

*** DrugScore-PPI 1.0 ***
Knowledge-based Scoring Function to
Predict Protein-Protein Interactions
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2009

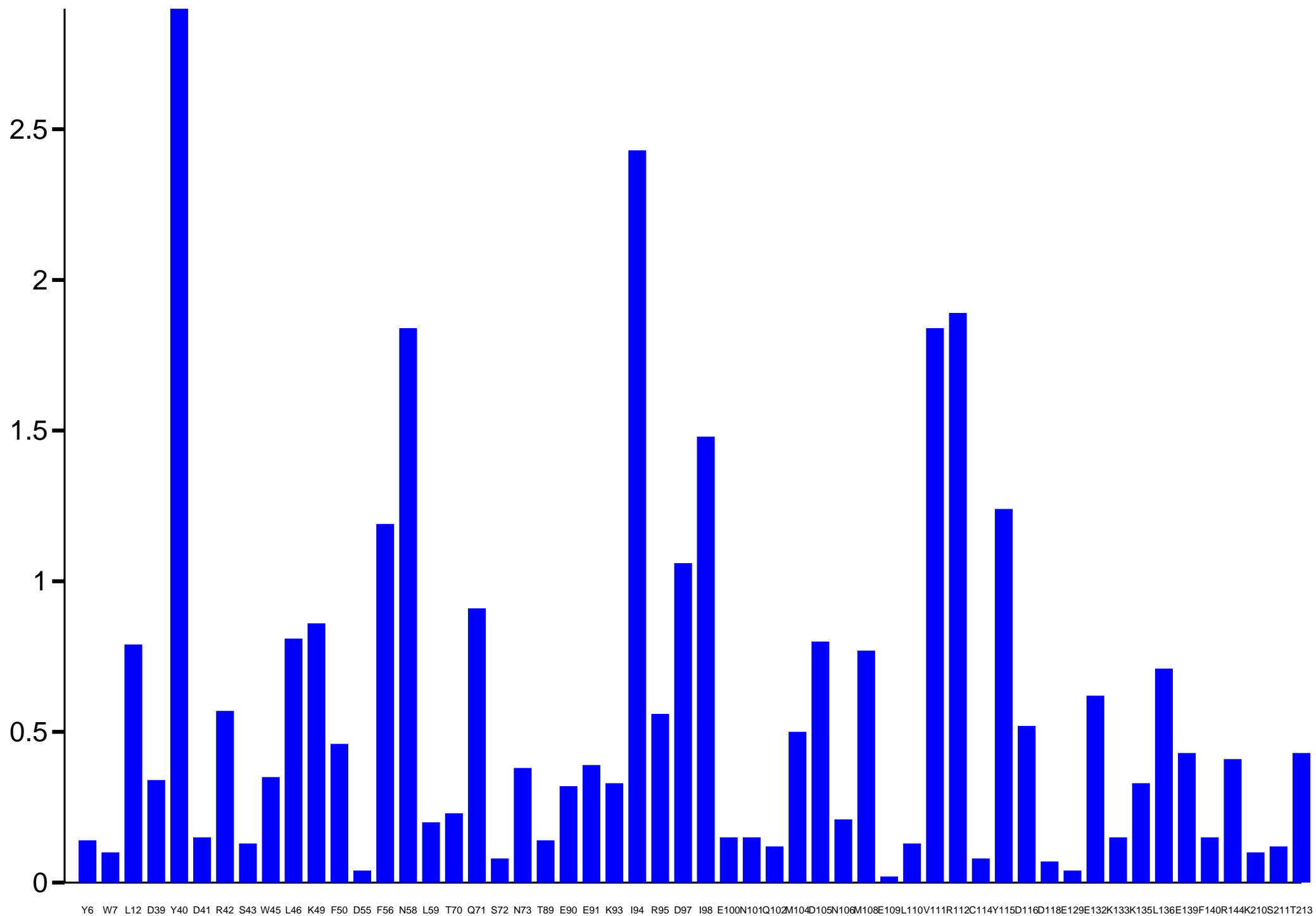
In silico alanine scanning on chain A for PDB-ID cluster3_1.
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Date: 2018-05-08 15:21:58

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
TYR6A	0.14	4.84	-
TRP7A	0.10	3.55	-
LEU12A	0.79	1.83	-
ASP39A	0.34	1.29	-
TYR40A	2.93	5.57	-
ASP41A	0.15	5.07	-
ARG42A	0.57	5.06	-
SER43A	0.13	4.62	-
TRP45A	0.35	5.58	-
LEU46A	0.81	4.56	-
LYS49A	0.86	5.82	-
PHE50A	0.46	2.60	-
ASP55A	0.04	1.29	-
PHE56A	1.19	4.14	-
ASN58A	1.84	11.70	-
LEU59A	0.20	5.55	-
THR70A	0.23	4.82	-
GLN71A	0.91	6.95	-
SER72A	0.08	1.60	-
ASN73A	0.38	8.87	-
THR89A	0.14	4.89	-
GLU90A	0.32	5.24	-
GLU91A	0.39	4.17	-
LYS93A	0.33	4.14	-
ILE94A	2.43	4.50	-
ARG95A	0.56	7.63	X
ASP97A	1.06	6.21	-
ILE98A	1.48	4.50	-
GLU100A	0.15	5.18	-
ASN101A	0.15	5.82	-
GLN102A	0.12	3.99	-
MET104A	0.50	6.09	-
ASP105A	0.80	7.57	X
ASN106A	0.21	7.10	-
MET108A	0.77	5.45	-
GLU109A	0.02	5.24	-
LEU110A	0.13	4.56	-
VAL111A	1.84	3.22	-
ARG112A	1.89	3.86	-
CYS114A	0.08	2.64	-
TYR115A	1.24	4.84	-
ASP116A	0.52	3.78	-
ASP118A	0.07	2.50	-
GLU129A	0.04	2.09	-
GLU132A	0.62	4.23	-
LYS133A	0.15	5.00	-
LYS135A	0.33	6.64	-
LEU136A	0.71	6.39	-
GLU139A	0.43	7.33	-
PHE140A	0.15	5.10	-
ARG144A	0.41	6.84	X
LYS210A	0.10	3.32	-
SER211A	0.12	4.11	-

THR213A 0.43 10.96 -

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



AA