



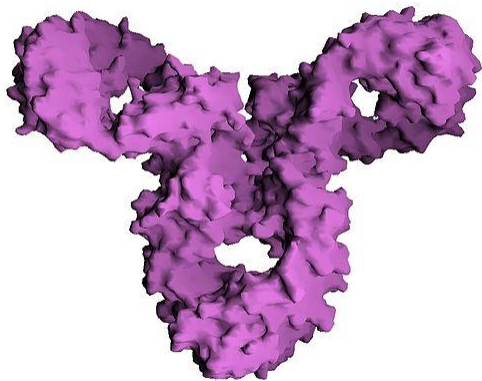
# **Analiza strukturalna białek**

Semestr Letni 2018

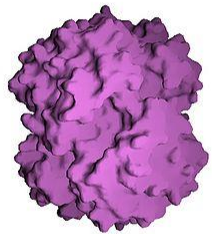
Magdalena Mozolewska

# 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.*



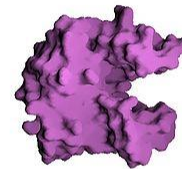
Przeciwciało (IgG)



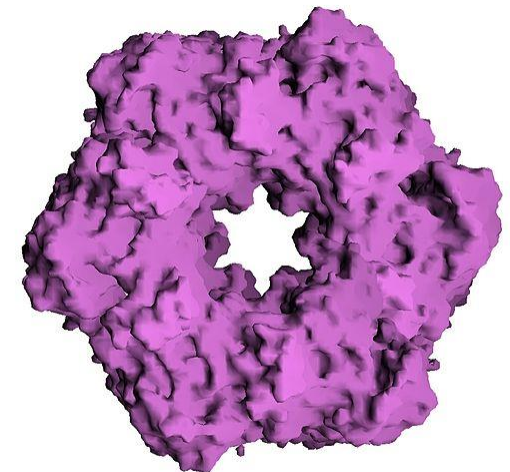
Hemoglobina



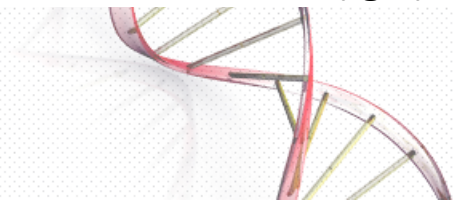
Insulina



Kinaza AK1



Ligaza glutaminy



# Białka

- Stanowią aż 75% suchej masy tkanek miękkich naszego ciała
- Zróżnicowanie właściwości fizykochemicznych poszczególnych reszt aminokwasowych umożliwia tworzenie niezwykle różnorodnych struktur białek o skomplikowanej topologii i różnych funkcjach



# Białka

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## 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

## ODPOIMUNIZACYJNE

To białka układu odpornościowego (np. immunoglobuliny, białka chorobotwórcze)

## FUNKCJE BIAŁEK

## ENZYMATYCZNE

przyspieszające specyficzne reakcje chemiczne

## TRANSPORTUJĄCE

To białka uczestniczące w transportowaniu różnych substancji odżywczych jak np. hemoglobina uczestnicząca w transporcie tlenu i CO<sub>2</sub>.

## 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

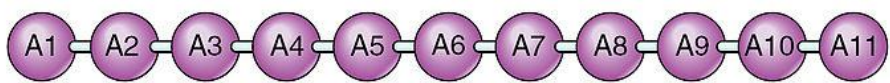


Hummus



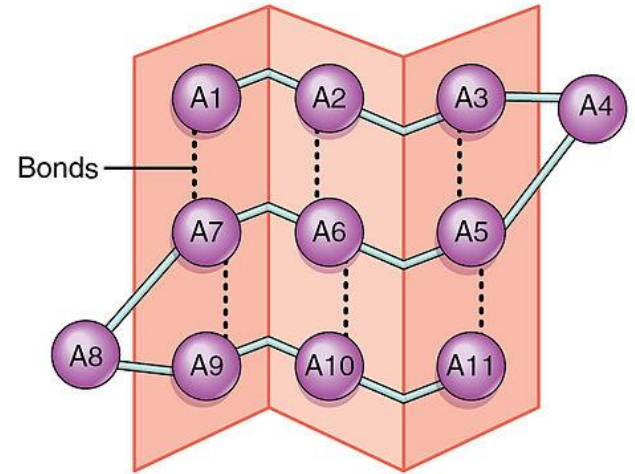
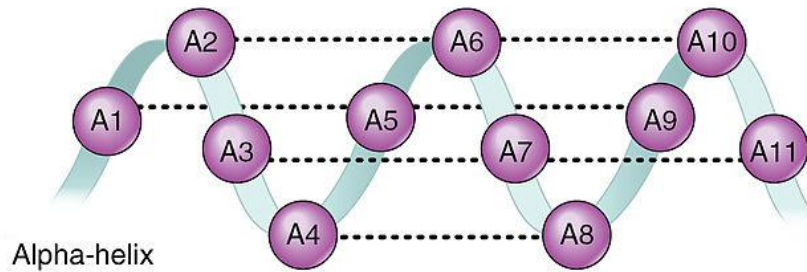
Nuts and seeds

©Nutrientsreview.com



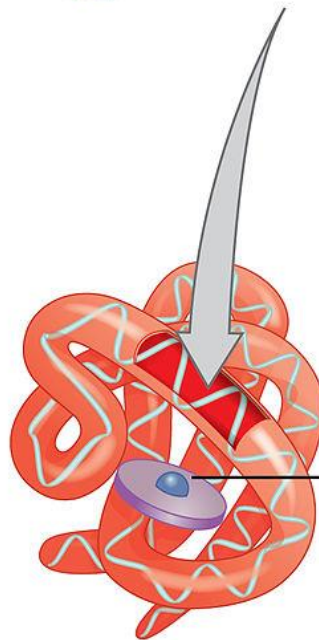
(a) Primary structure

Chain of amino acids



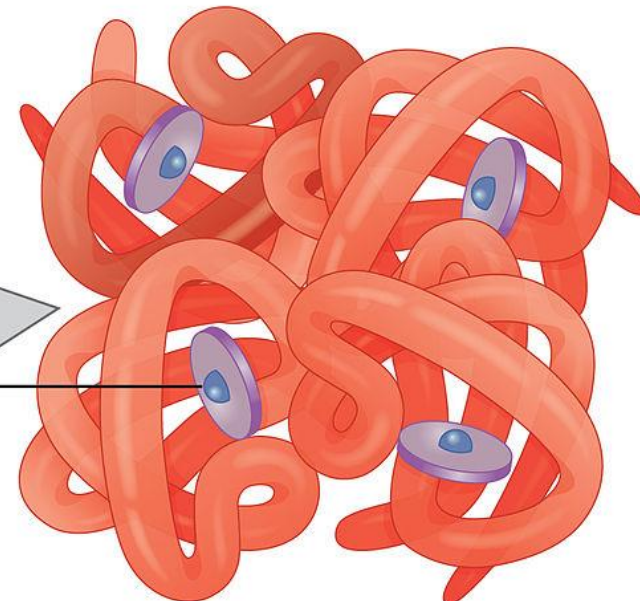
OR

(b) Secondary structure (pleated sheet)



(c) Tertiary structure

Heme units

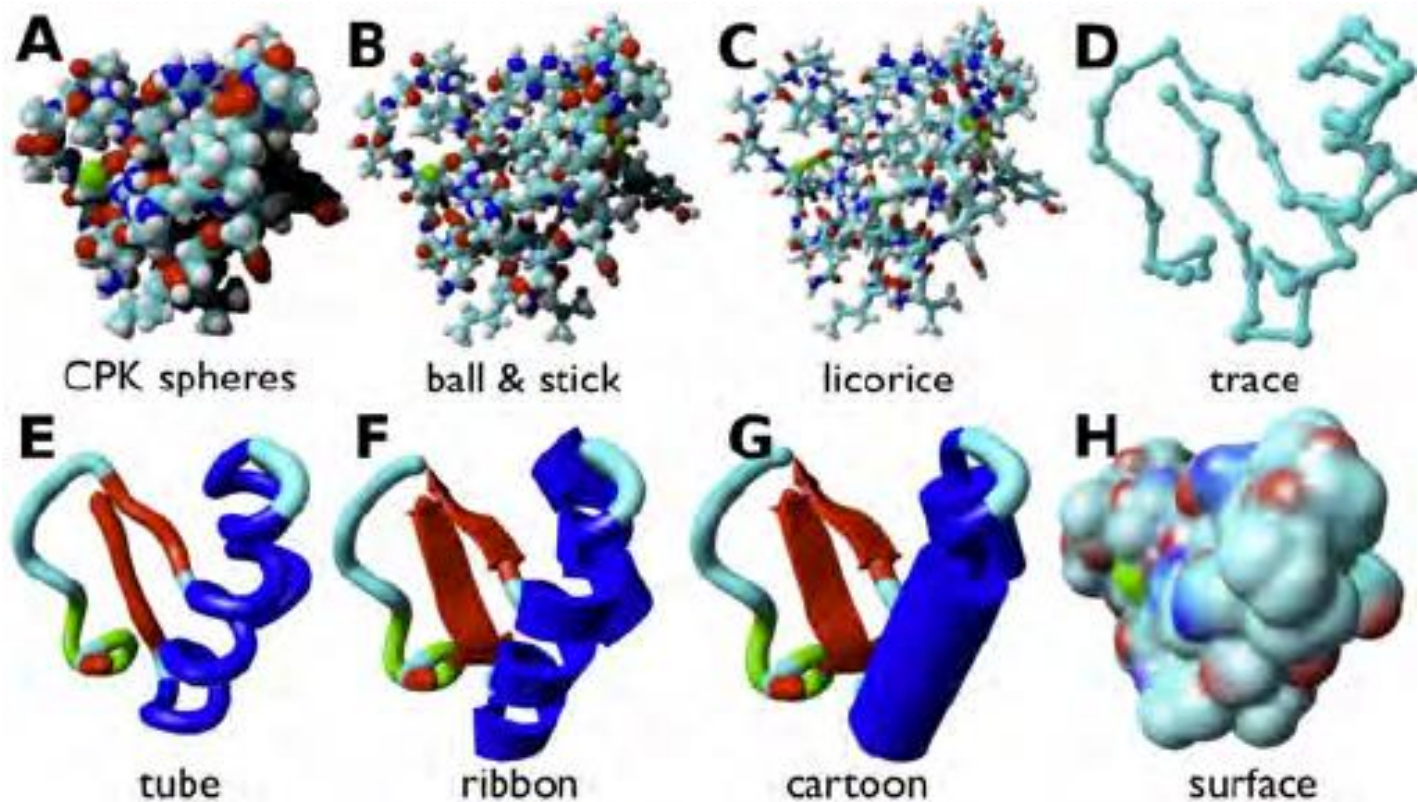


(d) Quaternary structure

Hemoglobin  
(globular protein)



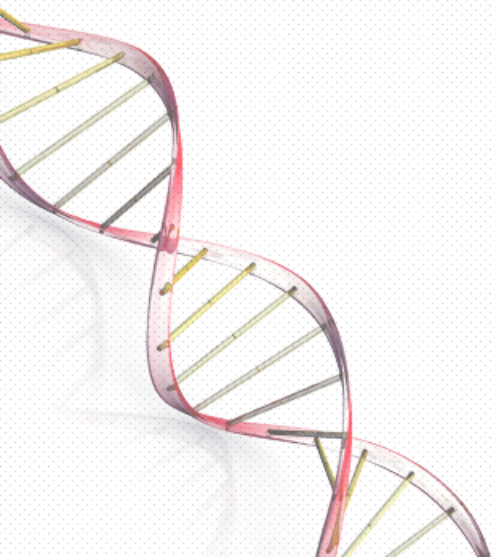
# Sposoby przedstawiania struktury białek



# I rzędowa struktura

MATQVMGQSSGGGGLFTSSGNIGMALPNDMYDLHDLSKAELAAPQLIMLANV  
ALTGEVNGSCCDYLVGEERQMAELMPVGDNNFSDSEEGEGLEESADIKGEPHG  
LENMELRSLELSVVEPQPVFEASGAPDIYSSNKDLPPETPGAEDKGKSSKTKPFRC  
KPCQYEAEESEQFVHHIRV

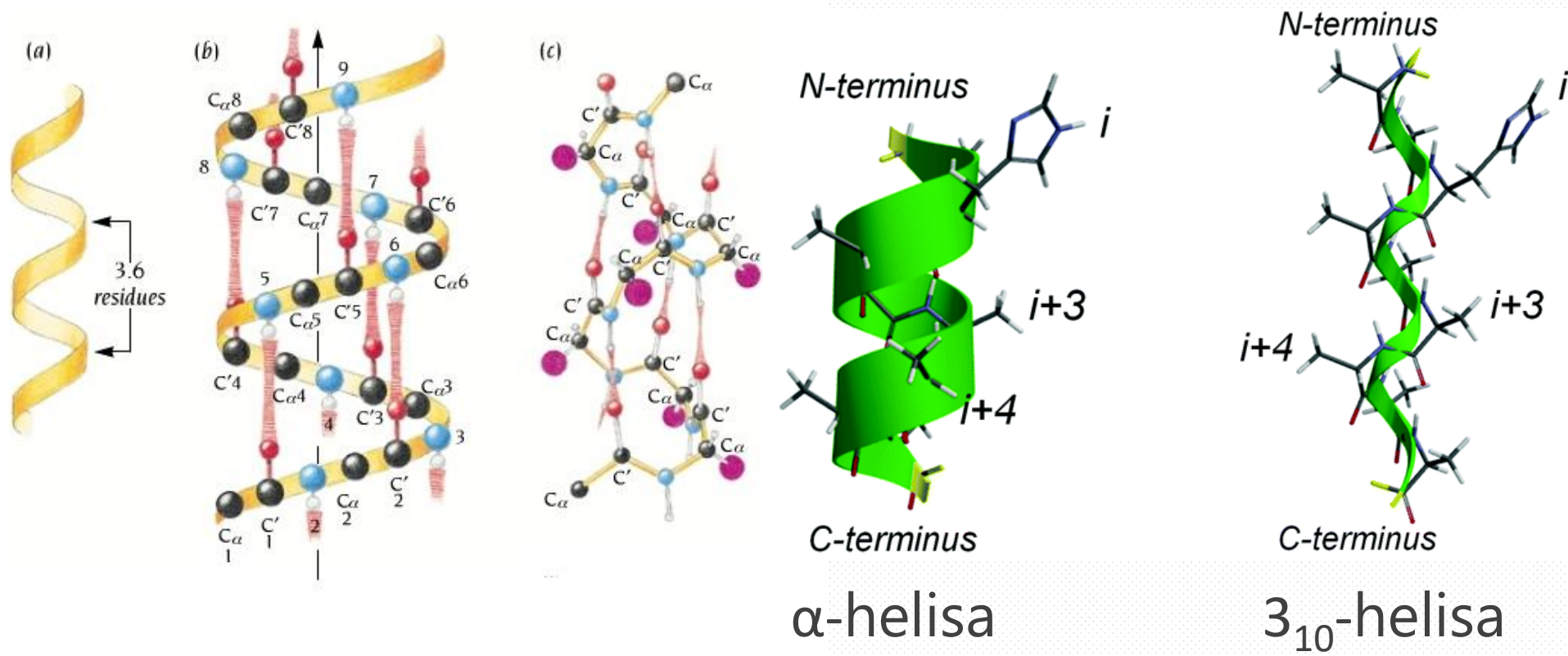
Czasami zalicza się tutaj także mostki disulfidowe, jako że są to wiązania kowalencyjne.

