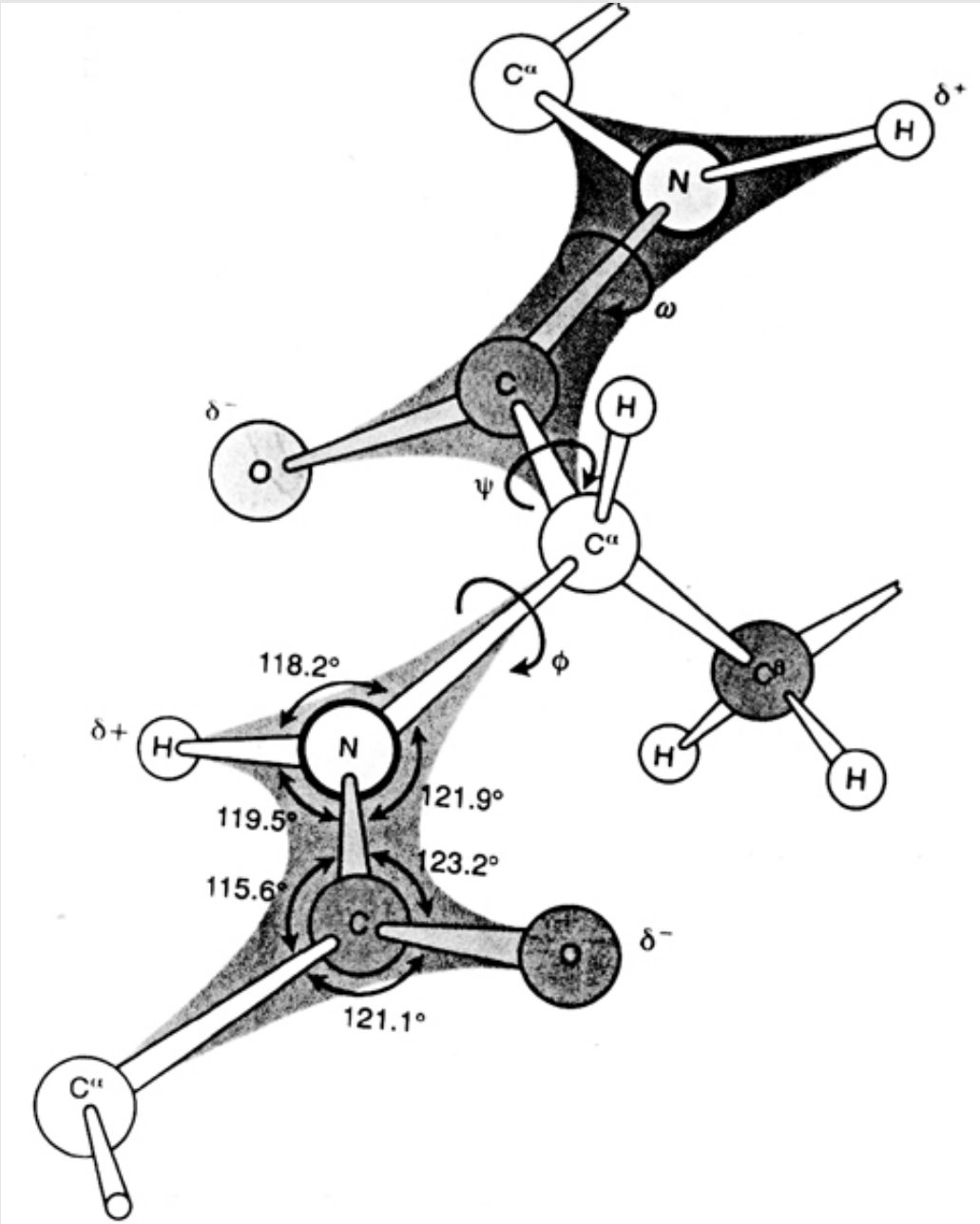
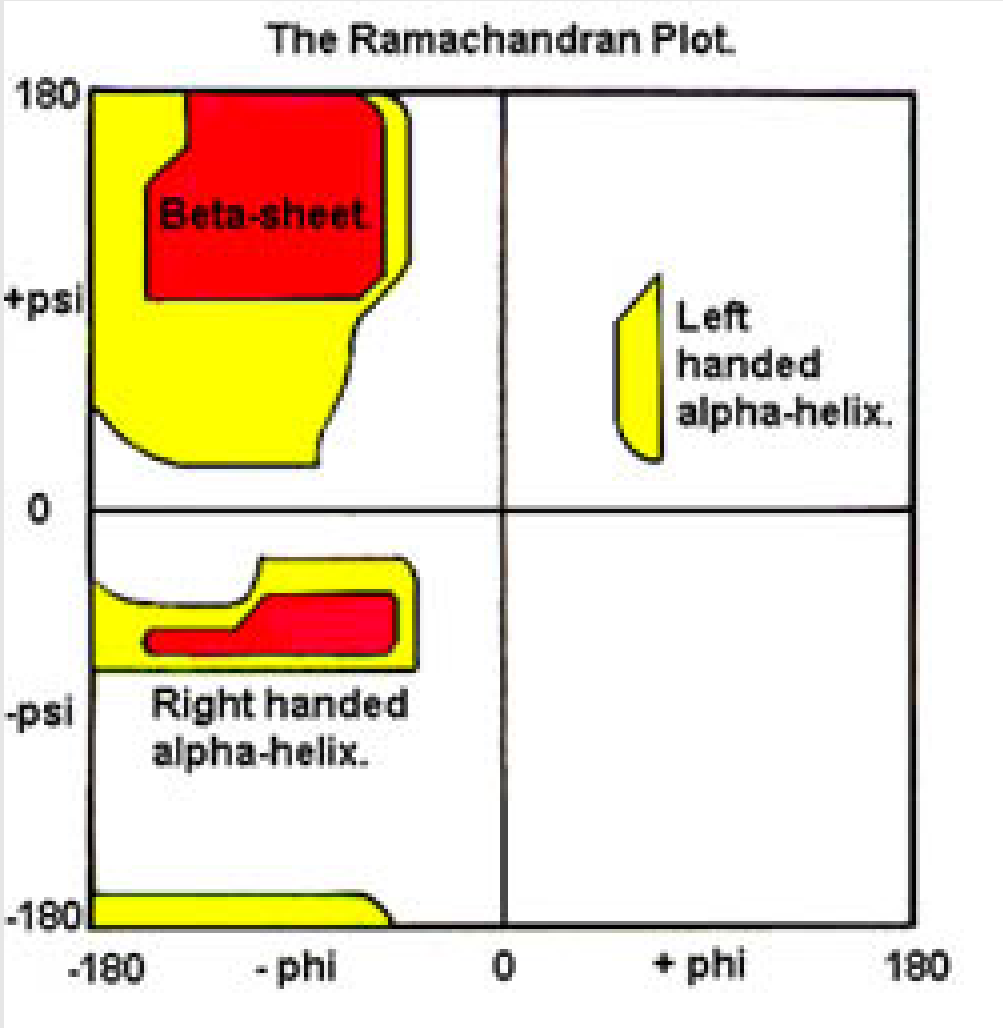
Makromolekulák

