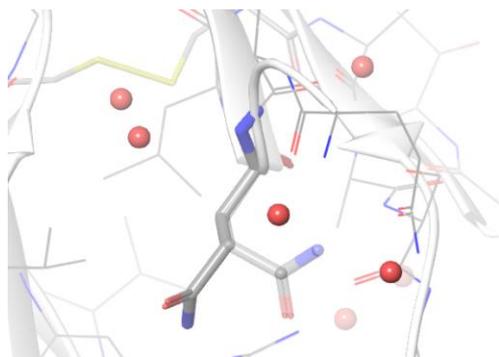
# Неупорядоченные белки

Intrinsically disordered proteins - «нарушители» догмы «структура определяет функцию»



# Структурные файлы. \*.pdb

Descriptor		Conformation index					Atom element					
Atom number		Residue name		Residue number			Beta-factor		Occupancy			
Atom name		Chain name										
...	ATOM	22	CG	AGLN	A	3	-30.506	25.807	16.125	0.50	43.30	C
	ATOM	23	CD	AGLN	A	3	-29.018	25.546	15.959	0.50	43.01	C
	ATOM	24	OE1	AGLN	A	3	-28.187	26.374	16.332	0.50	43.76	O
	ATOM	25	NE2	AGLN	A	3	-28.675	24.391	15.403	0.50	41.73	N
	ATOM	26	N	BGLN	A	3	-33.005	25.819	17.852	0.50	45.16	N
	ATOM	27	CA	BGLN	A	3	-32.788	24.834	16.796	0.50	44.25	C
	ATOM	28	C	BGLN	A	3	-33.529	23.510	17.024	0.50	43.75	C
...	HETATM	4140	C1	F09	C1131		-21.017	-3.092	-1.563	1.00	60.56	C
	HETATM	4141	C2	F09	C1131		-21.015	-1.597	-1.357	1.00	60.40	C



X



Y



Z coordinates in Å

# Задание поворота в пространстве

Матрица поворота:

$$M_x(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha & -\sin \alpha \\ 0 & \sin \alpha & \cos \alpha \end{pmatrix}$$

$$M_y(\alpha) = \begin{pmatrix} \cos \alpha & 0 & \sin \alpha \\ 0 & 1 & 0 \\ -\sin \alpha & 0 & \cos \alpha \end{pmatrix}$$

$$M_z(\alpha) = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Любое вращение в трехмерном пространстве может быть представлено как композиция поворотов вокруг трех ортогональных осей.

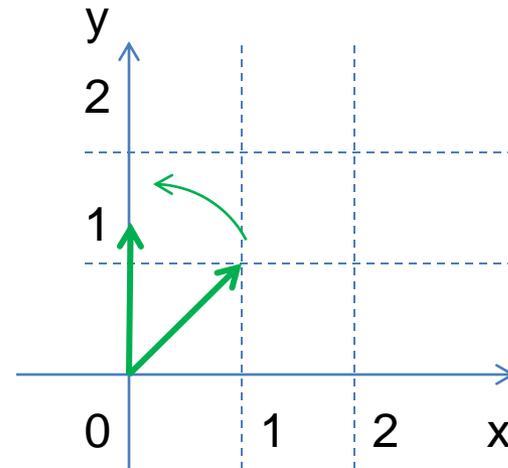
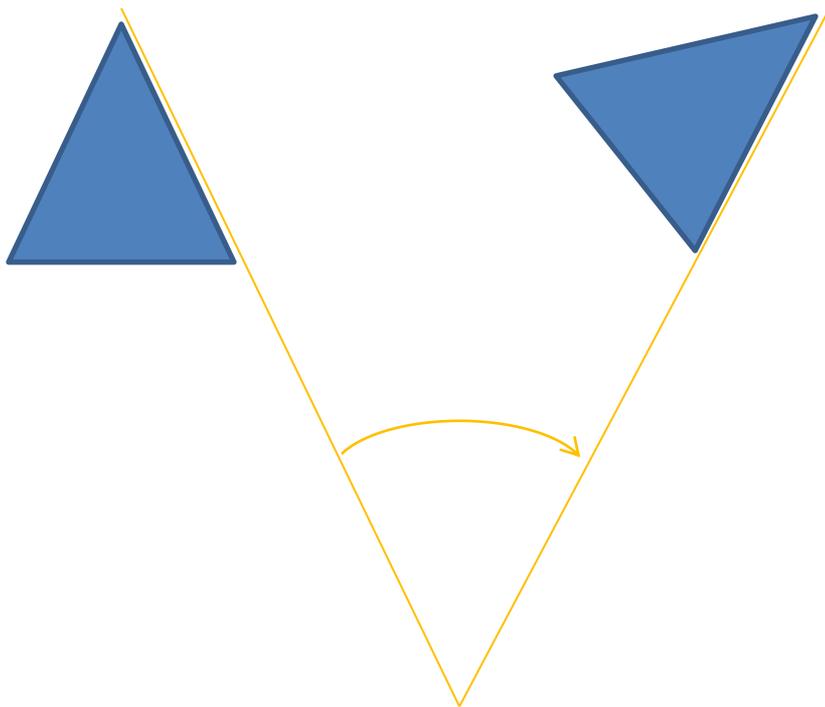
Недостатки: 1) громоздкость вычислений

