FUNCTIONALLY SIGNIFICANT AMINO ACID MOTIFS OF HEAT SHOCK PROTEINS:
STRUCTURAL AND BIOINFORMATIC ANALYSIS OF HSP60/HSP10 OF FIVE CHORDATES CLASSES

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Captions

Supplementary_OligHsp60

LEU22	Non-structured amino acid residues are marked in gray. Data was obtained using FoldUnfold.
2,05	Alkyl / Pi-alkyl - interaction between CH-groups (hydrophobic interaction) or between CH-donor and pi-acceptor groups (weak hydrogen bond) of amino acid side chains.
2,05	Carbon - weak hydrogen bond between CH-group and COOH-group of amino acid side chain.
2,05	Salt / charge-charge - salt-bridges and electrostatic interactions.
2,05	H-H - hydrogen bonds

Supplementary_PID

Color map

PID% (simple colors)	30 65 100
PID% (gradient)	10 20 30 40 50 60 70 80 90 100

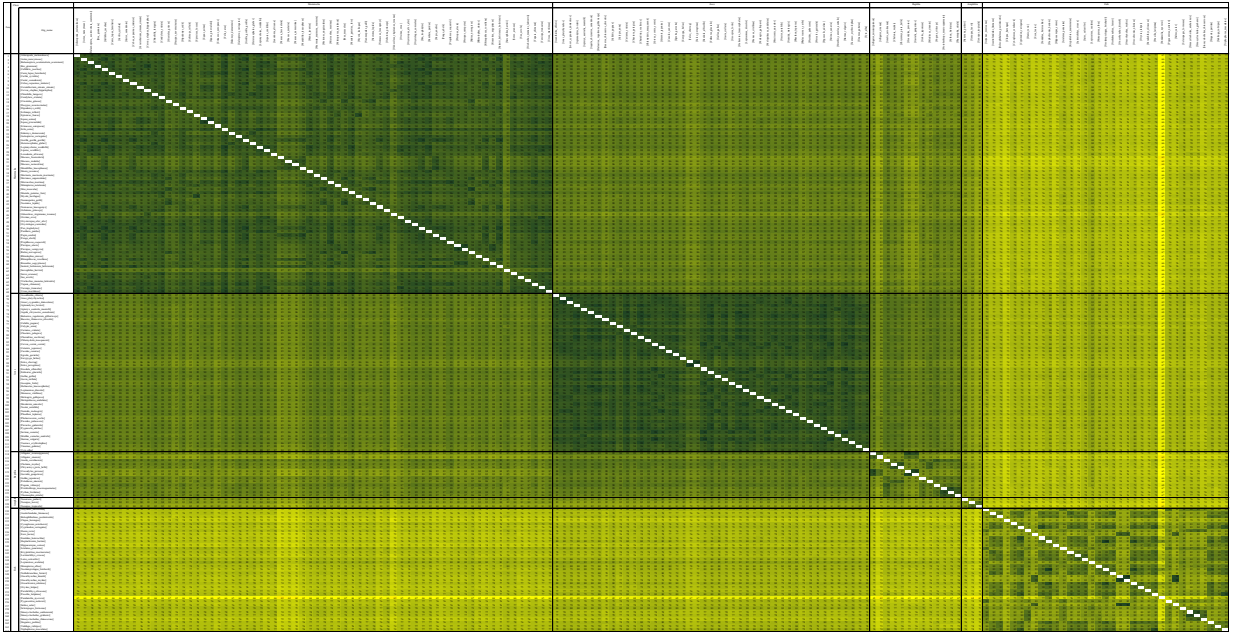
Equation for PID

$PID\% = (N_{eq} \times 100\%)/(N_1 + N_2 - N_{eq})$

N_{eq} is the number of equivalent aligned non-gapped characters; N_1 and N_2 are the length of aligned sequences.

