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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 cluster1_1.
(file uploaded by user)

Date: 2018-05-08 15:23:47

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
LYS44A	0.05	1.68	-
SER46A	0.23	7.74	-
CYS47A	0.23	7.85	-
LEU48A	0.64	0.94	-
TYR49A	2.45	7.23	-
LYS54A	0.31	4.14	-
GLN56A	0.14	4.90	-
ASP59A	-0.48	2.50	-
LEU60A	1.09	4.56	-
THR61A	0.33	6.08	-
LEU62A	0.67	2.72	-
TYR63A	0.12	7.23	-
GLN64A	0.13	3.99	-
THR67A	0.37	4.89	-
ARG70A	0.33	6.80	-
HIS71A	0.27	5.78	-
ARG74A	0.89	4.56	-
THR75A	0.11	3.63	-
TYR79A	0.16	5.62	-
LYS81A	0.10	3.32	-
ASP82A	0.19	6.35	-
GLN83A	0.16	1.03	-
GLN84A	1.61	7.98	-
GLU85A	0.18	6.26	-
LEU88A	0.77	4.56	-
ASP90A	0.31	7.49	-
MET91A	0.73	4.56	-
VAL92A	0.09	3.22	-
ASP94A	0.03	3.78	-
VAL96A	0.19	6.43	-
ASP98A	4.97	8.71	-
LEU99A	0.11	3.61	-
LYS102A	0.48	5.77	-
GLN125A	0.43	3.99	-
LYS127A	0.07	2.50	-
THR131A	0.20	4.89	-
LEU132A	0.18	3.61	-
GLN135A	-0.03	2.96	-

