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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 15:43:26

| Residue | ddGcalc [kcal/mol] | Degree Of Buriedness | Possible Saltbridges |
|---------|-----------------------|-------------------------|-------------------------|
| LEU41A | 0.14 | 4.61 | - |
| SER42A | 0.18 | 6.32 | - |
| ASP43A | 0.30 | 2.57 | - |
| ASN49A | 0.21 | 7.10 | - |
| LEU51A | 1.00 | 2.78 | - |
| LYS52A | 0.78 | 7.45 | - |
| LYS53A | 0.77 | 4.14 | - |
| VAL54A | 0.12 | 4.27 | - |
| ASP59A | 0.23 | 6.35 | X |
| ASP61A | 0.06 | 3.78 | - |
| PHE62A | 0.63 | 3.32 | - |
| THR63A | 0.07 | 1.26 | - |
| LEU64A | 0.61 | 4.56 | - |
| THR65A | 0.16 | 4.89 | - |
| GLU66A | 0.27 | 4.17 | - |
| VAL68A | 0.17 | 2.23 | - |
| ILE70A | 0.08 | 2.72 | - |
| LEU72A | 0.57 | 4.56 | - |
| TYR73A | 1.77 | 7.23 | - |
| THR75A | 0.15 | 4.89 | - |
| ARG76A | 3.12 | 6.80 | X |
| LYS77A | 0.63 | 5.87 | - |
| LYS79A | 0.60 | 4.23 | - |
| ASP82A | 0.77 | 3.78 | - |
| TYR85A | 0.50 | 2.44 | - |
| GLN87A | 0.30 | 5.01 | - |
| ASP88A | -0.09 | 3.86 | - |
| LEU89A | 0.63 | 3.77 | - |
| ARG92A | 0.49 | 6.84 | - |
| ASP96A | 0.26 | 3.71 | - |
| HIS103A | 0.14 | 3.85 | - |
| THR104A | 0.26 | 2.44 | - |
| ARG107A | 0.77 | 6.10 | - |
| LYS230A | 0.07 | 2.50 | - |
| MET232A | 0.05 | 1.83 | - |
| TRP234A | 0.42 | 3.47 | - |
| LEU236A | 0.61 | 4.61 | - |
| MET238A | 0.20 | 3.67 | - |
| ILE239A | 0.08 | 2.78 | - |
| ARG240A | 2.20 | 4.52 | X |

