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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 15:13:29

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
TYR9A	0.75	7.70	-
ILE12A	0.19	4.20	-
ARG13A	0.13	4.56	-
ARG15A	2.28	4.52	X
GLU39A	0.32	4.17	-
LEU41A	0.22	3.72	-
ASP42A	2.35	7.57	-
LYS43A	0.17	4.14	-
ARG45A	0.56	7.63	-
ASN46A	1.00	7.17	-
ASP47A	-0.17	6.28	-
TYR49A	0.07	2.39	-
LEU50A	0.13	4.61	-
MET51A	0.12	1.89	-
PHE52A	0.78	4.77	-
GLN53A	0.28	6.95	-
GLN54A	1.80	9.00	-
VAL55A	0.66	3.28	-
GLN67A	0.39	3.02	-
THR68A	0.34	3.63	-
ARG69A	0.59	3.82	-
ASN73A	0.37	7.03	-
TYR82A	0.28	9.63	-
ASP93A	0.57	4.92	-
MET94A	0.10	2.72	-
TYR95A	0.07	2.39	-
ILE96A	0.13	4.56	-
GLU97A	0.87	8.46	X
ASP101A	0.99	4.92	-
GLU104A	0.41	7.39	-
MET105A	0.13	4.56	-
LEU107A	0.39	4.50	-
LEU108A	0.64	5.45	-
PHE111A	0.98	5.00	-
LYS120A	0.33	4.14	-
LYS127A	0.24	4.68	-
TYR132A	0.09	3.18	-
SER216A	0.13	4.62	-
PHE220A	0.33	3.32	-
ARG221A	0.80	2.77	-
PHE222A	0.36	4.14	-

