



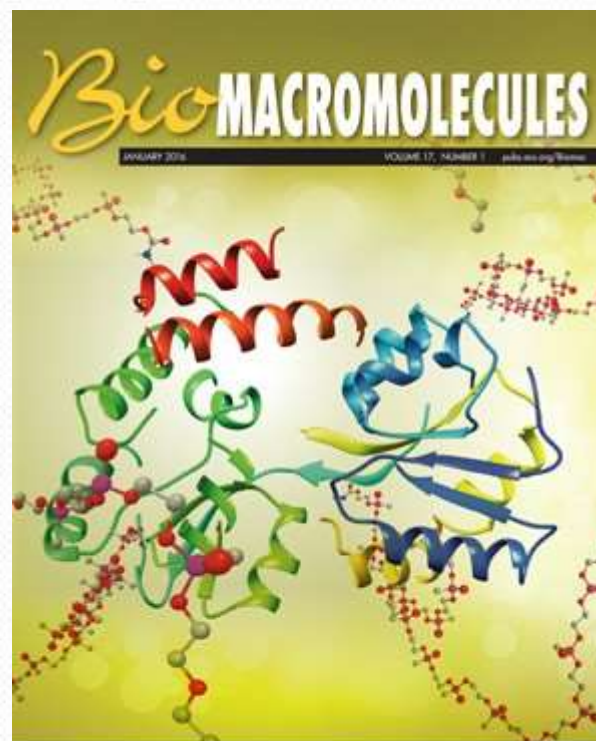
Analiza baz sekwencyjnych biomakromolekuł

Semest Letni 2017

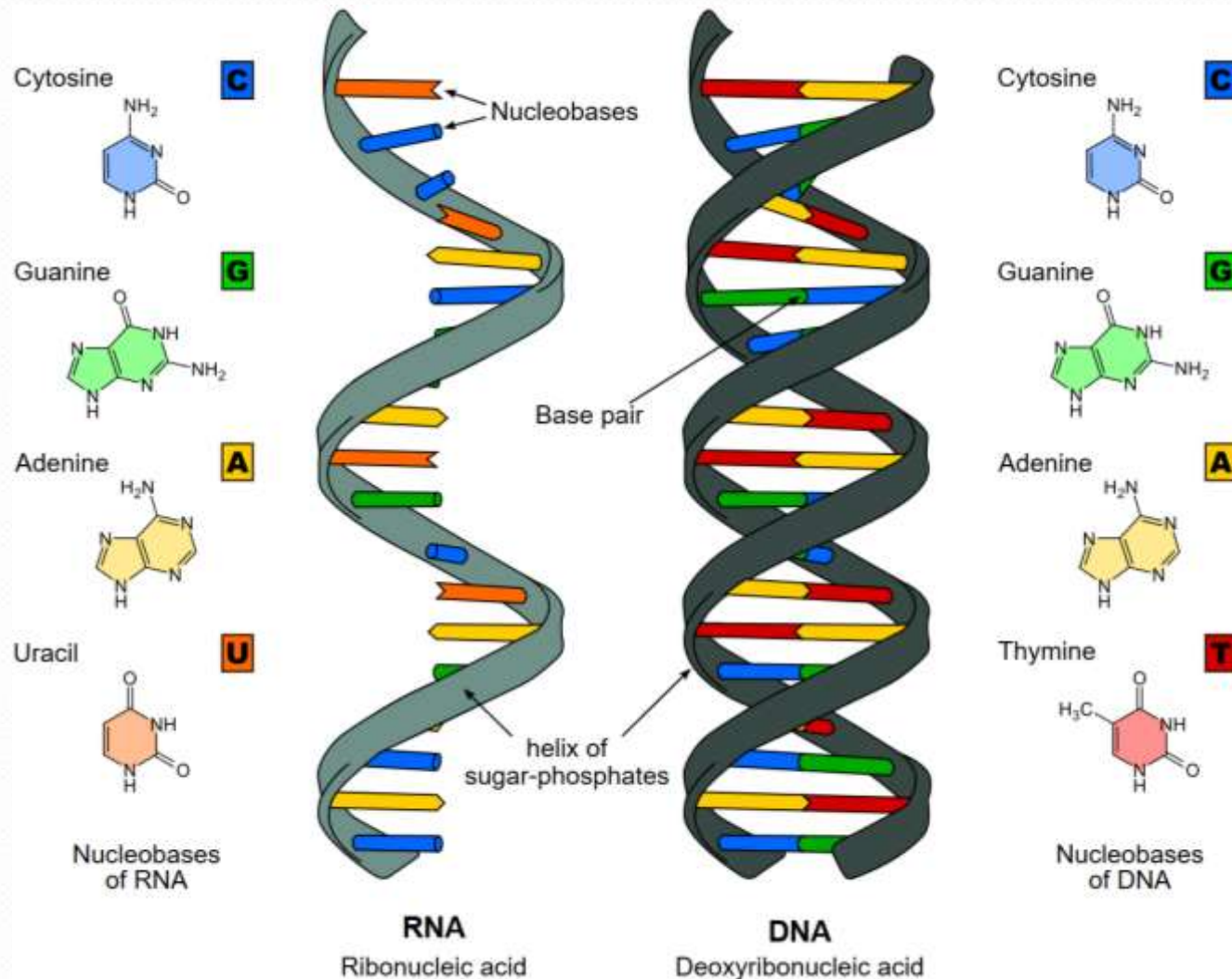
Magdalena Mozolewska

Biomacromolecules

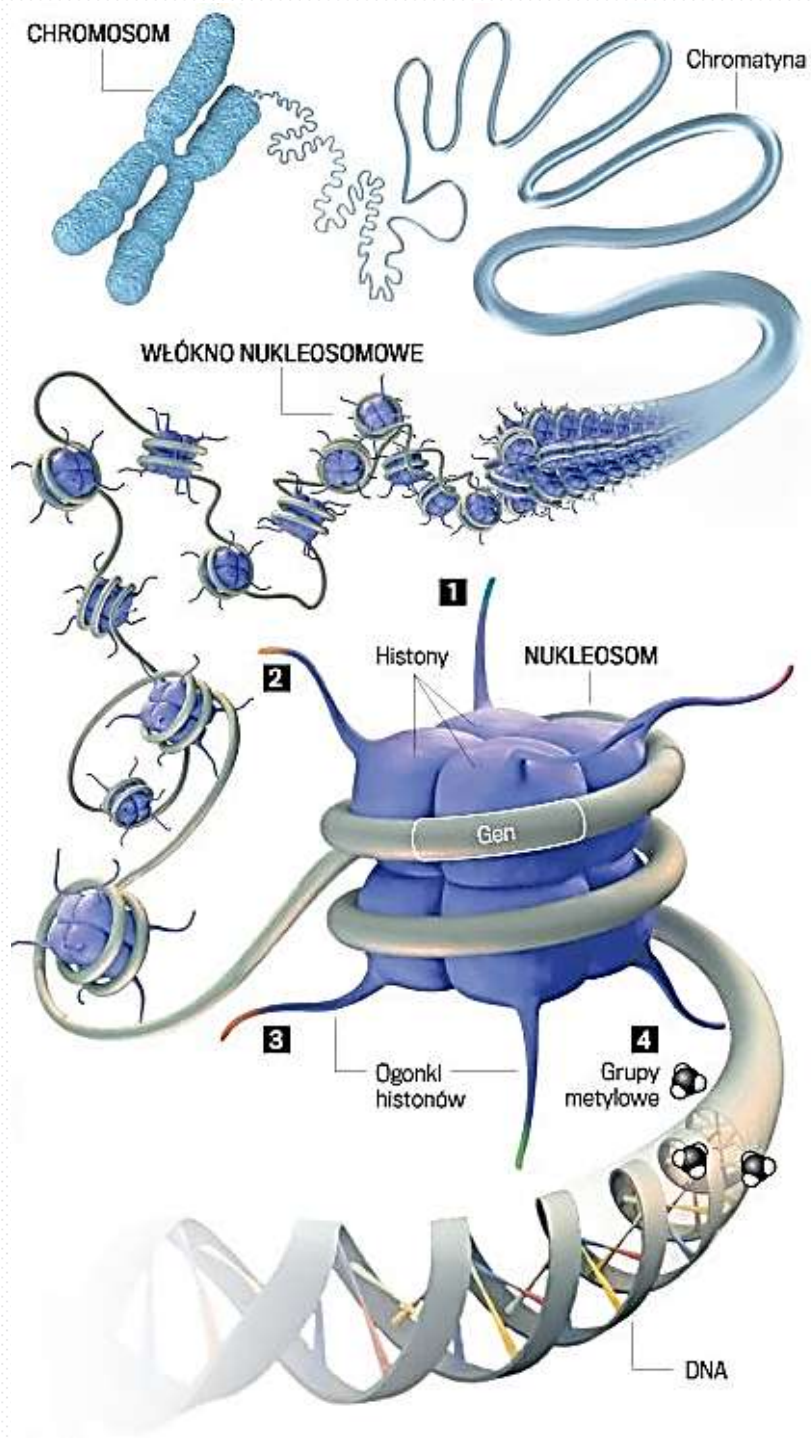
- Proteins
- Nucleic acids
- Polysaccharides
- Lipids (?)