Simon István

A peptid kötés

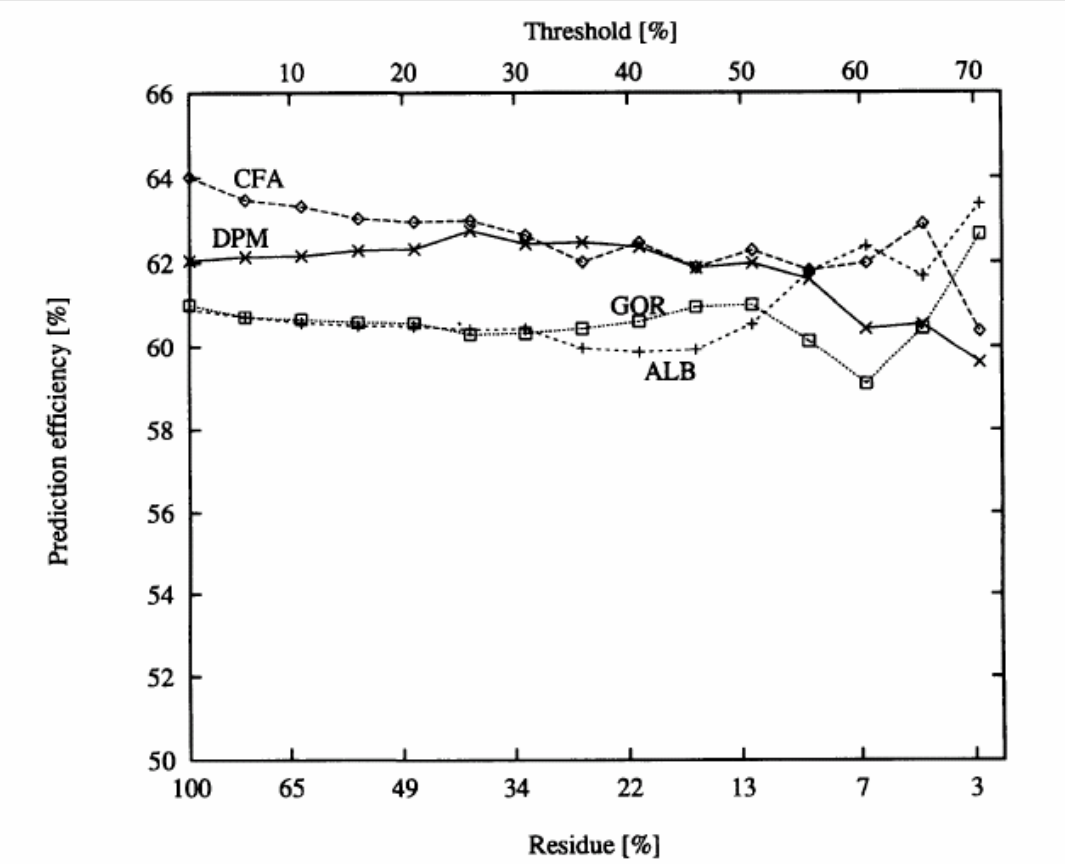



The Ramachandran Plot.
180
+psi
0
-psi
-180
Beta-sheet.
Left
handed
alpha-helix.
Right handed
alpha-helix.
-180
- phi
0
+ phi
180

Chou-Fasman Paraméterek

Aminosav	P(a)	P(b)
Alanine	142	83
Arginine	98	93
Aspartic Acid	101	54
Asparagine	67	89
Cysteine	70	119
Glutamic Acid	151	037
Glutamine	111	110
Glycine	57	75
Histidine	100	87
Isoleucine	108	160
Leucine	121	130
Lysine	114	74
Methionine	145	105
Phenylalanine	113	138
Proline	57	55
Serine	77	75
Threonine	83	119
Tryptophan	108	137
Tyrosine	69	147
Valine	106	170

Másodlagos szerkezetbecslő módszerek pontossága



Másodlagos szerkezetbecslő módszerek pontossága

	Accuracy of prediction methods			
	Chou–Fasman	Deléage	GOR	ALB
Helices	65.57%	68.63%	66.17%	70.61%
	65.37%	68.78%	65.84%	69.94%
	64.45%	**67.62%**	**64.47%**	**74.19%**
	ref. 65 70%	*ref 67.18%*	*ref. 65.41%*	*ref. 70.28%*
	δ = 0.83%	*δ = 0.85%*	*δ = 0.86%*	*δ = 0.88%*
Sheets	63.07%	65.02%	65.46%	59.06%
	62.15%	62.68%	64.57%	58.85%
	60.01%	**64.18%**	**62.97%**	**57.69%**
	ref. 63 39%	*ref. 65.50%*	*ref. 65.24%*	*ref. 58.96%*
	δ = 0.81%	*δ = 0.79%*	*δ = 0 79%*	*δ = 0.71%*
Turns		53.12%	57.54%	58.55%
		52.90%	57.09%	58.29%
		53.03%	**60.62%**	**58.83%**
		ref. 53.33%	*ref. 57.93%*	*ref. 59.33%*
	63.39%	*δ = 0.81%*	*δ = 0 99%*	*δ = 1.04%*
	63.94%			
	60.66%	61.44%	54.88%	55.37%
Coils	*ref. 63.20%*	61.20%	54.76%	57.18%
	δ = 0.77%	**61.32%**	**54.85%**	**49.35%**
		ref. 60.53%	*ref. 54 69%*	*ref. 53.92%*
		δ = 0.74%	*δ = 0 47%*	*δ = 0.77%*

