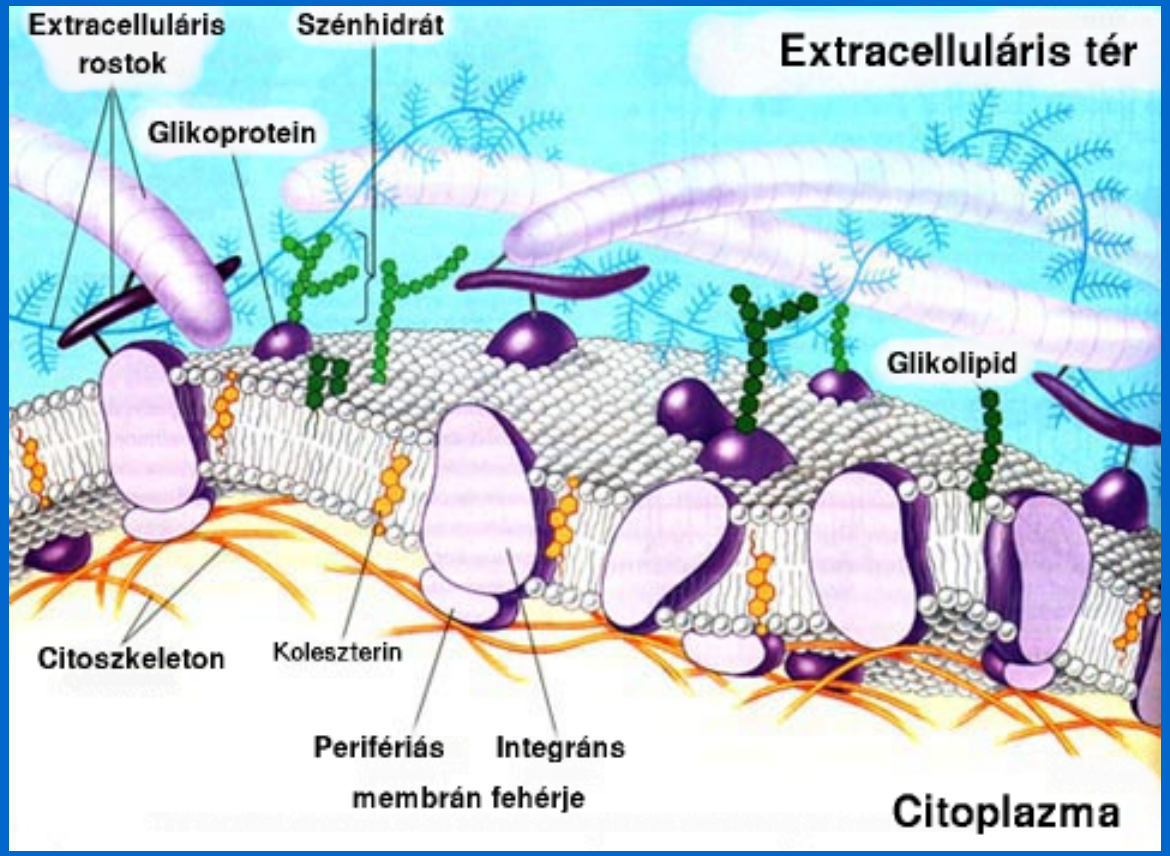
Makromolekulák

Simon István

Transzmembrán fehérjék



Anyagcsere folyamatok

Transzporterek

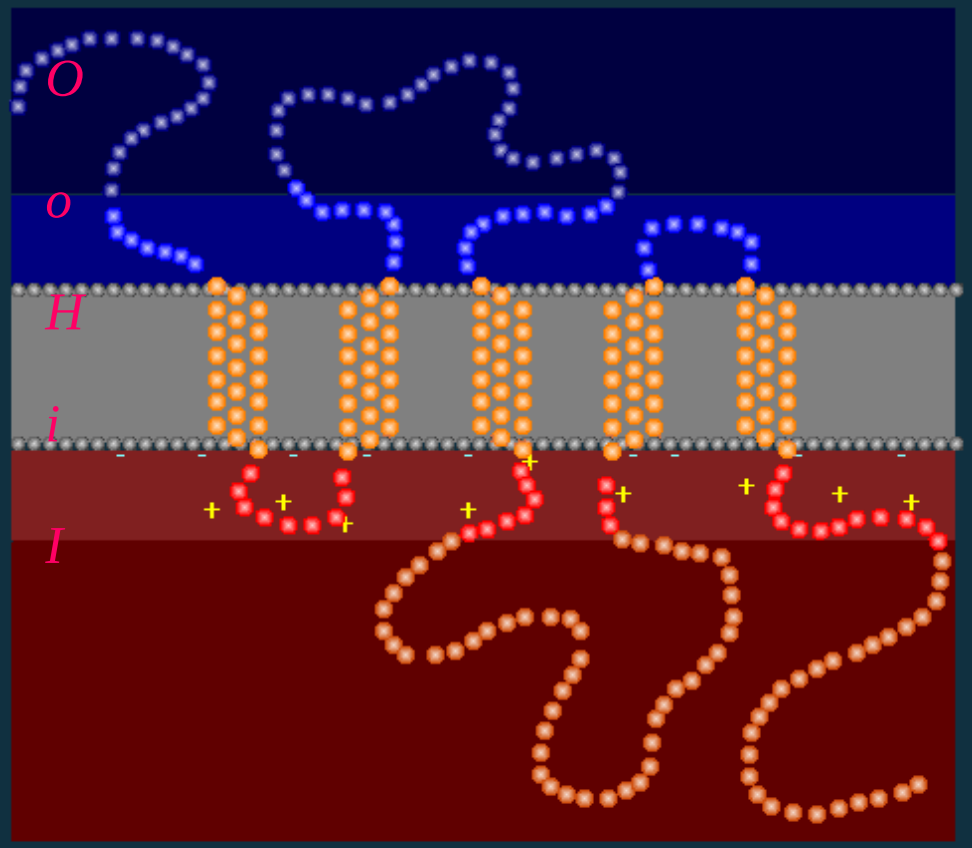
Ion csatornák

Hordozók

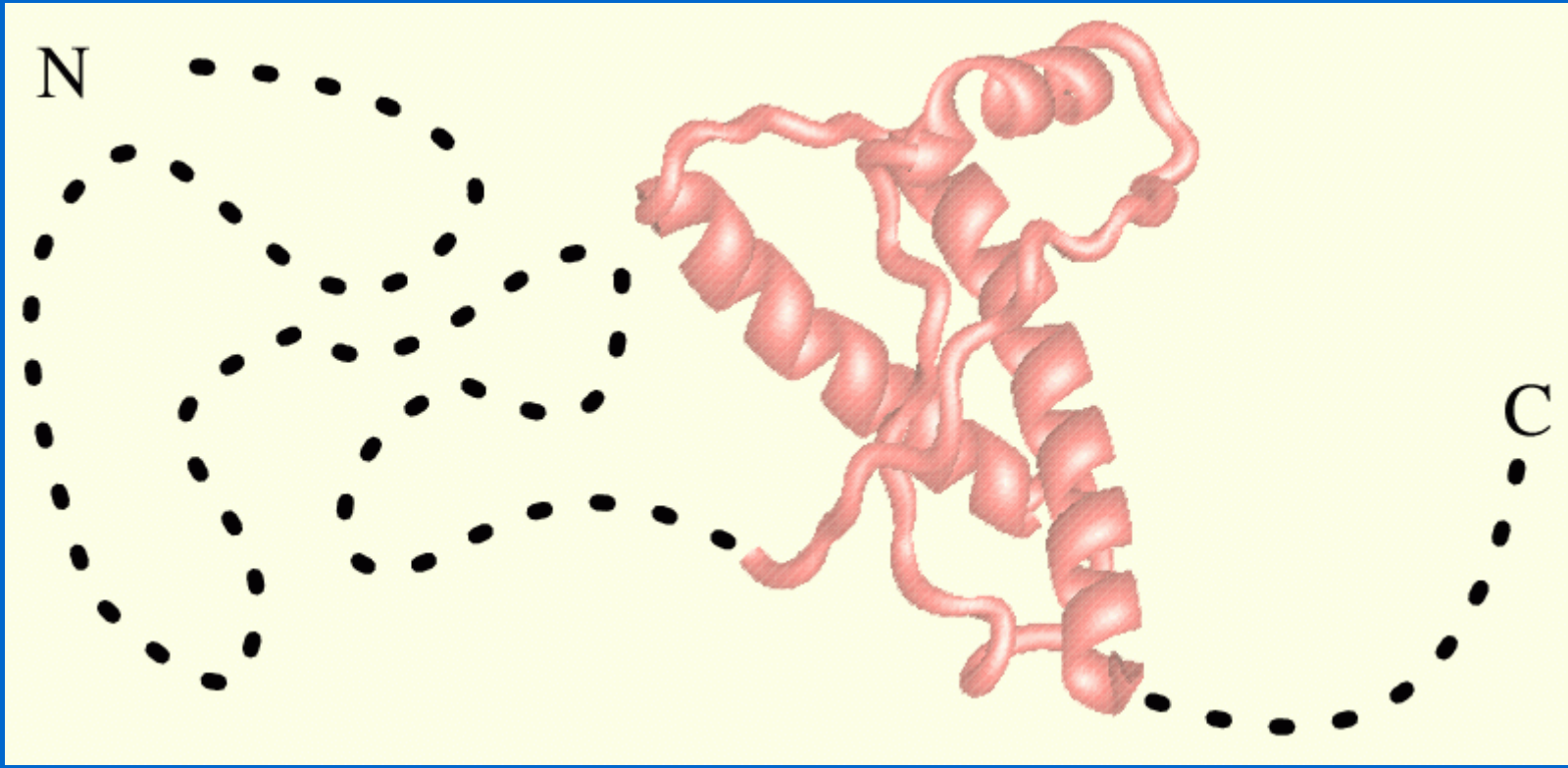