2) неустойчивость вычислений (ошибки округления)

# Задание поворота в пространстве. Пример

Матрица поворота:

$$M_z(\alpha) = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

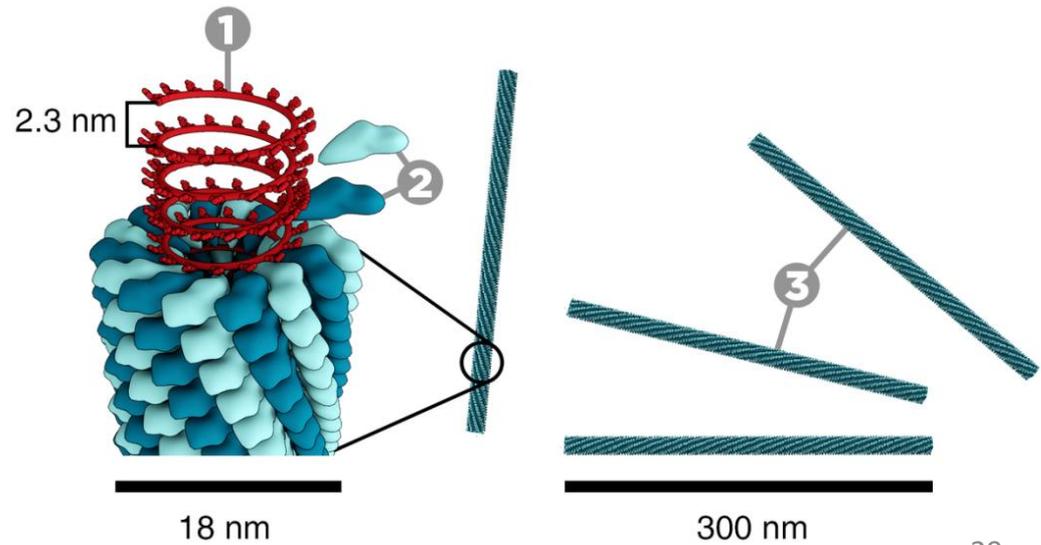
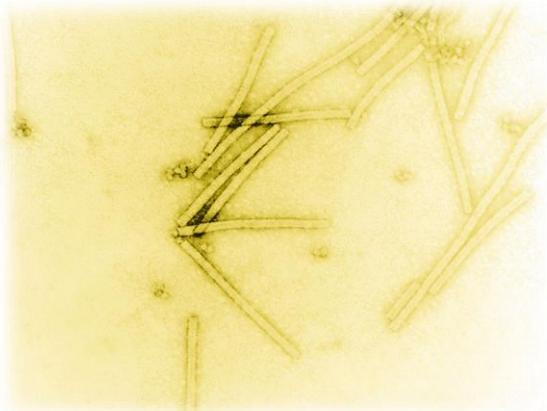
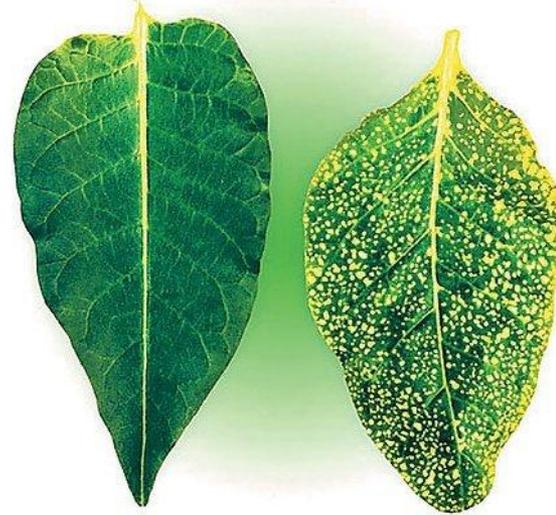


$$\begin{pmatrix} 0 \\ \sqrt{2} \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

# Вирус табачной мозаики



Д.И. Ивановский  
(1864 — 1920)



# Вирус табачной мозаики

REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN  
 REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE  
 REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS  
 REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND  
 REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.

REMARK 350

REMARK 350 BIOMOLECULE: 1

REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, R

REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000

REMARK 350 BIOMT2 1 0.000000 1.000000 -0.000000

REMARK 350 BIOMT3 1 0.000000 -0.000000 1.000000

REMARK 350 BIOMT1 2 0.923478 -0.383651 0.000000

REMARK 350 BIOMT2 2 0.383651 0.923478 -0.000000

REMARK 350 BIOMT3 2 0.000000 -0.000000 1.000000

...