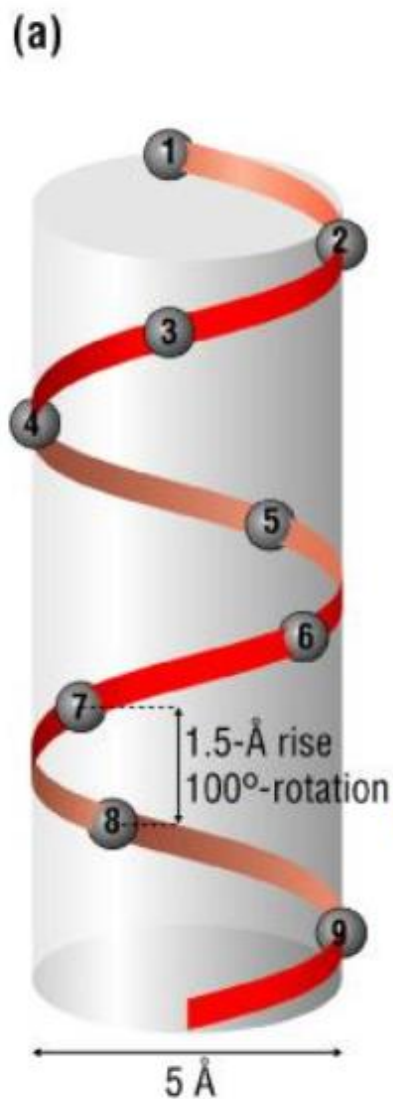




# II rzędowa struktura

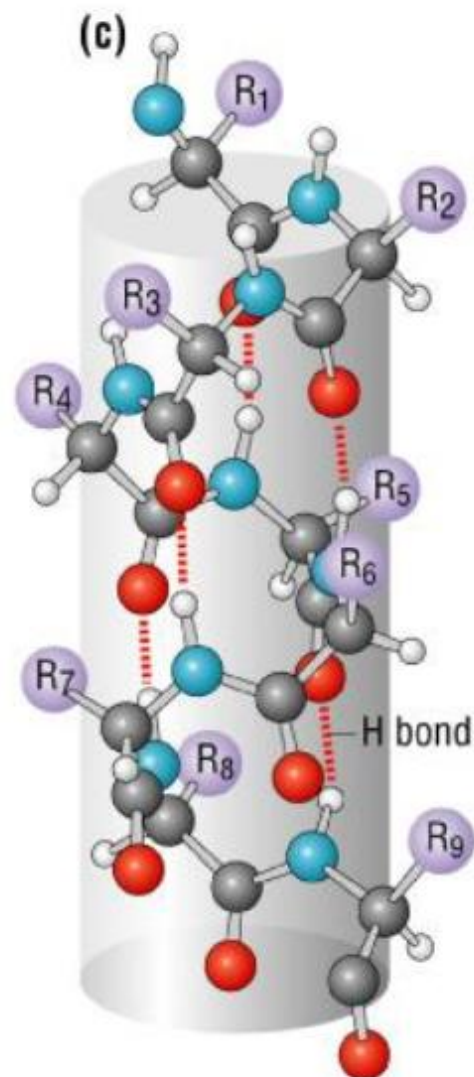
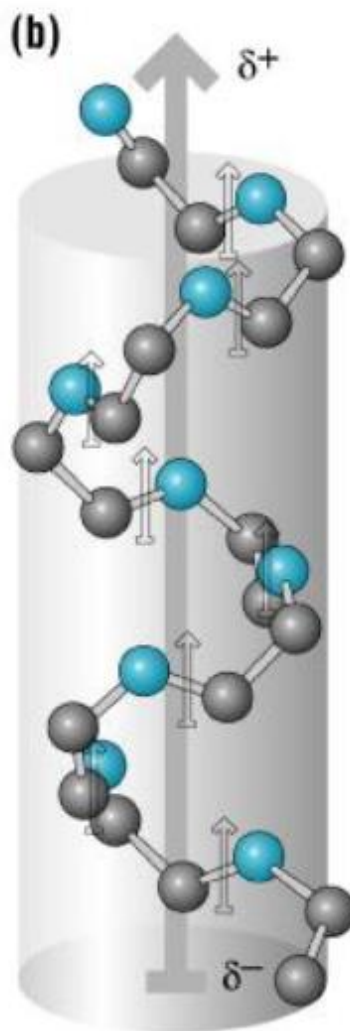
- Helisy





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3.6 reszty  
na skręt

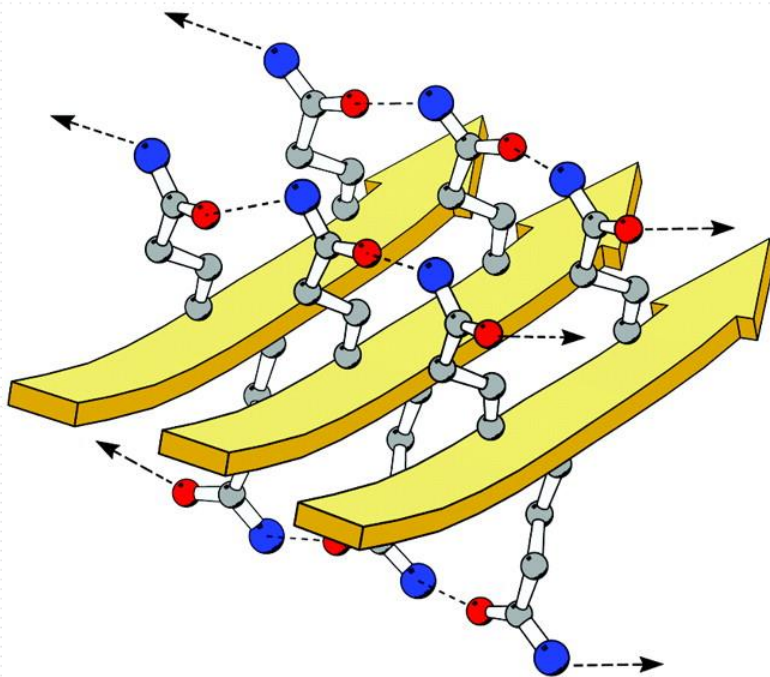


wiązania wodorowe pomiędzy C=O i N-H  
znajdującymi się blisko siebie w sekwencji

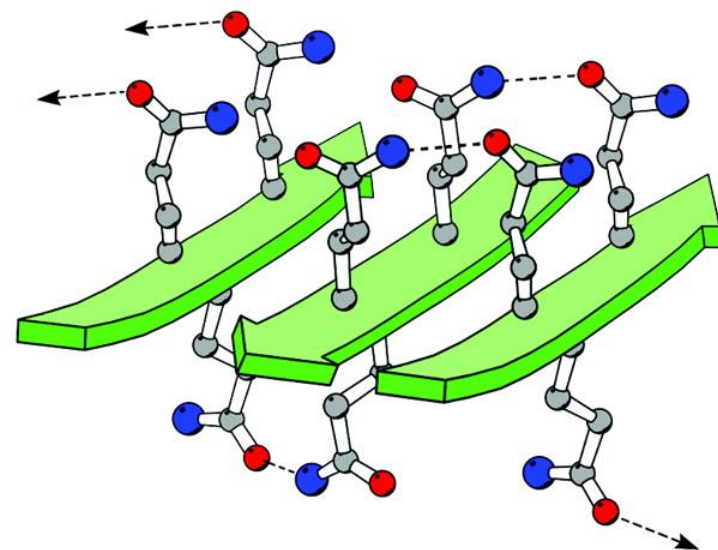
$n+4$

# II rzędowa struktura

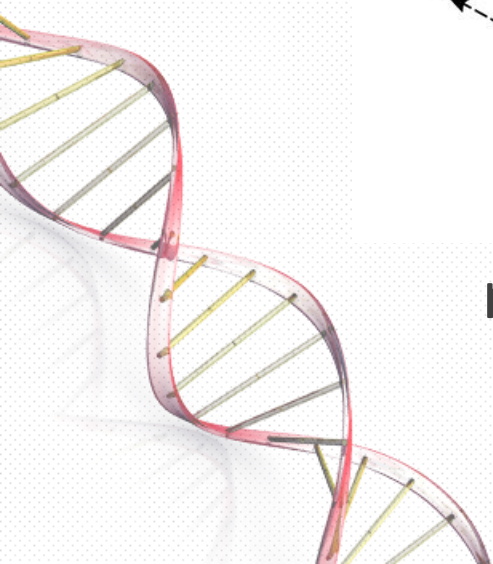
- Beta-kartki



równoległe



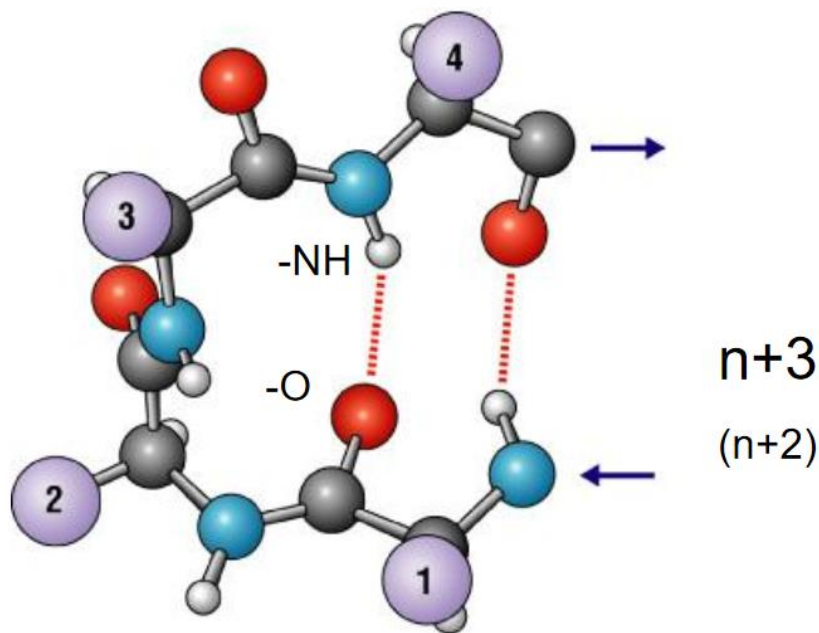
anty równoległe



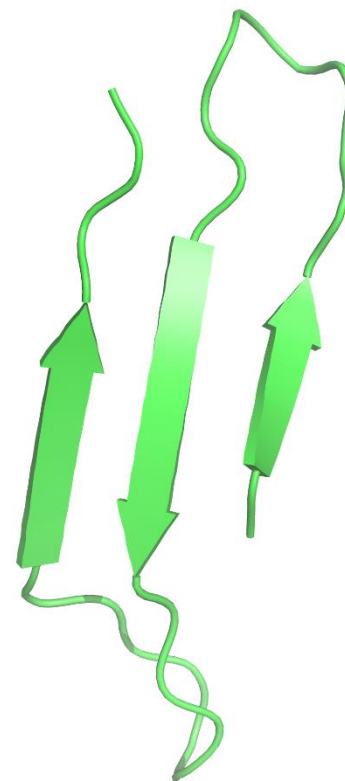


# II rzędowa struktura

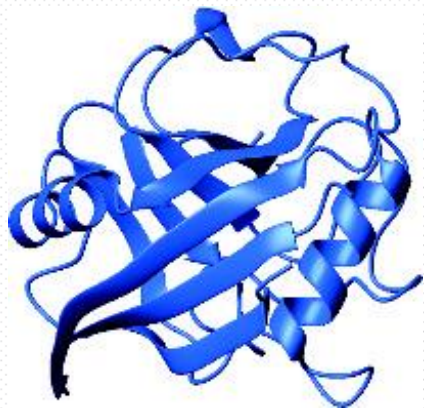
- Obecność zgięć beta pozwala ograniczyć rozmiary białka i nadać mu bardziej zwartą strukturę



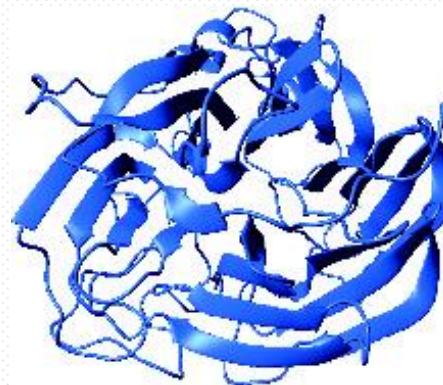
Część grup C=O i N-H nie tworzy HB w obrębie łańcucha, dlatego zgięcia występują najczęściej na powierzchni cząsteczki białka gdzie tworzą HB z wodą



