|  |  |  |  |
| --- | --- | --- | --- |
| Protein 1 (PDB) | Protein 2 (PDB) | Complex | MODEL (PDB) |
| TGF-β 3  (1TGJ) | TGF-β Type II Receptor  (1M9Z) | 1KTZ | TGF-β Type II Receptor/ TGF-β 3  (1tgj\_1m9z\_1ktz) |
| TEM-1 β-lactamase  (1ZG4) | β-lactamase inhibitor protein-I  (3GMU) | 1JTG | β-lactamase inhibitor protein-I/ TEM-1 β-lactamase  (1zg4\_3gmu\_1jtg) |
| Fragment B of protein A  (2JWD) | IgG1  (4DZ8) | 1FC2 | IgG1/Fragment B of protein A  (2jwd\_4dz8\_1fc2) |
| Cytochrome C peroxidase  (3R99) | Iso-1-cytochrome C  (1NMI) | 2PCC | Iso-1-Cytochrome C/ Cytochrome C peroxidase  (3r99\_1nmi\_2pcc) |

**Table S1**. List of reconstructed dimers from ZEMu [1] dataset. The origin ZEMu dataset contains 4 dimers and 11 trimers. Only the four dimers are used for benchmarking BindProfX, which only consider dimeric interaction.

|  |  |  |
| --- | --- | --- |
| Number of mutations | ZEMu | Profile-score |
| 1 | 0.046 | 0.311 |
| 2 or more | 0.068 | 0.100 |
| All mixed | 0.118 | 0.454 |

**Table S2**. Summary of the correlation coefficient between predicted and experimental values by ZEMu and by BindProfX profile score. The values predicted by ZEMu was directed taken from the supplementary material of the ZEMu paper [1]. 87 mutations were excluded from the ZEMu dataset because their native amino acid types reported in the paper were found to be inconsistent with the actual structure.

[1] Dourado DFAR, Flores SC. Modeling and fitting protein-protein complexes to predict change of binding energy. Sci Rep-Uk. 2016;6.