REMARK 350 BIOMT1 49 0.926988 0.375092 0.000000

REMARK 350 BIOMT2 49 -0.375092 0.926988 -0.000000

REMARK 350 BIOMT3 49 0.000000 -0.000000 1.000000

матрица поворота

вектор переноса

0.00000

0.00000

0.00000

-0.00000

0.00000

-67.58400

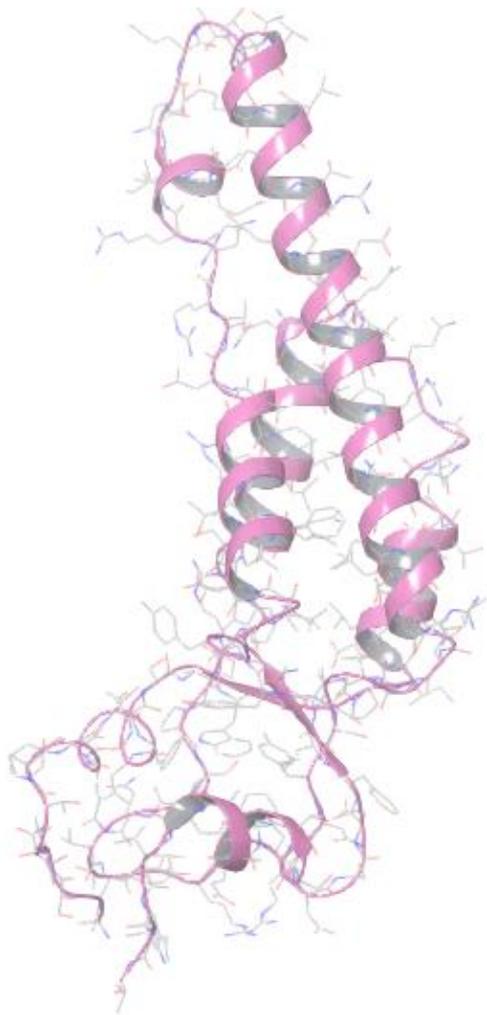
-0.00000

0.00000

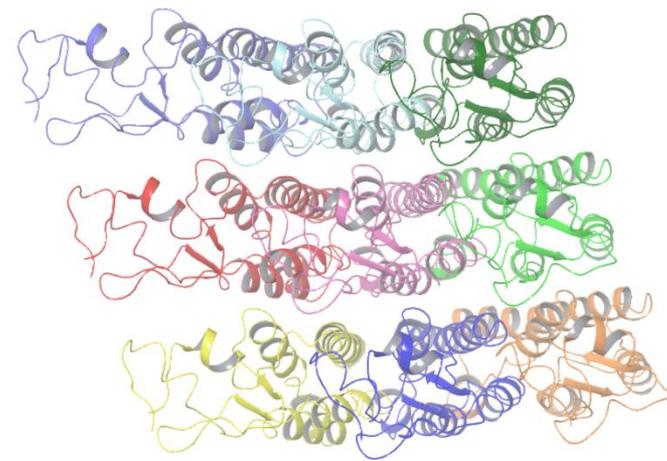
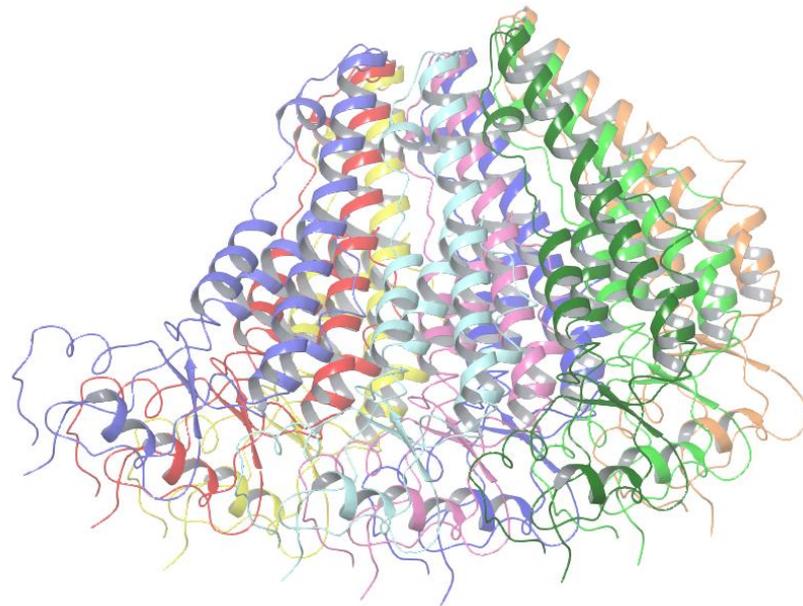
-1.40800

$$\begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix} = \begin{pmatrix} BIOMT1_{2x} & BIOMT1_{2y} & BIOMT1_{2z} \\ BIOMT2_{2x} & BIOMT2_{2y} & BIOMT2_{2z} \\ BIOMT3_{2x} & BIOMT3_{2y} & BIOMT3_{2z} \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} + \begin{pmatrix} BIOMT1_{2s} \\ BIOMT2_{2s} \\ BIOMT3_{2s} \end{pmatrix}$$

