

# Molekulafizika

## előadás

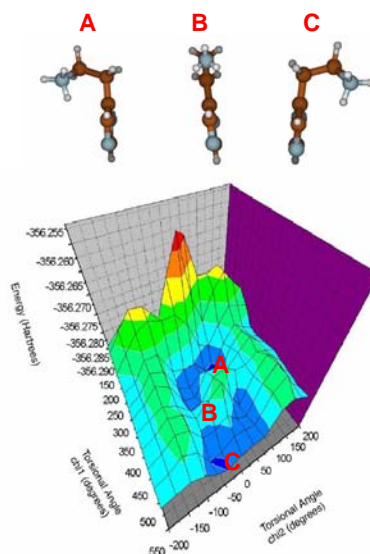
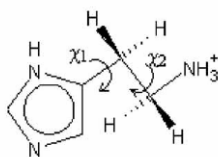
2006. december 14.

Bogár Ferenc  
MTA Fehérjekémiai Kutatócsoport  
SZTE



## Többatomos molekulák

- Koordináták (3N-6)
  - Descartes, belső
- Kötési energia, atomizációs energia
- Minimális bázis
  - C: 1s,2s,2px,2py,2pz
- PES, lokális minimumok, konformáció



# CH<sub>4</sub>

•T<sub>d</sub>

•Minimális bázis

C: 1s, 2s, 2p<sub>x</sub>, 2p<sub>y</sub>, 2p<sub>z</sub>

H: 1s<sub>H1</sub>, 1s<sub>H2</sub>, 1s<sub>H3</sub>, 1s<sub>H4</sub>

•Szimmetria függvények:

A<sub>1</sub>: a<sub>1</sub>1s<sub>H</sub> = 1s<sub>H1</sub> + 1s<sub>H2</sub> + 1s<sub>H3</sub> + 1s<sub>H4</sub>, 1s, 2s

F<sub>2</sub>: f<sub>21</sub>1s<sub>H</sub> = 1s<sub>H1</sub> + 1s<sub>H2</sub> - 1s<sub>H3</sub> - 1s<sub>H4</sub>, 2p<sub>x</sub>

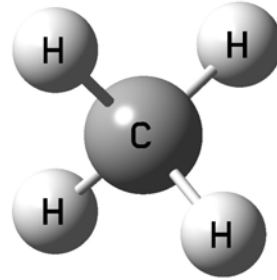
f<sub>21</sub>1s<sub>H</sub> = 1s<sub>H1</sub> + 1s<sub>H2</sub> - 1s<sub>H3</sub> - 1s<sub>H4</sub>, 2p<sub>y</sub>

f<sub>21</sub>1s<sub>H</sub> = 1s<sub>H1</sub> + 1s<sub>H2</sub> - 1s<sub>H3</sub> - 1s<sub>H4</sub>, 2p<sub>z</sub>

•A Fock mátrix 9 × 9-es

•A szimmetria bázisban szétbomlik

egy 3×3-as és egy 6 × 6-os blokkra



## CH<sub>4</sub> kanonikus pályák



1:A<sub>1</sub>



2:A<sub>1</sub>



3:F<sub>2</sub>



4:F<sub>2</sub>



5:F<sub>2</sub>



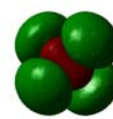
6:F<sub>2</sub>



7:F<sub>2</sub>



8:F<sub>2</sub>



9:A<sub>1</sub>

# NH<sub>3</sub>

•T<sub>d</sub>

•Minimális bázis

N: 1s, 2s, 2p<sub>x</sub>, 2p<sub>y</sub>, 2p<sub>z</sub>

H: 1s<sub>H1</sub>, 1s<sub>H2</sub>, 1s<sub>H3</sub>

•Szimmetria függvények:

A<sub>1</sub>: a<sub>1</sub>1s<sub>H</sub> = 1s<sub>H1</sub> + 1s<sub>H2</sub> + 1s<sub>H3</sub>, 1s, 2s, 2p<sub>z</sub>