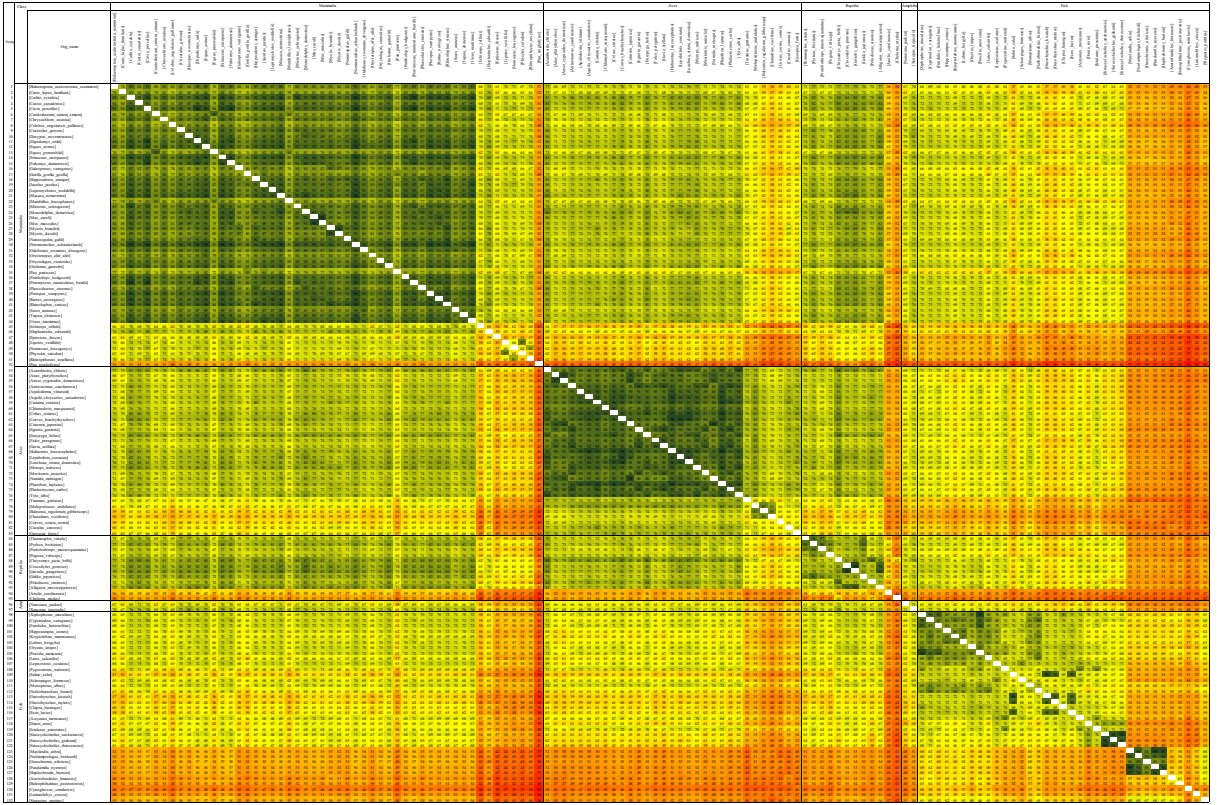
Supplementary_PID

Hsp60



Supplementary_PID

Hsp10



Supplementary_OligHsp60

The map of amino acid residues involved in oligomerization of Hsp60 monomers (Hsp60 sequence PDB 4PJ1)

№AA		1	2	3	4	5	6	6	6	6	7	7	7	8	9	9	9	10	11	11	12	12	13	14	15	16	16	17	18	19	20	21	21
	Subunit_1 / Subunit_2	LEU22	ALA26	VAL29	PRO33(O)	LYS34(NZ)	ARG36(CD)	ARG36(NH1)	ARG36(NH2)	ARG36	THR37(N)	THR37(O)	THR37(OG1)	VAL38	ILE39(N)	ILE39(O)	ILE39	ILE40	GLU41(N)	GLU41(OE1)	SER46(CB)	SER46(OG)	PRO47	VAL49	ILE60	ASP61(O)	ASP61(OD2)	LYS63	ASN153(O)	ASP155(OD2)	THR385(OG1)	GLU389(OE1)	GLU389(OE2)
1	GLY1(N)																										2,9						
2	ALA3																											4,5					
3	LYS4(N)																									3,2							
4	VAL6	5,3																							5,2								
5	PHE8		5,3																														
6	LYS65(NZ)																			3,8													
7	ILE69																5,2						4,4										
8	LEU73																						5,0										
9	ASP76(OD1)																				3,5												
9	ASP76(OD2)																					3,1											
10	SER108(O)								2,9																								
11	LYS109(O)								3,2																								
12	ALA111(O)								2,9																								
13	ASN112(ND2)				3,3																												
14	PRO113									4,6																							
15	ARG117(NH1)																																5,3
15	ARG117(NH2)																															2,9	
16	ARG118(NH2)																												2,8	5,3			
17	ASP436(OD2)					3,7																											
18	ASP507(CA)																														3,6		
19	LEU514																							4,4									
20	THR517(O)										3,1																						
20	THR517(OG1)												2,5																				
21	ALA518																4,5																
22	GLU519(N)											2,9																					
22	GLU519(OE1)						3,6	2,9																									
23	VAL520(O)														3,1				2,9														
23	VAL520		4,7	5,1										4,5																			
24	VAL521																4,8																
25	VAL522(N)															2,9																	
25	VAL522																	4,9							5,0								
26	GLU524(N)																			3,1													

Remark. The bond lengths are represented in the map cells.