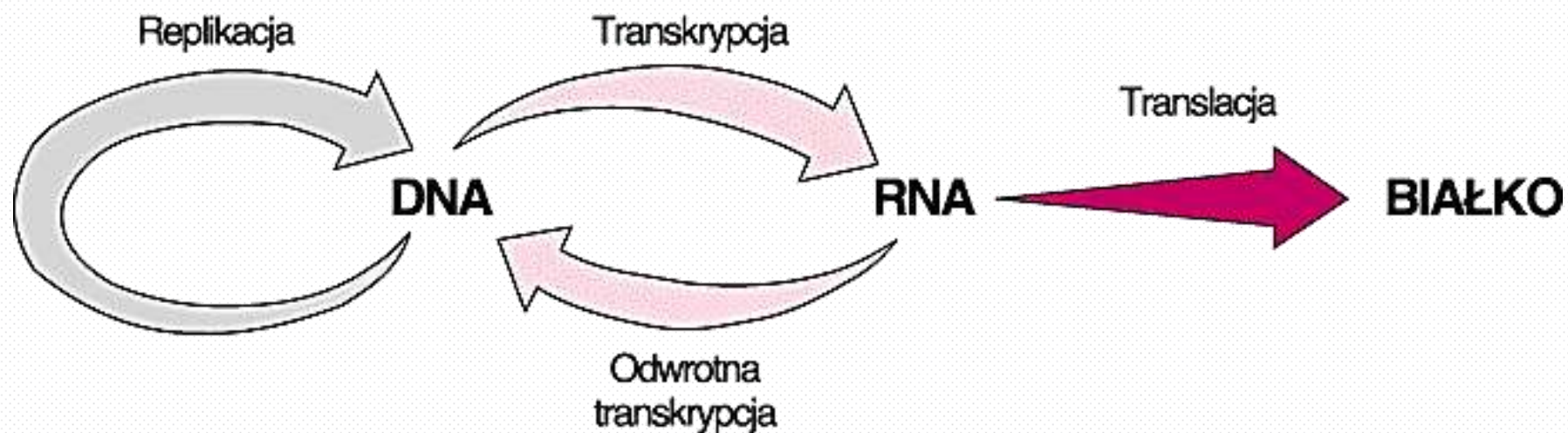
Nucleic acids



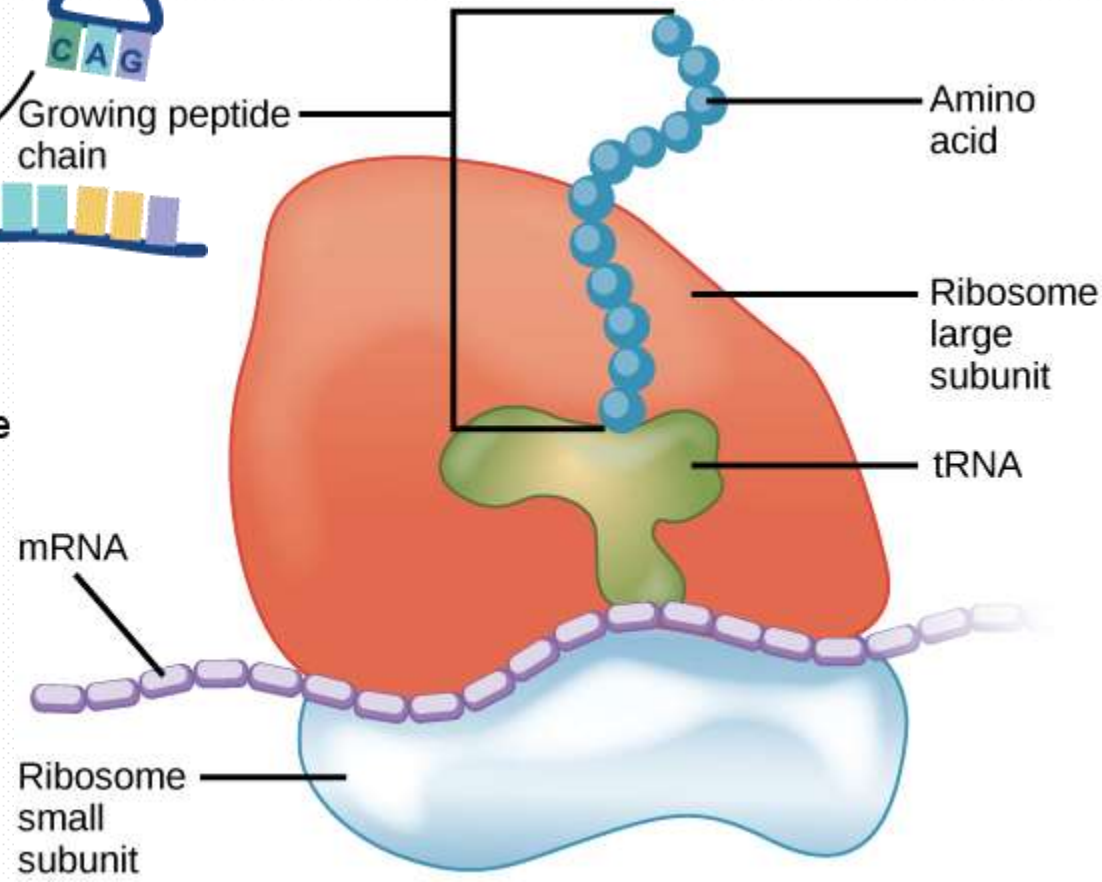
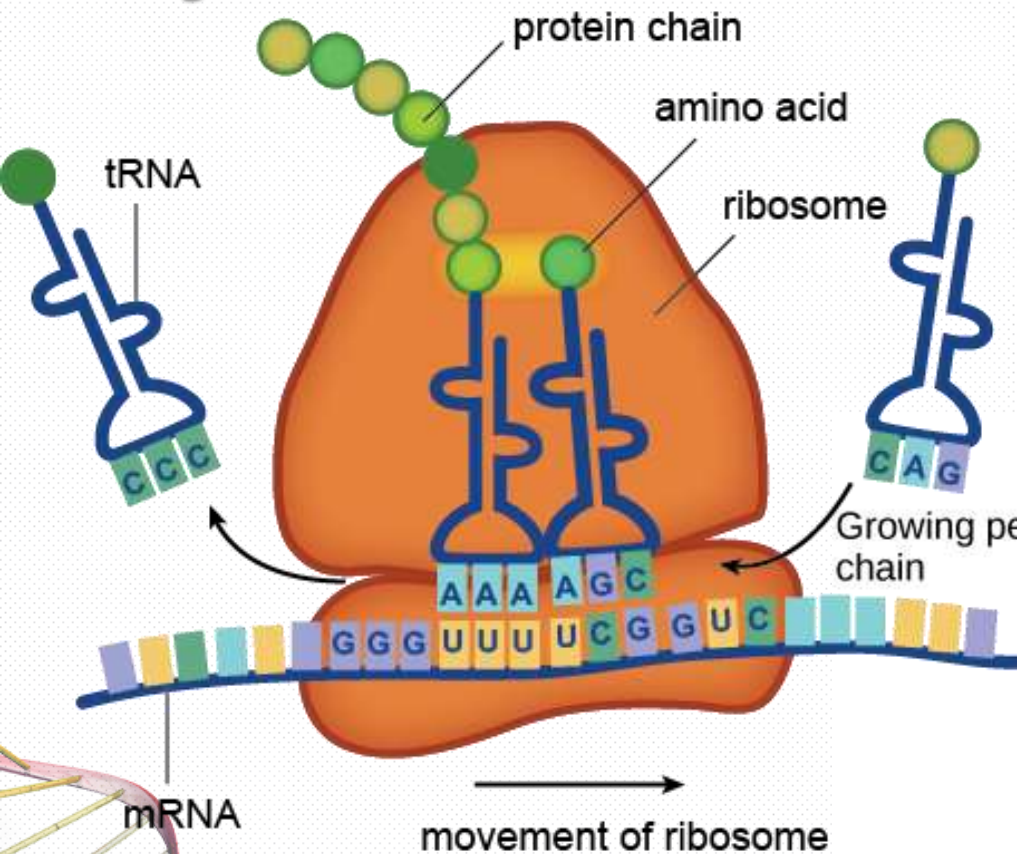
DNA



Od DNA do Białka

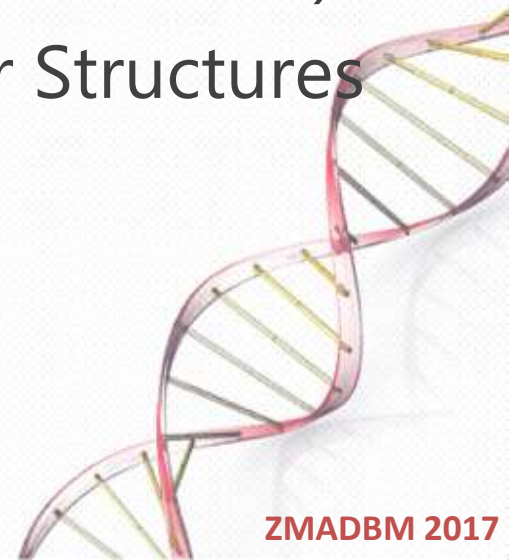


Rybosom



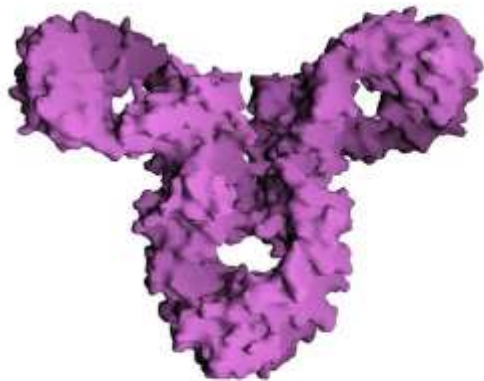
Proteins

- 20 types of natural amino-acid types
- Peptides (from 2 to 50 or 100 residues)
- Proteins (from 20 to 34350 (or more) amino-acid residues)
- Protein DataBank (PDB) – database with protein structures marked by pdb codes (4 letter codes)
 - 134 983 Biological Macromolecular Structures (and increasing every day)



Białka

- *Wielkocząsteczkowe (masa cząsteczkowa od ok. 10 000 do kilku mln Daltonów) biopolimery, a właściwie biologiczne polikondensaty, zbudowane z reszt aminokwasów połączonych ze sobą wiązaniami peptydowymi -CONH-. Występują we wszystkich żywych organizmach oraz wirusach.*



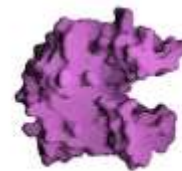
Przeciwciało (IgG)



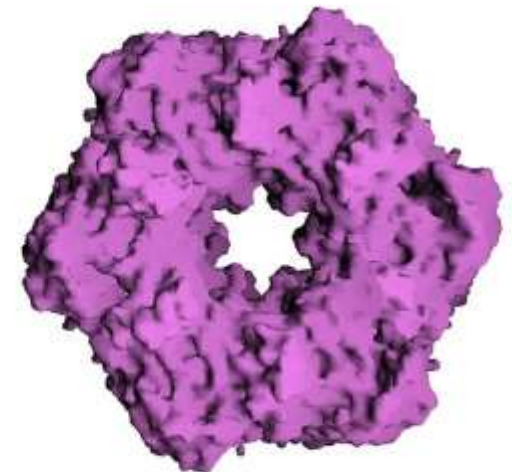
Hemoglobina



Insulina



Kinaza AK1



Ligaza glutaminy



STRUKTURALNE

Odpowiedzialne za mechaniczną stabilność narządów i tkanek. Do białek strukturalnych zalicza się także histony pełniące kluczową rolę w upakowaniu DNA w chromatynie

ZAPASOWE

Niektóre białka budujące mięśnie mogą być wykorzystywane jako materiał energetyczny; także wiele białek roślinnych pełni funkcję zapasową

ODPOI

To białka układu (np. immunologicznego) organizmowi chronią przed chorobami

FUNKCJE BIAŁEK

ENZYMATYCZNE

przyspieszające specyficzne reakcje chemiczne

TRANSPORTUJĄCE

To białka uczestniczące w transportowaniu różnych substancji odżywczych jak np. hemoglobina uczestnicząca w transporcie tlenu i CO₂.