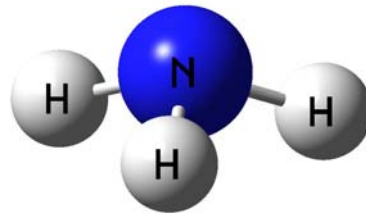
E<sub>1</sub>: e<sub>11</sub>1s<sub>H</sub> = 1s<sub>H1</sub> - 1/2(1s<sub>H2</sub> + 1s<sub>H3</sub>), 2p<sub>x</sub>

e<sub>12</sub>1s<sub>H</sub> = (1s<sub>H2</sub> - 1s<sub>H3</sub>), 2p<sub>y</sub>

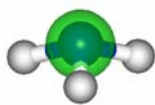
•A Fock mátrix 8 × 8-as

•A szimmetria bázisban szétbomlik

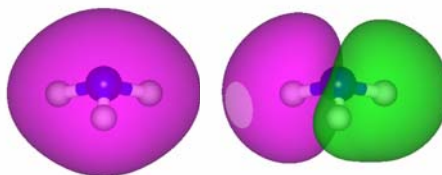
két 4×4-es blokkra



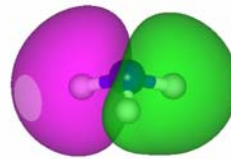
## NH<sub>3</sub> kanonikus pályák



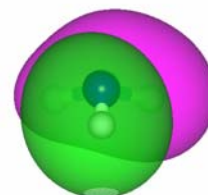
1:A<sub>1</sub>



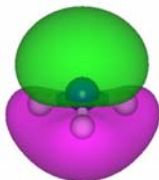
2:A<sub>1</sub>



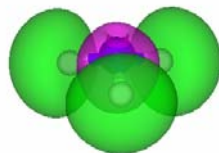
3:E<sub>1</sub>



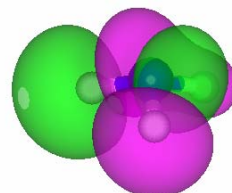
4:E<sub>1</sub>



5:A<sub>1</sub>



6:A<sub>1</sub>

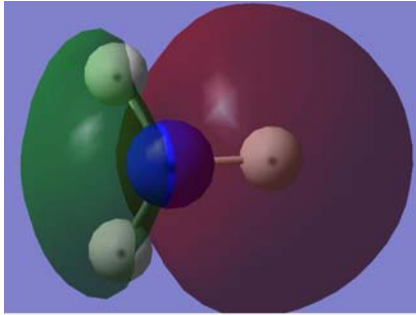


7:E<sub>1</sub>

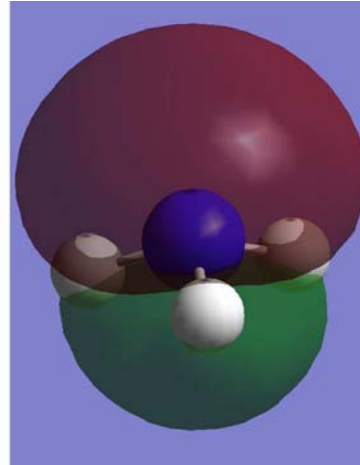


8:E<sub>1</sub>

## NH<sub>3</sub> lokalizált pályák



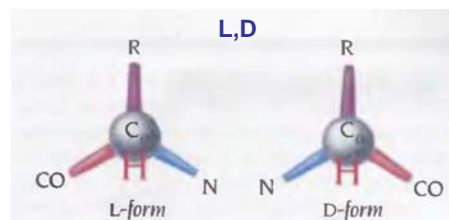
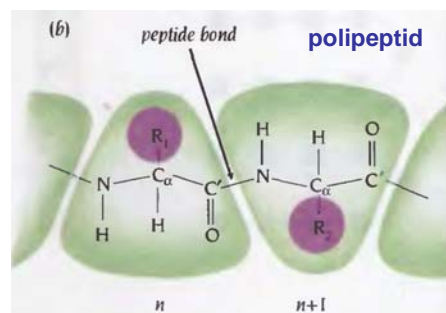
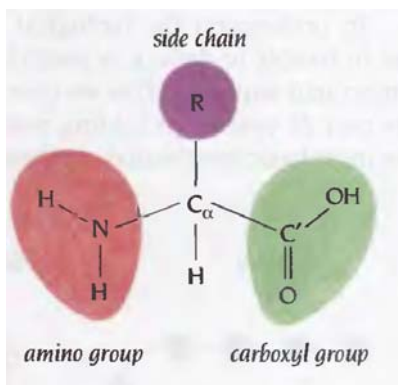
NH kötés



