**Supplementary Table R3-Q3-2. Calculation of the prediction ratio for the scores of the docking poses**

The prediction ratio () is defined in *Marillet et al.* (reference) as the percentage of cases such that the difference between the experimental and predicted free energies is equal or smaller than a specified amount δ. We have calculated the prediction ratio for the standard case of δ equal to 2.8 Kcal/mol. We have also added the absolute number of predictions for the prediction ratio in the column *abs*. We have used the scores of the native conformation of the complexes and also the averages with all the poses from a docking search with PatchDock. Several scores are used, some taken from our analysis and others from the CCHarPPI server.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | δ (KCal/mol) | AB2 | | | | AB2 Rigid | | | | AB2 Flexible | | | |
| Native | | All decoys | | Native | | All decoys | | Native | | All decoys | |
| % | abs | % | abs | % | abs | % | abs | % | abs | % | abs |
| FiberDock | 2.8 | 68.09 | 64 | 71.28 | 67 | 56.25 | 27 | 64.58 | 31 | 80.43 | 37 | 78.26 | 36 |
| 2.8 | 31.91 | 30 | 28.72 | 27 | 43.75 | 21 | 35.42 | 17 | 19.57 | 9 | 21.74 | 10 |
| aVdW | 2.8 | 67.02 | 63 | 64.89 | 61 | 60.42 | 29 | 56.25 | 27 | 73.91 | 34 | 73.91 | 34 |
| 2.8 | 32.98 | 31 | 35.11 | 33 | 39.58 | 19 | 43.75 | 21 | 26.09 | 12 | 26.09 | 12 |
| rVdW | 2.8 | 58.51 | 55 | 64.89 | 61 | 45.83 | 22 | 54.17 | 26 | 71.74 | 33 | 76.09 | 35 |
| 2.8 | 41.49 | 39 | 35.11 | 33 | 54.17 | 26 | 45.83 | 22 | 28.26 | 13 | 23.91 | 11 |
| aElec | 2.8 | 61.70 | 58 | 70.21 | 66 | 52.08 | 25 | 62.50 | 30 | 71.74 | 33 | 78.26 | 36 |
| 2.8 | 38.30 | 36 | 29.79 | 28 | 47.92 | 23 | 37.50 | 18 | 28.26 | 13 | 21.74 | 10 |
| rElec | 2.8 | 60.64 | 57 | 69.15 | 65 | 50.00 | 24 | 60.42 | 29 | 71.74 | 33 | 78.26 | 36 |
| 2.8 | 39.36 | 37 | 30.85 | 29 | 50.00 | 24 | 39.58 | 19 | 28.26 | 13 | 21.74 | 10 |
| laElec | 2.8 | 60.64 | 57 | 69.15 | 65 | 52.08 | 25 | 62.50 | 30 | 69.57 | 32 | 76.09 | 35 |
| 2.8 | 39.36 | 37 | 30.85 | 29 | 47.92 | 23 | 37.50 | 18 | 30.43 | 14 | 23.91 | 11 |
| lrElec | 2.8 | 56.38 | 53 | 70.21 | 66 | 45.83 | 22 | 62.50 | 30 | 67.39 | 31 | 78.26 | 36 |
| 2.8 | 43.62 | 41 | 29.79 | 28 | 54.17 | 26 | 37.50 | 18 | 32.61 | 15 | 21.74 | 10 |
| HB | 2.8 | 67.02 | 63 | 57.45 | 54 | 60.42 | 29 | 45.83 | 22 | 73.91 | 34 | 69.57 | 32 |
| 2.8 | 32.98 | 31 | 42.55 | 40 | 39.58 | 19 | 54.17 | 26 | 26.09 | 12 | 30.43 | 14 |
| EPAIR | 2.8 | 62.77 | 59 | 68.09 | 64 | 50.00 | 24 | 62.50 | 30 | 76.09 | 35 | 73.91 | 34 |
| 2.8 | 37.23 | 35 | 31.91 | 30 | 50.00 | 24 | 37.50 | 18 | 23.91 | 11 | 26.09 | 12 |
| ES3DC | 2.8 | 65.96 | 62 | 73.40 | 69 | 56.25 | 27 | 70.83 | 34 | 76.09 | 35 | 76.09 | 35 |
| 2.8 | 34.04 | 32 | 26.60 | 25 | 43.75 | 21 | 29.17 | 14 | 23.91 | 11 | 23.91 | 11 |
| E3D | 2.8 | 67.02 | 63 | 58.51 | 55 | 58.33 | 28 | 47.92 | 23 | 76.09 | 35 | 69.57 | 32 |
| 2.8 | 32.98 | 31 | 41.49 | 39 | 41.67 | 20 | 52.08 | 25 | 23.91 | 11 | 30.43 | 14 |
| ZRANK | 2.8 | 63.83 | 60 | - | - | 52.08 | 25 | - | - | 76.09 | 35 | - | - |
| 2.8 | 36.17 | 34 | - | - | 47.92 | 23 | - | - | 23.91 | 11 | - | - |
| ZRANK2 | 2.8 | 60.64 | 57 | - | - | 52.08 | 25 | - | - | 69.57 | 32 | - | - |
| 2.8 | 39.36 | 37 | - | - | 47.92 | 23 | - | - | 30.43 | 14 | - | - |
| ROSSETADOCK | 2.8 | 67.02 | 63 | - | - | 60.42 | 29 | - | - | 73.91 | 34 | - | - |
| 2.8 | 32.98 | 31 | - | - | 39.58 | 19 | - | - | 26.09 | 12 | - | - |
| PyDock | 2.8 | 60.64 | 57 | - | - | 52.08 | 25 | - | - | 69.57 | 32 | - | - |
| 2.8 | 39.36 | 37 | - | - | 47.92 | 23 | - | - | 30.43 | 14 | - | - |
| PISA | 2.8 | 65.96 | 62 | - | - | 58.33 | 28 | - | - | 73.91 | 34 | - | - |
| 2.8 | 34.04 | 32 | - | - | 41.67 | 20 | - | - | 26.09 | 12 | - | - |
| PIE | 2.8 | 64.89 | 61 | - | - | 56.25 | 27 | - | - | 73.91 | 34 | - | - |
| 2.8 | 35.11 | 33 | - | - | 43.75 | 21 | - | - | 26.09 | 12 | - | - |
| SIPPER | 2.8 | 63.83 | 60 | - | - | 56.25 | 27 | - | - | 71.74 | 33 | - | - |
| 2.8 | 36.17 | 34 | - | - | 43.75 | 21 | - | - | 28.26 | 13 | - | - |