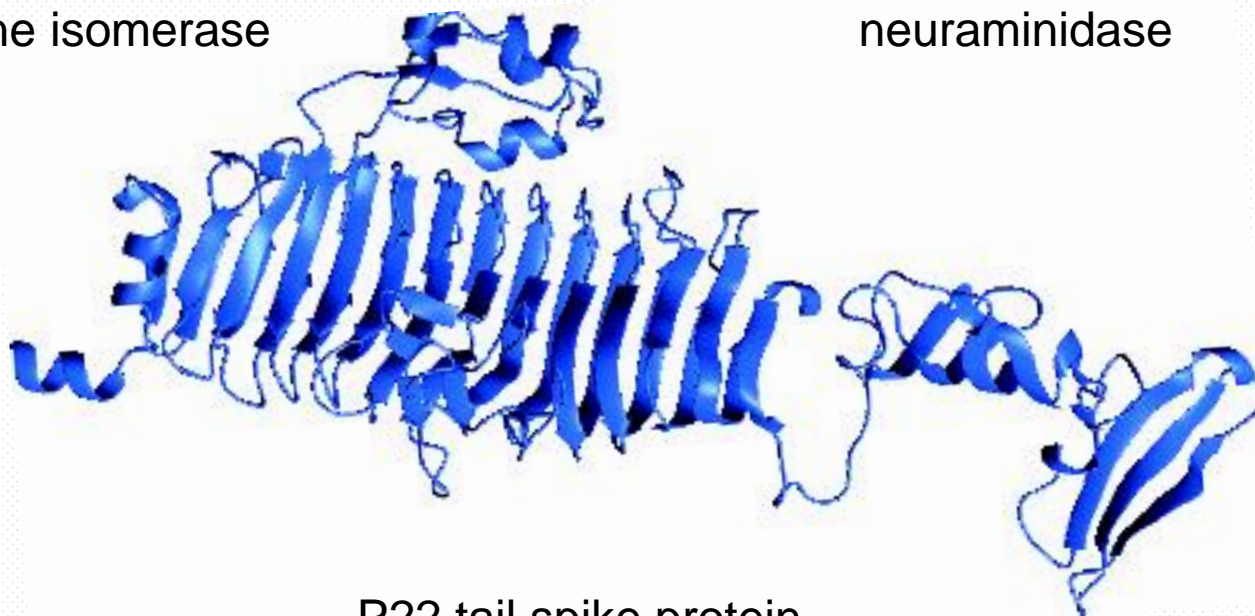
# III rzędowa struktura



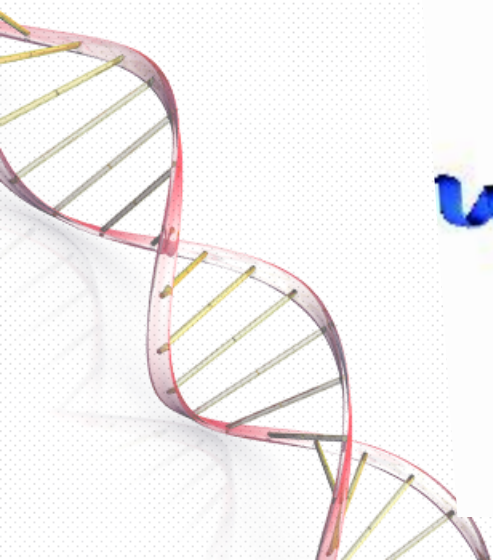
cis-trans proline isomerase



neuraminidase

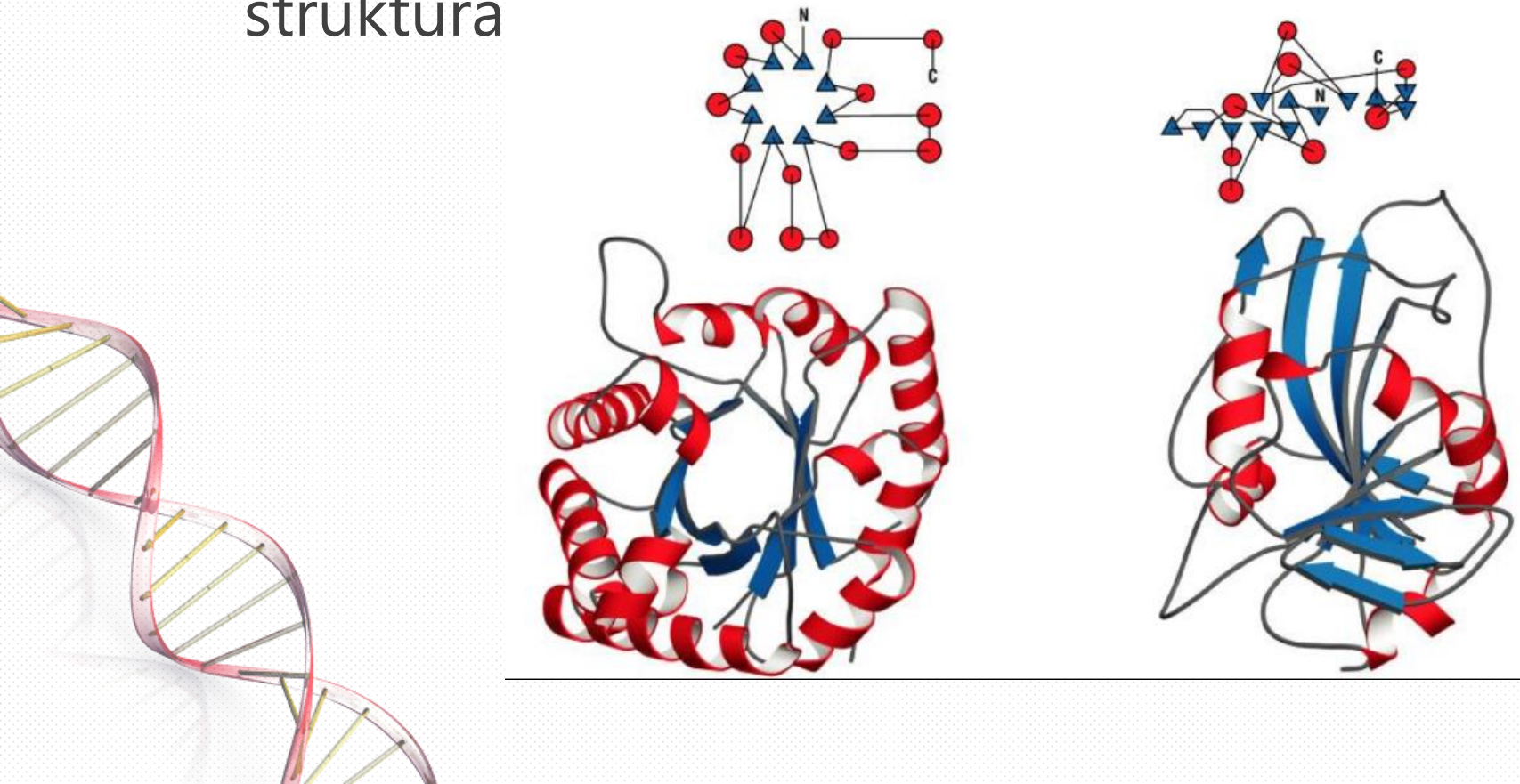


P22 tail spike protein



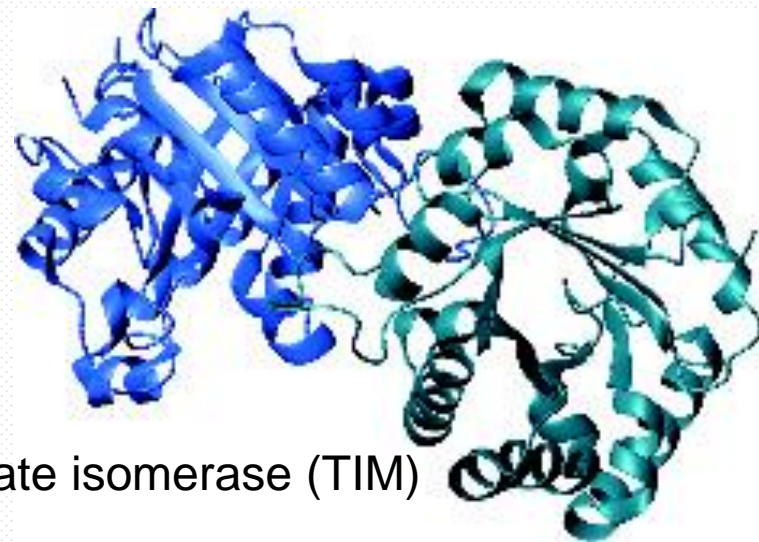
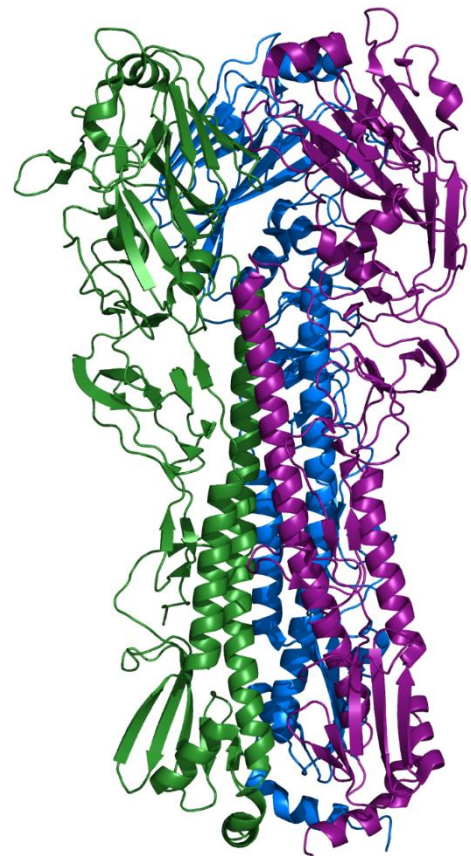
# III rzędowa struktura

- podobne elementy struktury drugorzędowej mogą tworzyć białka o całkiem różnych strukturach

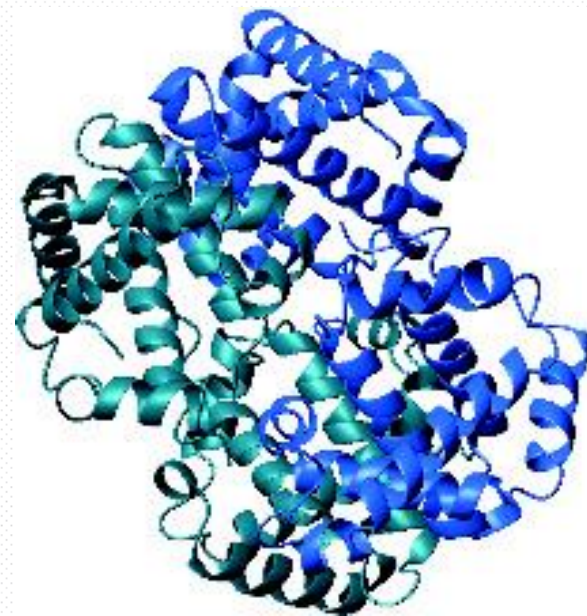




# VI rzędowa struktura



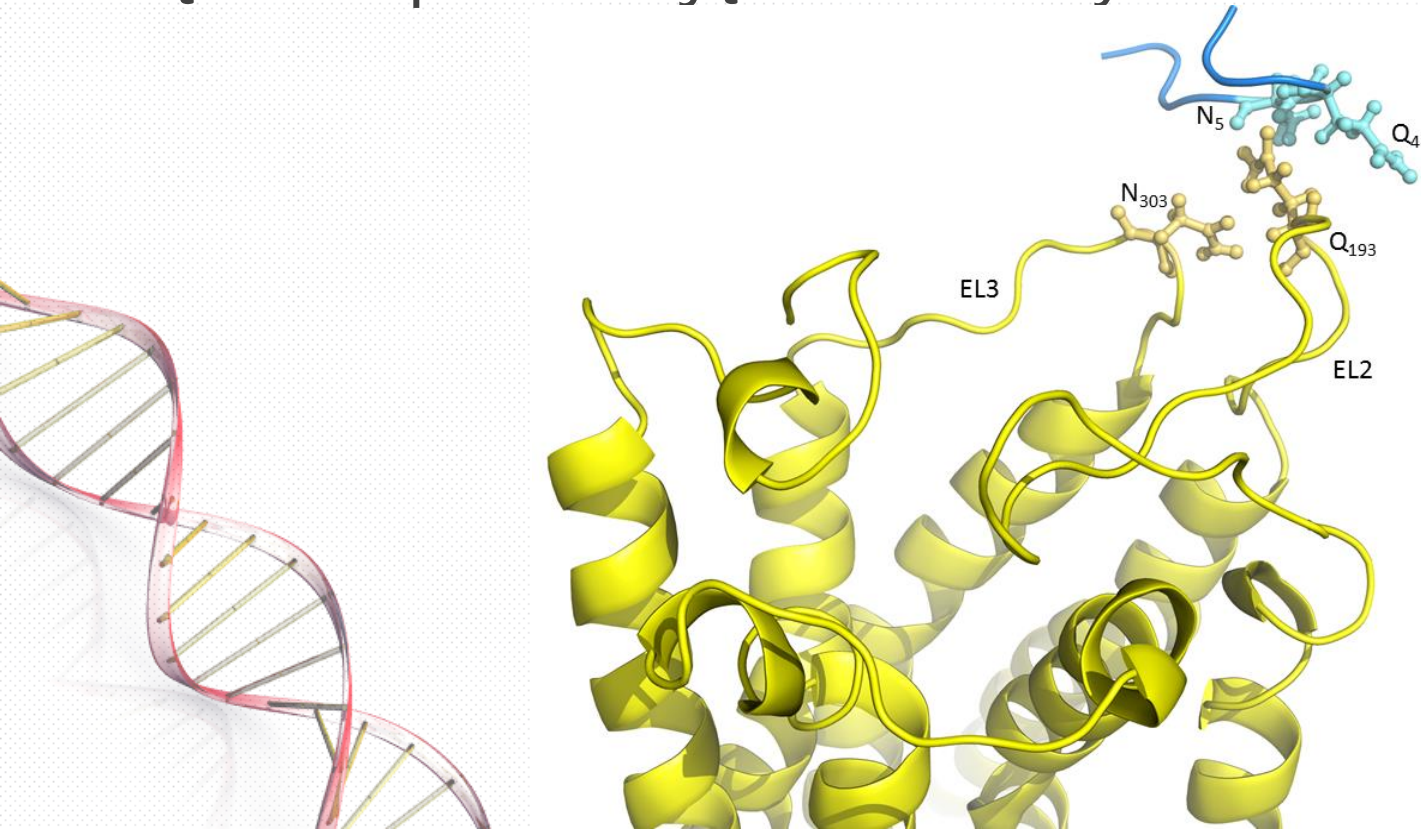
Triose phosphate isomerase (TIM)



Haemoglobin

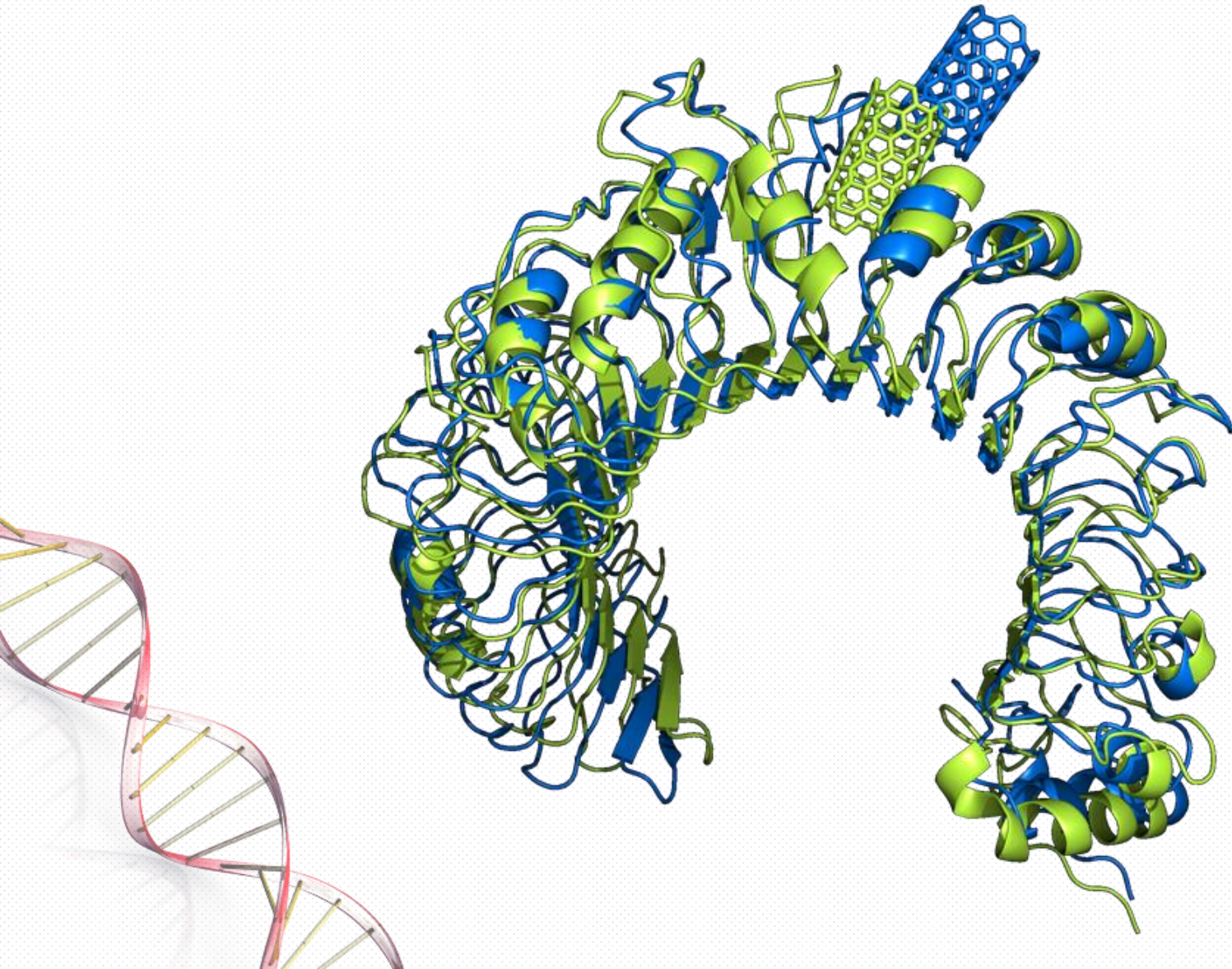
# Pętle

- Zwykle są na powierzchni, eksponowane do rozpuszczalnika
- Bardzo ruchliwe
- Często odpowiadają za oddziaływania z ligandem