Aminosav helyettesítési mátrix

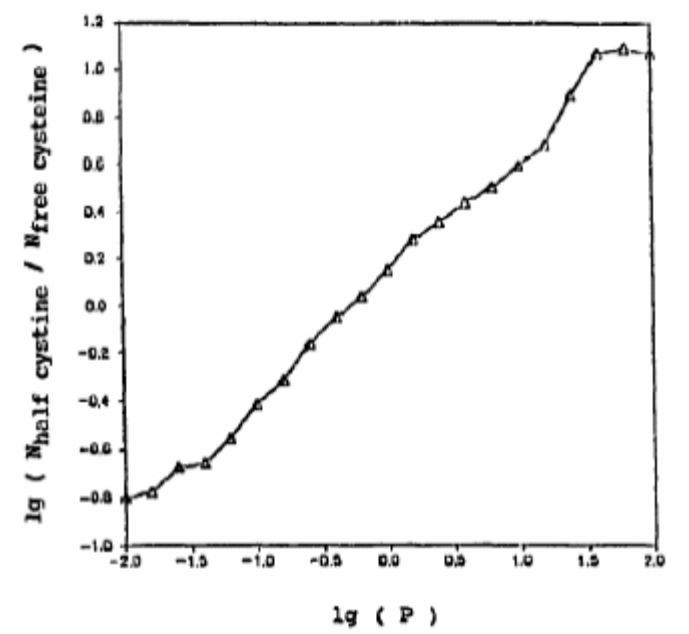
	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W
C	0.04																		
D	−0.08	−0.24																	
E	0.08	−0.51	0.37																
F	−0.25	0.30	−0.40	−0.50															
G	0.11	0.25	0.11	−0.23	−0.09														
H	−0.11	0.18	0.22	−0.19	−0.06	0.18													
I	−0.10	0.26	−0.54	−0.51	0.60	−0.22	−0.14												
K	−0.07	−0.43	0.18	0.54	−0.41	−0.23	−0.09	−0.40											
L	0.20	0.23	−0.55	−0.45	0.44	−0.14	−0.12	0.60	−0.34										
M	0.15	0.10	−0.25	−0.14	0.22	−0.01	−0.19	0.36	−0.16	0.38									
N	−0.14	−0.14	0.56	0.13	−0.33	0.22	0.32	−0.37	0.22	−0.39	−0.11								
P	−0.07	0.02	0.09	−0.11	−0.12	0.25	0.05	−0.19	−0.17	−0.20	−0.17	0.05							
Q	−0.01	−0.29	0.19	0.51	−0.44	−0.13	0.05	−0.43	0.52	−0.30	−0.18	0.20	−0.03						
R	−0.07	−0.20	−0.01	0.34	−0.31	−0.11	0.13	−0.29	0.47	−0.20	−0.17	0.12	−0.17	0.57					
S	0.14	0.10	0.22	−0.17	−0.01	0.29	0.14	−0.27	−0.24	−0.19	−0.17	0.14	0.27	−0.06	−0.16				
T	0.11	0.14	0.23	−0.27	0.02	−0.02	0.08	0.00	−0.24	−0.04	−0.02	0.13	0.20	−0.15	−0.32	0.45			
V	0.06	0.33	−0.48	−0.44	0.47	−0.12	−0.18	0.70	−0.36	0.49	0.23	−0.46	−0.17	−0.38	−0.29	−0.18	0.07		
W	−0.25	0.18	−0.41	−0.22	0.41	−0.08	−0.11	0.36	−0.22	0.22	0.16	−0.39	−0.13	−0.17	−0.03	−0.17	−0.12	0.29	
Y	−0.36	0.21	−0.34	−0.32	0.54	−0.24	0.08	0.43	−0.20	0.17	0.07	−0.27	−0.23	−0.28	−0.03	−0.21	−0.14	0.31	0.43