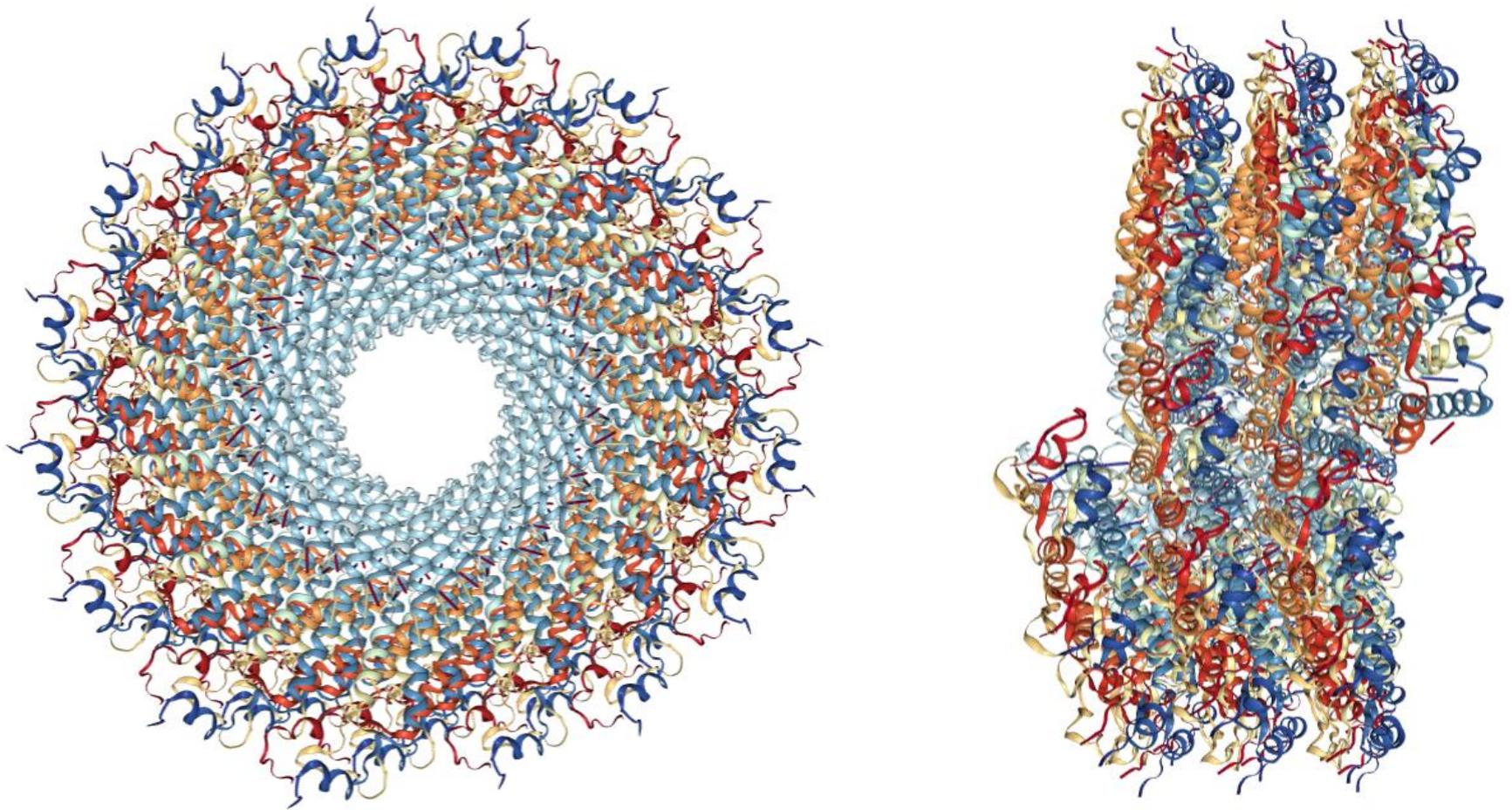
# Вирус табачной мозаики



(pdb-код 4udv)



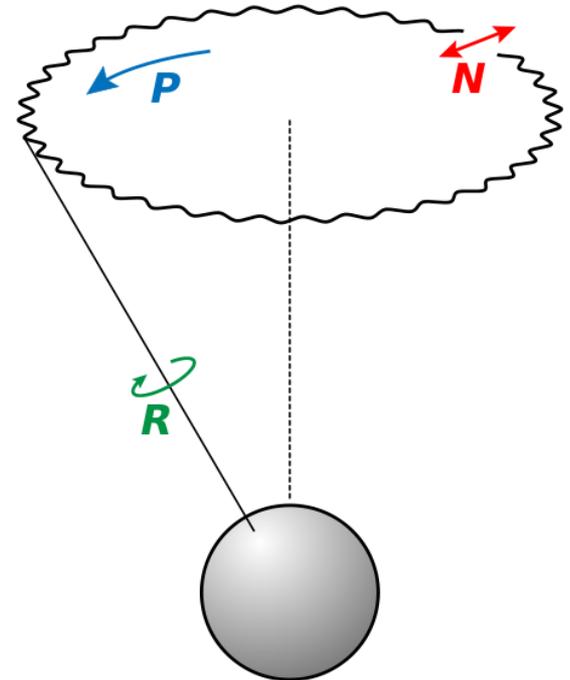
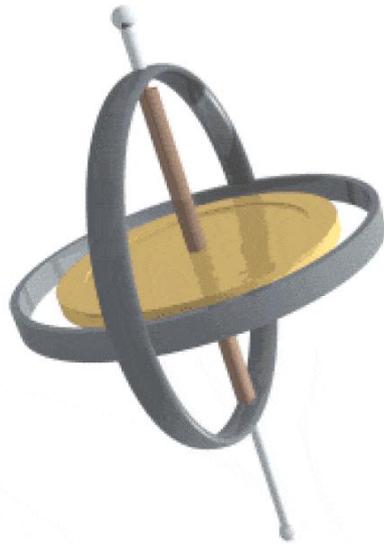
# Вирус табачной мозаики



(pdb-код 4udv)

