**Supplementary Table R3-Q3-1. 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 cases of δ equal to 1.4, 2.8, and 4.2 Kcal/mol. We have introduced the results in non-cumulative rows for a better comprehension. We have also added the absolute number of predictions for each 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 | 1.4 | 38.30 | 36 | 39.36 | 37 | 29.17 | 14 | 29.17 | 14 | 47.83 | 22 | 50.00 | 23 |
| 1.4 δ 2.8 | 29.79 | 28 | 31.91 | 30 | 27.08 | 13 | 35.42 | 17 | 32.61 | 15 | 28.26 | 13 |
| 2.8δ 4.2 | 17.02 | 16 | 14.89 | 14 | 31.25 | 15 | 20.83 | 10 | 2.17 | 1 | 8.70 | 4 |
| 4.2 | 14.89 | 14 | 13.83 | 13 | 12.50 | 6 | 14.58 | 7 | 17.39 | 8 | 13.04 | 6 |
| aVdW | 1.4 | 41.49 | 39 | 36.17 | 34 | 35.42 | 17 | 33.33 | 16 | 47.83 | 22 | 39.13 | 18 |
| 1.4 δ 2.8 | 25.53 | 24 | 28.72 | 27 | 25.00 | 12 | 22.92 | 11 | 26.09 | 12 | 34.78 | 16 |
| 2.8δ 4.2 | 20.21 | 19 | 20.21 | 19 | 27.08 | 13 | 27.08 | 13 | 13.04 | 6 | 13.04 | 6 |
| 4.2 | 12.77 | 12 | 14.89 | 14 | 12.50 | 6 | 16.67 | 8 | 13.04 | 6 | 13.04 | 6 |
| rVdW | 1.4 | 38.30 | 36 | 35.11 | 33 | 33.33 | 16 | 31.25 | 15 | 43.48 | 20 | 39.13 | 18 |
| 1.4 δ 2.8 | 20.21 | 19 | 29.79 | 28 | 12.50 | 6 | 22.92 | 11 | 28.26 | 13 | 36.96 | 17 |
| 2.8δ 4.2 | 23.40 | 22 | 18.09 | 17 | 33.33 | 16 | 25.00 | 12 | 13.04 | 6 | 10.87 | 5 |
| 4.2 | 18.09 | 17 | 17.02 | 16 | 20.83 | 10 | 20.83 | 10 | 15.22 | 7 | 13.04 | 6 |
| aElec | 1.4 | 37.23 | 35 | 41.49 | 39 | 33.33 | 16 | 33.33 | 16 | 41.30 | 19 | 50.00 | 23 |
| 1.4 δ 2.8 | 24.47 | 23 | 28.72 | 27 | 18.75 | 9 | 29.17 | 14 | 30.43 | 14 | 28.26 | 13 |
| 2.8δ 4.2 | 19.15 | 18 | 13.83 | 13 | 25.00 | 12 | 22.92 | 11 | 13.04 | 6 | 4.35 | 2 |
| 4.2 | 19.15 | 18 | 15.96 | 15 | 22.92 | 11 | 14.58 | 7 | 15.22 | 7 | 17.39 | 8 |
| rElec | 1.4 | 37.23 | 35 | 39.36 | 37 | 35.42 | 17 | 29.17 | 14 | 39.13 | 18 | 50.00 | 23 |
| 1.4 δ 2.8 | 23.40 | 22 | 29.79 | 28 | 14.58 | 7 | 31.25 | 15 | 32.61 | 15 | 28.26 | 13 |
| 2.8δ 4.2 | 21.28 | 20 | 14.89 | 14 | 29.17 | 14 | 25.00 | 12 | 13.04 | 6 | 4.35 | 2 |
| 4.2 | 18.09 | 17 | 15.96 | 15 | 20.83 | 10 | 14.58 | 7 | 15.22 | 7 | 17.39 | 8 |