Diszulfid becslő potenciál

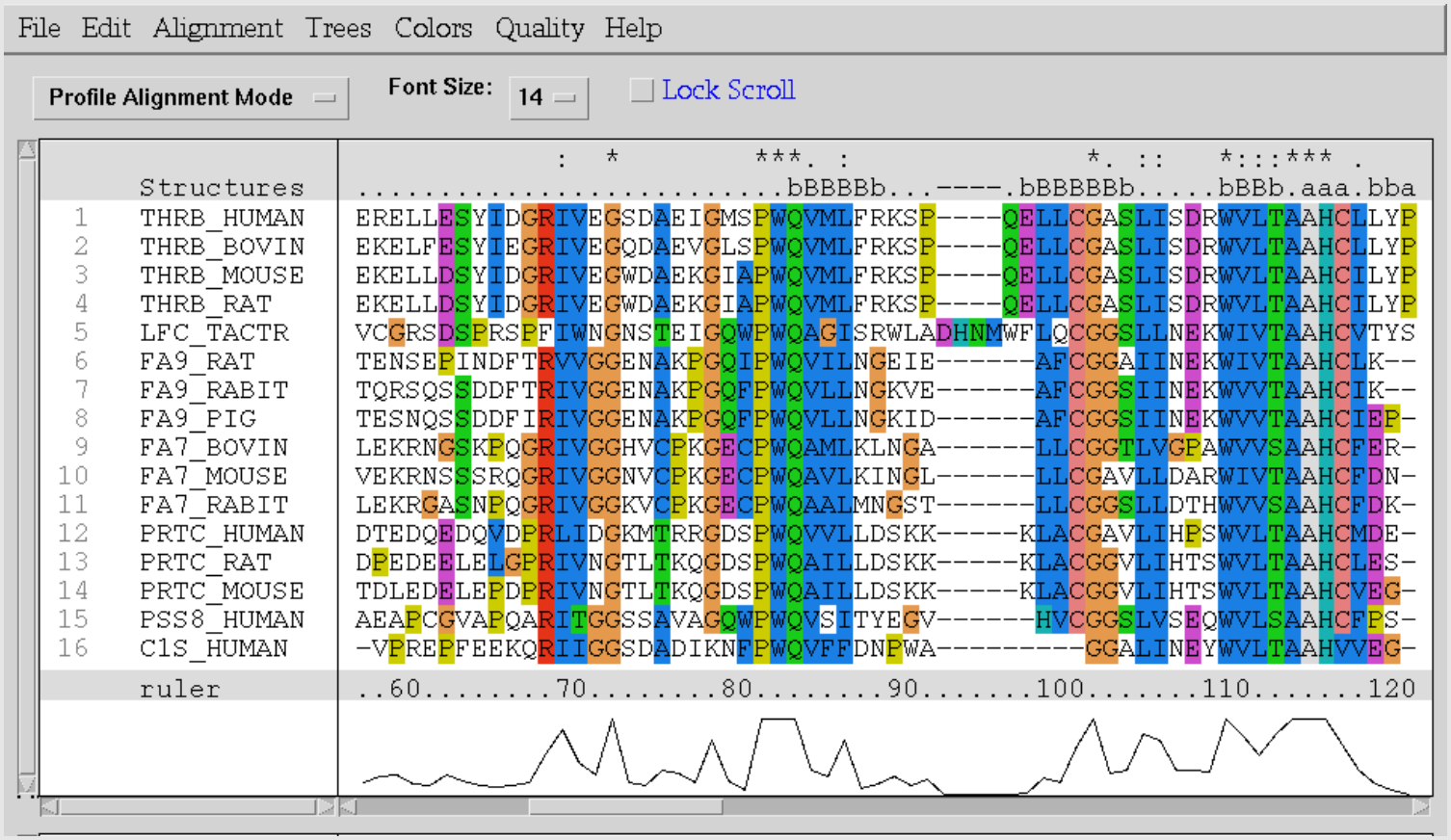
Ratio of the normalized abundances of various residues in a given position in the vicinity of half cystines and 'free' cysteines

	−10	−9	−8	−7	−6	−5	−4	−3	−2	−1	Cys	1	2	3	4	5	6	7	8	9	10
A	1.50	0.73	1.44	0.72	0.59	0.99	0.99	1.18	1.17	1.12		1.74	1.26	0.95	1.15	0.65	0.88	0.70	0.63	0.74	1.54
C	0.77	1.64	0.62	1.65	1.25	1.44	1.44	0.50	0.44	0.69		0.81	0.41	0.61	1.33	1.54	1.30	1.79	0.78	1.39	0.87
D	0.94	0.81	1.16	1.60	1.94	0.62	0.82	1.42	1.08	1.04		0.90	0.73	1.17	1.60	1.35	1.06	1.09	1.16	1.31	1.28
E	0.66	1.27	0.51	1.88	1.27	1.06	1.03	1.25	0.81	0.97		0.94	0.81	0.71	0.44	0.74	0.53	0.57	0.59	0.49	0.46
F	0.90	0.17	0.41	0.43	0.88	0.49	0.52	0.79	0.65	0.80		0.97	0.49	0.99	0.41	1.21	0.59	1.11	0.75	0.96	1.08
G	1.55	2.07	1.35	1.08	1.18	1.94	1.90	1.25	1.24	1.29		1.95	1.75	1.38	1.53	1.04	1.46	1.54	1.25	0.92	1.53
H	0.78	0.72	0.68	0.43	0.43	0.67	0.22	1.00	1.08	1.31		0.22	0.23	0.78	2.25	0.76	0.69	0.35	0.54	0.51	0.44
I	0.70	0.98	0.58	0.96	1.16	1.06	0.47	0.65	1.30	1.02		0.42	1.31	0.94	0.76	1.30	1.31	0.90	1.36	1.13	0.78
K	0.67	0.77	0.87	1.08	0.81	1.26	0.67	0.90	1.11	0.72		1.00	0.94	1.15	0.79	1.16	0.64	1.12	1.02	1.01	0.87
L	0.60	0.57	0.71	0.54	0.44	0.56	0.61	0.21	0.78	0.50		0.48	0.59	0.35	0.74	0.45	0.46	0.94	0.81	0.80	0.61
M	0.66	0.80	0.34	0.53	0.76	0.62	0.33	0.46	1.99	0.44		0.54	0.75	0.48	0.53	0.37	0.59	0.54	0.36	0.57	0.44
N	1.60	1.44	1.55	0.87	1.06	0.88	1.91	2.08	2.03	1.25		1.80	1.58	1.65	1.47	1.07	2.35	1.89	1.52	1.17	1.03
P	0.93	0.72	1.18	1.03	0.87	0.59	0.99	0.89	0.33	0.81		0.70	0.61	0.70	0.74	0.84	1.14	1.38	1.05	0.81	1.57
Q	0.79	1.18	0.82	1.13	1.17	0.92	1.03	1.07	0.40	0.72		1.05	1.11	0.91	0.84	1.24	0.65	0.73	0.88	1.34	0.53
R	0.95	1.12	0.99	1.09	0.94	0.50	0.53	0.72	1.10	0.73		0.77	0.88	0.61	0.47	0.49	0.77	0.90	0.68	0.99	0.41
S	1.51	0.94	1.55	0.98	1.06	1.09	1.00	1.53	0.83	0.98		1.69	1.40	1.52	1.16	1.29	1.23	0.92	1.38	0.96	1.12
T	0.80	1.03	1.21	1.12	1.03	2.04	1.23	1.43	1.10	1.86		0.73	1.40	1.53	0.87	0.98	1.36	0.56	1.32	1.24	1.27
V	1.05	1.26	0.71	0.69	1.29	1.05	1.12	0.81	0.73	1.08		0.62	1.25	0.95	0.57	1.02	0.63	0.56	0.61	1.14	1.27
W	0.81	0.17	2.57	1.63	1.25	1.15	1.66	0.14	0.51	1.67		0.78	0.36	1.17	1.28	1.77	1.24	1.42	1.00	2.15	1.34
Y	1.63	1.28	2.05	1.55	1.11	1.03	1.37	1.25	2.73	1.81		2.21	0.89	1.81	1.60	2.22	1.63	1.36	2.50	1.59	1.03