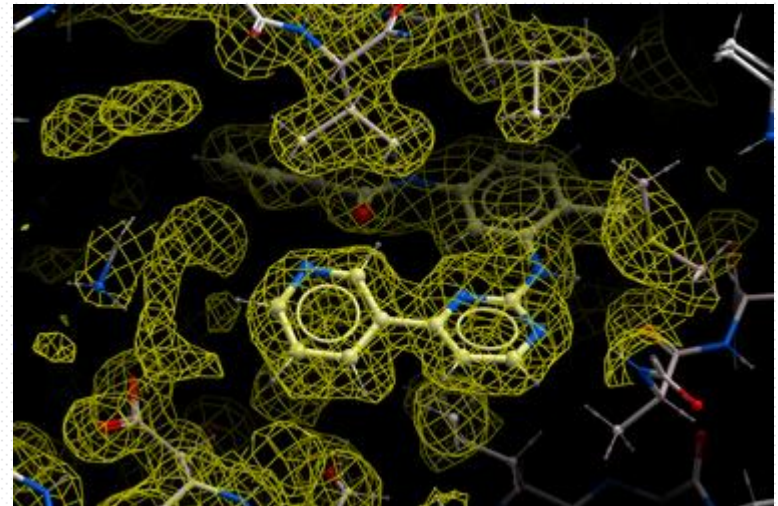
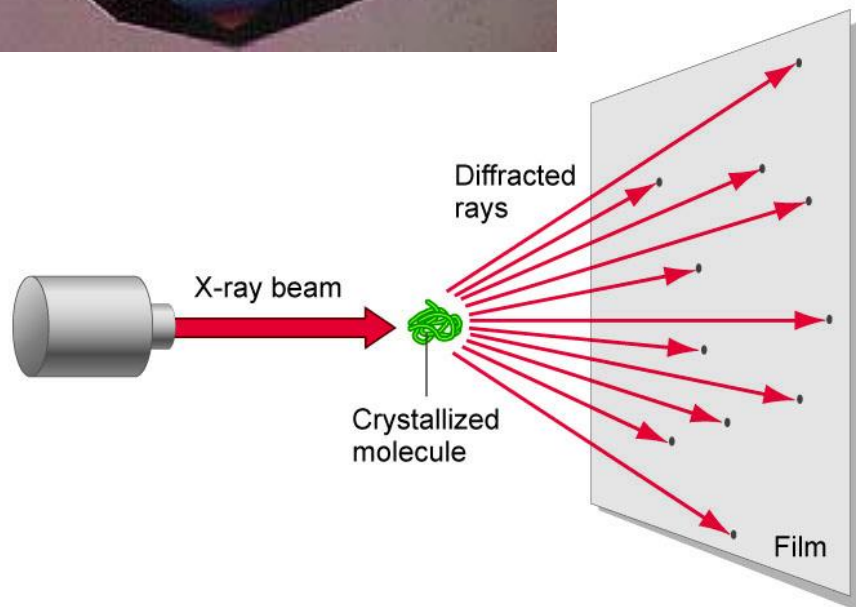
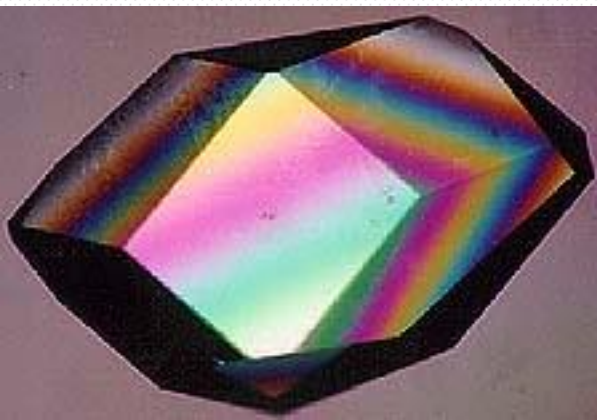


# Pętle

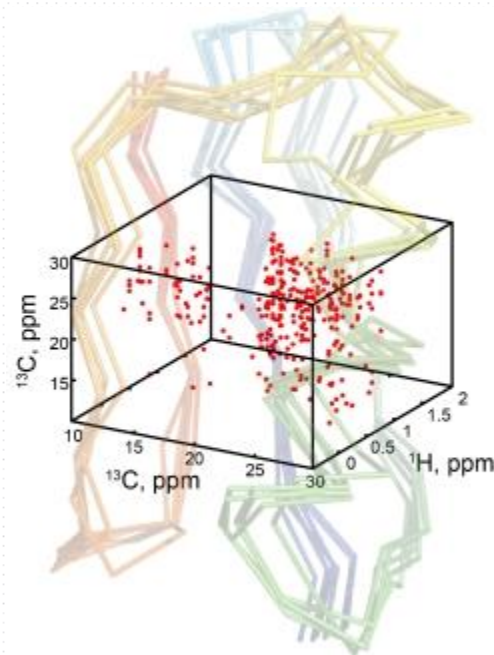
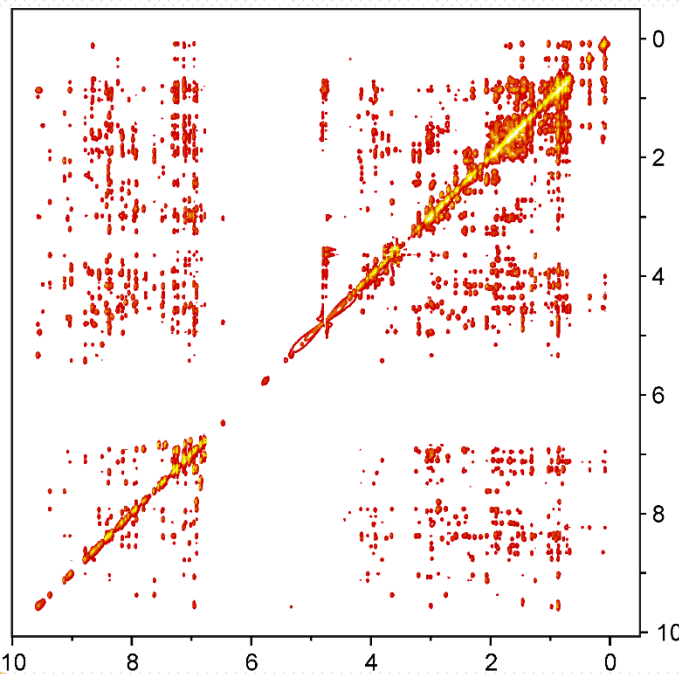




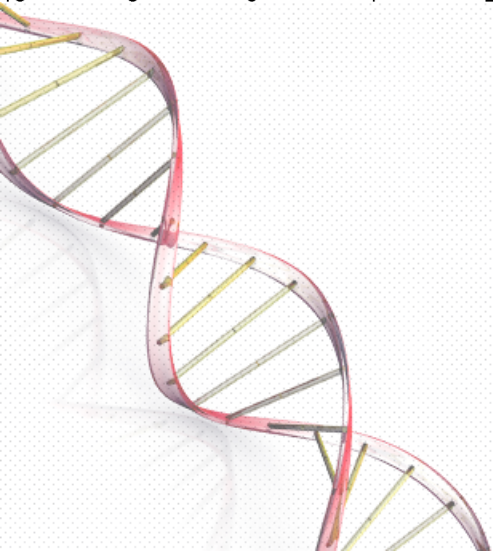
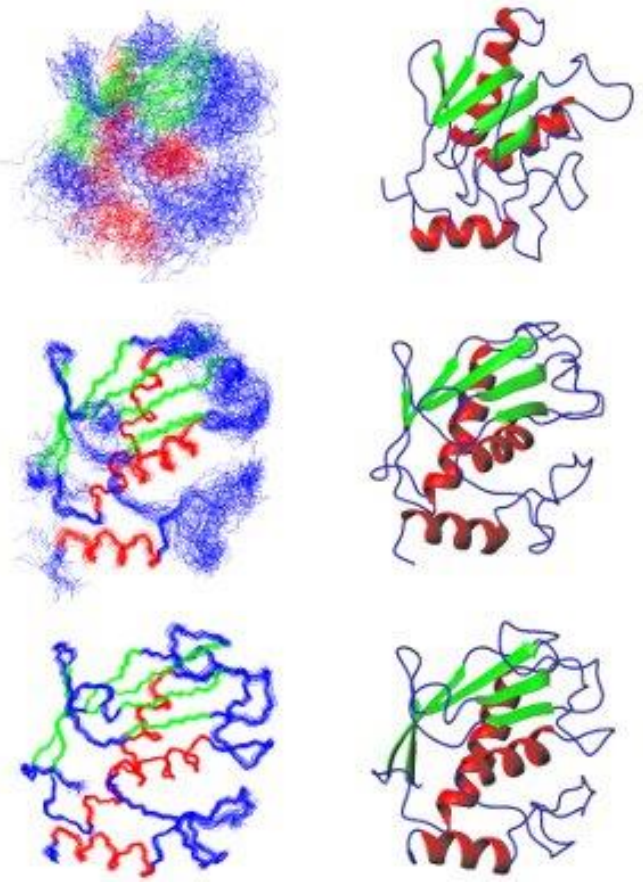
# **Eksperymentalne metody otrzymywania struktur białek - krystalografia rentgenowska**



# NMR – jądrowy rezonans magnetyczny

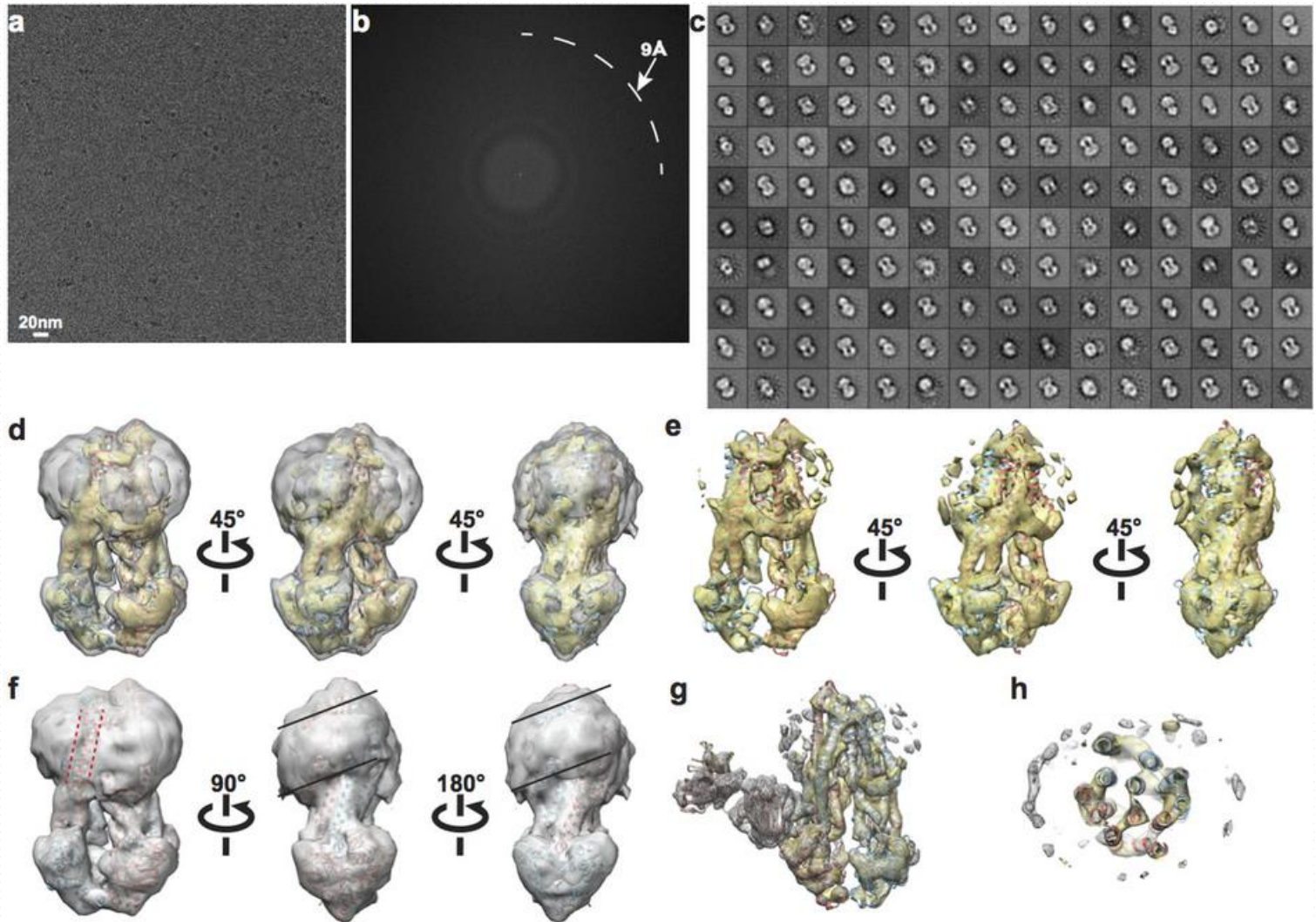


MMP-1 NMR Structure as a Function of the Total Number of Restraints used in the Simulation



