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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 cluster2_1.
(file uploaded by user)

Date: 2018-05-08 15:41:12

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
PHE8A	0.05	1.68	-
ARG13A	-0.06	5.01	-
VAL35A	0.09	3.22	-
TRP38A	0.49	5.31	-
GLN39A	0.09	1.03	-
SER42A	0.15	4.62	-
LEU43A	0.11	3.61	-
LYS44A	0.78	5.87	-
SER46A	0.27	8.74	-
CYS47A	0.23	7.85	-
LEU48A	1.21	4.56	-
TYR49A	1.18	5.62	-
GLN51A	1.07	5.01	-
LEU52A	0.15	3.72	-
LYS54A	0.45	3.37	-
PHE55A	0.10	3.32	-
GLN56A	0.39	3.93	-
ASP57A	0.11	3.78	-
ASP59A	1.74	3.78	-
LEU60A	1.07	4.56	-
THR61A	0.55	6.08	-
LEU62A	0.17	1.83	-
TYR63A	1.32	3.69	-
GLN64A	0.01	4.90	-
ASN66A	0.74	5.95	-
THR67A	0.28	4.82	-
ARG70A	0.09	6.05	-
HIS71A	0.20	4.73	-
LEU72A	0.05	1.83	-
ARG74A	1.64	7.59	X
THR75A	0.39	8.52	-
TYR79A	0.94	2.44	-
LYS81A	0.12	4.14	-
ASP82A	-0.44	7.57	-
GLN83A	0.48	9.06	-
GLN84A	-0.04	2.96	-
ASP90A	0.18	6.28	-
ASP94A	0.65	6.35	-
GLU97A	0.26	8.00	-
ILE104A	0.40	5.55	-
TYR108A	0.17	5.67	-