# Задание поворота в пространстве

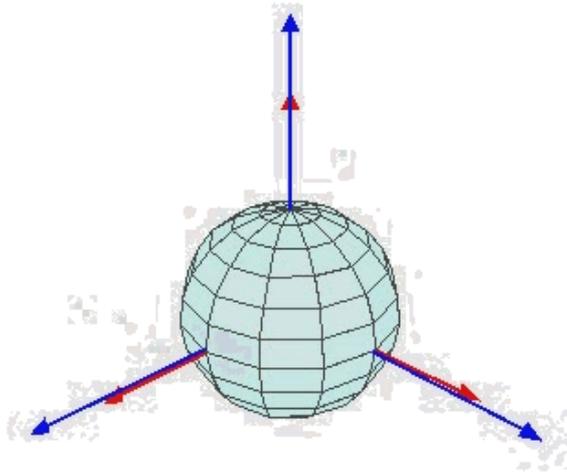
Гироскоп: прецессия, нутация и собственное вращение



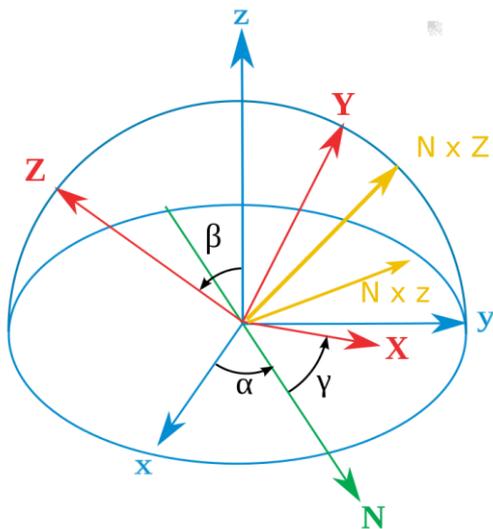
<https://www.youtube.com/watch?v=kgcM7MmBj40>

# Задание поворота в пространстве

Прецессия гироскопа:



Леонард Эйлер  
(1707 – 1783)



$x, y, z$  – исходные оси

$X, Y, Z$  – конечные оси

$N$  – линия узлов

# Задание поворота в пространстве

**Углы Эйлера (1776):**

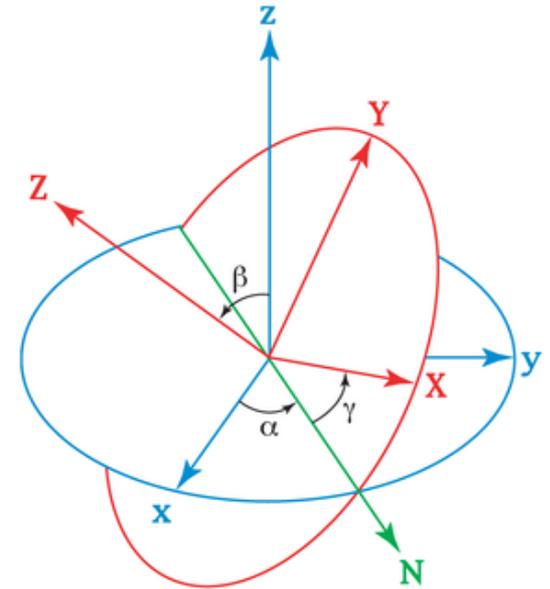
$x, y, z$  — исходные оси

$X, Y, Z$  — конечные оси

Угол  $\alpha$  между осью  $x$  и линией узлов — угол прецессии (поворот вокруг оси  $z$ ).

Угол  $\beta$  между осями  $z$  и  $z'$  — угол нутации (поворот вокруг оси  $x' =$  линии узлов).

Угол  $\gamma$  между осью  $x'$  и линией узлов — угол собственного вращения (поворот вокруг оси  $z'' = Z$ ).



Такие повороты **некоммутативны** и конечное положение системы зависит от порядка, в котором совершаются повороты.

**Недостатки: сложность вычислений при комбинации вращений, «складывание рамок карданова подвеса» ( $\beta=0$ ).**

**Используются в ЭМ, ЯМР, ЭПР.**

# Задание поворота в пространстве

Карданов подвес



# Задание поворота в пространстве

**Кватернионы** (1843): система гиперкомплексных чисел, образующая векторное пространство размерностью четыре над полем вещественных чисел.

$$q = a + bi + cj + dk$$

$$\bar{q} = a - bi - cj - dk$$

$$|q|^2 = a^2 + b^2 + c^2 + d^2$$

$$q^{-1} = \frac{\bar{q}}{|q|^2}$$

×	<b>1</b>	<b>i</b>	<b>j</b>	<b>k</b>
<b>1</b>	1	<i>i</i>	<i>j</i>	<i>k</i>
<b>i</b>	<i>i</i>	-1	<i>k</i>	- <i>j</i>
<b>j</b>	<i>j</i>	- <i>k</i>	-1	<i>i</i>
<b>k</b>	<i>k</i>	<i>j</i>	- <i>i</i>	-1



Уильям Роуэн Гамильтон  
(1805 — 1865)