| laElec | 1.4 | 37.23 | 35 | 42.55 | 40 | 33.33 | 16 | 35.42 | 17 | 41.30 | 19 | 50.00 | 23 |
| 1.4 δ 2.8 | 23.40 | 22 | 26.60 | 25 | 18.75 | 9 | 27.08 | 13 | 28.26 | 13 | 26.09 | 12 |
| 2.8δ 4.2 | 21.28 | 20 | 15.96 | 15 | 27.08 | 13 | 22.92 | 11 | 15.22 | 7 | 8.70 | 4 |
| 4.2 | 18.09 | 17 | 14.89 | 14 | 20.83 | 10 | 14.58 | 7 | 15.22 | 7 | 15.22 | 7 |
| lrElec | 1.4 | 38.30 | 36 | 41.49 | 39 | 33.33 | 16 | 33.33 | 16 | 43.48 | 20 | 50.00 | 23 |
| 1.4 δ 2.8 | 18.09 | 17 | 28.72 | 27 | 12.50 | 6 | 29.17 | 14 | 23.91 | 11 | 28.26 | 13 |
| 2.8δ 4.2 | 25.53 | 24 | 14.89 | 14 | 33.33 | 16 | 22.92 | 11 | 17.39 | 8 | 6.52 | 3 |
| 4.2 | 18.09 | 17 | 14.89 | 14 | 20.83 | 10 | 14.58 | 7 | 15.22 | 7 | 15.22 | 7 |
| HB | 1.4 | 37.23 | 35 | 38.30 | 36 | 31.25 | 15 | 33.33 | 16 | 43.48 | 20 | 43.48 | 20 |
| 1.4 δ 2.8 | 29.79 | 28 | 19.15 | 18 | 29.17 | 14 | 12.50 | 6 | 30.43 | 14 | 26.09 | 12 |
| 2.8δ 4.2 | 15.96 | 15 | 25.53 | 24 | 16.67 | 8 | 35.42 | 17 | 15.22 | 7 | 15.22 | 7 |
| 4.2 | 17.02 | 16 | 17.02 | 16 | 22.92 | 11 | 18.75 | 9 | 10.87 | 5 | 15.22 | 7 |
| EPAIR | 1.4 | 32.98 | 31 | 41.49 | 39 | 29.17 | 14 | 35.42 | 17 | 36.96 | 17 | 47.83 | 22 |
| 1.4 δ 2.8 | 29.79 | 28 | 26.60 | 25 | 20.83 | 10 | 27.08 | 13 | 39.13 | 18 | 26.09 | 12 |
| 2.8δ 4.2 | 19.15 | 18 | 15.96 | 15 | 29.17 | 14 | 16.67 | 8 | 8.70 | 4 | 15.22 | 7 |
| 4.2 | 18.09 | 17 | 15.96 | 15 | 20.83 | 10 | 20.83 | 10 | 15.22 | 7 | 10.87 | 5 |
| ES3DC | 1.4 | 38.30 | 36 | 46.81 | 44 | 33.33 | 16 | 39.58 | 19 | 43.48 | 20 | 54.35 | 25 |
| 1.4 δ 2.8 | 27.66 | 26 | 26.60 | 25 | 22.92 | 11 | 31.25 | 15 | 32.61 | 15 | 21.74 | 10 |
| 2.8δ 4.2 | 19.15 | 18 | 9.57 | 9 | 27.08 | 13 | 10.42 | 5 | 10.87 | 5 | 8.70 | 4 |
| 4.2 | 14.89 | 14 | 17.02 | 16 | 16.67 | 8 | 18.75 | 9 | 13.04 | 6 | 15.22 | 7 |
| E3D | 1.4 | 36.17 | 34 | 38.30 | 36 | 33.33 | 16 | 31.25 | 15 | 39.13 | 18 | 45.65 | 21 |
| 1.4 δ 2.8 | 30.85 | 29 | 20.21 | 19 | 25.00 | 12 | 16.67 | 8 | 36.96 | 17 | 23.91 | 11 |
| 2.8δ 4.2 | 20.21 | 19 | 24.47 | 23 | 29.17 | 14 | 31.25 | 15 | 10.87 | 5 | 17.39 | 8 |
| 4.2 | 12.77 | 12 | 17.02 | 16 | 12.50 | 6 | 20.83 | 10 | 13.04 | 6 | 13.04 | 6 |