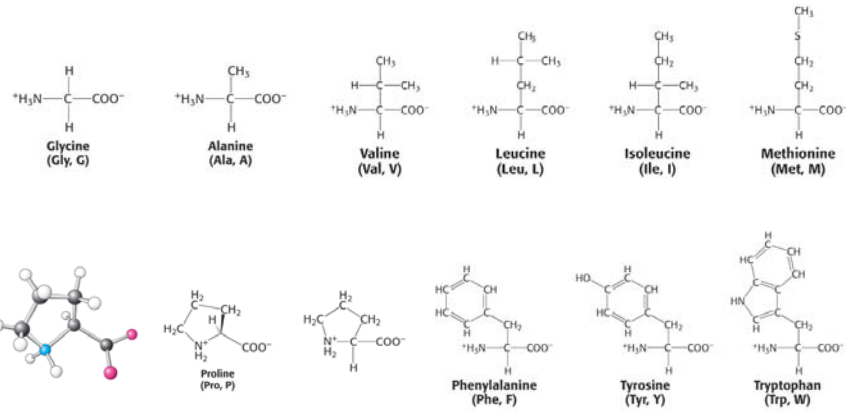
Magányos pár

## Peptidek; fehérjék

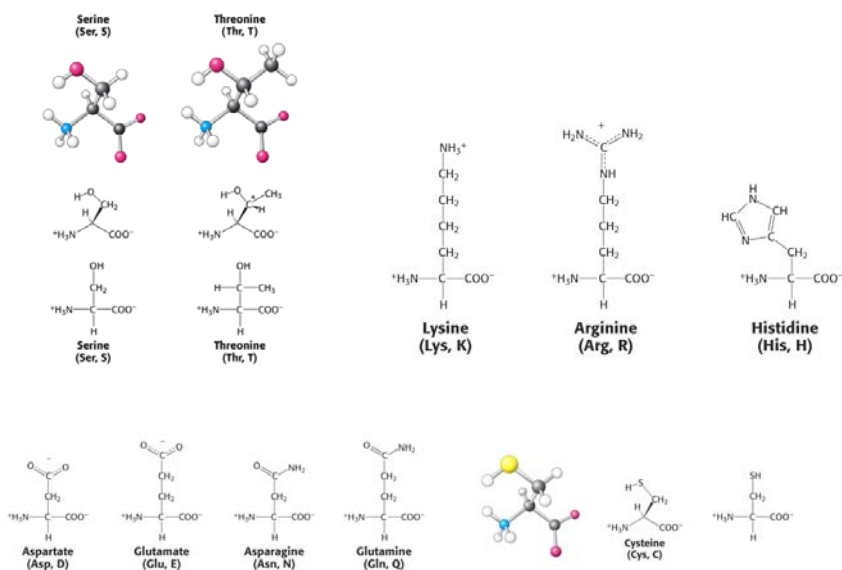
aminosav



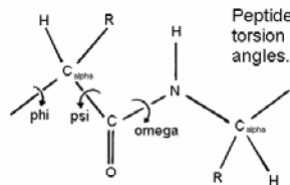
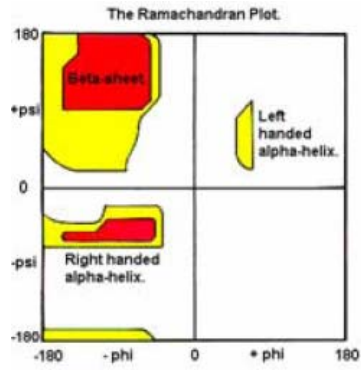
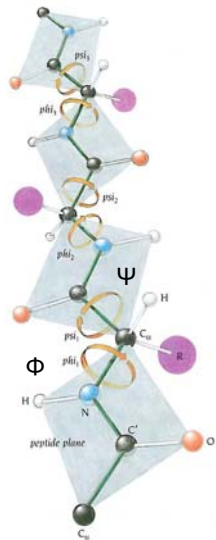
# Alifás és aromás aminosavak