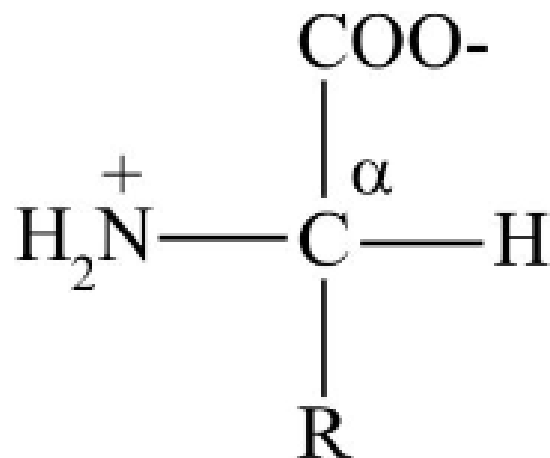


# Kriomikroskopia elektronowa



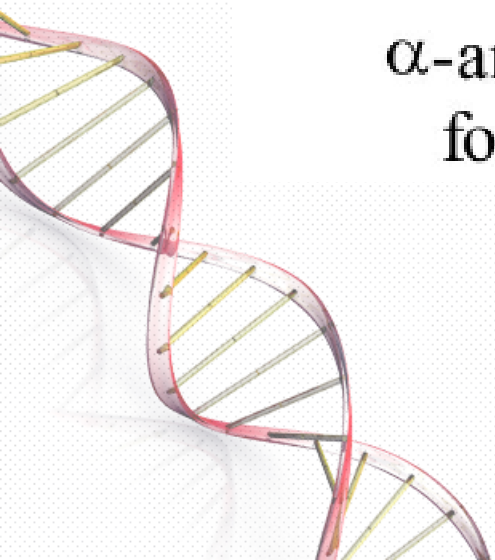


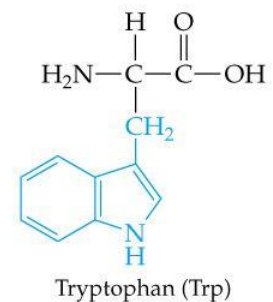
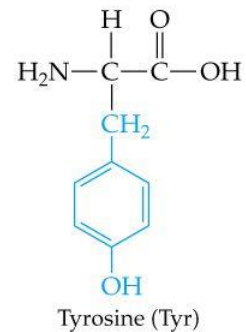
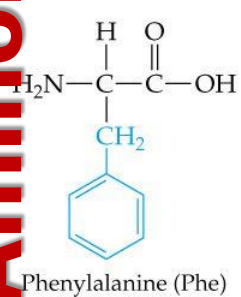
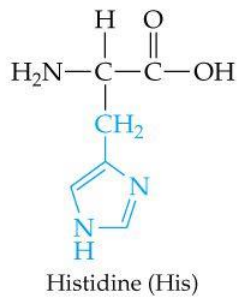
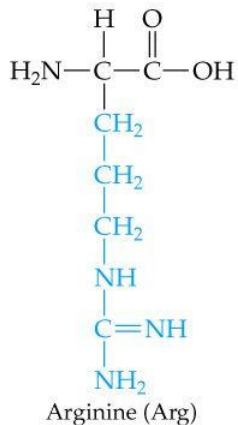
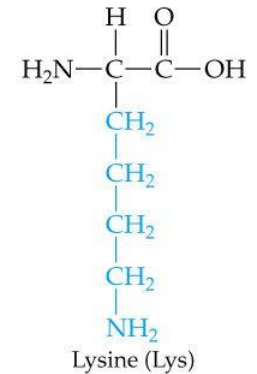
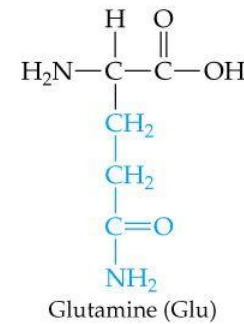
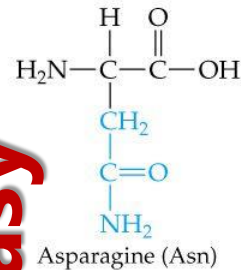
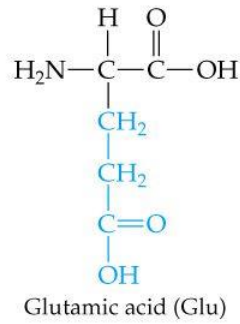
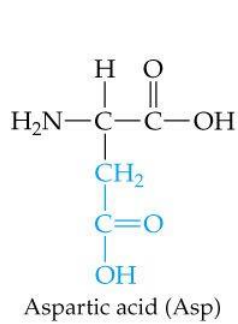
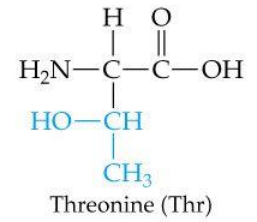
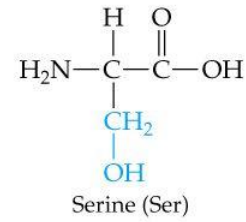
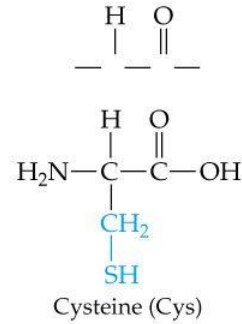
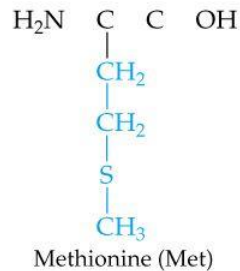
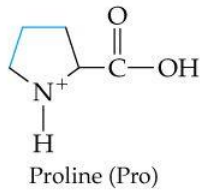
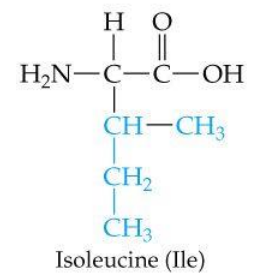
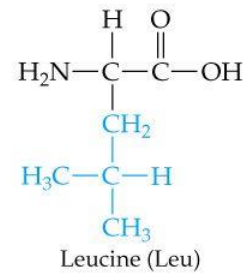
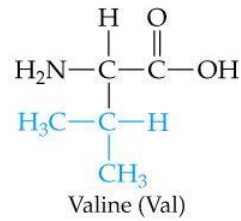
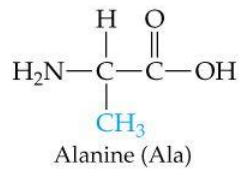
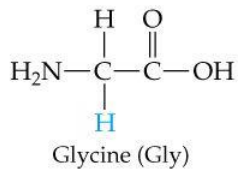
# Aminokwasy



$\alpha$ -aminokwas  
forma L

Znanych jest ponad 300 aminokwasów występujących naturalnie. W skład białek wszystkich organizmów żywych wchodzi głównie 20 podstawowych aminokwasów





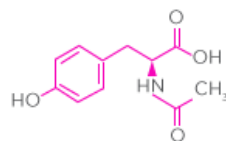
# Aminokwasy



# Aminokwasy

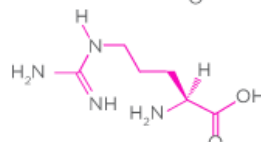
## Acetyl Tyrosine

Highly bio-available form of L-Tyrosine, a building block protein



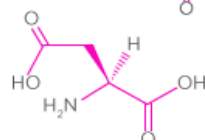
## Arginine

May speed the healing of skin cell damage and wounds



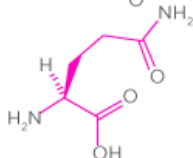
## Aspartic Acid

Involved in building skin cell DNA (genetic structure in the nucleolus)



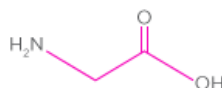
## Glutamine

Help prevent muscle and tissue breakdown. May also improve wound healing



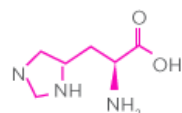
## Glycine

Help prevent muscle and tissue breakdown. May also improve wound healing



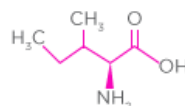
## Histidine

Antioxidant, neutralizes free radicals; may help boost UV protection. L-Histidine may also help prevent against certain types of skin infections



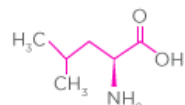
## Isoleucine

May be important in protein synthesis and tissue repair. May also promote the natural production of anti-microbial peptides



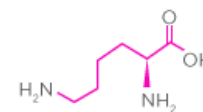
## Leucine

May improve wrinkles when used in conjunction with glycine and proline



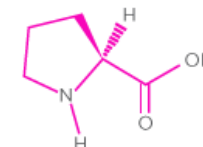
## Lysine

This is an amino acid that actually does hydrate, though it also may be involved in collagen production



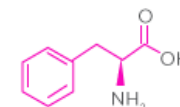
## Proline

Has been shown to improve the appearance of fine lines and wrinkles around the eyes when used with glycine and leucine ("crow's feet") in at least one independent study



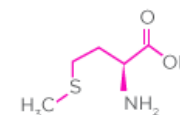
## Phenylalanine

Building blocks for various proteins



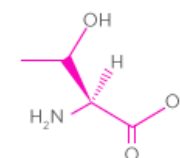
## Methionine

Neutralizes free radicals and fights skin aging



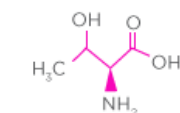
## Serine

Important in formation of cell membranes.



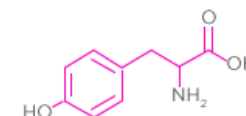
## Threonine

Important for the formation of collagen and elastin



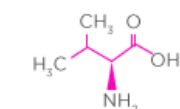
## Tyrosine

Helps protein and other agents penetrate the skin



## Valine

Branched chain amino acid. Important for muscular and tissue strength.