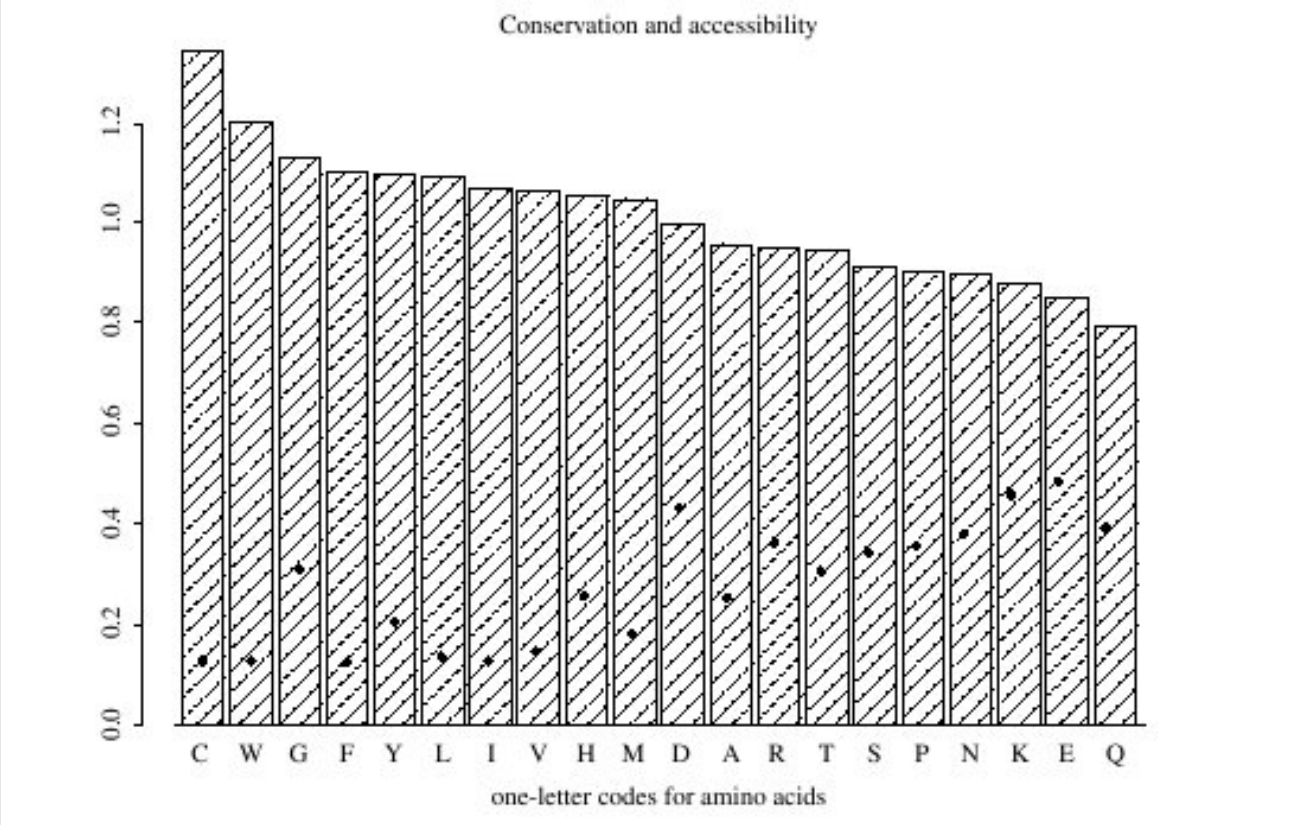
Diszulfid becslés pontossága



Szerin proteázok szekvenciáinak összehasonlítása



Aminosavak konzervativitása és eltemetettsége



Diszulfid hidak előfordulása másodlagos szerkezet szerint

Table 2. Conservation and frequency of bonded and non-bonded cysteines in secondary structural elements. The first column refers to overall database statistics considering all type of residues

Secondary structures	All residues frequency %	Non-bonded Cys		Bonded Cys	
		Frequency %	Conservation	Frequency %	Conservation
Helix	32	31	1.137	25.0	1.770
Sheet	23	26	1.033	28.7	1.444
Coil	45	42	1.350	47.0	1.587

http://manaslu.aecom.yu.edu/cysredox.html

Predicting the redox state of cysteins in proteins from multiple sequence alignments

A. Fiser & I. Simon, Bioinformatics, *16*, 291-325 (2000)

A. Fiser & I. Simon, Methods Enzym., *353*, 10-21 (2002)

Paste your protein sequence in the window ... (use one letter codes)

or upload your sequence file: Browse...

Cutoff for Cystein covalent state prediction 1.27 (range (0.00;unlimited))