# Задание поворота в пространстве

Описание поворота через кватернион:

$$q = w + x\mathbf{i} + y\mathbf{j} + z\mathbf{k} = w + (x, y, z) = \cos(\alpha/2) + \mathbf{u} \sin(\alpha/2)$$

$$\vec{t} = q\vec{v}q^{-1} = \frac{q\vec{v}\bar{q}}{|q|^2}$$

-результат поворота вектора  $\mathbf{v}$   
вокруг вектора  $\mathbf{u}$  на угол  $\alpha$

$$T = QVQ^{-1} = \frac{QVQ^T}{\sqrt{\det(Q)}}$$

- он же в матричном виде

Преимущества: а) интуитивно понятный смысл и отсутствие «складывания рамок»  
б) возможность использования векторной алгебры  
в) легкость выполнения интерполяции

$$q(t) = (1-t)q_1 + tq_2, \quad 0 < t < 1$$

# Задание поворота в пространстве

Пример: поворот вектора  $\mathbf{v}$   $(1, 0, 0)$  вокруг вектора  $\mathbf{u}$   $(1, 1, 1)$  на угол  $120^\circ$ .

Кватернион поворота

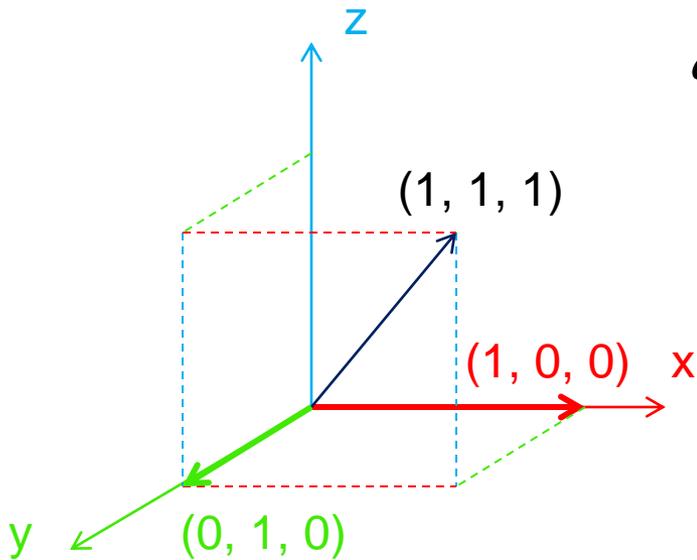
$$q = \cos\left(\frac{\pi}{3}\right) + \sin\left(\frac{\pi}{3}\right)\vec{i} + \sin\left(\frac{\pi}{3}\right)\vec{j} + \sin\left(\frac{\pi}{3}\right)\vec{k}$$

Вектор  $\mathbf{u}$  должен быть единичным, поэтому переобозначим

$$\mathbf{u} = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$$

и для кватерниона получаем

$$q = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{1}{2}(1, 1, 1, 1)$$



# Задание поворота в пространстве

In quaternion form

$$q = \frac{1}{2}(1, 1, 1, 1) \quad q^{-1} = \frac{1}{2}(1, -1, -1, -1) \quad \vec{v} = (0, 1, 0, 0)$$

Note that  $|q|^2 = 1$

$$\vec{t} = q\vec{v}q = \frac{1}{4}(1, 1, 1, 1)(0, 1, 0, 0)(1, -1, -1, -1) = \frac{1}{4}(1 + \vec{i} + \vec{j} + \vec{k})(\vec{i})(1 - \vec{i} - \vec{j} - \vec{k}) =$$

$$= \frac{1}{4}(1 + \vec{i} + \vec{j} + \vec{k})(\vec{i} + 1 - \vec{k} + \vec{j}) =$$

$$= \frac{1}{4}((1 + \vec{i} + \vec{j} - \vec{k}) + \vec{i}(1 + \vec{i} + \vec{j} - \vec{k}) + \vec{j}(1 + \vec{i} + \vec{j} - \vec{k}) + \vec{k}(1 + \vec{i} + \vec{j} - \vec{k})) =$$

$$= \frac{1}{4}(1 + \vec{i} + \vec{j} - \vec{k} + \vec{i} - 1 + \vec{k} + \vec{j} + \vec{j} - \vec{k} - 1 - \vec{i} + \vec{k} + \vec{j} - \vec{i} + 1) =$$

$$= \frac{1}{4}(0 + 0\vec{i} + 4\vec{j} + 0\vec{k}) = (0, 0, 1, 0)$$

that corresponds to a vector  $\vec{t} = (0, 1, 0)$

$\times$	<b>1</b>	<b>i</b>	<b>j</b>	<b>k</b>
<b>1</b>	1	i	j	k
<b>i</b>	i	-1	k	-j
<b>j</b>	j	-k	-1	i
<b>k</b>	k	j	-i	-1