REGULACYJNE

To niektóre hormony, a także receptory uczestniczące w percepcji różnych cząsteczek sygnałowych; białkami regulatorowymi są także czynniki transkrypcyjne, regulujące ekspresję genów

Foods High in Protein



Meat and fish



Cheese



Eggs



Beans



Bread



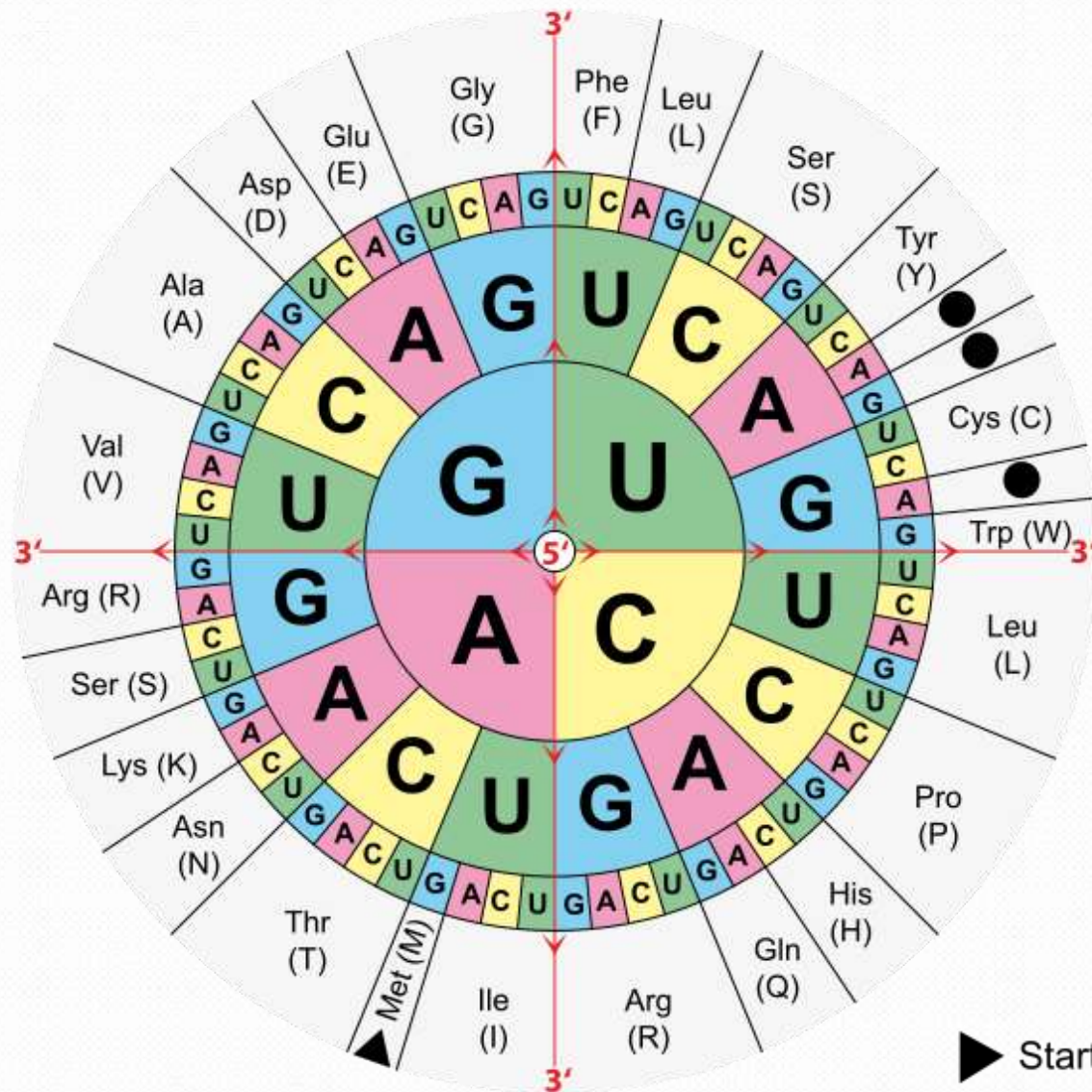
Hummus



Nuts and seeds

©Nutrientsreview.com

Tabela kodonów



► Start
● Stop





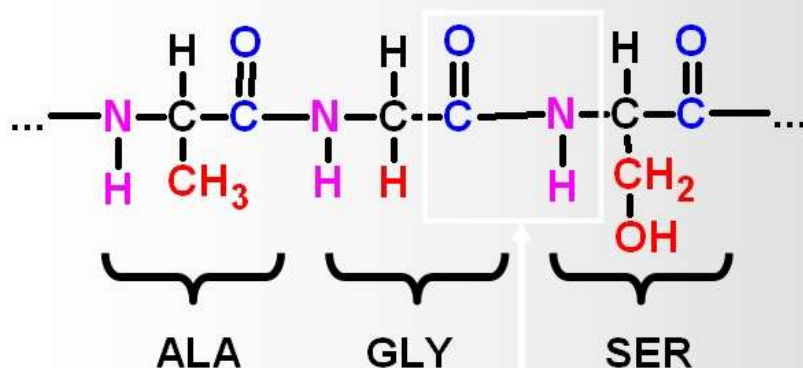
BUDOWA BIAŁEK

Białka są to złożone związki o skomplikowanych wzorach chemicznych.

Białka składają się z połączonych ze sobą aminokwasów tworzących długi łańcuch.

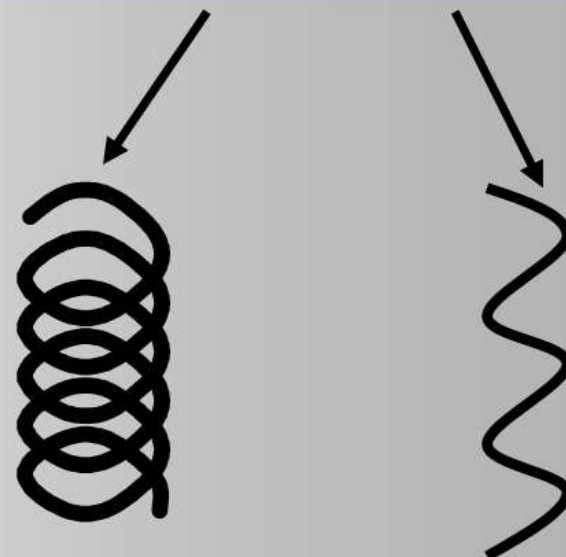


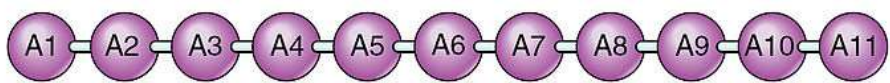
WZÓR FRAGMENTU BIAŁKA, KTÓRY ZAWIERA TRZY AMINOKWASY:



WIAZANIE
PEPTYDOWE

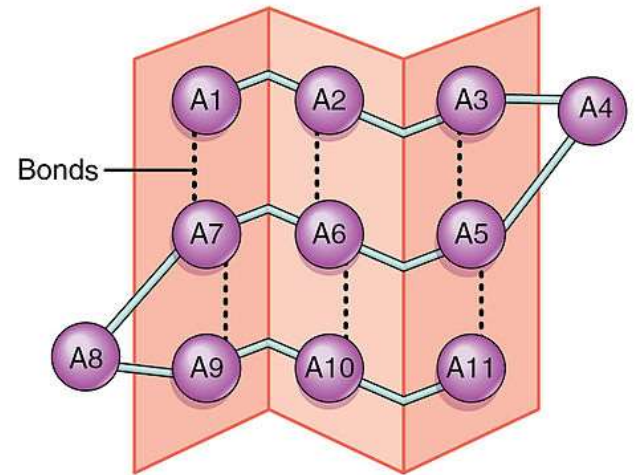
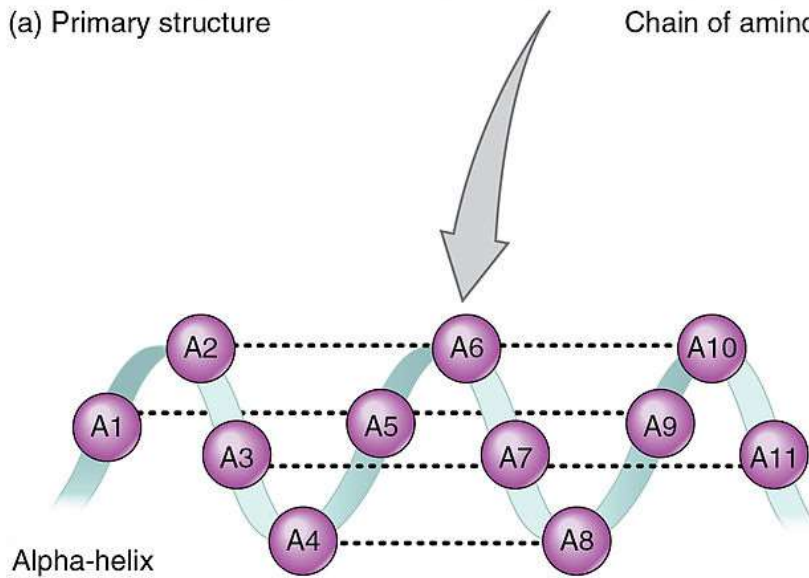
ŁAŃCUCHY AMINOKWASÓW MOGĄ MIEĆ STRUKTURĘ HELISY LUB HARMONIJKI.