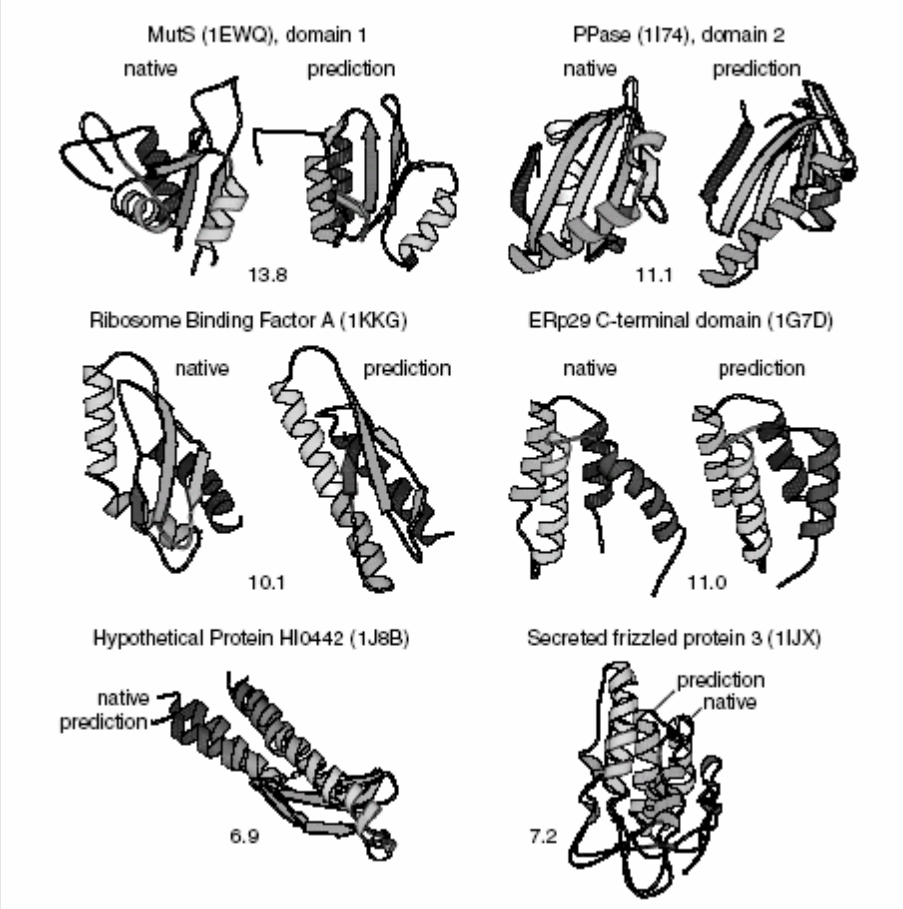
Fraction of gaps to eliminate per position 0.15 (range (0.00;1.00))

Number of sequences to consider from the Psi-Blast search 40 (range(2,50))

Your name (optional)

PROCESS RESET

A rozetta módszer



Homológia meghatározása

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P450cam   PPHVPEHLVFDFDMYNPSNLSAGVQEAWAVLQESNVPDLVWTRCNGGHWIATR-GQLIRE   73
P450BM-3  IKEMPQPKTFGELKNLPLLNTDKPVQALMKIADELGEIFKFEAPGRVTRYLS-SQRLIKE   60
P450 2C5  KLPPGPTPFPIIGNILQIDAKD-ISKSLTKFSECYGPVFTVYLGMKPTVVLH-GYEAVKE   67
P450 2B4  GKLPPGPSPLPVLGNLLQMDRKGLLRSFLRLREKYGDVFTVYLGSRPVVVLC-GTDAIRE   67
                                     A                                B

P450cam   AYED-YPHFSSECPFIPREAGEAY-DFIPTSMDPPE--QRQFRALANQVVG--MPVVDKL  127
P450BM-3  ACD--ESRFDKNLSQALKFVRDFA-GDGLFTSWTHEKNWKKAHNILLPSFSQQA--MKGY  115
P450 2C5  ALVD-LGEEFAGRGSVPILEKVSK-GLGIAFSNA--KTWKEMRRFSLMTLRNFGMGKRSI  123
P450 2B4  ALVDQAEAFSGRGKIAVVDPIFQGYGVIFAN----GERWRALRRFSLATMRDFGMGKRSV  123
                                B'                                C

P450cam   ENRIQELACSLIESLRPQ---GQCNFTEDYAEPFPIRIFMLLAGLP----------EEDI  174
P450BM-3  HAMMVDIAVQLVQKWERLNADEHIE-VPEDMTRLTLDTIGLCGFNYRFNSFYRDQPHPFI  174
P450 2C5  EDRIQEEARCLVEELRKT-NASPCDP-TFILGCAPCNVICSVIFH-NRFDYKDEEFLKLM  180
P450 2B4  EERIQEEARCLVEELRKSKG-ALLDN-TLLFHSITSNIICSIVFGKRFDY-KDPVFLRLL  180
              D                                E

P450cam   PHLKYLTDQMTRPDGSMT----------------FAEAKEALYDYLIPIIEQRRQK----  214
P450BM-3  TSMVRALDEAMNKLQRAN----PDDPAYDENKRQFQEDIKVMNDLVDKIIADRKASGE--  228
P450 2C5  ESLHENVELLGTPWLQVYNNFPALLDYFPGIHKTLLKNADYIKNFIMEKVKEHQKLLDVN  240
P450 2B4  DLFFQSFSLISSFSSQVFELFSGFLKHFPGTHRQIYRNLQEINTFIGQSVEKHRATLDPS  240
            F                                G

P450cam   PGTDAISIVAN-GQVN-G---RPITSDEAKRMCGLLLVGGLDTVVNFLSFSMEFLAKSPE  269
P450BM-3  QSDDLLTHMLNGKDPETG---EPLDDENIRYQIITFLIAGHETTSGLLSFALYFLVKNPH  285
P450 2C5  NPRDFIDCFLIKMEQENN---LEFTLESLVIAVSDLFGAGTETTSTTLRYSLLLLKHPE  297
P450 2B4  NPRDFIDVYLLRMEKDKSDPSSEFHNQNLILTVLSLFFAGTETTSTTLRYGFLLMLKYPN  300
                H                                I

P450cam   HRQELIERP-----------------ERIPAACEELLRRFS-LVADGR-ILTSDYEF-H  308
P450BM-3  VLQKAAEEAARVLV-DPVPSYKQVKQLKYVGMVLNEALRLWPTAPAFSL-YAKEDTVLGG  343
P450 2C5  VAARVQEEIERVIGKHRSPCMQDRSRMPYTDAVIHEIQRFIDLLPTNLPHAVTRDVRF-R  356
P450 2B4  VTERVQKEIEQVIGSHRPPALQDRAKMPYTDAVIHEIQRLGDLIPFGVPHTVTKDTQF-R  359
            J                                K

P450cam   GVQLKKGDQILLPQMLSGLDERENACPMHVDFSRQKV---------SHTTFGHGSHLCLG  359
P450BM-3  EYPLEKGDELMVLIPQLHRDKTIWGDDVEEFRPERFENP-SAIPQHAFKPFGNGQRACIG  402
P450 2C5  NYFIPKGTDIITSLTSVLHDEKAFPNPKVFDPGHFLDESGNFKKSDYFMPFSAGKRMCVG  416
P450 2B4  GYVIPKNTEVFFVLSSALHDPRYFETPNTFNPGHFLDANGALKRNEGFMPFSLGKRICLG  419
                     K'                                 *