# Aminokwasy

Niepolarne

=

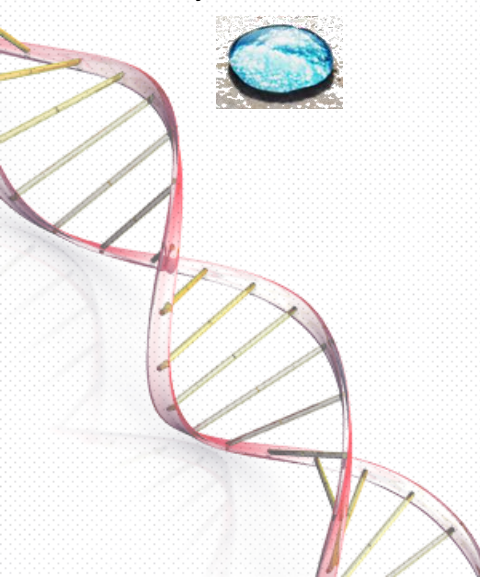
Hydrofobowe



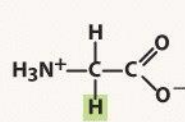
Polarne

=

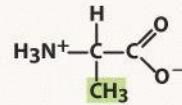
Hydrofilowe



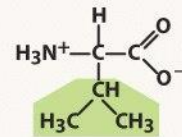
**Nonpolar  
side chains**



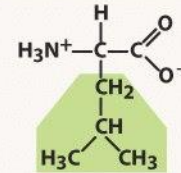
Glycine (G)  
Gly



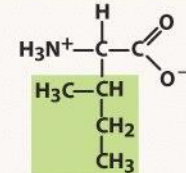
Alanine (A)  
Ala



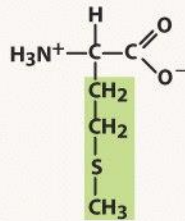
Valine (V)  
Val



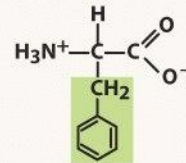
Leucine (L)  
Leu



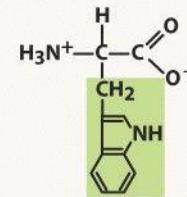
Isoleucine (I)  
Ile



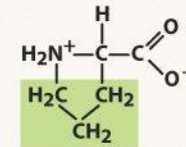
Methionine (M)  
Met



Phenylalanine (F)  
Phe

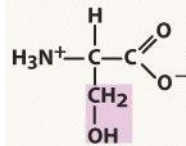


Tryptophan (W)  
Trp

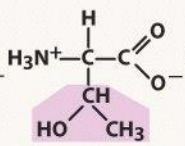


Proline (P)  
Pro

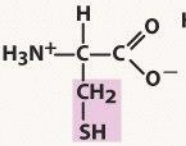
**Polar side  
chains**



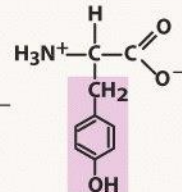
Serine (S)  
Ser



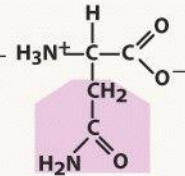
Threonine (T)  
Thr



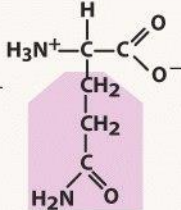
Cysteine (C)  
Cys



Tyrosine (Y)  
Tyr

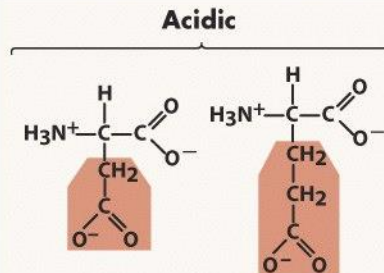


Asparagine (N)  
Asn



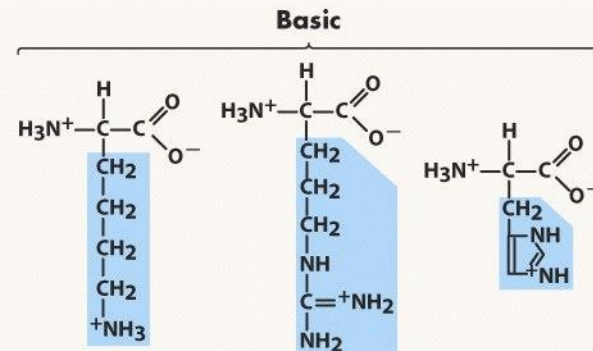
Glutamine (Q)  
Gln

**Electrically  
charged  
side chains**



Aspartate (D)  
Asp

Glutamate (E)  
Glu



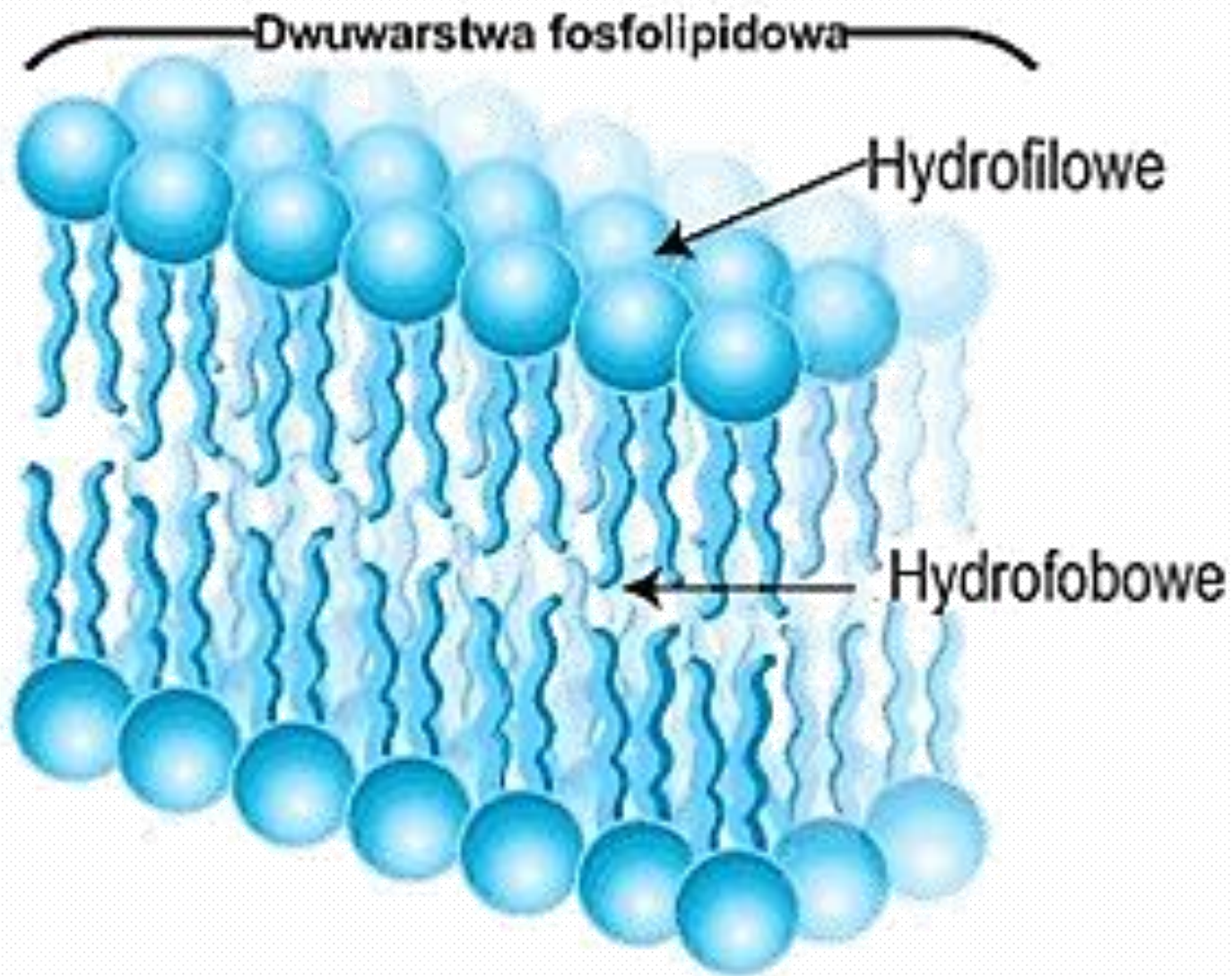
Lysine (K)  
Lys

Arginine (R)  
Arg

Histidine (H)  
His

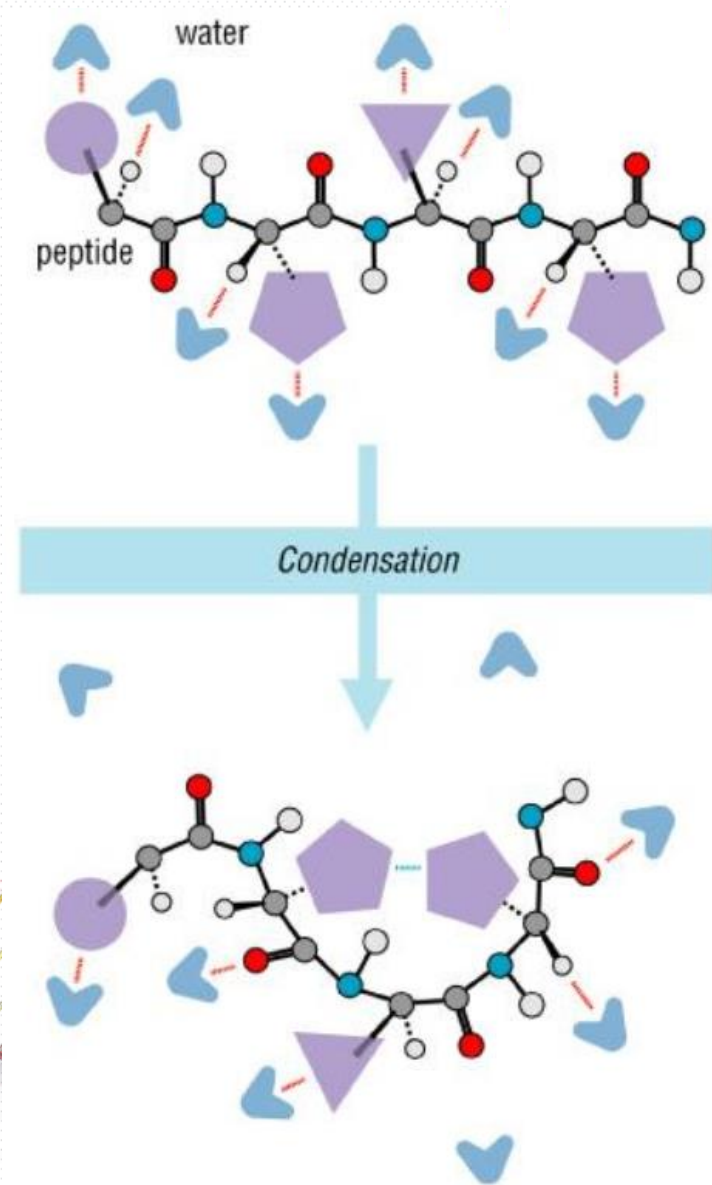
Figure 3-5 Biological Science, 2/e

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# Hydrofobowość



- minimalizacja powierzchni hydrofobowej dostępnej dla rozpuszczalnika

- zbliżenie polaryzowalnych grup hydrofobowych umożliwia powstanie między nimi oddziaływań van der Waalsa

- tym samym „wciągnięcie” polarnych grup C=O i N-H łańcucha głównego staje się siłą sprawczą powstania struktur drugorzędowych



hydrophobic: AGILMPV    white

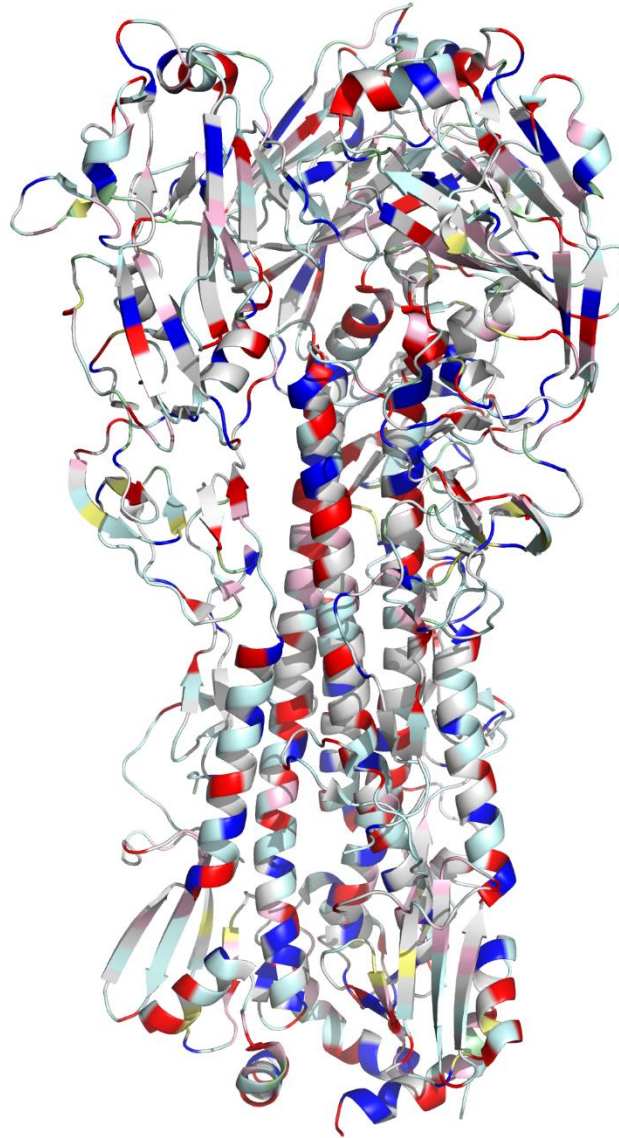
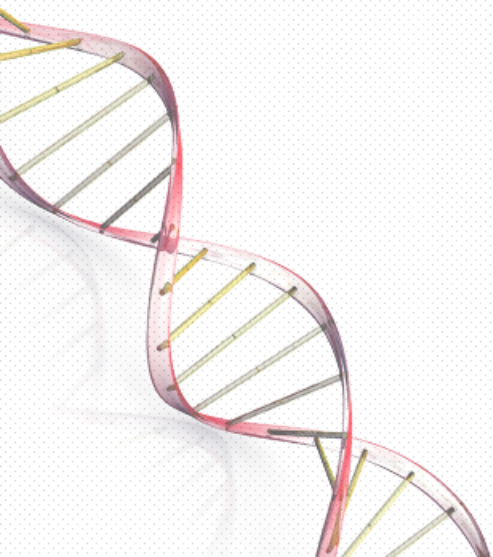
semipolar: C            yellow

polar: HNQST          cyan

positive: KR            blue

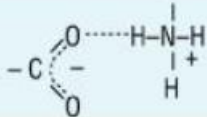

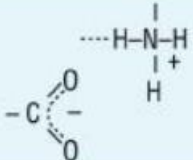
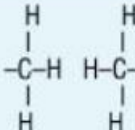
negative: DE            red

aromatic: FWY          magenta



# Oddziaływania stabilizujące białko

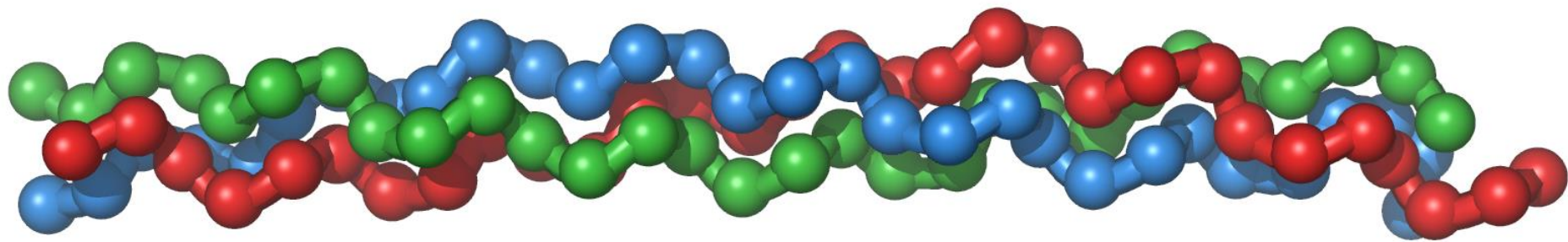
## Chemical Interactions that Stabilize Polypeptides

| Interaction                          | Example                                                                             | Distance dependence                                                               | Typical distance | Free energy (bond dissociation enthalpies for the covalent bonds)                                                                                                    |
|--------------------------------------|-------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Covalent bond                        | $\text{-C}_\alpha\text{-C-}$                                                        | -                                                                                 | 1.5 Å            | 356 kJ/mole<br>(610 kJ/mole for a C=C bond)                                                                                                                          |
| Disulfide bond                       | $\text{-Cys-S-S-Cys-}$                                                              | -                                                                                 | 2.2 Å            | 167 kJ/mole                                                                                                                                                          |
| Salt bridge                          |    | Donor (here N), and acceptor (here O) atoms <3.5 Å                                | 2.8 Å            | 12.5–17 kJ/mole; may be as high as 30 kJ/mole for fully or partially buried salt bridges (see text), less if the salt bridge is external                             |
| Hydrogen bond                        |    | Donor (here N), and acceptor (here O) atoms <3.5 Å                                | 3.0 Å            | 2–6 kJ/mole in water; 12.5–21 kJ/mole if either donor or acceptor is charged                                                                                         |
| Long-range electrostatic interaction |   | Depends on dielectric constant of medium. Screened by water. 1/r dependence       | Variable         | Depends on distance and environment. Can be very strong in nonpolar region but very weak in water                                                                    |
| Van der Waals interaction            |  | Short range. Falls off rapidly beyond 4 Å separation. 1/r <sup>6</sup> dependence | 3.5 Å            | 4 kJ/mole (4–17 in protein interior) depending on the size of the group (for comparison, the average thermal energy of molecules at room temperature is 2.5 kJ/mole) |



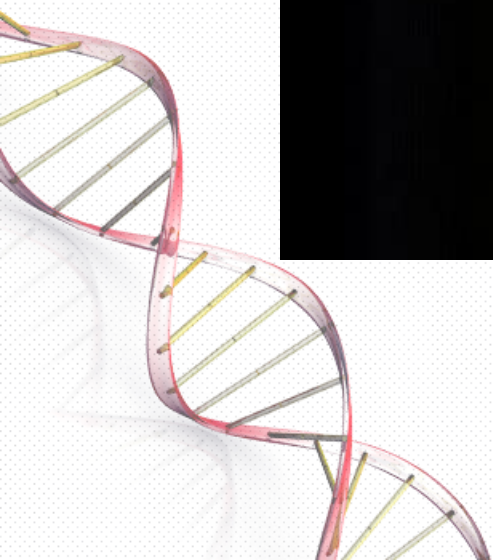
# Funkcje

- Kolagen
  - Bardzo wysoka odporność na rozciąganie
  - Elastyczność skóry
  - Ścięgna
  - Rogówka oka





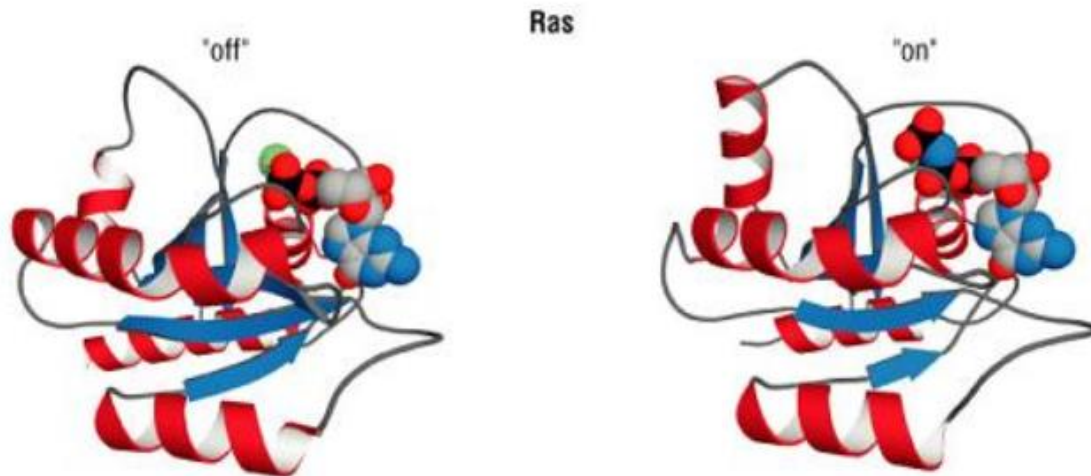
# Zmiana struktury



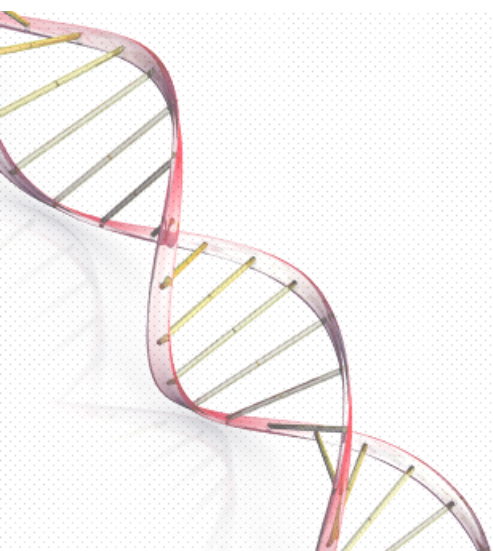
# Zmiana struktury

## Molekularny przełącznik -

zmiana konformacyjna  
pod wpływem pH  
lub wiązania liganda  
przełącza funkcję

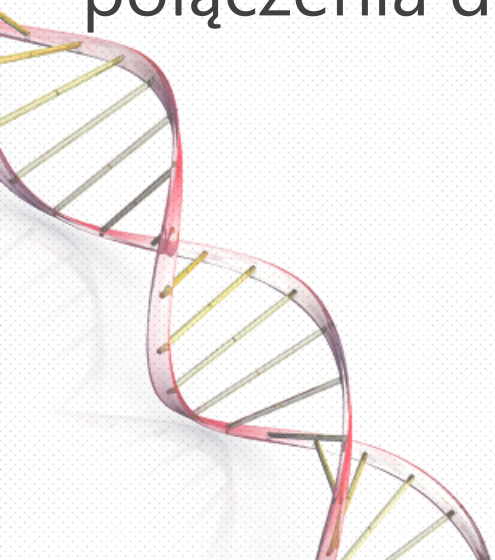


The GDP-bound ("off"; PDB 1pll) state of Ras differs significantly from the GTP-bound ("on"; PDB 121p) state. This difference causes the two states to be recognized by different proteins in signal transduction pathways.