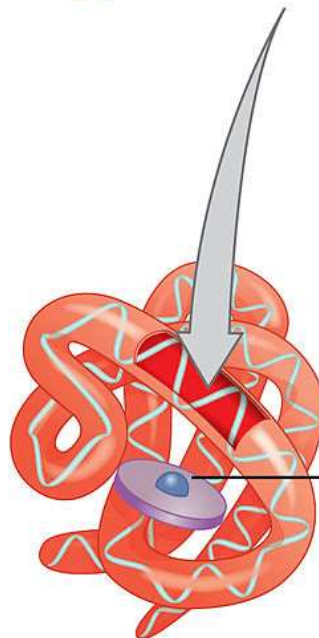
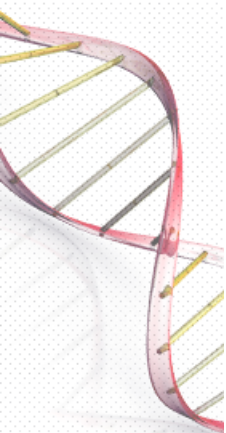


(a) Primary structure

Chain of amino acids

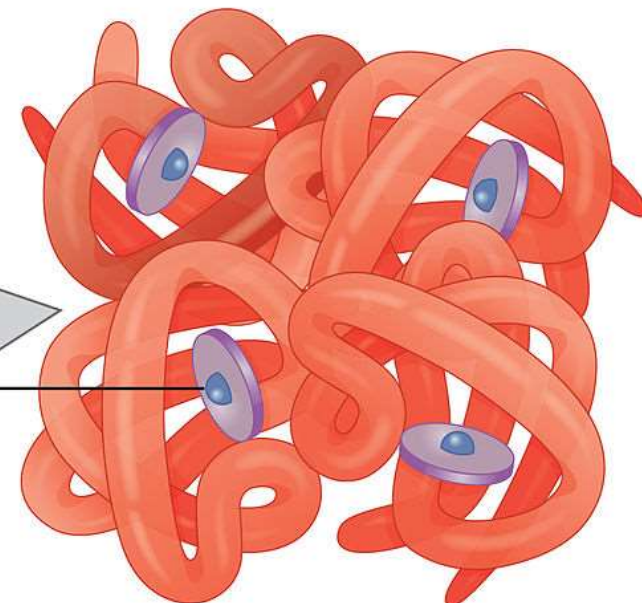


(b) Secondary structure (pleated sheet)



(c) Tertiary structure

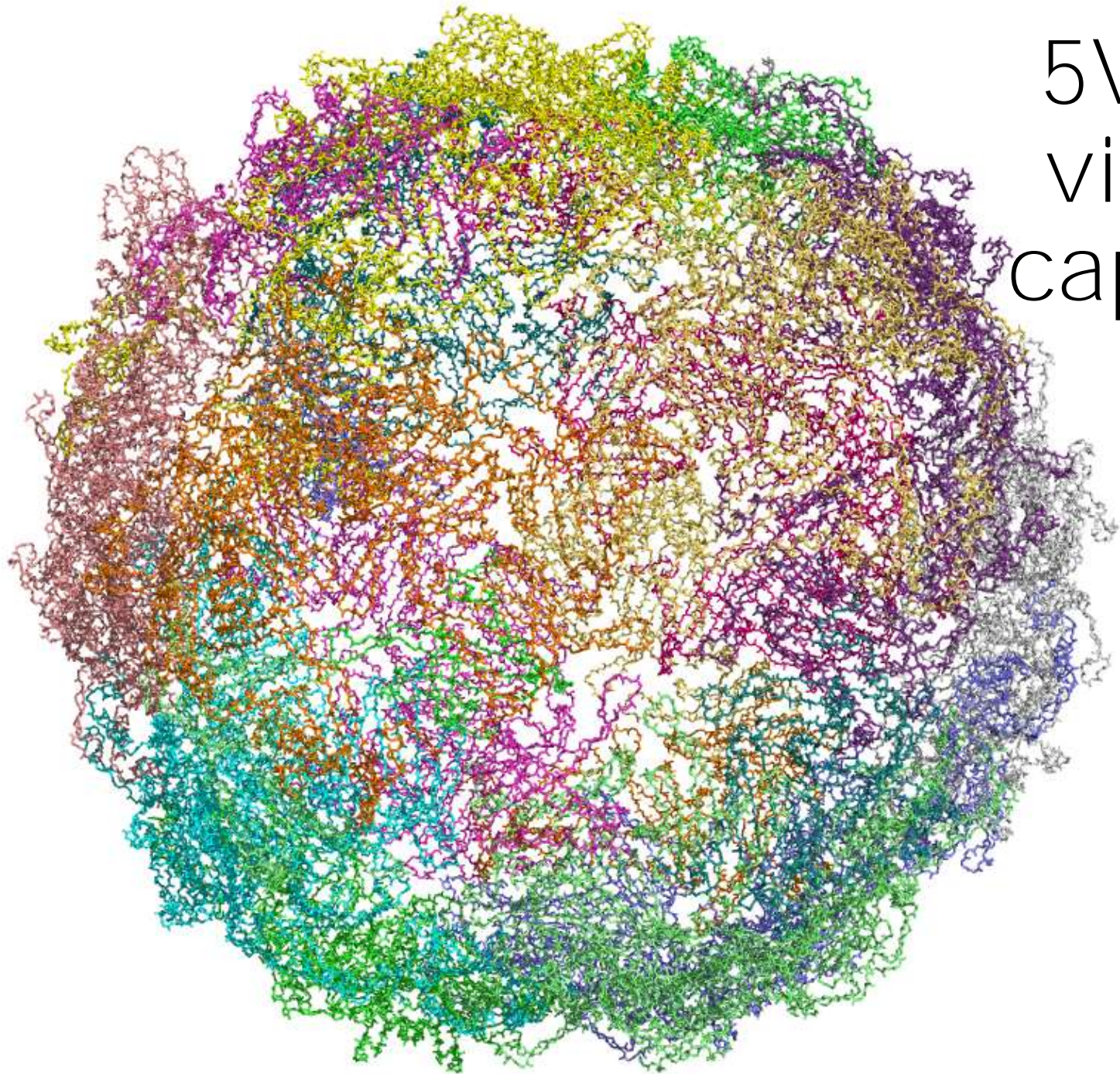
Heme units



(d) Quaternary structure

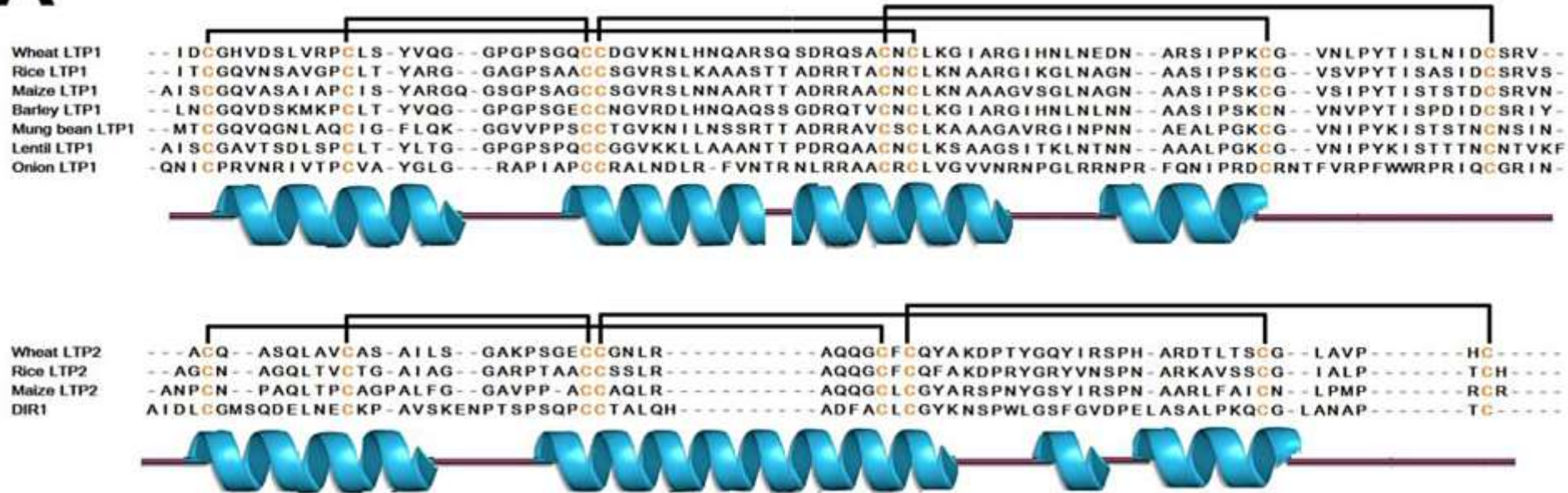
Hemoglobin
(globular protein)

5VLZ virial capsid

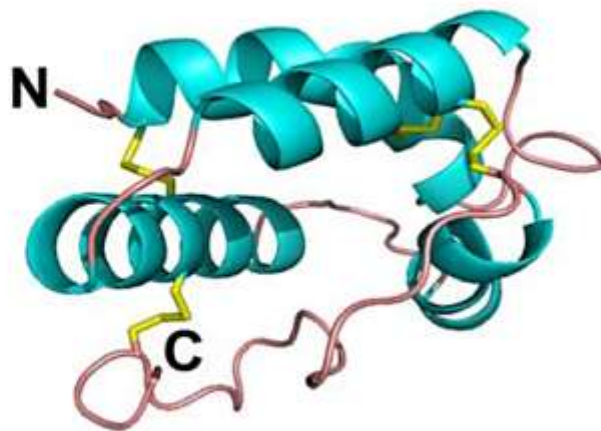


Wiązania disulfidowe

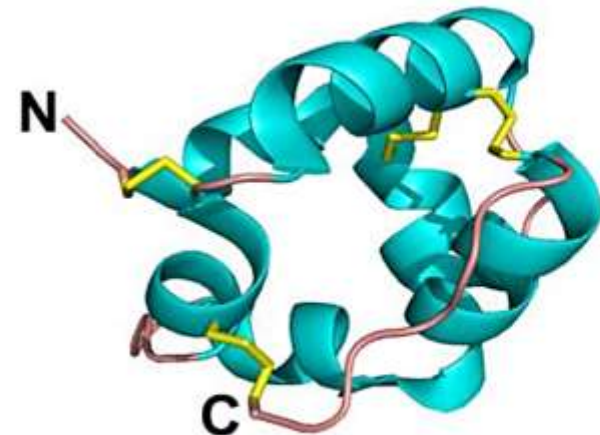
A



B



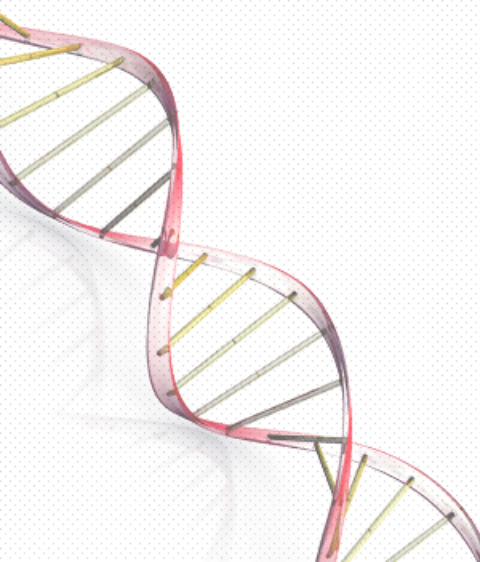
Maize LTP1



Wheat LTP2

Bazy biatek

- RCSB PDB - <http://www.rcsb.org>



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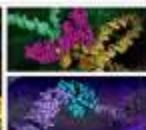
A Structural View of Biology

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.