Információ csere

Receptorok

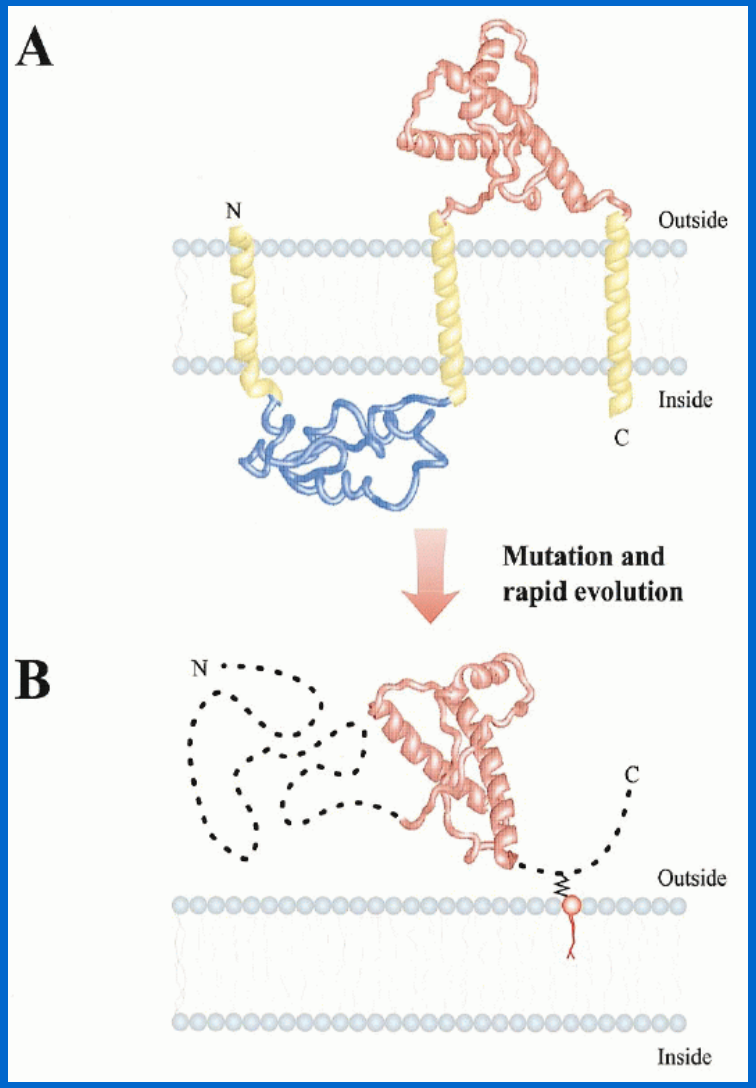
A HMMTOP eljárás



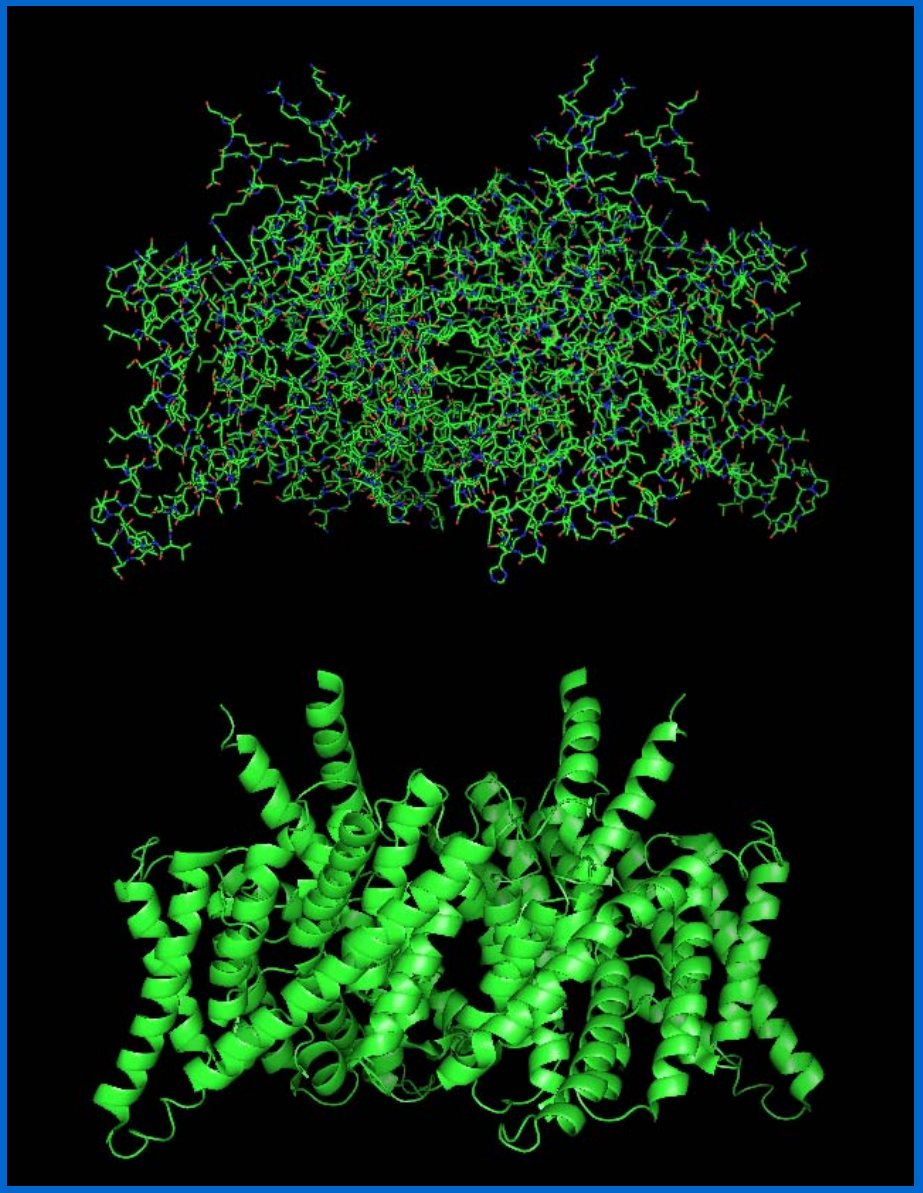
Prion protein



Prion fehérje

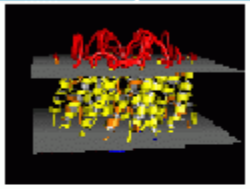