# Poláros aminosavak

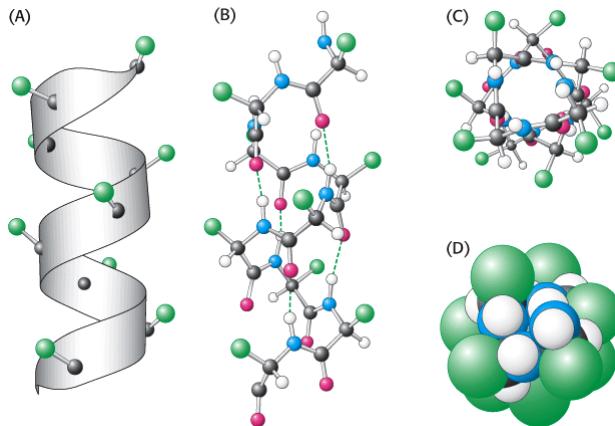


# Másodlagos szerkezet

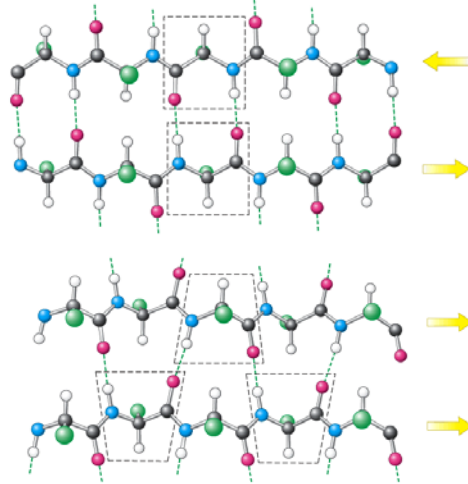


Branden & Tooze, Introduction to protein structure

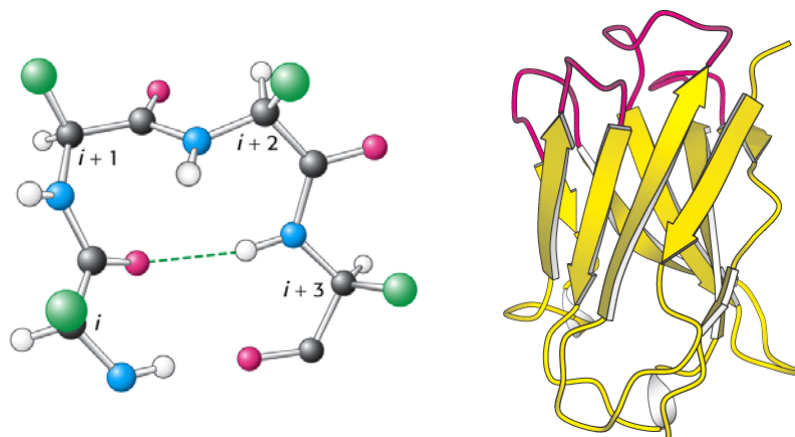
# Alfa hélix



## Béta redő

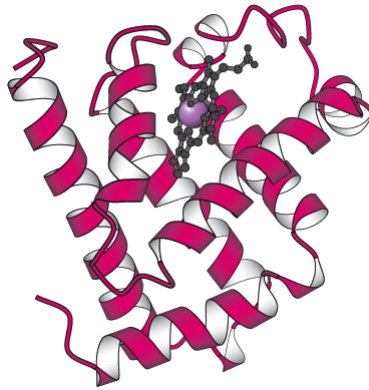


## Kanyar

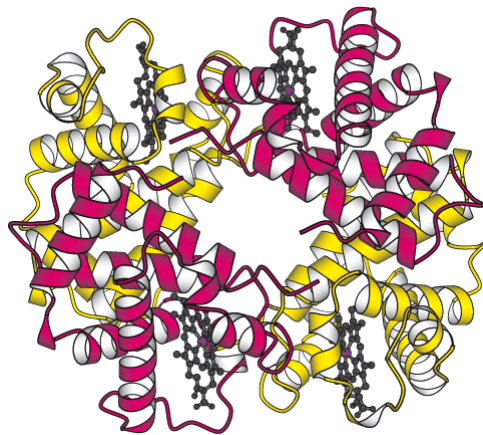


## Harmadlagos szerkezet

(B)

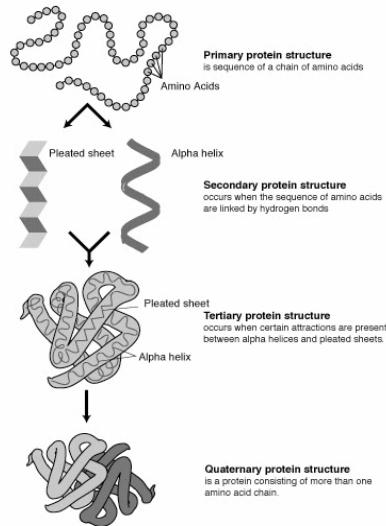


## Negyedleges szerkezet

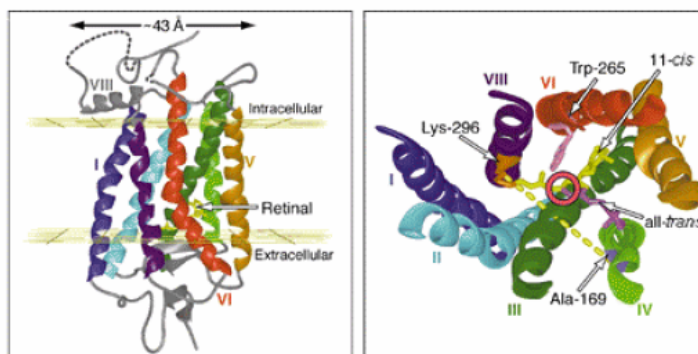




# Szerveződési szintek



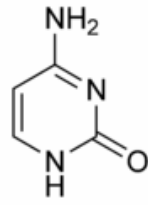
# Membránban kötött receptorok



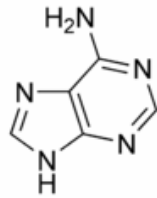
**Two views of rhodopsin. (Left)** The seven  $\alpha$  helices of the GPCR rhodopsin weave back and forth through the membrane lipid bilayer (yellow lines) from the extracellular environment (bottom) to the cytoplasm (top). **(Right)** The chromophore, retinal, is nestled among the transmembrane helices (loops not shown; enlargement viewed from the cytoplasm). Retinal is shown in its 11-*cis* dark form (yellow) and its all-*trans* light form (magenta, where the two differ). Roman numerals indicate numbered helices; the red circle indicates the position about which isomerization of retinal (from *cis* to *trans*) occurs.

