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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 cluster3_1.
(file uploaded by user)

Date: 2018-05-08 15:35:33

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
TYR6A	0.85	5.57	-
TRP7A	1.12	4.18	-
ILE9A	0.21	7.33	-
LEU12A	0.49	3.67	-
MET34A	0.28	6.03	-
TYR40A	0.15	5.26	-
ARG42A	0.94	5.31	X
TRP45A	0.16	2.79	-
LEU46A	0.08	2.78	-
LYS49A	0.38	5.00	-
PHE50A	0.20	1.68	-
ASP55A	0.04	1.29	-
PHE56A	0.63	4.14	-
ASN58A	2.36	6.96	-
LEU59A	0.42	5.50	-
THR70A	0.21	6.00	-
GLN71A	1.15	4.90	-
ASN73A	0.81	6.58	-
ARG77A	0.11	5.26	-
ARG81A	0.07	2.28	-
ASP97A	0.90	6.28	-
GLU100A	0.56	6.38	-
ASN101A	1.53	11.84	-
GLN102A	0.06	3.93	-
PHE103A	0.05	1.68	-
MET104A	0.23	5.50	-
ASP105A	0.76	6.28	-
ARG107A	0.15	5.01	-
MET108A	0.69	5.09	-
GLN109A	0.04	5.54	-
LYS112A	1.00	5.77	-
LEU113A	0.05	1.83	-
CYS114A	0.15	5.21	-
TYR115A	3.45	4.79	-
ASP116A	2.36	6.28	-
ASP118A	0.89	3.78	-
GLU120A	0.03	1.07	-
LYS121A	0.10	3.32	-
LEU122A	0.32	3.61	-
GLU125A	0.10	2.09	-
PHE208A	0.28	3.32	-
MET211A	0.42	6.98	-