A Molecular View of HIV Therapy



2016 FASEB BioArt Winner
View animation on PDB-101


March Molecule of the Month



Photoactive Yellow Protein

Latest Entries

As of Tuesday Mar 07



5UQS [PDB Entry](#)

Cryo-EM structure of the Mediator-RNAPII

Features & Highlights

View Validation in 3D
Visualizing structure quality metrics in three dimensions » 10/11

Explore Ligand Interactions in 3D
Analyze small molecule interactions with NGL » 10/11

New Images for Transmembrane Proteins
Access multiple high resolution images that highlight orientation in membranes » 10/11

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Publications ▶

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[wwPDB News: The paper describing wwPDB OneDep system is now available](#) » 02/09

[Download Lists of PDB IDs](#) » 02/07

```
HEADER      DE NOVO PROTEIN                25-FEB-02   1L2Y
TITLE       NMR STRUCTURE OF TRP-CAGE MINIPROTEIN CONSTRUCT TC5B
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: TC5B;
COMPND      3 CHAIN: A;
COMPND      4 ENGINEERED: YES
SOURCE      MOL_ID: 1;
SOURCE      2 SYNTHETIC: YES;
SOURCE      3 OTHER_DETAILS: THE PROTEIN WAS SYNTHESIZED USING STANDARD
SOURCE      4 FMOC SOLID-PHASE SYNTHESIS METHODS ON AN APPLIED
SOURCE      5 BIOSYSTEMS 433A PEPTIDE SYNTHESIZER.
KEYWDS      MINIPROTEIN, TWO-STATE FOLDING, TRP-CAGE, DE NOVO PROTEIN
EXPDTA      SOLUTION NMR
NUMMDL      38
AUTHOR      J.W.NEIDIGH,R.M.FESINMEYER,N.H.ANDERSEN
REVDAT      2   24-FEB-09 1L2Y   1   VERSN
REVDAT      1   29-MAY-02 1L2Y   0
JRNL        AUTH      J.W.NEIDIGH,R.M.FESINMEYER,N.H.ANDERSEN
JRNL        TITL      DESIGNING A 20-RESIDUE PROTEIN.
JRNL        REF       NAT.STRUCT.BIOL.                V.    9    425 2002
JRNL        REFN      ISSN 1072-8368
JRNL        PMID      11979279
JRNL        DOI       10.1038/NSB798
REMARK      1
REMARK      2
REMARK      2 RESOLUTION. NOT APPLICABLE.
REMARK      3
REMARK      3 REFINEMENT.
REMARK      3   PROGRAM      : AMBER 6.0
REMARK      3   AUTHORS     : KOLLMAN
REMARK      3
REMARK      3 OTHER REFINEMENT REMARKS: 169 NOE DISTANCE CONSTRAINTS WERE
REMARK      3 EMPLOYED. CNS WAS EMPLOYED FOR S.A., FOLLOWED BY MINIMIZATION
REMARK      3 USING THE SANDER MODULE OF AMBER.
REMARK      4
REMARK      4 1L2Y COMPLIES WITH FORMAT V. 3.15, 01-DEC-08
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 28-FEB-02.
REMARK 100 THE RCSB ID CODE IS RCSB015598.
REMARK 210
REMARK 210 EXPERIMENTAL DETAILS
REMARK 210 EXPERIMENT TYPE           : NMR
REMARK 210 TEMPERATURE                (KELVIN) : 282
REMARK 210 PH                        : 7
REMARK 210 IONIC STRENGTH             : NULL
REMARK 210 PRESSURE                   : AMBIENT
REMARK 210 SAMPLE CONTENTS            : 1.0-1.8 MM TC5B
REMARK 210
REMARK 210 NMR EXPERIMENTS CONDUCTED : 2D NOESY
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← Name and PDB code

PDB file

← Article with description

← Refinement (by MD simulation)

← Experimental details