P450cam   QHLARREIIVTLKEWLTRIPDFSIAP---GAQIQHKS-GIVSGVQALPLVWDPATTKAV  414
P450BM-3  QQFALHEATLVLGMMLKHFDFEDHT----NYELDIKE-TLTLKPEGFVVKAKSKKIPLG  456
P450 2C5  EGLARMELFLFLTSILQNFKLQSLVEP-KDLDITAVVNGFVSVPPSYQLCFIPI-----  469
P450 2B4  EGIARTELFLFFTTILQNFSIASPVPPEDIDLTPRES-GVGNVPPSYQIRFLAR-----  472
                L
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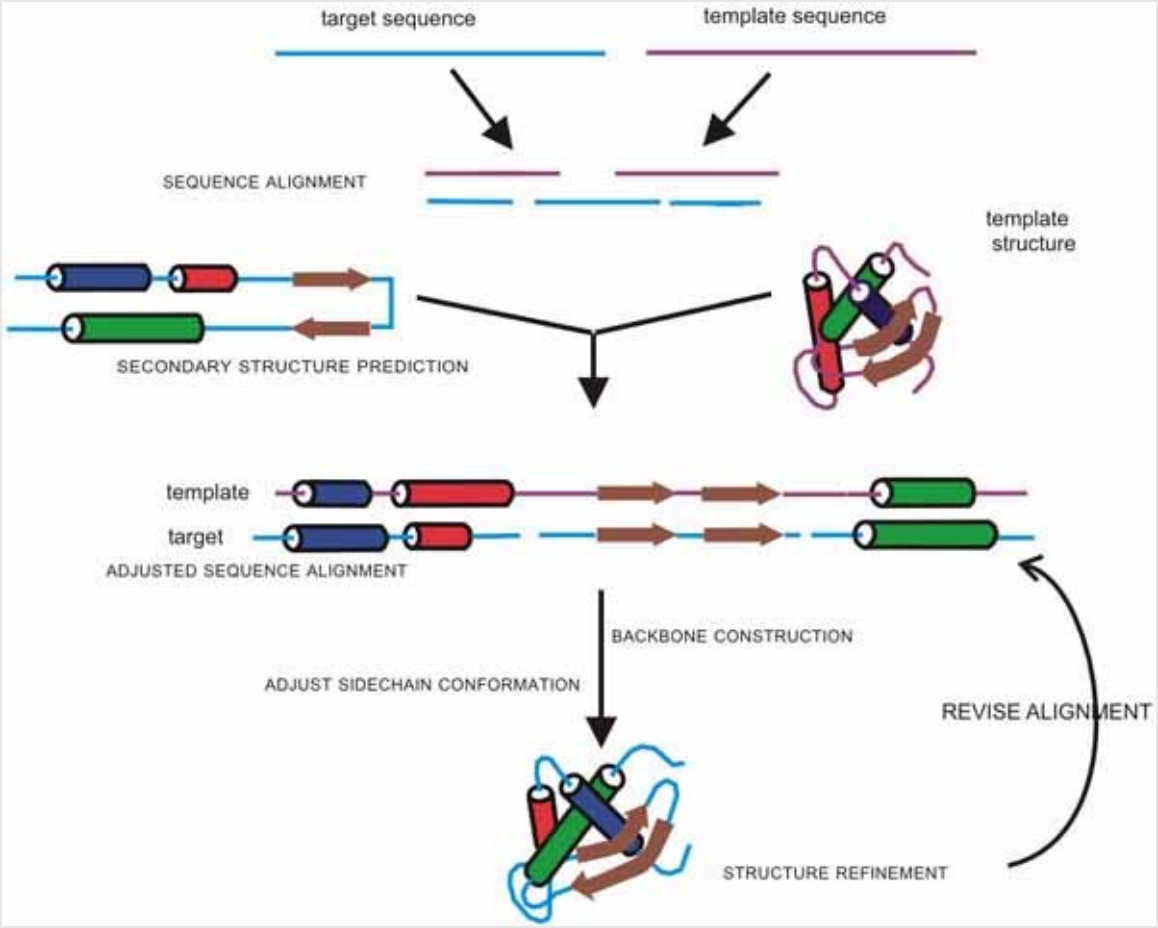
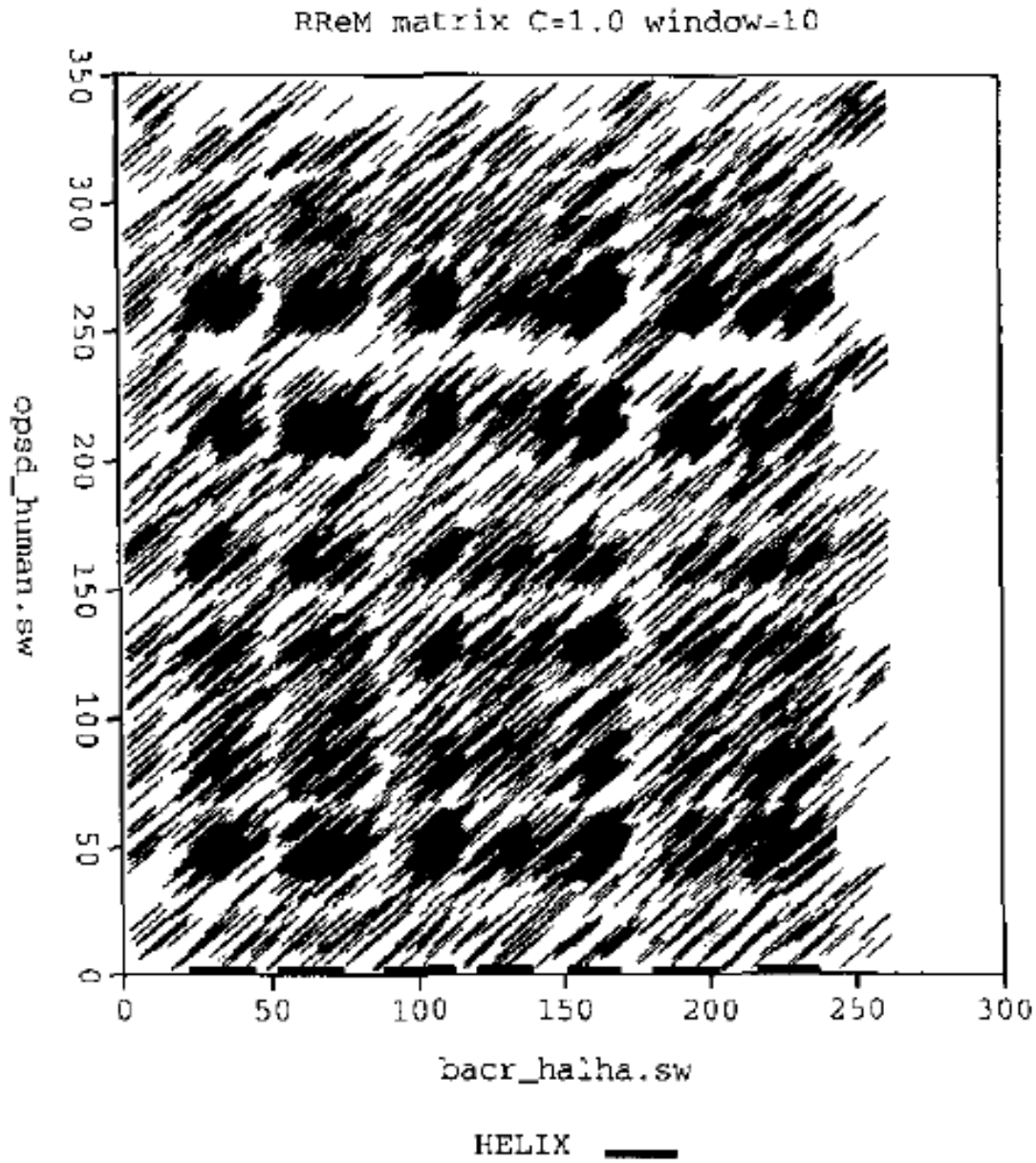
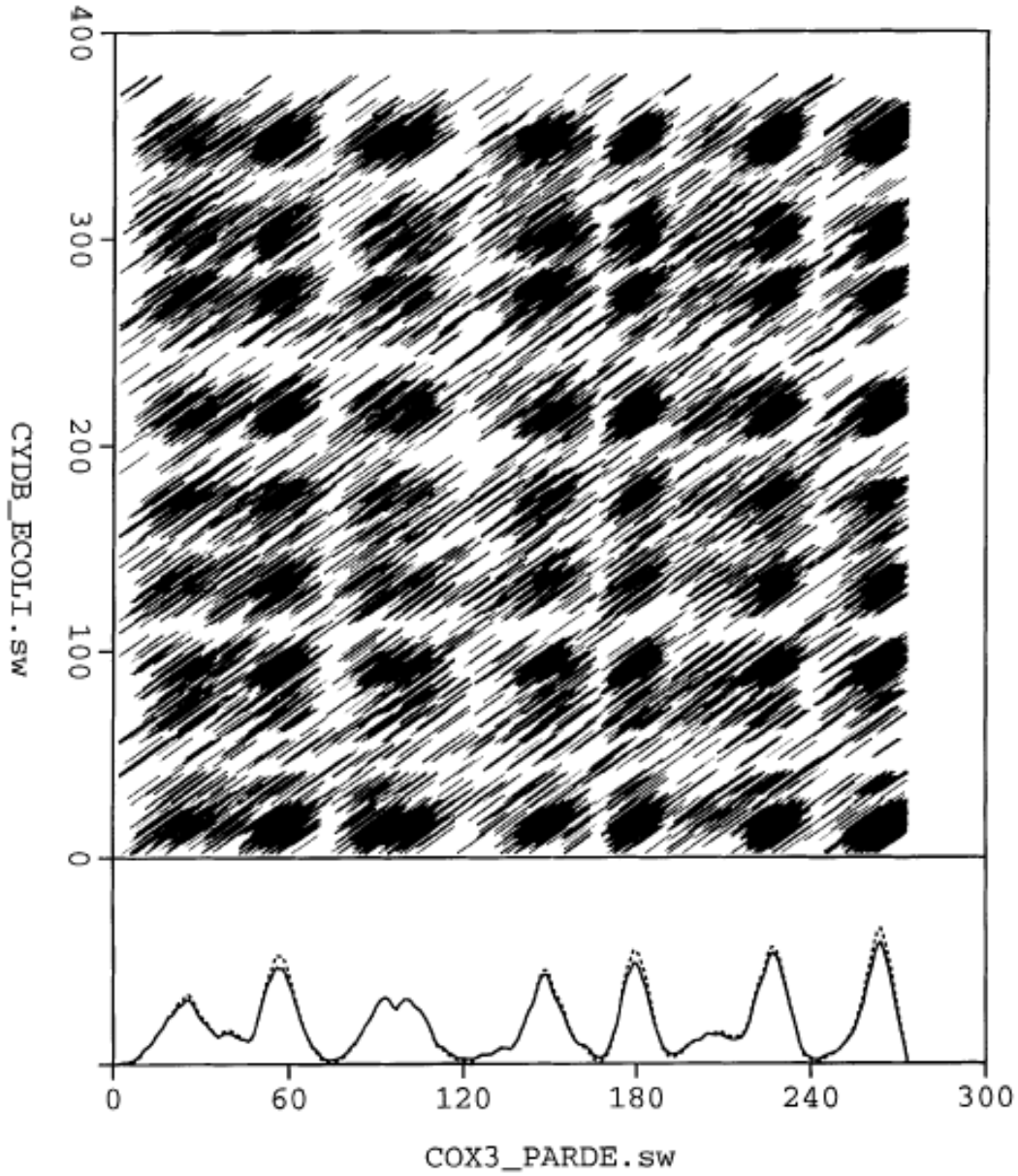
Szerkezetbecslés homológia alapján



Az emberi rodopszin és a bakteriorodopszin aminosav-sorrendjeinek összehasonlítása



A DAS szerver algoritmusa