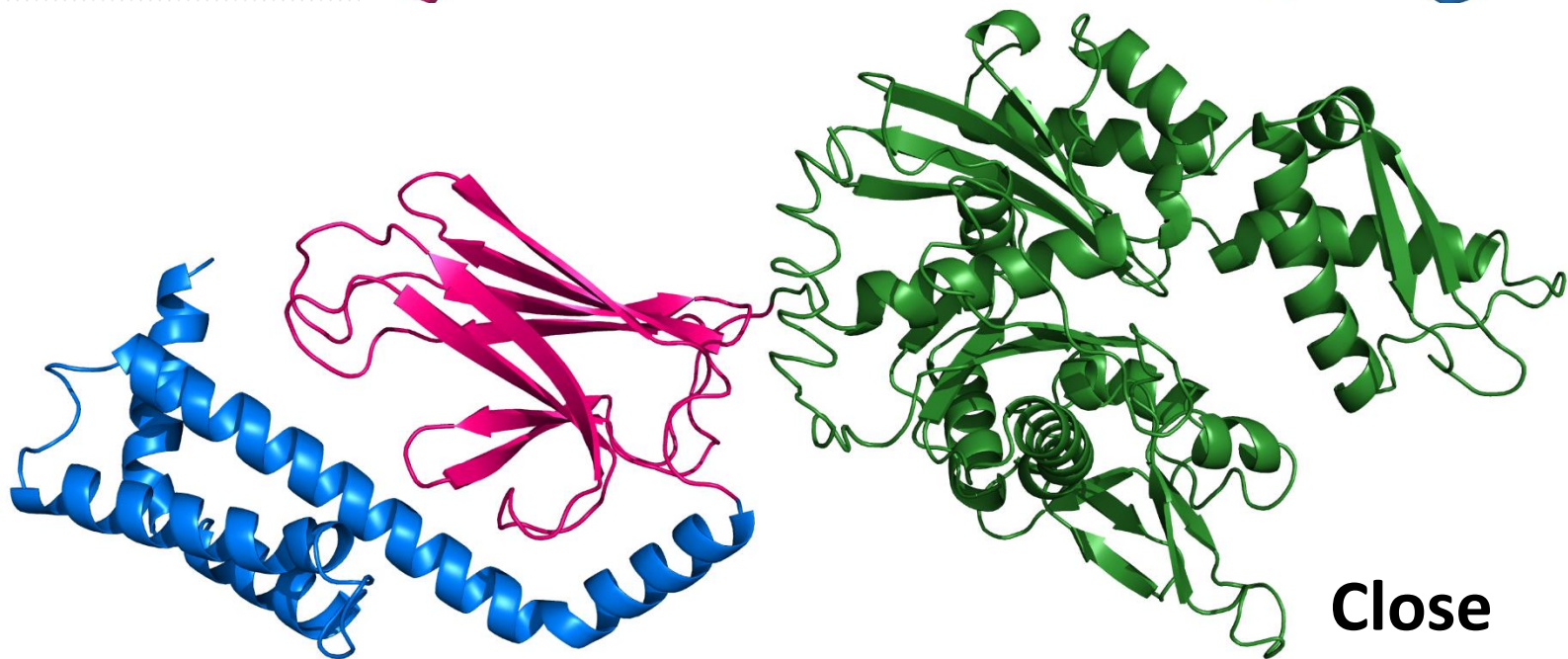
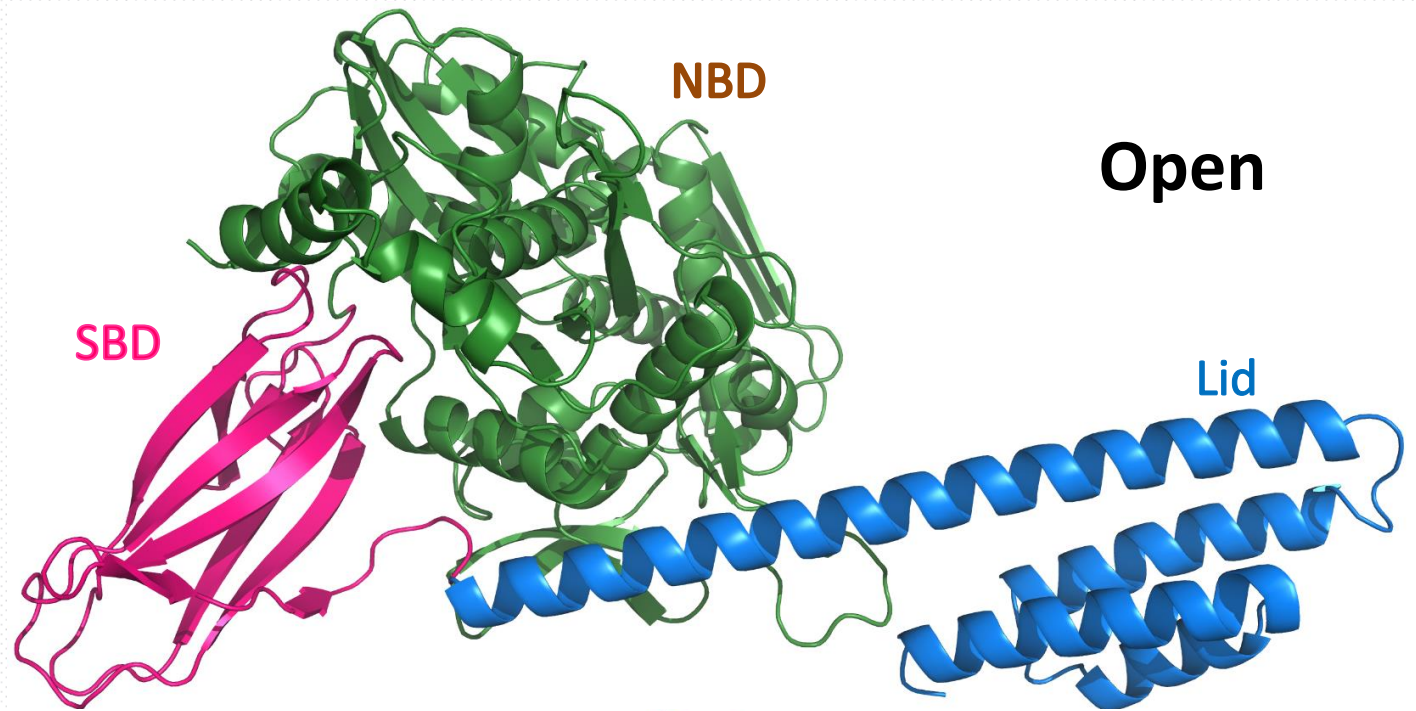


# Ruchliwość białek

- Domeny białek są połączone elastycznym łącznikiem
- Ruchliwość jest konieczna do spełnienia określonych funkcji biologicznych
- Miejsca wiążące znajdują się często w okolicy połączenia domen

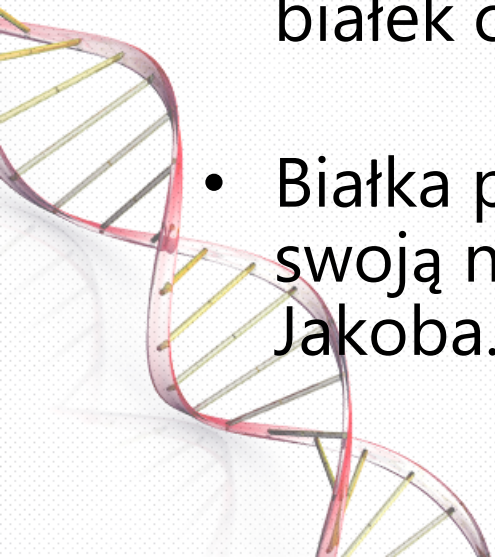


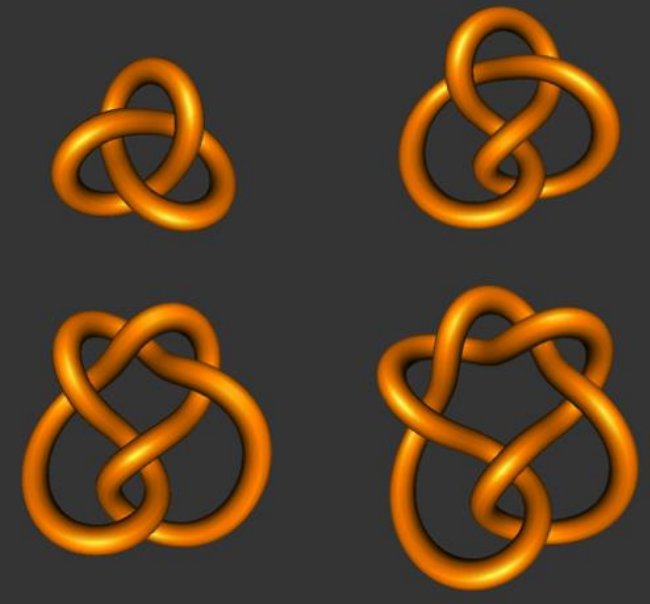




# Zaburzenia w strukturach białek

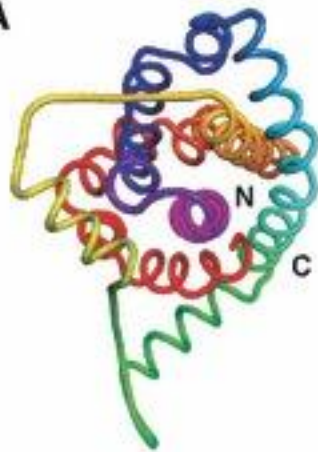
- Choroba Alzheimera – związek pomiędzy poziomem tlenku azotu, co wpływa negatywnie na zwijanie białka, odkładanie blaszek starczych w skład których wchodzi białko beta amyloid ( $A\beta$ ) o błędnej strukturze.
- Choroba Parkinsona – obumieranie komórek produkujących dopaminę, zaburzenie homeostazy białek co prowadzi do ich agregacji.
- Białka prionowe – infekcyjne białka, które zmieniają swoją natywną strukturę np. choroba Creutzfeldta-Jakoba.