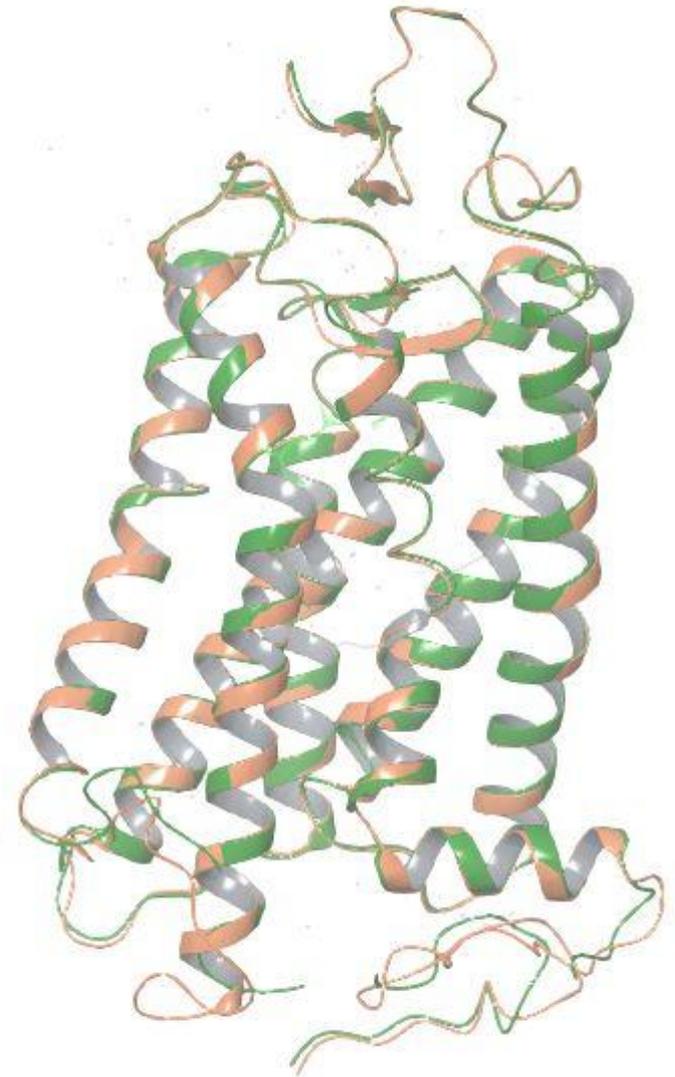
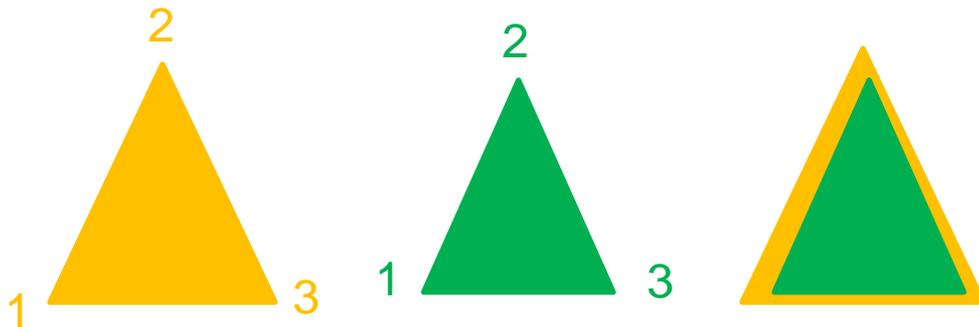
# Структурные выравнивания

Варианты задачи:

1) Взаимное соответствие атомов известно заранее:

$$p_i \leftrightarrow q_i, i = 1, \dots, N$$

(различные структуры или модели одной и той же последовательности или близко гомологичных последовательностей одинаковой длины);



Совмещение структур зрительного родопсина (pdb-коды 1u19 и 1f88)

# Структурные выравнивания

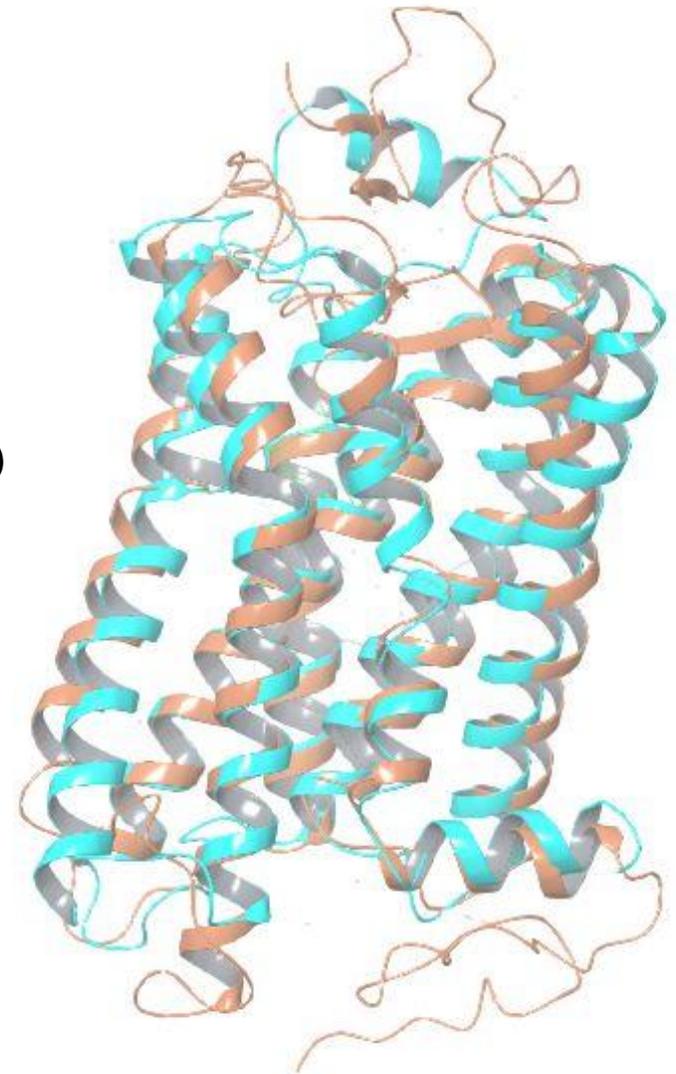
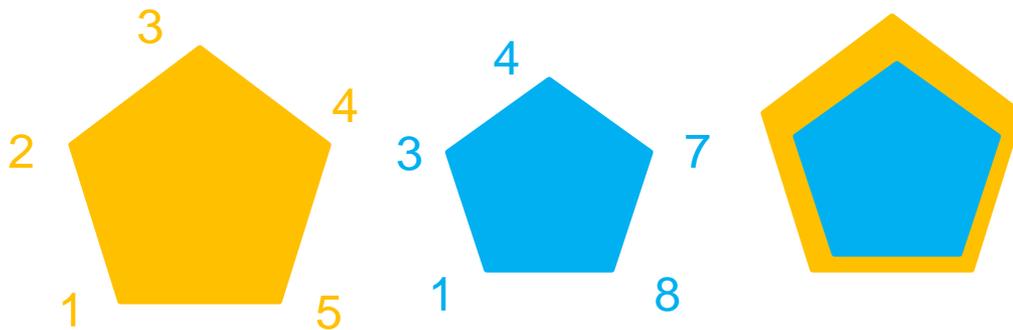
Варианты задачи:

2) Соответствие неизвестно, но известен порядок следования:

$$P_{i(k)} \leftrightarrow q_{j(k)}, i = 1, \dots, K \leq N, M,$$

$$\text{причем } k_1 > k_2 \Leftrightarrow i(k_1) > i(k_2), j(k_1) > j(k_2)$$

(структуры последовательностей разной длины, имеющие вставки в выравнивании последовательностей);



Совмещение структур зрительного родопсина (pdb-код 1u19) и  $\beta$ 2-адренэргического рецептора (pdb-код 2rh1)

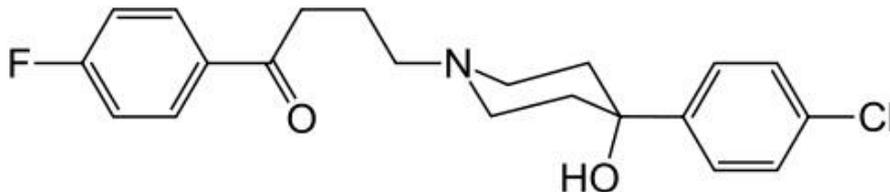
# Структурные выравнивания

Варианты задачи:

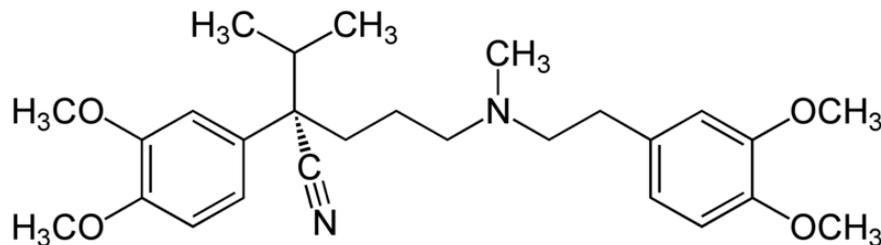
3) Неизвестно ни соответствие, ни порядок следования:

$$P_{i(k)} \leftrightarrow q_{j(k)}, i = 1, \dots, K \leq N, M$$

(фармакофоры)



Галоперидол  
(блокатор дофаминовых  
рецепторов)



Верапамил  
(блокатор потенциал-зависимых  
кальциевых каналов)

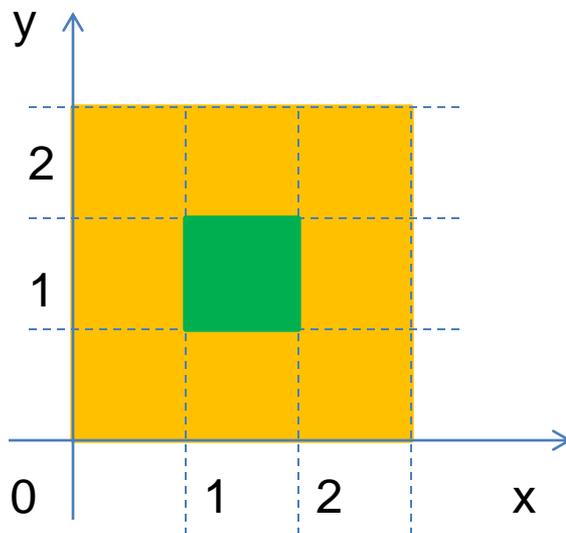
Оба проявляют активность в отношении калиевых каналов

# Структурные выравнивания

Мера близости (для структур с заранее известным взаимным соответствием атомов) - **среднеквадратичное отклонение атомов (СКО):**

$$СКО = \sqrt{\frac{\sum_i \left( (x_i - x_i^0)^2 + (y_i - y_i^0)^2 + (z_i - z_i^0)^2 \right)}{n}}$$

(обычно рассчитывается для Са-атомов, но в случае очень близких гомологов – для всех тяжелых атомов)



$$СКО = \sqrt{2}$$

Продолжение следует...