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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 15:30:49

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
GLU3A	0.12	4.23	-
TYR9A	0.15	4.79	-
ARG15A	0.82	6.14	-
ASP42A	1.26	10.14	-
LEU44A	0.11	3.67	-
ARG45A	0.19	4.56	-
ASN46A	0.22	3.52	-
ASP47A	0.13	3.71	-
TYR49A	0.16	5.57	-
LEU50A	0.11	3.67	-
MET51A	0.45	1.89	-
PHE52A	1.39	7.60	-
GLN53A	0.35	6.04	-
GLN54A	0.15	4.96	-
ILE60A	0.19	6.34	-
ASP61A	1.76	6.21	-
MET63A	0.93	7.33	-
LYS64A	0.30	5.49	-
LEU65A	0.82	3.61	-
VAL66A	0.81	4.27	-
GLN67A	0.11	3.99	-
ARG69A	-0.13	3.82	-
ILE71A	0.13	4.50	-
ASN73A	0.00	5.89	-
TYR74A	0.20	4.01	-
SER77A	0.11	3.11	-
LYS78A	0.10	3.32	-
LYS84A	0.12	4.14	-
ASP85A	0.18	6.35	-
ILE86A	1.71	1.83	-
LYS87A	1.10	5.00	-
LEU91A	0.32	2.72	-
MET94A	0.20	2.72	-
GLU97A	0.25	5.24	-
ASP101A	0.88	4.92	-
GLU104A	0.22	7.39	X
MET105A	0.11	3.61	-
LEU107A	0.38	5.45	-
LEU108A	1.07	4.50	-
PHE111A	0.23	4.19	-
THR112A	0.31	7.26	-
GLN113A	0.43	1.03	-
GLU116A	0.06	2.09	-
LYS120A	0.07	2.50	-
LEU213A	0.11	3.61	-
SER216A	0.13	4.62	-
ARG217A	0.47	4.52	X
PHE220A	0.05	1.68	-
ARG221A	0.46	4.56	-
PHE222A	0.59	2.50	-

