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*** DrugScore-PPI 1.0 ***
Knowledge-based Scoring Function to
Predict Protein-Protein Interactions
D. M. Krüger, H. Gohlke
2009

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In silico alanine scanning on chain A for PDB-ID cluster7_1.
(file uploaded by user)

Date: 2018-05-08 15:19:17

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
TRP7A	0.16	2.83	-
ASP39A	0.60	2.57	-
TYR40A	0.84	5.52	-
ARG42A	1.68	6.05	-
TRP45A	0.51	3.43	-
LEU46A	0.79	2.72	-
ASN47A	-0.24	3.52	-
GLU48A	0.15	5.18	-
LYS49A	0.69	4.95	-
PHE50A	1.32	7.55	-
LYS51A	0.40	3.32	-
LEU54A	0.16	2.72	-
ASP55A	2.69	7.57	-
PHE56A	0.92	4.19	-
ASN58A	1.07	9.47	-
LEU59A	0.34	4.61	-
THR66A	0.09	1.26	-
HIS67A	0.35	5.72	-
LYS68A	0.29	3.32	-
ILE69A	0.57	3.67	-
THR70A	0.38	9.63	-
GLN71A	0.15	5.98	-
ASN73A	0.44	4.74	-
ARG77A	0.69	6.05	-
TYR78A	0.84	6.45	-
ARG81A	-0.13	2.28	-
LYS82A	0.51	5.77	-
GLU90A	0.20	3.22	-
LYS91A	0.05	1.68	-
GLN93A	1.06	7.92	-
ILE94A	0.72	3.61	-
GLU96A	0.15	5.24	-
ASP97A	4.74	11.42	X
ILE98A	0.13	2.72	-
GLU100A	0.49	9.42	-
ASN101A	0.89	9.40	-
MET108A	0.12	4.20	-
LYS112A	0.79	3.37	-
LEU113A	0.11	3.61	-
TYR115A	0.77	3.96	-
ASP116A	2.68	10.06	X
ASP118A	1.28	5.00	-

PHE119A	0.07	2.50	—
LYS121A	0.09	2.50	—
LEU122A	0.25	3.61	—
MET211A	0.21	2.72	—