```

REMARK 900 1JRJ IS AN ANALOUS C-TERMINAL STRUCTURE.
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SEQRES 2 A 20 SER GLY ARG PRO PRO PRO SER
HELIX 1 1 ASN A 1 ASP A 9 1
HELIX 2 2 GLY A 10 GLY A 15 5
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ORIGX1 1.000000 0.000000 0.000000 0.000000
ORIGX2 0.000000 1.000000 0.000000 0.000000
ORIGX3 0.000000 0.000000 1.000000 0.000000
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SCALE2 0.000000 1.000000 0.000000 0.000000
SCALE3 0.000000 0.000000 1.000000 0.000000
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ATOM 3 C ASN A 1 -7.117 2.964 -1.897 1.00 0.00 C
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ATOM 6 CG ASN A 1 -10.915 3.130 -2.611 1.00 0.00 C
ATOM 7 OD1 ASN A 1 -11.269 2.700 -1.524 1.00 0.00 O
ATOM 8 ND2 ASN A 1 -11.806 3.406 -3.543 1.00 0.00 N
ATOM 9 H1 ASN A 1 -8.330 3.957 0.261 1.00 0.00 H
ATOM 10 H2 ASN A 1 -8.740 5.068 -0.889 1.00 0.00 H
ATOM 11 H3 ASN A 1 -9.877 4.041 -0.293 1.00 0.00 H
ATOM 12 HA ASN A 1 -8.930 2.162 -1.239 1.00 0.00 H
ATOM 13 HB2 ASN A 1 -9.310 4.417 -3.193 1.00 0.00 H
ATOM 14 HB3 ASN A 1 -9.108 2.719 -3.679 1.00 0.00 H
ATOM 15 HD21 ASN A 1 -11.572 3.791 -4.444 1.00 0.00 H
ATOM 16 HD22 ASN A 1 -12.757 3.183 -3.294 1.00 0.00 H
ATOM 17 N LEU A 2 -6.379 4.031 -2.228 1.00 0.00 N
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ATOM 19 C LEU A 2 -4.136 3.187 -1.404 1.00 0.00 C
ATOM 20 O LEU A 2 -3.391 2.274 -1.760 1.00 0.00 O
ATOM 21 CB LEU A 2 -4.411 5.450 -2.619 1.00 0.00 C
ATOM 22 CG LEU A 2 -4.795 6.450 -1.495 1.00 0.00 C
ATOM 23 CD1 LEU A 2 -3.612 6.803 -0.599 1.00 0.00 C
ATOM 24 CD2 LEU A 2 -5.351 7.748 -2.084 1.00 0.00 C
ATOM 25 H LEU A 2 -6.821 4.923 -2.394 1.00 0.00 H
ATOM 26 HA LEU A 2 -4.750 3.494 -3.403 1.00 0.00 H
ATOM 27 HB2 LEU A 2 -3.340 5.414 -2.672 1.00 0.00 H
ATOM 28 HB3 LEU A 2 -4.813 5.817 -3.564 1.00 0.00 H
ATOM 29 HG LEU A 2 -5.568 6.022 -0.858 1.00 0.00 H
ATOM 30 HD11 LEU A 2 -3.207 5.905 -0.146 1.00 0.00 H
ATOM 31 HD12 LEU A 2 -2.841 7.304 -1.183 1.00 0.00 H
ATOM 32 HD13 LEU A 2 -3.929 7.477 0.197 1.00 0.00 H
ATOM 33 HD21 LEU A 2 -4.607 8.209 -2.736 1.00 0.00 H
ATOM 34 HD22 LEU A 2 -6.255 7.544 -2.657 1.00 0.00 H
ATOM 35 HD23 LEU A 2 -5.592 8.445 -1.281 1.00 0.00 H

```

← Sequence (full)


PDB file

← Coordinates



Inne bazy

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The mission of UniProt is to provide the scientific community with a comprehensive, high-quality and freely accessible resource of protein sequence and functional information.

UniProtKB

UniProt Knowledgebase

Swiss-Prot (553,655)

Manually annotated and reviewed.

Records with information extracted from literature and curator-evaluated computational analysis.

TrEMBL (77,483,538)

Automatically annotated and not reviewed.

Records that await full manual annotation.

UniRef

The UniProt Reference Clusters (UniRef) provide clustered sets of sequences from the UniProt Knowledgebase (including isoforms) and selected UniParc records.


UniParc


UniParc is a comprehensive and non-redundant database that contains most of the publicly available protein sequences in the world.


Proteomes


A proteome is the set of proteins thought to be expressed by an organism. UniProt provides proteomes for species with completely sequenced genomes.


Supporting data


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[Subcellular locations](#)


[Cross-ref. databases](#)


[Diseases](#)


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News

[Forthcoming changes](#)
Planned changes for UniProt

[UniProt release 2017_02](#)
Freshwater fish see red | Cross-references to Araport, TAIR and IMGT/Gene-DB | Removal of sequence similarity annotations for domains

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Sheen in wolves' clothing | Change of the UniRef FASTA header


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Find regions of similarity between your sequences

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Protein spotlight



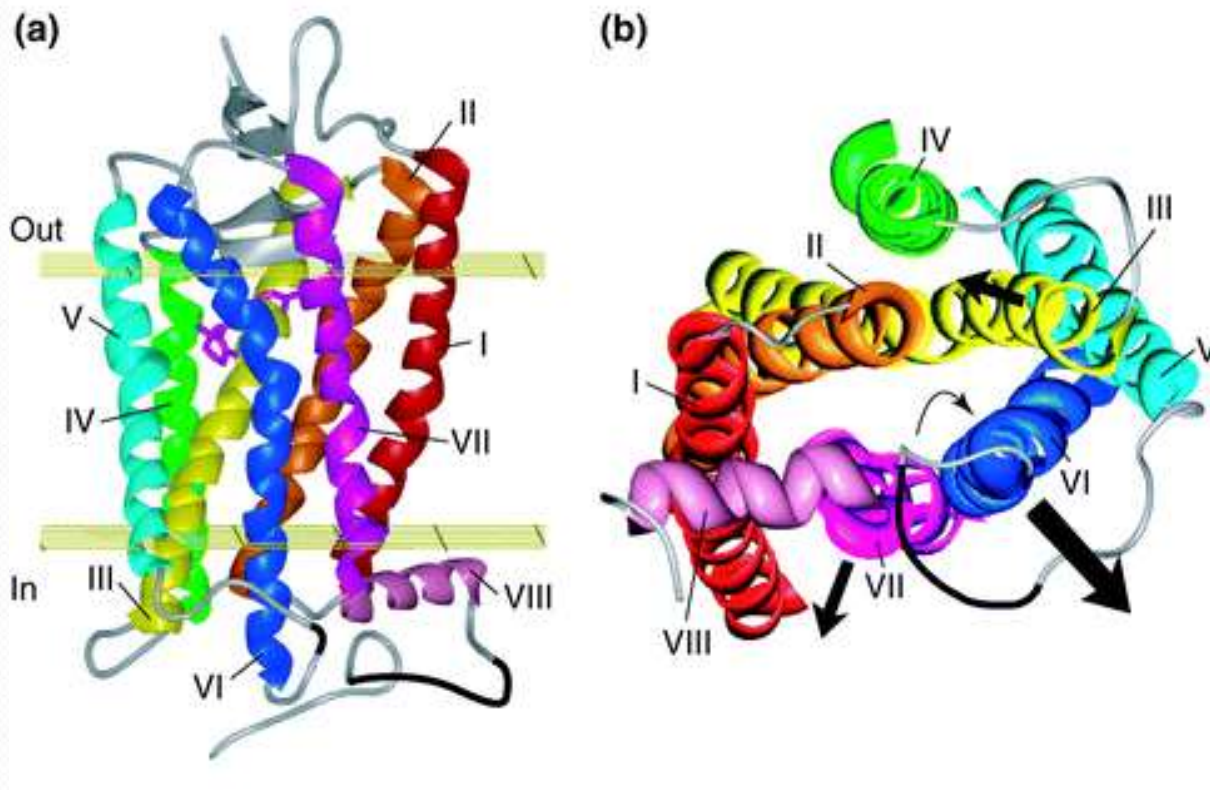
A Walk On The Rough Side

February 2017

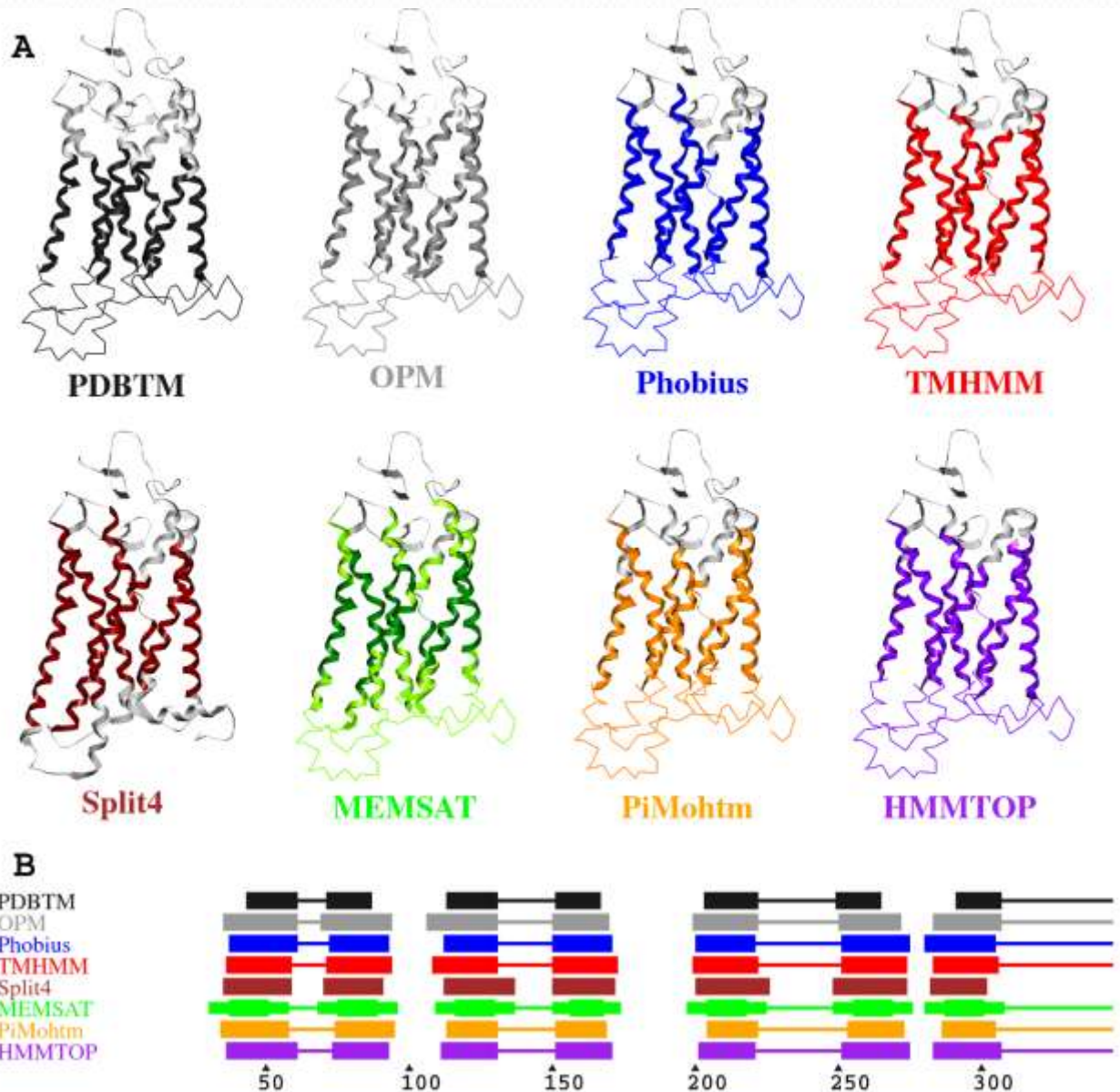
Life can be hard. There are times when you find yourself in the most unfriendly circumstances and, more often than not, the best way to deal with the situation is to find your own solution and wriggle your own way out. Living species are the most imaginative of beings when it comes to designing defence mechanisms. Some release nasty smells to ward off predators, or melt into the landscape and become invisible to them...