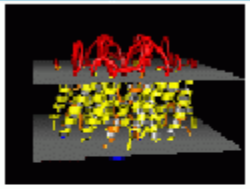
E. Coli klorid csatorna fehérje



Membrán pozíció lokalizálása transzmembrán fehérjékben

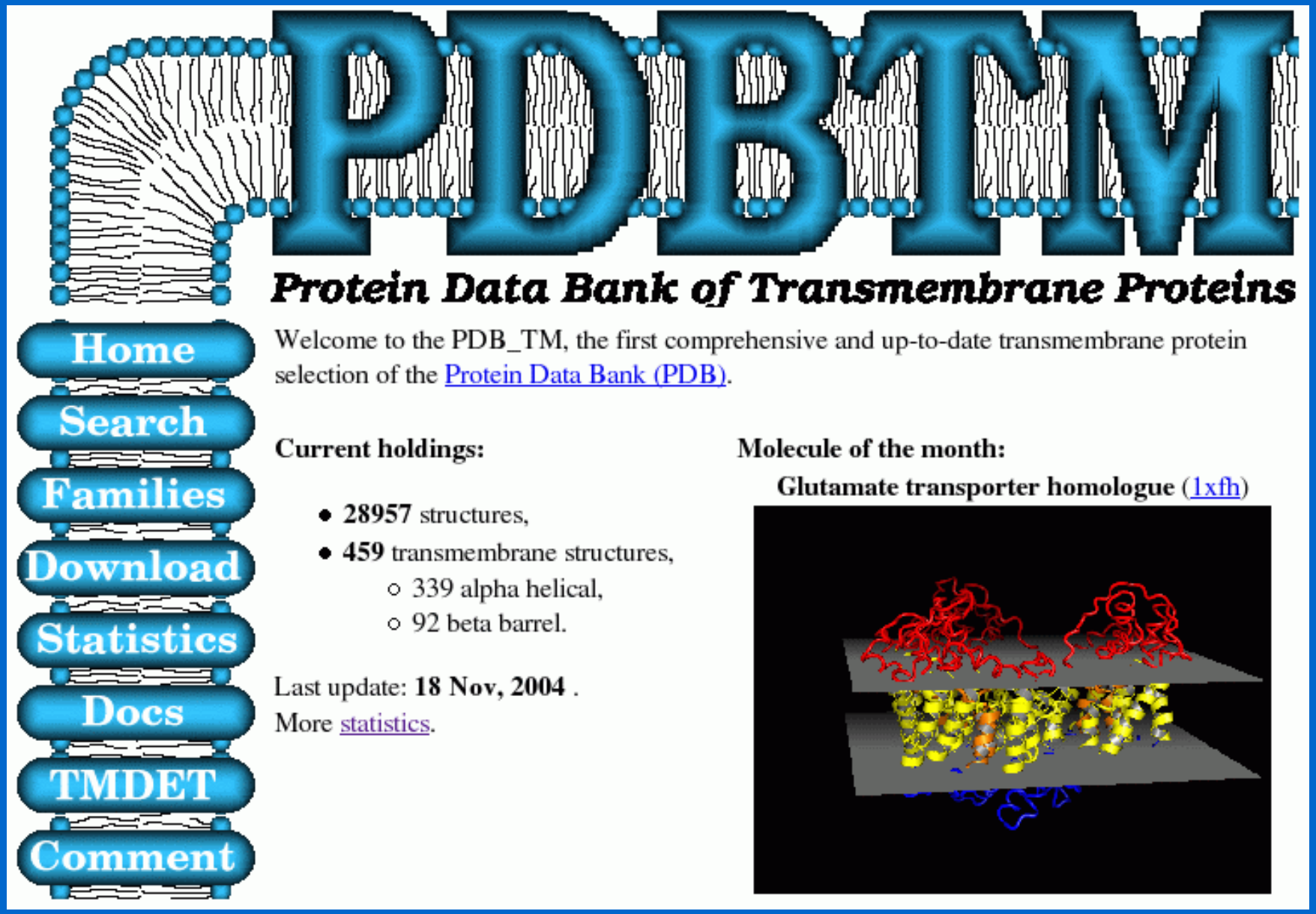
1fqy	Alpha helical protein



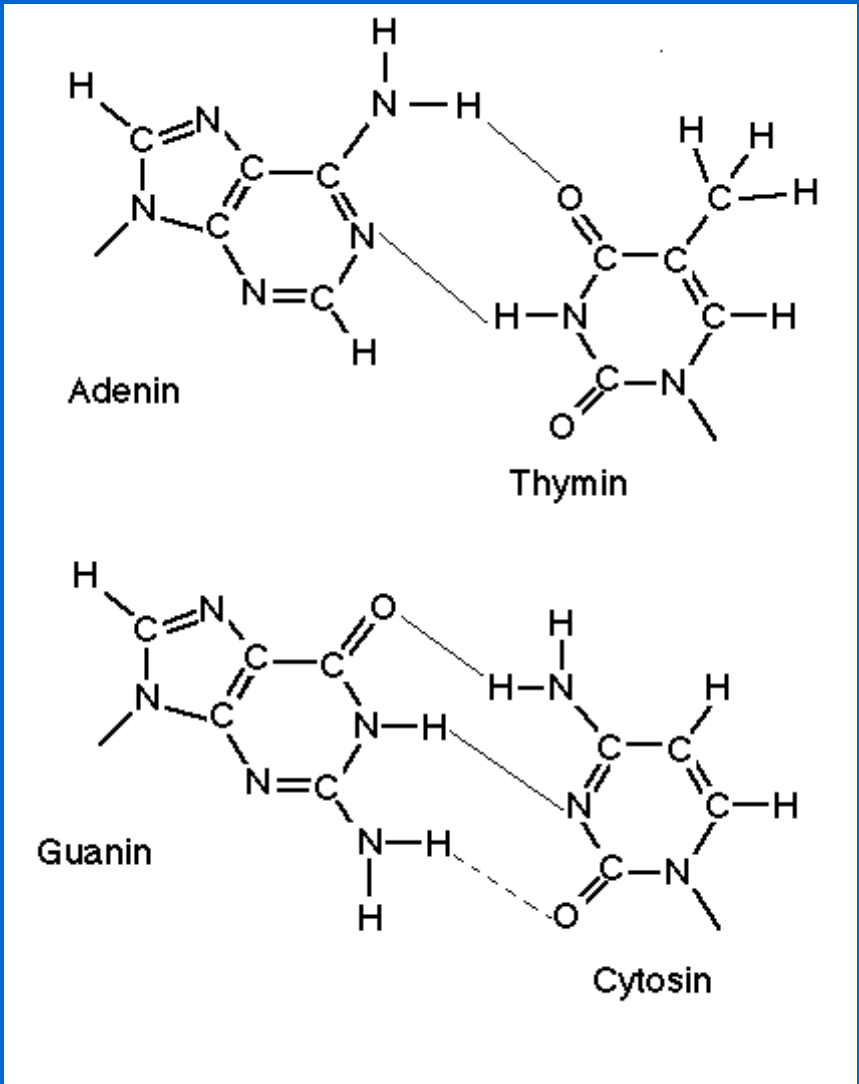