<http://www.biochem.wisc.edu/biochem630/pdfs/8bourne.pdf>

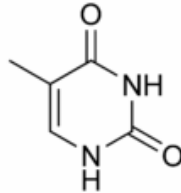
# A DNS építőkövei



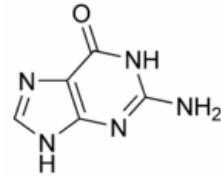
Citozin



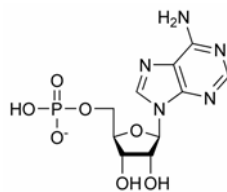
Adenin



Timin

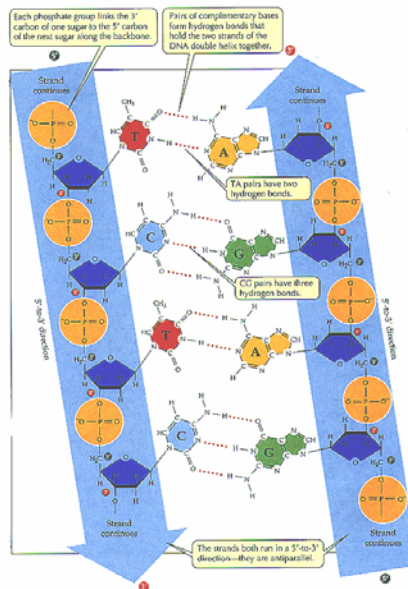


Guanin



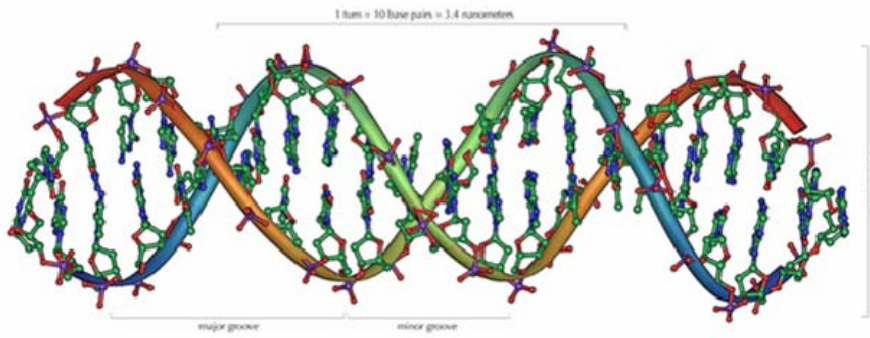
Nukleotid

# A DNS felépítése



Taken from [http://www.bio.utk.edu/bio140/structure\\_of\\_dna\\_and\\_rna.htm](http://www.bio.utk.edu/bio140/structure_of_dna_and_rna.htm)

# Térszerkezet



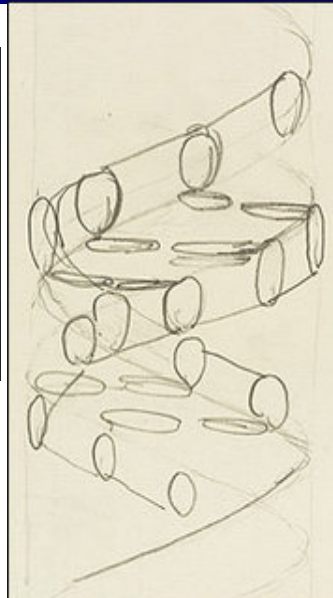
# Történet



James Watson  
Cavendish Laboratory  
University of Cambridge



Francis Crick



# Források

## DNS:

[en.wikipedia.org/wiki/DNA](https://en.wikipedia.org/wiki/DNA)

[www.blc.arizona.edu/Molecular\\_Graphics/DNA\\_Structure/DNA\\_Tutorial.HTML#Purine](http://www.blc.arizona.edu/Molecular_Graphics/DNA_Structure/DNA_Tutorial.HTML#Purine)

## Fehérjék:

[en.wikipedia.org/wiki/Protein\\_structure](https://en.wikipedia.org/wiki/Protein_structure)

[webhost.bridgew.edu/fgorga/proteins/default.htm](http://webhost.bridgew.edu/fgorga/proteins/default.htm)