Sekwencje białek

- Białka homologiczne?

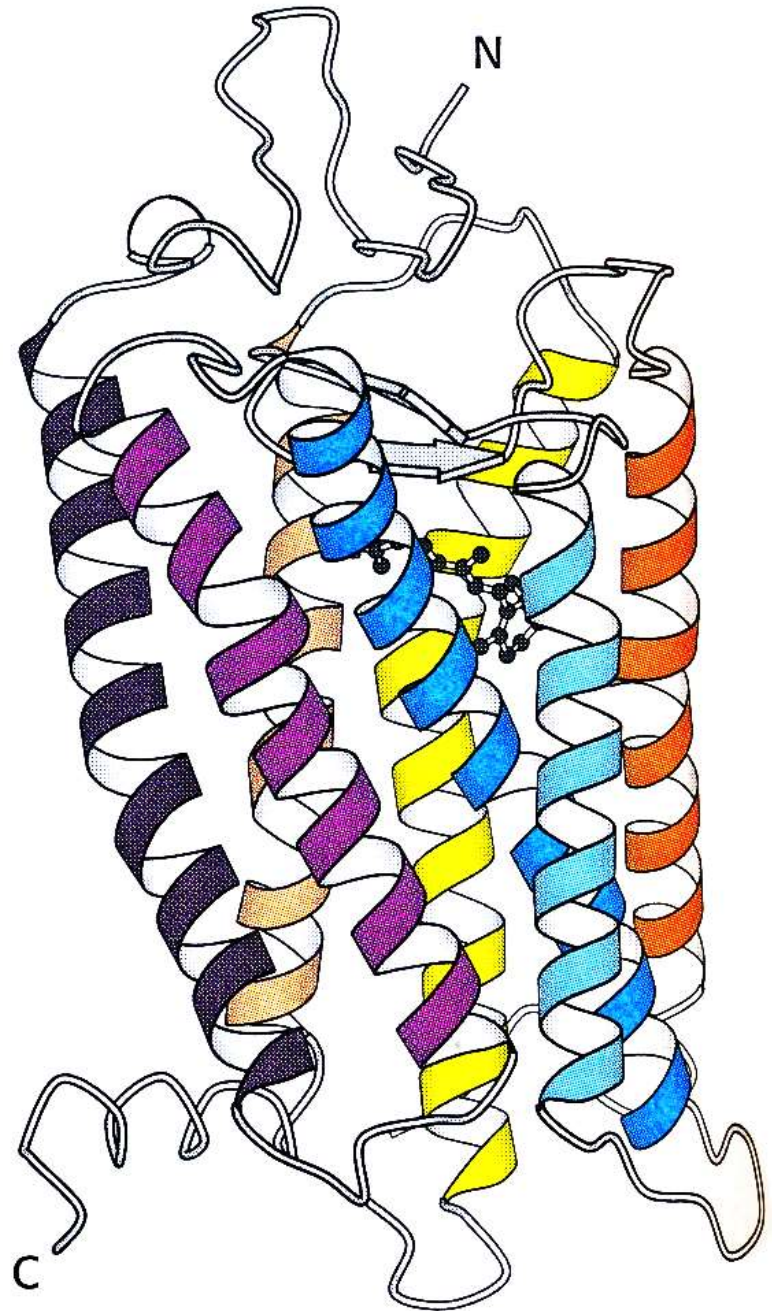


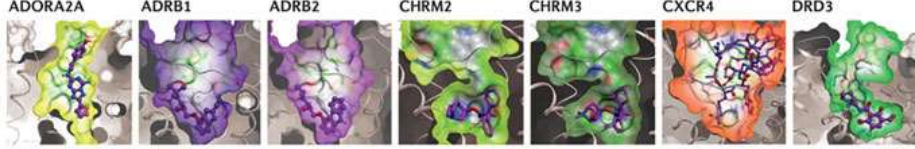
GPCR



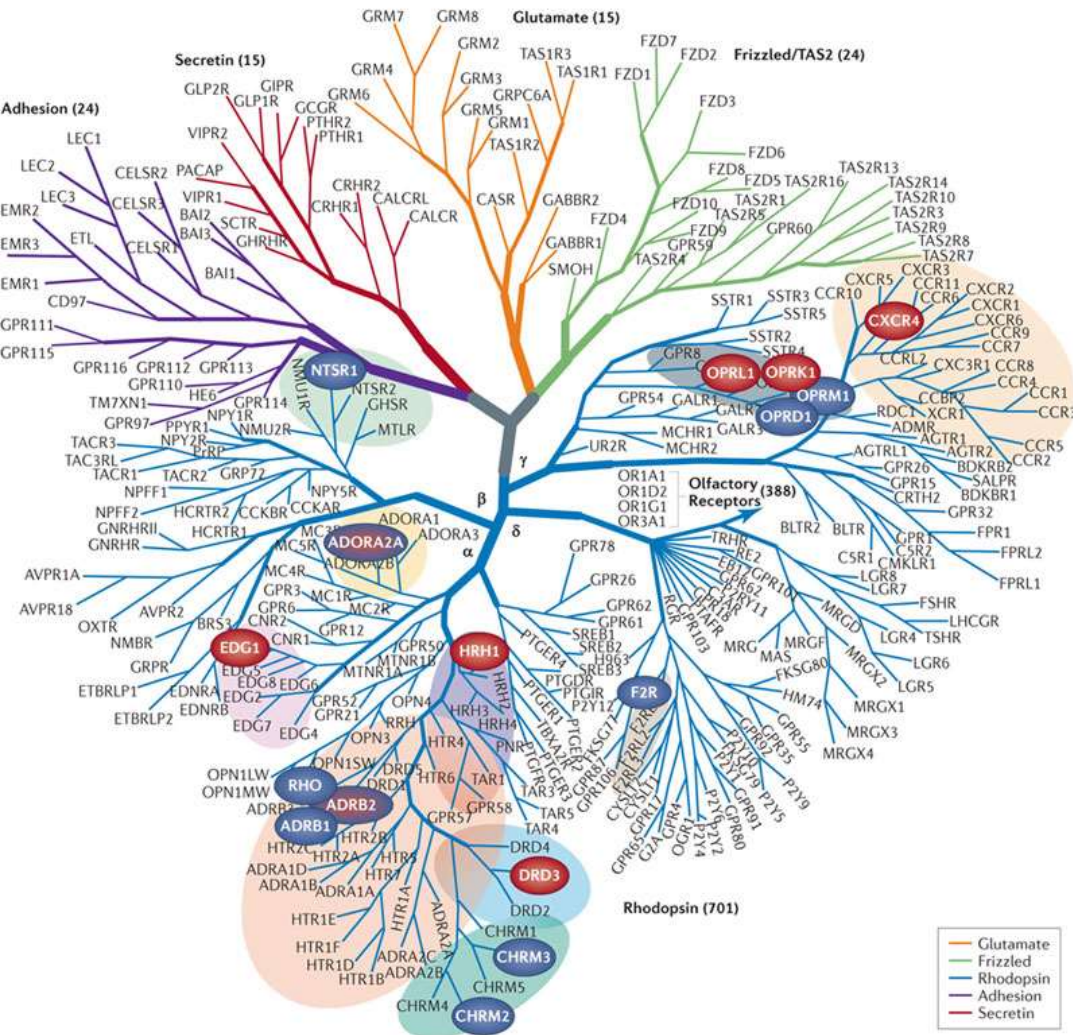
Receptory 7TM, czyli receptory o siedmiu helisach transbłonowych są liczną grupą receptorów, które pośredniczą w m.in.:

- węchu
- smaku
- wzroku
- neurotransmisji
- wydzielaniu hormonów
- chemotaksji
- egzocytozie
- regulacji ciśnienia krwi
- embriogenezie
- wzroście i różnicowaniu komórki
- rozwoju
- infekcjach wirusowych

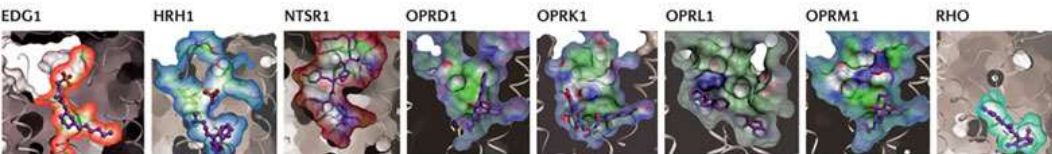




GPCR

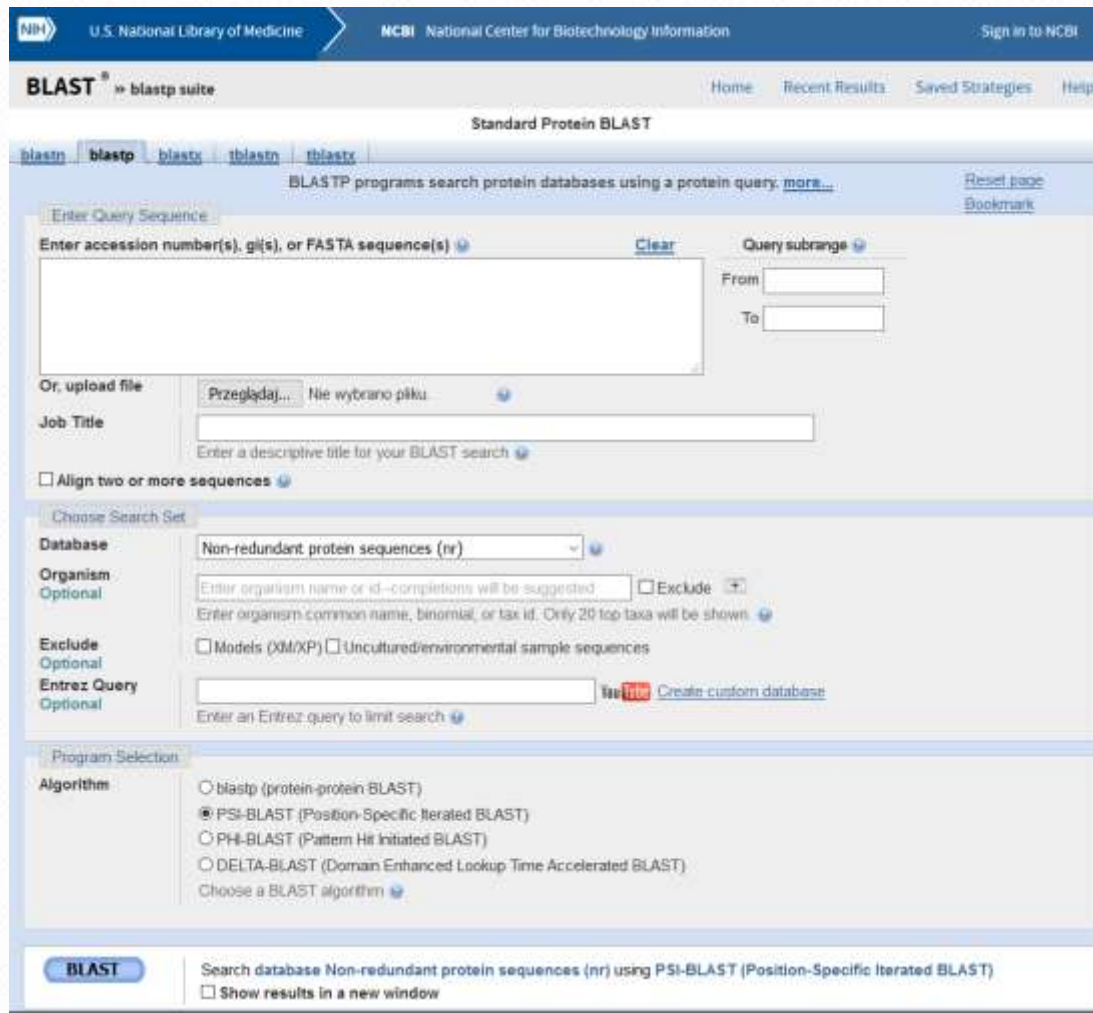


- 30–40% leków oddziałują z GPCR
- Miliardy USD rocznie przeznaczane jest na znajdowanie nowych leków – ligandów GPCR



Białka sekwencyjnie podobne

- PSI-BLAST - <https://blast.ncbi.nlm.nih.gov/>



The screenshot displays the NCBI BLAST web interface for a Standard Protein BLAST search. The header includes the NIH logo, "U.S. National Library of Medicine", "NCBI National Center for Biotechnology Information", and a "Sign in to NCBI" link. The main title is "BLAST® » blastp suite". Navigation links for "Home", "Recent Results", "Saved Strategies", and "Help" are present. The "Standard Protein BLAST" section features tabs for "blastn", "blastp", "blastx", "tblastn", and "tblastx", with "blastp" selected. Below the tabs, a text box for "Enter Query Sequence" is followed by a "Clear" button and a "Query subrange" section with "From" and "To" input fields. An "Or, upload file" section shows a "Przeglądaj..." button and a message "Nie wybrano pliku". A "Job Title" field is also present. The "Choose Search Set" section includes a "Database" dropdown set to "Non-redundant protein sequences (nr)", an "Organism" field with a suggestion icon, and an "Exclude" section with checkboxes for "Models (XM/XP)" and "Uncultured/environmental sample sequences". An "Entrez Query" field is also available. The "Program Selection" section shows the "Algorithm" dropdown set to "PSI-BLAST (Position-Specific Iterated BLAST)". At the bottom, a "BLAST" button and a summary line "Search database Non-redundant protein sequences (nr) using PSI-BLAST (Position-Specific Iterated BLAST)" are visible, along with a checkbox for "Show results in a new window".



CASP

C
A
S
P
12



- The Critical Assessment of protein Structure Prediction
- Ponad 100 grup przewiduje struktury białek tylko na podstawie ich sekwencji
- Pomimo 12 edycji (24 lat) problem ten nie jest i nie będzie szybko całkowicie rozwiązany
- Przewidywane białka oznaczane są kodami T0XXX.



T0763

Sequence analysis results for job: T0763

ID: 1f822970-d609-11e3-82eb-00163e110593

Summary

PSIPRED

Downloads

Secondary Structure Map

Feature predictions are colour coded onto the sequence according to the sequence feature key shown below.

1 M K K T N K I I F I V F I V I F I G L S Y R H F T N T D K A R M E I S S L S S I D V F K F N S F S K 50
51 F S N D K I G V I Y D E E K L S K F K V I M N S L D T S E G I K K I E V P K D A N I E S F K Y S Y H 100
101 I Q P N L K Y V E D N N V Y D G Y F L L Y I L V G D S E G K S Y I I F S G T E L S Y V L D K N N T N 150
151 I L K E I F L N V K K Q Q

Key

Annotations

Helix

M

Sheet

L

Disordered

E

Dompred Boundary

A

DomSSEA Boundary

D

Sequence Resubmission

Start

1

Stop

163

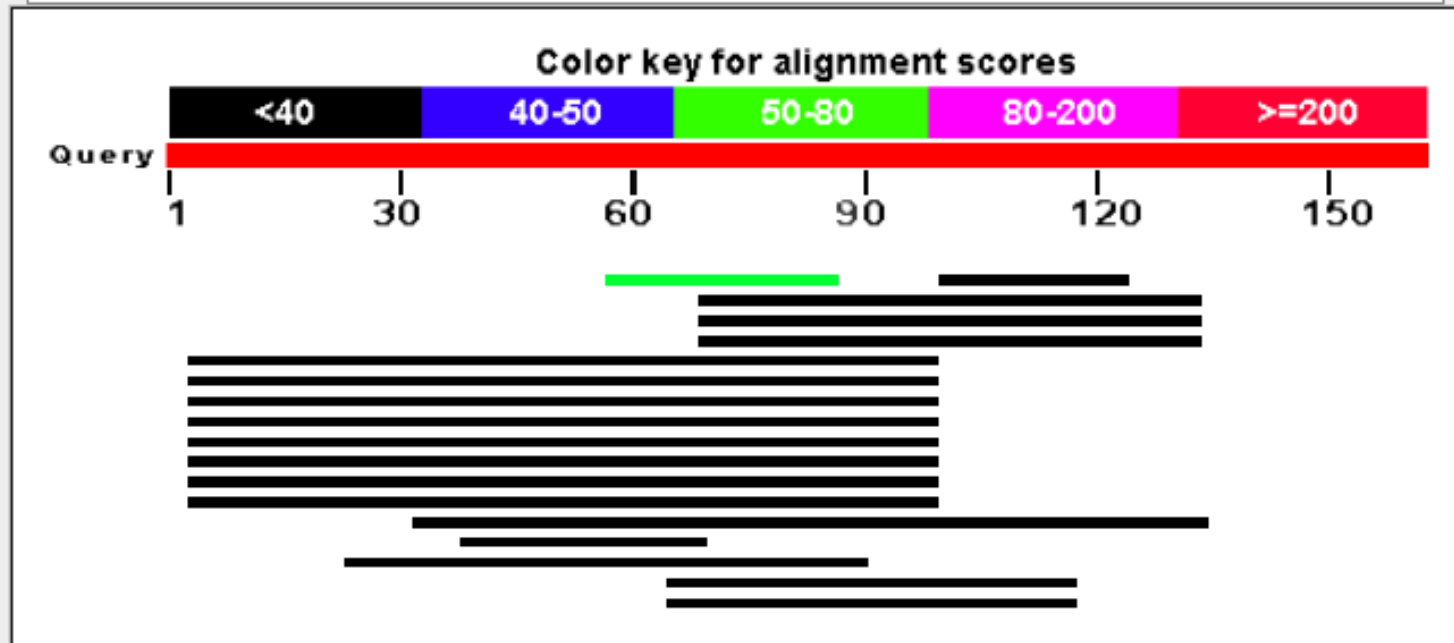
Select Methods



T0763

Distribution of 18 Blast Hits on the Query Sequence [?](#)

Mouse over to see the define, click to show alignments



T0763

Sequences with E-value WORSE than threshold

Select: [All](#) [None](#) Selected: 0

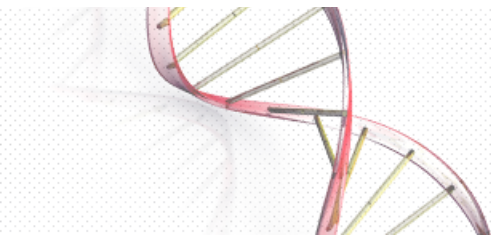
[Alignments](#) [Download](#) [Contact Us](#) [Privacy Policy](#) [Terms of Use](#) [Help](#)

	Description	Max score	Total score	Query cover	E value	Ident	Accession	Select for PSI blast