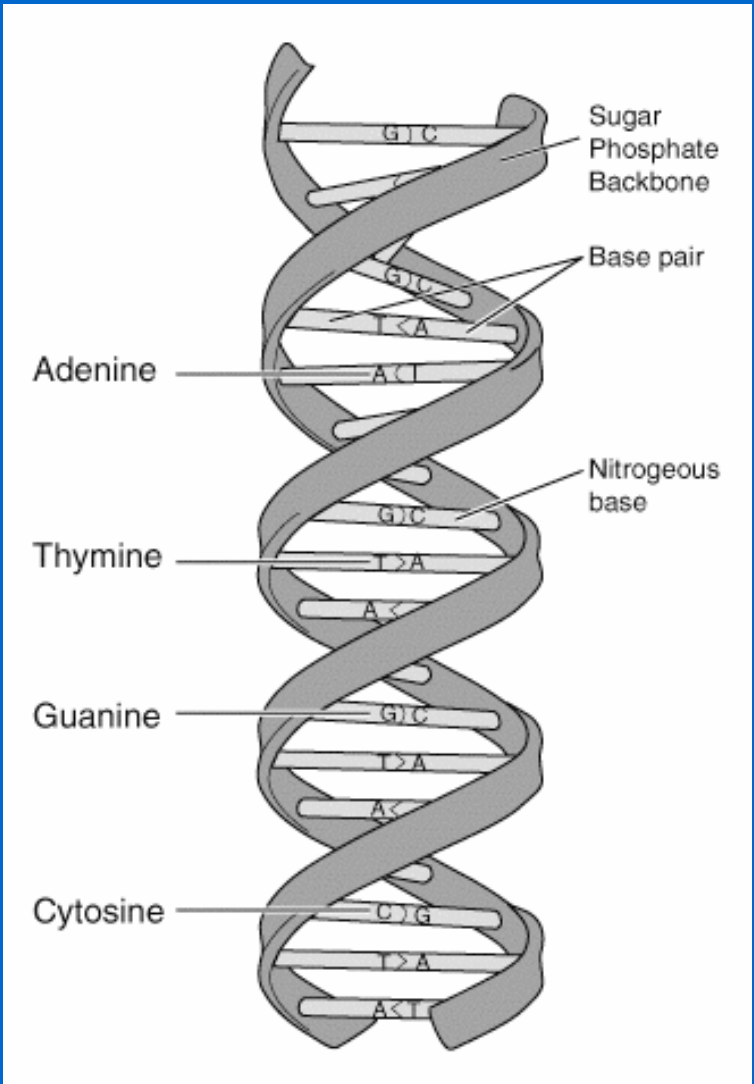
Chain 'A' has 6 transmembrane segments:	
Unknown	1-7 (MASEFKK)
Side 2	8-10 (KLF)
Transmembrane	11-31 (WRAVVAEFL..LFVFISIGS)
Side 1	32-49 (ALGFKYPVGNNQTAVQDN)
Transmembrane	50-69 (VKVSLAFGLSIATLAQSVGH)
Side 2	70-70 (I)
Membrane loop	71-85 (SGAHLNPAVTLGLLL)
Side 2	86-91 (SCQISI)
Transmembrane	92-112 (FRALMYIIA..GAIVATAIL)
Side 1	113-137 (SGITSSLTG..LADGVNSGQ)
Transmembrane	138-156 (GLGIEIIGTLQLVLCVLAT)
Side 2	157-165 (TDRRRRDLG)
Transmembrane	166-184 (GSAPLAIGLSVALGHLLAI)
Side 1	185-187 (DYT)
Membrane loop	188-201 (GCGINPARSFGSAV)
Side 1	202-207 (ITHNFS)
Transmembrane	208-230 (NHWIFWVGP..LAVLIYDFI)
Side 2	231-233 (LAP)
Unknown	234-269 (RSSDLTDRV..NSRVEMKPK)