| ZRANK | 1.4 | 38.30 | 36 | - | - | 35.42 | 17 | - | - | 41.30 | 19 | - | - |
| 1.4 δ 2.8 | 25.53 | 24 | - | - | 16.67 | 8 | - | - | 34.78 | 16 | - | - |
| 2.8δ 4.2 | 22.34 | 21 | - | - | 33.33 | 16 | - | - | 10.87 | 5 | - | - |
| 4.2 | 13.83 | 13 | - | - | 14.58 | 7 | - | - | 13.04 | 6 | - | - |
| ZRANK2 | 1.4 | 38.30 | 36 | - | - | 35.42 | 17 | - | - | 41.30 | 19 | - | - |
| 1.4 δ 2.8 | 22.34 | 21 | - | - | 16.67 | 8 | - | - | 28.26 | 13 | - | - |
| 2.8δ 4.2 | 24.47 | 23 | - | - | 31.25 | 15 | - | - | 17.39 | 8 | - | - |
| 4.2 | 14.89 | 14 | - | - | 16.67 | 8 | - | - | 13.04 | 6 | - | - |
| RosettaDock | 1.4 | 37.23 | 35 | - | - | 33.33 | 16 | - | - | 41.30 | 19 | - | - |
| 1.4 δ 2.8 | 29.79 | 28 | - | - | 27.08 | 13 | - | - | 32.61 | 15 | - | - |
| 2.8δ 4.2 | 17.02 | 16 | - | - | 20.83 | 10 | - | - | 13.04 | 6 | - | - |
| 4.2 | 15.96 | 15 | - | - | 18.75 | 9 | - | - | 13.04 | 6 | - | - |
| PyDock | 1.4 | 38.30 | 36 | - | - | 29.17 | 14 | - | - | 47.83 | 22 | - | - |
| 1.4 δ 2.8 | 22.34 | 21 | - | - | 22.92 | 11 | - | - | 21.74 | 10 | - | - |
| 2.8δ 4.2 | 25.53 | 24 | - | - | 35.42 | 17 | - | - | 15.22 | 7 | - | - |
| 4.2 | 13.83 | 13 | - | - | 12.50 | 6 | - | - | 15.22 | 7 | - | - |
| PISA | 1.4 | 35.11 | 33 | - | - | 25.00 | 12 | - | - | 45.65 | 21 | - | - |
| 1.4 δ 2.8 | 30.85 | 29 | - | - | 33.33 | 16 | - | - | 28.26 | 13 | - | - |
| 2.8δ 4.2 | 21.28 | 20 | - | - | 33.33 | 16 | - | - | 8.70 | 4 | - | - |
| 4.2 | 12.77 | 12 | - | - | 8.33 | 4 | - | - | 17.39 | 8 | - | - |
| PIE | 1.4 | 41.49 | 39 | - | - | 33.33 | 16 | - | - | 50.00 | 23 | - | - |
| 1.4 δ 2.8 | 23.40 | 22 | - | - | 22.92 | 11 | - | - | 23.91 | 11 | - | - |
| 2.8δ 4.2 | 19.15 | 18 | - | - | 29.17 | 14 | - | - | 8.70 | 4 | - | - |
| 4.2 | 15.96 | 15 | - | - | 14.58 | 7 | - | - | 17.39 | 8 | - | - |
| SIPPER | 1.4 | 41.49 | 39 | - | - | 31.25 | 15 | - | - | 52.17 | 24 | - | - |
| 1.4 δ 2.8 | 22.34 | 21 | - | - | 25.00 | 12 | - | - | 19.57 | 9 | - | - |
| 2.8δ 4.2 | 20.21 | 19 | - | - | 25.00 | 12 | - | - | 15.22 | 7 | - | - |
| 4.2 | 15.96 | 15 | - | - | 18.75 | 9 | - | - | 13.04 | 6 | - | - |