

*** DrugScore-PPI 1.0 ***
Knowledge-based Scoring Function to
Predict Protein-Protein Interactions
D. M. Krüger, H. Gohlke
2009

In silico alanine scanning on chain A for PDB-ID cluster2_1.
(file uploaded by user)

Date: 2018-05-08 15:16:07

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
TYR6A	0.32	4.84	-
TRP7A	0.06	2.11	-
LEU12A	0.19	3.72	-
ASP39A	-0.40	2.57	-
TYR40A	0.93	6.40	-
ASP41A	0.58	5.00	-
ARG42A	0.28	6.05	X
TRP45A	0.34	2.79	-
LEU46A	0.88	6.34	-
LYS49A	0.67	4.14	-
PHE50A	0.40	2.50	-
ASP55A	0.28	1.29	-
PHE56A	1.48	5.00	-
ASN58A	0.90	7.10	-
LEU59A	0.12	3.67	-
GLN71A	0.28	3.99	-
ASN73A	0.10	3.52	-
GLU91A	0.44	5.24	-
ILE94A	0.61	2.72	-
ARG95A	0.44	9.87	X
ASP97A	1.08	3.71	-
ILE98A	0.95	4.56	-
ASN101A	0.12	2.37	-
GLN102A	1.15	8.89	-
MET104A	0.17	2.72	-
ASP105A	1.18	7.57	X
ASN106A	0.24	8.18	-
MET108A	0.74	3.67	-
GLN109A	0.20	6.95	-
MET112A	0.42	5.50	-
ILE113A	0.12	4.20	-
TYR115A	2.35	5.57	-
ASN116A	0.21	7.10	-
GLU118A	0.08	4.17	-
LYS125A	0.21	3.32	-
GLU128A	0.09	3.10	-
GLU129A	0.21	6.32	-
GLU132A	1.30	5.31	-
LYS133A	0.20	6.69	-
LYS135A	0.07	2.50	-
LEU136A	0.08	2.72	-
GLU139A	0.00	3.10	-
PHE140A	0.41	5.05	-
LEU141A	0.16	5.39	-
ARG144A	-0.23	6.84	X
PHE208A	0.18	6.31	-
SER209A	0.17	5.62	-
LYS210A	0.14	4.68	-
MET211A	0.50	3.72	-
VAL213A	0.16	5.38	-