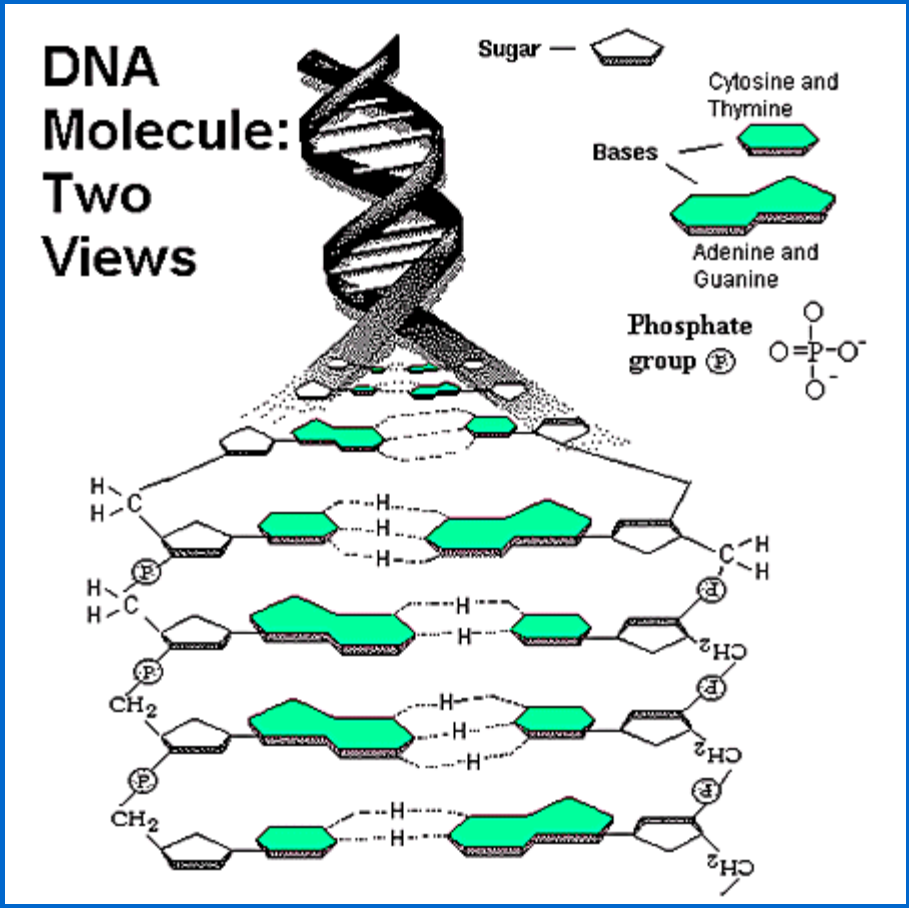
A PDB_TM adatbázis



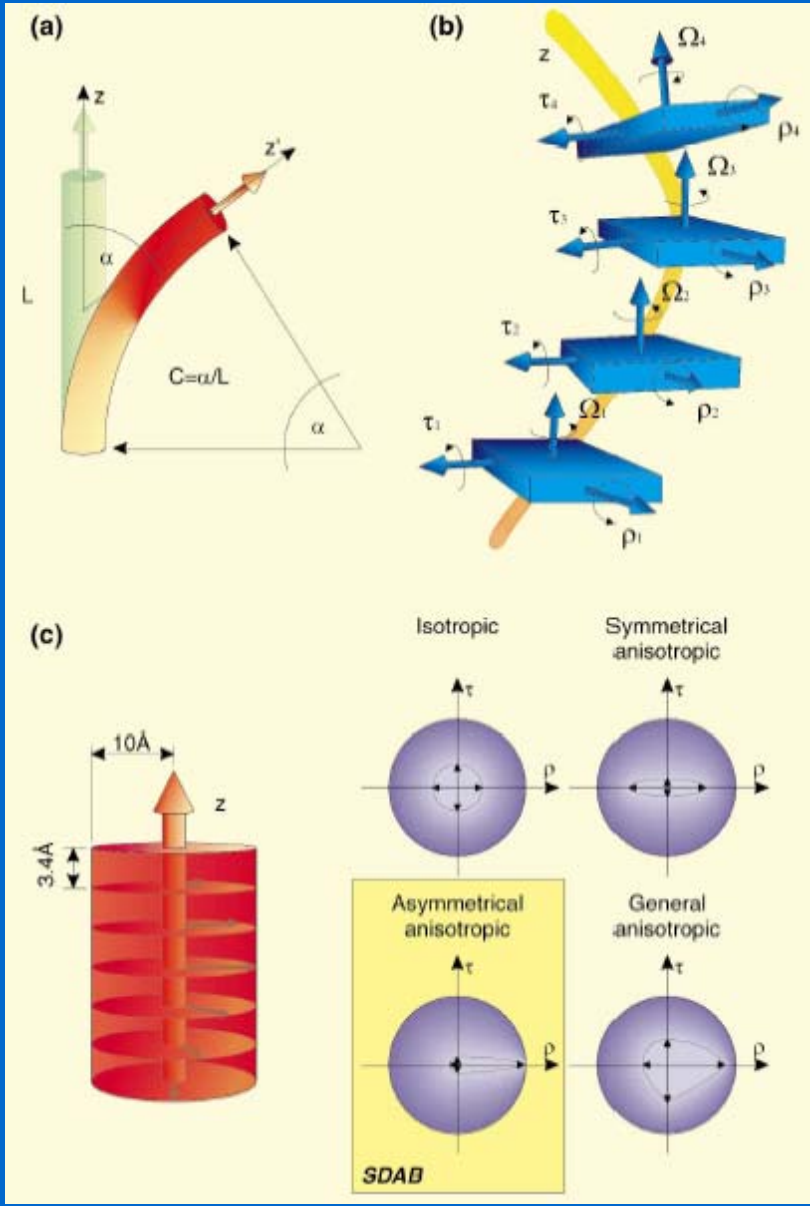
DNS


Adenin
Thymin
Guanin
Cytosin

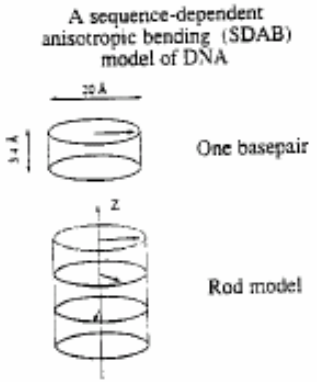

Sugar
Phosphate
Backbone
Base pair
Adenine
Nitrogeous
base
Thymine
Guanine
Cytosine


DNA Molecule: Two Views
Sugar
Cytosine and Thymine
Bases
Adenine and Guanine
Phosphate group

