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

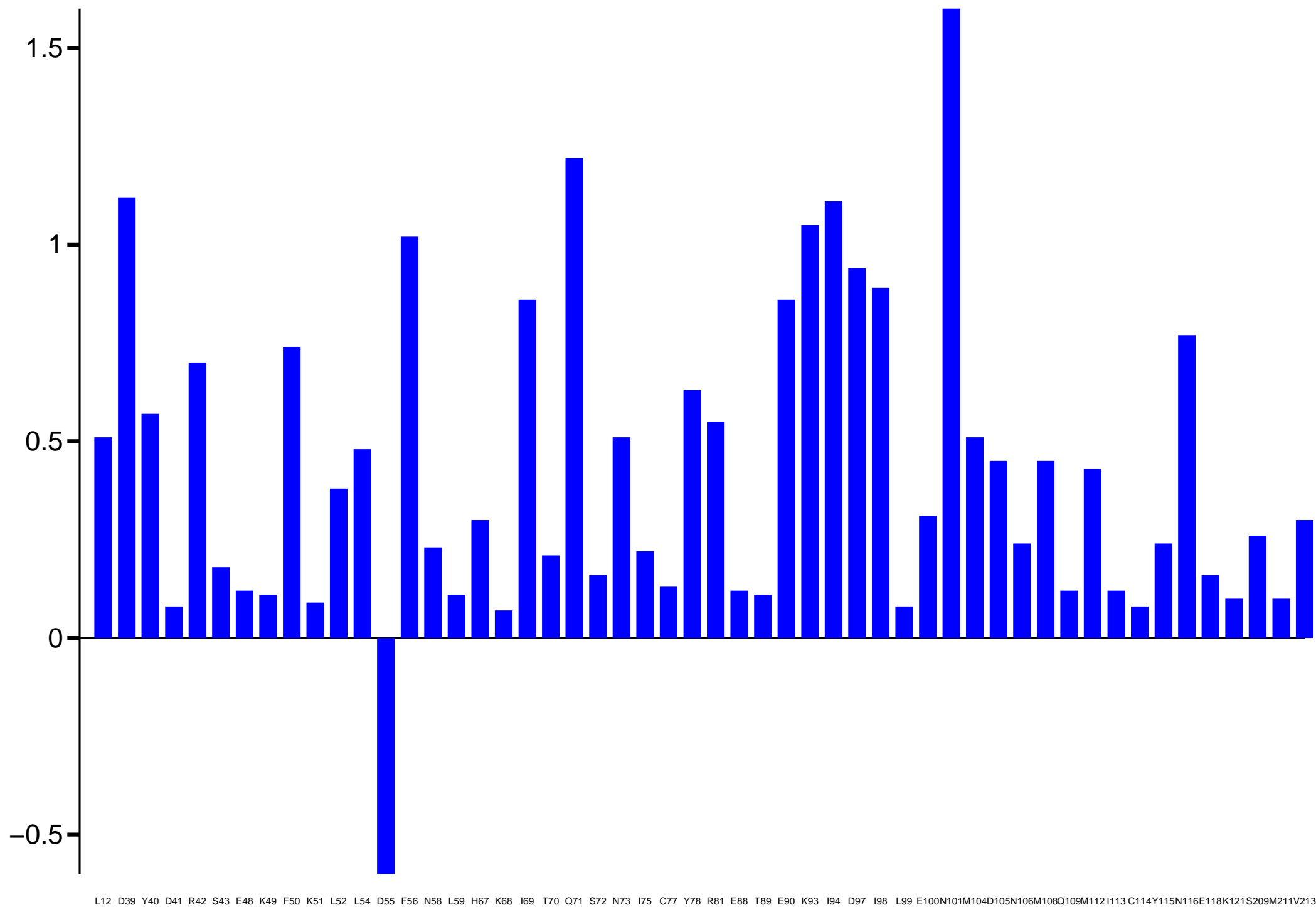
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In silico alanine scanning on chain A for PDB-ID cluster1_1.
(file uploaded by user)

Date: 2018-05-08 15:33:24

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
LEU12A	0.51	5.14	-
ASP39A	1.12	2.57	X
TYR40A	0.57	6.40	-
ASP41A	0.08	5.07	-
ARG42A	0.70	3.07	-
SER43A	0.18	6.23	-
GLU48A	0.12	4.11	-
LYS49A	0.11	3.32	-
PHE50A	0.74	2.50	-
LYS51A	0.09	2.50	-
LEU52A	0.38	5.45	-
LEU54A	0.48	5.45	-
ASP55A	-0.61	3.78	-
PHE56A	1.02	5.82	-
ASN58A	0.23	4.74	-
LEU59A	0.11	3.67	-
HIS67A	0.30	4.73	-
LYS68A	0.07	2.50	-
ILE69A	0.86	4.56	-
THR70A	0.21	7.26	-
GLN71A	1.22	4.96	-
SER72A	0.16	3.11	-
ASN73A	0.51	4.67	-
ILE75A	0.22	5.45	-
CYS77A	0.13	3.93	-
TYR78A	0.63	4.84	-
ARG81A	0.55	4.26	-
GLU88A	0.12	4.17	-
THR89A	0.11	3.70	-
GLU90A	0.86	7.39	X
LYS93A	1.05	6.64	-
ILE94A	1.11	5.55	-
ASP97A	0.94	6.21	-
ILE98A	0.89	3.61	-
LEU99A	0.08	2.72	-
GLU100A	0.31	5.85	-
ASN101A	1.65	9.40	-
MET104A	0.51	3.61	-
ASP105A	0.45	7.57	-
ASN106A	0.24	8.25	-
MET108A	0.45	3.61	-
GLN109A	0.12	8.94	-
MET112A	0.43	3.61	-
ILE113A	0.12	4.20	-
CYS114A	0.08	2.64	-
TYR115A	0.24	4.05	-
ASN116A	0.77	5.89	-
GLU118A	0.16	3.16	-
LYS121A	0.10	3.32	-
SER209A	0.26	8.83	-
MET211A	0.10	1.83	-
VAL213A	0.30	6.49	-

$\Delta\Delta G_{\text{calc}}[\text{kcal/mol}]$



AA