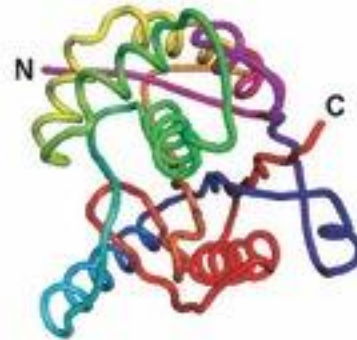


# roteins

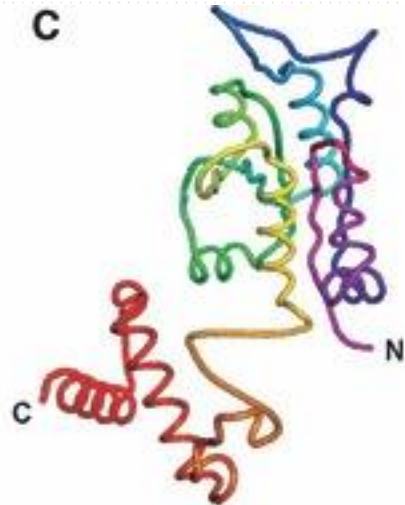
A



B



C



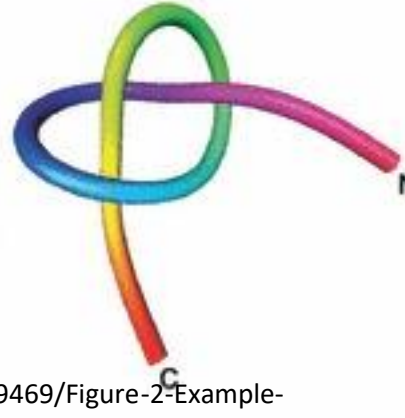
N



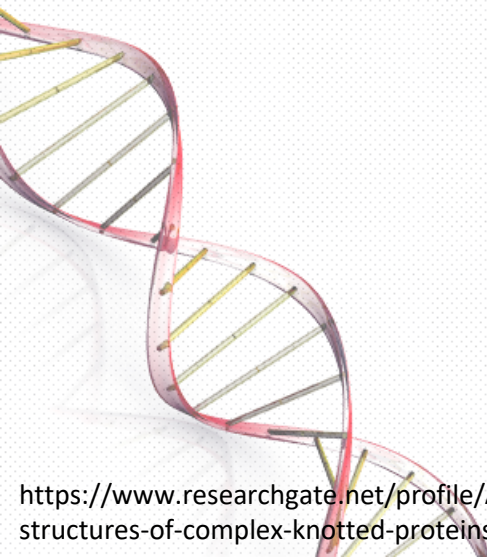
N



C



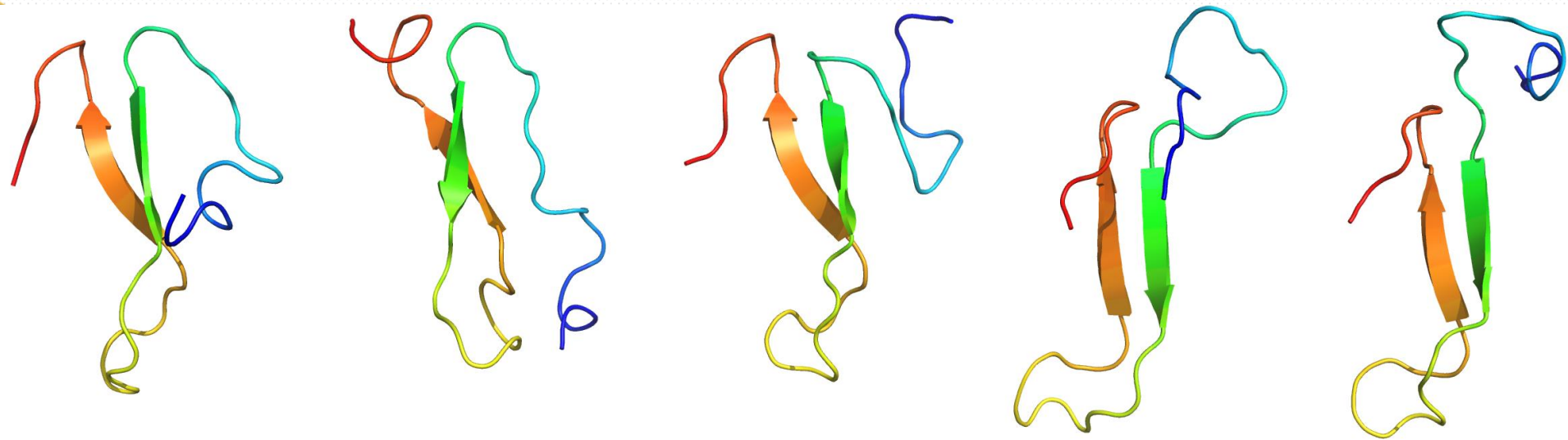
N



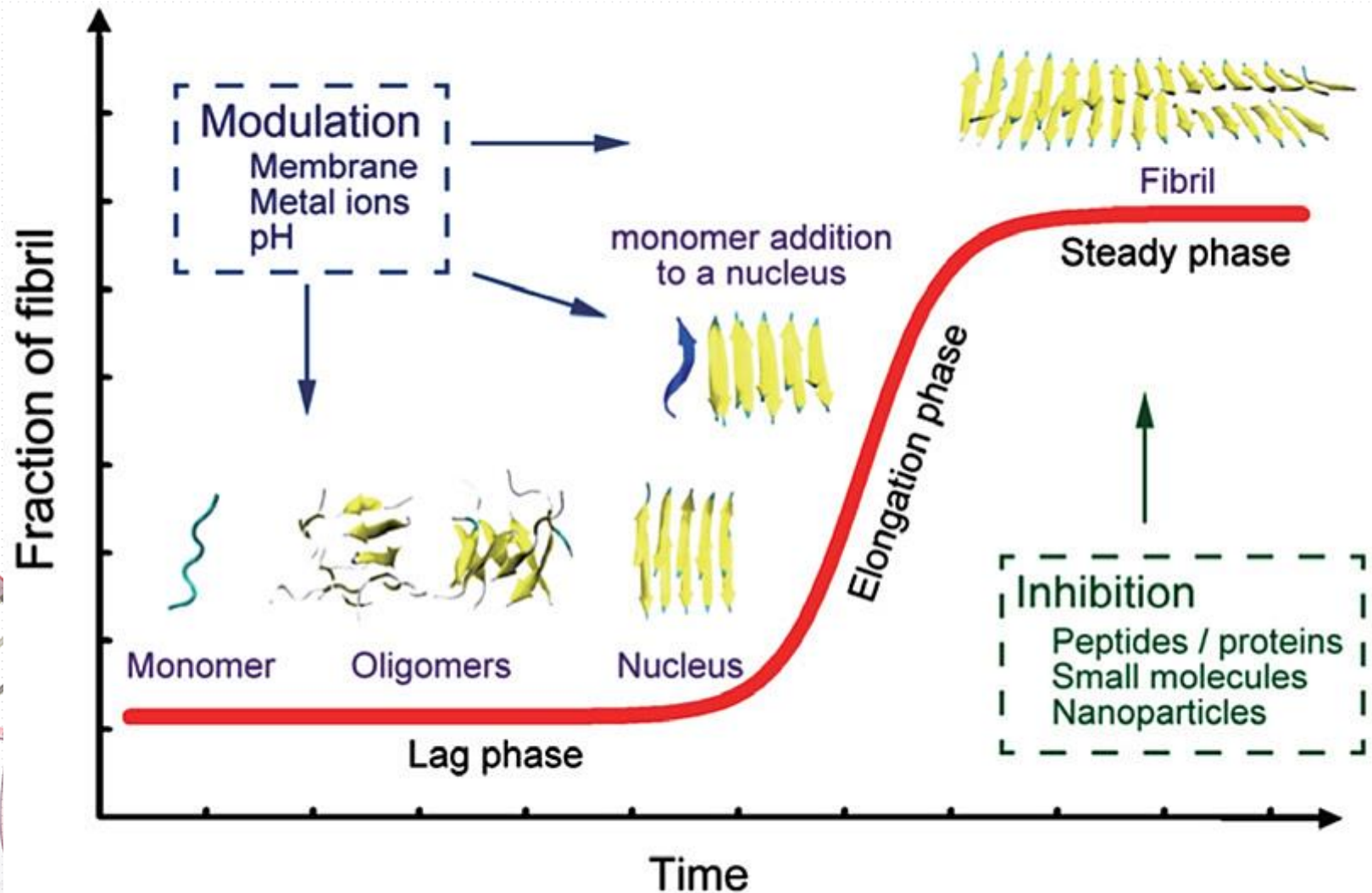


# Intrinsically disordered proteins (IDP)

- Proteins, which contain large unstructured fragments.
- Proteins lacking tertiary structure.
- E.g. monomeric A $\beta$ 40 and A $\beta$ 42.



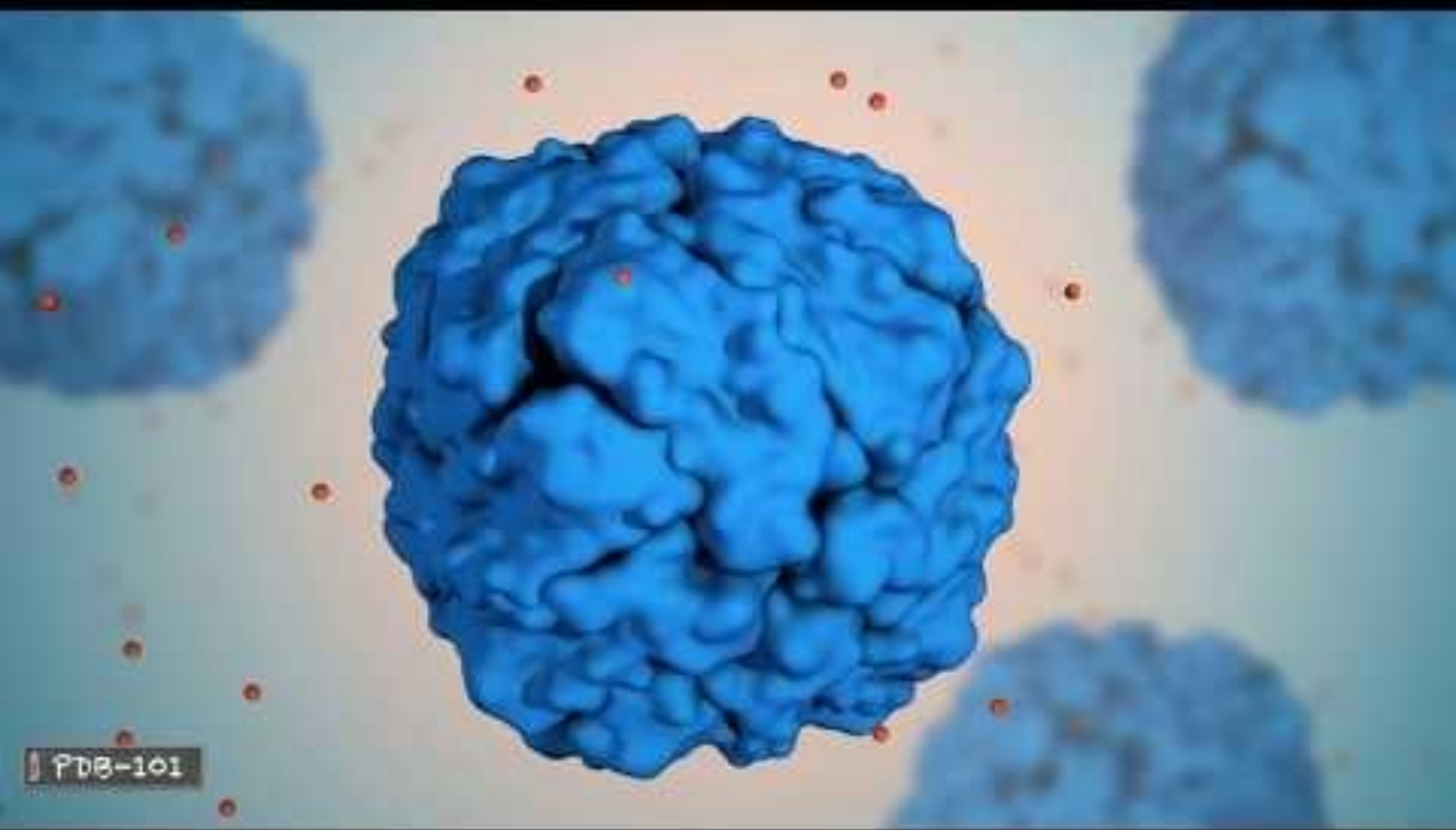
# Intrinsically disordered proteins (IDPs)



Science  
AAAS







PDB-101

```
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 ANALAGOUS C-TERMINAL STRUCTURE.

| DBREF  | 1L2Y     | A        | 1        | 20                                                  | PDB     | 1L2Y     | 1L2Y   | 1    | 20   |   |
|--------|----------|----------|----------|-----------------------------------------------------|---------|----------|--------|------|------|---|
| SEQRES | 1        | A        | 20       | ASN LEU TYR ILE GLN TRP LEU LYS ASP GLY GLY PRO SER |         |          |        |      |      |   |
| 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      |      |      |   |
| CRYST1 | 1.000    | 1.000    | 1.000    | 90.00                                               | 90.00   | 90.00    | P 1    | 1    |      |   |
| 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 |        |      |      |   |
| SCALE1 | 1.000000 | 0.000000 | 0.000000 |                                                     |         | 0.000000 |        |      |      |   |
| SCALE2 | 0.000000 | 1.000000 | 0.000000 |                                                     |         | 0.000000 |        |      |      |   |
| SCALE3 | 0.000000 | 0.000000 | 1.000000 |                                                     |         | 0.000000 |        |      |      |   |
| MODEL  | 1        |          |          |                                                     |         |          |        |      |      |   |
| ATOM   | 1        | N        | ASN A    | 1                                                   | -8.901  | 4.127    | -0.555 | 1.00 | 0.00 | N |
| ATOM   | 2        | CA       | ASN A    | 1                                                   | -8.608  | 3.135    | -1.618 | 1.00 | 0.00 | C |
| ATOM   | 3        | C        | ASN A    | 1                                                   | -7.117  | 2.964    | -1.897 | 1.00 | 0.00 | C |
| ATOM   | 4        | O        | ASN A    | 1                                                   | -6.634  | 1.849    | -1.758 | 1.00 | 0.00 | O |
| ATOM   | 5        | CB       | ASN A    | 1                                                   | -9.437  | 3.396    | -2.889 | 1.00 | 0.00 | C |
| 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 |
| ATOM   | 18       | CA       | LEU A    | 2                                                   | -4.923  | 4.002    | -2.452 | 1.00 | 0.00 | C |
| 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

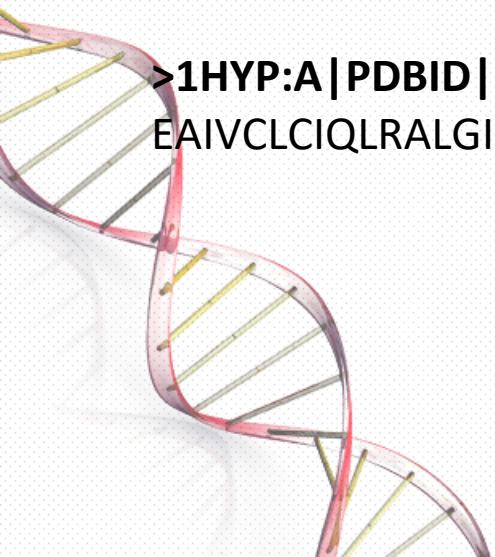


# Protein structure

- Primary
  - Sequence (from N- to C-terminus)
  - Sometimes also disulfide bonds

**FASTA format:**

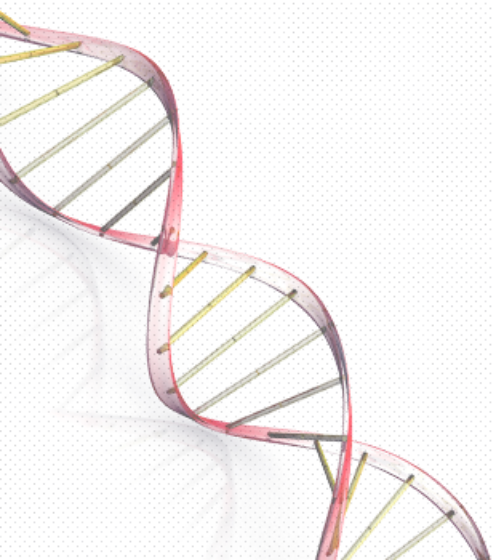
**>1HYP:A|PDBID|CHAIN|SEQUENCE**ALITRPSCPDLISICLNILGGSLGTVDDCCALIGGLGDI  
EAIVCLCIQLRALGILNLRNLQLILNSCGRSYPSNATCPRT



# Avogadro



- Program do budowy, wizualizacji i edycji cząsteczek chemicznych.
- Przeznaczony jest do stosowania w chemii obliczeniowej, modelowaniu molekularnym, inżynierii materiałowej czy też w bioinformatyce.



# Pytania i odpowiedzi na zadania

[m.mozolewska@ipipan.waw.pl](mailto:m.mozolewska@ipipan.waw.pl)

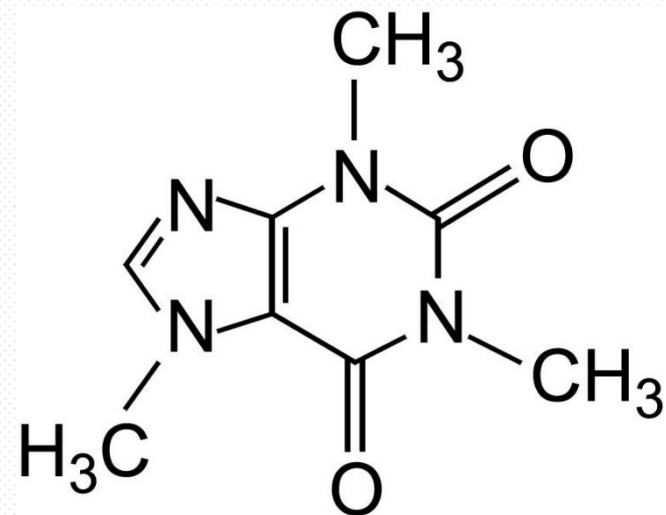
Zdjęcia, schematy i rysunki zostały zaczerpnięte z internetu.





# Zadania (maksymalnie 5 punktów)

1. Proszę zbudować cząsteczkę kofeiny w programie Avogadro.
  - a) Proszę obliczyć energię kofeiny przed optymalizacją energii.
  - b) Zoptymalizuj strukturę.
  - c) Proszę obliczyć energię kofeiny po optymalizacji energii.
  - d) Proszę obliczyć odległości pomiędzy atomami tlenu.
  - e) Proszę zapisać obrazek struktury.
  - f) Podaj do jakiej grupy związków chemicznych należy kofeina.



*Kofeina* C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>



# Zadania (maksymalnie 5 punktów)

2. Program R – baza bio3d
  - a) Zaimportuj z bazy PDB białko o kodzie 4Q21
  - b) Wyekstrahuj z pliku PDB sekwencję w postaci kodu trójliterowego i zamień go na kod jednoliterowy
  - c) Nałóż na siebie dwie struktury 4Q21 oraz 521P, zapisz wynik i obserwacje – czym się różnią?
  
3. Zaimportuj z bazy PDB białka:  
"1TND\_B", "1AGR\_A", "1FQJ\_A", "1TAG\_A", "1GG2\_A", "1KJY\_A"
  - a) Wyekstrahuj i nałóż na siebie interesujące nas łańcuchy
  - b) Oblicz podobieństwo sekwencyjne oraz RMSD