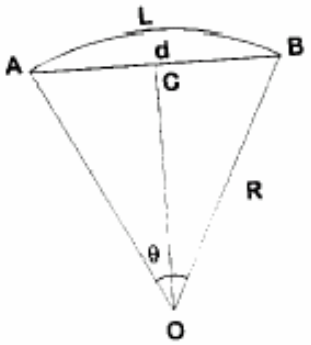
Inhomogén anizotróp rúd hajlítása



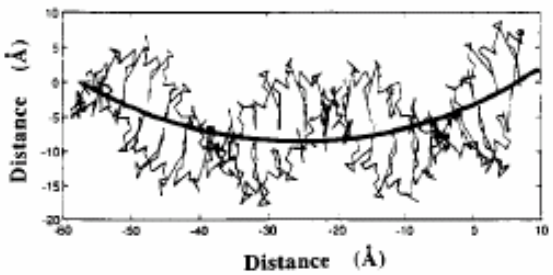
DNS hajlítás



a



b

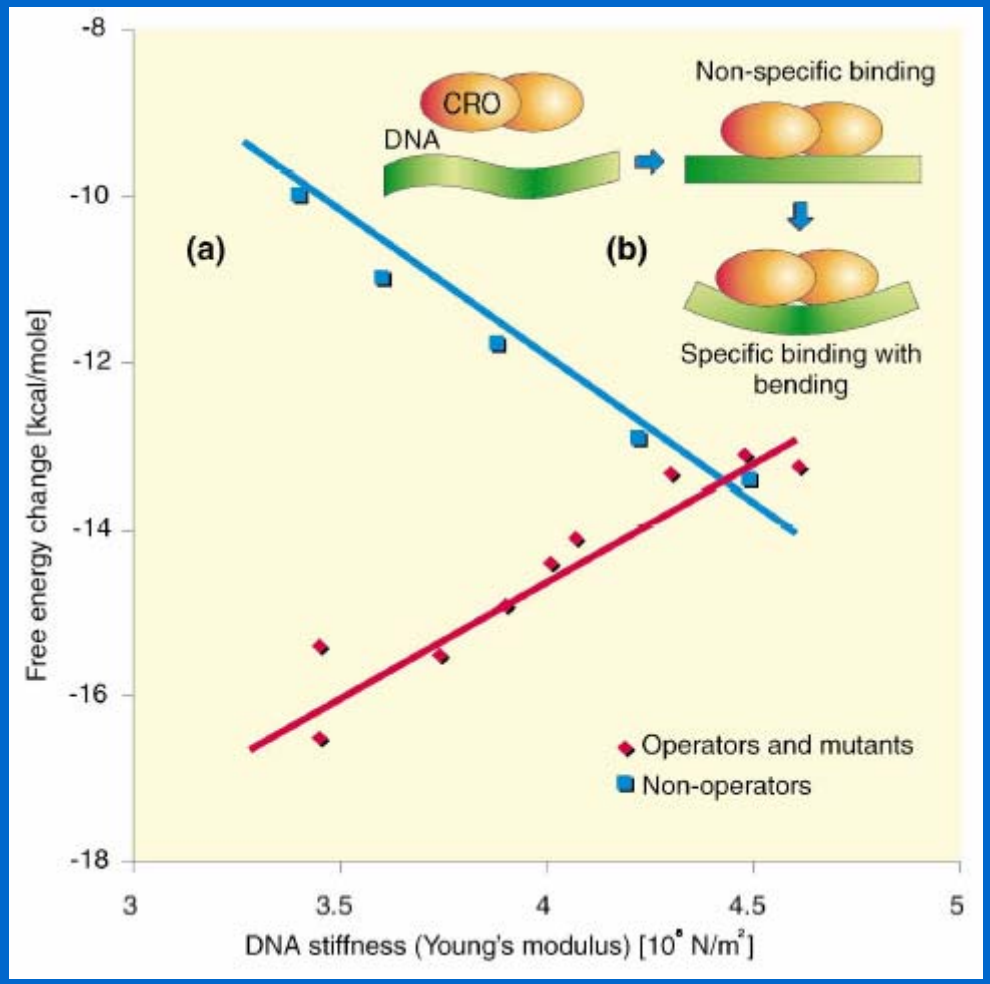


c

DNA stiffness (Young's modulus) scale for the trinucleotides in DNA [5]

Trinucleotide	Young's modulus, E (10^8 N/m^2)	Trinucleotide	Young's modulus, E (10^8 N/m^2)
AAA/TTT	7.176	CAG/CTG	1.668
AAC/GTT	6.272	CCA/TGG	6.813
AAG/CTT	4.736	CCC/GGG	3.868
AAT/ATT	7.237	CCG/CGG	5.440
ACA/TGT	3.810	CGA/TCG	3.810
ACC/GGT	4.156	CGC/GCG	4.678
ACG/CGT	4.156	CTA/TAG	2.673
ACT/AGT	6.033	CTC/GAG	3.353
AGA/TCT	3.410	GAA/TTC	4.214
AGC/GCT	3.524	GAC/GTC	3.925
AGG/CCT	4.445	GCA/TGC	2.842
ATA/TAT	1.613	GCC/GGC	2.448
ATC/GAT	5.087	GGA/TCC	3.581
ATG/CAT	2.169	GTA/TAC	3.467
CAA/TTG	3.581	TAA/TTA	2.955
CAC/GTG	3.239	TCA/TGA	1.447

Computed Young's modulus for Cro operators, mutants and non-operators

No.	Code	Sequences	E (10^8 N/m^2)	ΔG (kcal/mole)
Operators				
1	OR1	TACCTCTGGCGGTGATA	3.45	−15.4
2	OR2	CAACACGCACGGTGTTA	4.07	−14.1
3	OR3	TATCCCTTGCGGTGATA	3.45	−16.1
4	OL1	TACCACTGGCGGTGATA	3.74	−15.5
5	OL2	TATCTCTGGCGGTGTTG	3.90	−14.9
6	OL3	AACCATCTGCGGTGATA	4.01	−14.4
Operator mutants				
7	OM1	TTTACCTCTGGCGGTGATAAT	4.30	−13.33
8	OM2	TTTACCTCTGGCGGTATTAAT	4.48	-13.11
9	OM3	TTTACCTCTGGCGGAGTTAAT	4.61	−13.26
Non-operators				
10	N1	TAAAACACCTCACGAGTTAAT	4.49	−13.40
11	N2	TAAATCACTCCCGGGTATATT	4.22	−12.90
12	N3	TATATCAGTGGCAGTGTGAAT	3.60	−10.97
13	N4	TAGATCACCGCAGCGGTTGCT	3.88	−11.76
14	N5	TTCAGCACCGCTGATGCTGCT	3.40	−9.97

DNS-Cro fehérje kölcsönhatás