<input type="checkbox"/>	Chain A, Anti-EgHER3 FAB DL11 IN COMPLEX WITH DOMAINS 1-11 Of The Her3 Extracellular Region [Homo sapiens]	32.7	32.7	39%	0.12	23%	3P11_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain C, Crystal Structure Of Anti-her3 Fab Rq7116 In Complex With The Extracellular Domains Of Human Her3 (erbb3) [Homo sapiens]	32.7	32.7	39%	0.12	23%	4LEO_C	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Her3 Extracellular Domain In Complex With Fab Fragment Of Mor9825 [Homo sapiens]	32.7	32.7	39%	0.12	23%	4P55_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Structure Of The Her3 (Erbb3) Extracellular Domain [Homo sapiens] >pdh1M6BIB Chain B, Structure Of The Her3 (Erbb3) Extracellular Domain	32.7	32.7	39%	0.14	21%	1M6B_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Structure Determination Of A 16.1kDa Copper Protein Rusticyanin At 2.1a Resolution Using Anomalous Scattering Data With Direct Methods [Acidithiobacillus ferrooxidans]	29.6	29.6	59%	0.75	22%	1A8Z_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Crystal Structures Of Ser98asp And Met148leu Rusticyanin [Acidithiobacillus ferrooxidans] >pdh1GY1IB Chain B, Crystal Structures Of Ser98asp And Met148leu Rusticyanin	28.5	28.5	59%	1.7	21%	1GY1_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain V, Localization Of The Small Subunit Ribosomal Proteins Into A 5.5 A Cryo-em Map Of Triticum Aestivum Translating 80s Ribosome [Triticum aestivum]	27.3	27.3	15%	2.3	40%	3J68_V	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Crystal Structure Of Met148leu Rusticyanin [Acidithiobacillus ferrooxidans] >pdh1GY2IB Chain B, Crystal Structure Of Met148leu Rusticyanin	28.1	28.1	59%	2.5	22%	1GY2_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Crystal Structure Of The Met148gin Mutant Of Rusticyanin At 1.5 Angstrom Resolution [Acidithiobacillus ferrooxidans] >pdh1E30IB Chain B, Crystal Structure Of The Met148gin Mutant Of Rusticyanin At 1.5 Angstrom Resolution	28.1	28.1	59%	2.5	22%	1E30_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Rusticyanin (Rc) From Thiobacillus Ferrooxidans [Acidithiobacillus ferrooxidans]	28.1	28.1	59%	2.9	22%	1RCY_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Crystal Structure Of His143met Rusticyanin [Acidithiobacillus ferrooxidans]	28.1	28.1	59%	2.9	22%	2CAL_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Reduced Rusticyanin At 1.9 Angstroms [Acidithiobacillus ferrooxidans]	28.1	28.1	59%	2.9	22%	1A3Z_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Reduced Rusticyanin, Nmr [Acidithiobacillus ferrooxidans]	28.1	28.1	59%	2.9	22%	1OUR_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Structures Of Adenylosuccinate Synthetase From Triticum Aestivum And Arabidopsis Thaliana [Triticum aestivum] >pdh1D13IB Chain B, Structures Of Adenylosuccinate Synthetase From Triticum Aestivum And Arabidopsis Thaliana	28.5	28.5	63%	3.0	30%	1D13_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Crystal Structure Of The Kluyveromyces Lactis Urea Carboxylase [Kluyveromyces lactis NRRL Y-1140]	28.5	28.5	19%	3.5	41%	3VAZ_A	<input type="checkbox"/>
<input type="checkbox"/>	Chain A, Crystal Structure Of The Sheath Tail Protein Lin1278 From Listeria Innocua, Northeast Structural Genomics Consortium Target Lkr115 [Listeria innocua] >pdh3LMIB Chain B, Crystal Structure Of The Sheath Tail Protein Lin1278 From Listeria Innocua	27.7	27.7	41%	4.9	24%	3LM_A	<input type="checkbox"/>

Run PSI-Blast iteration 2 with max

500

Go



Pytania i odpowiedzi na zadania

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Zdjęcia, schematy i rysunki zostały zaczerpnięte z internetu.



Zadania (maksymalnie 10 punktów)

1. Proszę wyszukać na stronie <http://www.rcsb.org> jakie białko jest białkiem miesiąca marzec w 2017 roku.
 - a) Jakie funkcje w organizmie pełni te białko?
 - b) Jaki jest kod PDB tego białka?
 - c) Jaką metodą została otrzymana struktura tego białka?
 - d) Z jakiego organizmu pochodzi te białko?

2. Wyszukaj białko o kodzie PDB: **5H07**
 - a) Pod jakim kodem UNIPROT się kryje to białko?
 - b) Jaką funkcję pełni to białko?
 - c) Ile posiada alfa-helis a ile beta-kartek?
 - d) Do jakich białek sekwencja tego białka jest podobna? Wymień trzy.



Zadania (maksymalnie 10 punktów)

3. Wyszukaj w bazie UniProt białko „REST”.
 - a) Wybierz jedno białko i sprawdź czy jest dostępna dla niego struktura pdb.
 - b) Jaka jest funkcja tego białka?
 - c) Z jakich fragmentów składa się te białko?
 - d) Pobierz sekwencję białka oraz przeprowadź przewidywanie podobnych sekwencyjnie białek.
4. Wyszukaj i podaj jakie pakiety R mogą być pomocne przy analizie struktur białek np. obliczenie odległości pomiędzy atomami?
5. Znajdź pakiet do R, który będzie przeszukiwał bazę danych PDB. Wyszukaj w wszystkie białka, które posiadają mostki disulfidowe i kompleksy białko-DNA.

