# Supplementary Information

# Deep transfer learning for inter-chain contact predictions of transmembrane protein complexes

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**Running Title:** Inter-protein contact prediction for transmembrane protein complexes

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**Supplementary Table 1:** Comparison of the precisions (%) by DeepTMP, DeepHomo2.0, CDPred, GLINTER, and DeepHomo for top 1, 10, 25, 50, L/10, L/5, and L predicted contacts on the 296 soluble protein dimers from Homodimer300 test set when the experimental monomer structures (predicted monomer structures by AlphaFold2) are used as input.

| Method | Top 1 | Top 10 | Top 25 | Top 50 | Top L/10 | Top L/5 | Top L |
|---|---|---|---|---|---|---|---|
| DeepTMP | 71.3 (61.5) | 71.2 (62.7) | 70.5 (62.1) | 70.2 (61.0) | 70.9 (62.0) | 70.2 (61.5) | 65.1 (55.1) |
| DeepHomo2.0 | 73.3 (61.8) | 71.6 (61.7) | 70.5 (60.2) | 68.0 (57.8) | 70.3 (60.6) | 68.4 (58.1) | 56.3 (46.8) |
| CDPred | 74.7 (68.6) | 72.3 (67.3) | 70.2 (66.4) | 68.4 (64.5) | 70.1 (66.7) | 68.3 (64.7) | 58.7 (54.7) |
| GLINTER | 68.6 (61.5) | 64.4 (57.4) | 60.4 (54.8) | 56.6 (51.6) | 61.3 (55.2) | 57.5 (52.2) | 43.3 (39.5) |
| DeepHomo | 61.1 (55.4) | 57.2 (49.6) | 53.8 (46.4) | 50.1 (44.0) | 54.6 (47.6) | 51.6 (44.6) | 38.8 (33.6) |

**Supplementary Table 2:** Comparison of the precisions (%) by DeepTMP and DeepTMP$\alpha$ for top 1, 10, 25, 50, L/10, L/5, and L predicted contacts on the three types of topologies when the experimental monomer structures (predicted monomer structures by AlphaFold2) are used as input.

| Method | Topology | Top 1 | Top 10 | Top 25 | Top 50 | Top L/10 | Top L/5 | Top L |
|---|---|---|---|---|---|---|---|---|
| DeepTMP | Alpha | 76.3 (71.1) | 76.6 (70.0) | 74.8 (67.7) | 72.5 (64.9) | 76.2 (68.8) | 73.7 (66.4) | 62.1 (56.4) |
| | Beta | 100 (100) | 100 (96.7) | 98.7 (94.7) | 98.7 (90.0) | 97.7 (96.6) | 98.3 (90.2) | 87.9 (74.3) |
| | Alpha+Beta | 100 (90.9) | 97.3 (93.6) | 97.8 (93.8) | 98.0 (90.9) | 97.9 (92.3) | 96.9 (89.0) | 85.0 (79.7) |
| DeepTMP$\alpha$ | Alpha | 65.8 (68.4) | 70.8 (67.1) | 68.7 (66.6) | 67.1 (65.1) | 70.8 (66.3) | 68.6 (64.1) | 58.2 (54.0) |
| | Beta | 100 (100) | 96.7 (96.7) | 84.0 (92.0) | 82.0 (87.3) | 84.2 (90.8) | 83.0 (87.3) | 74.5 (65.7) |
| | Alpha+Beta | 90.9 (90.9) | 94.5 (89.1) | 93.8 (90.2) | 91.8 (88.9) | 92.2 (89.4) | 89.5 (88.2) | 76.9 (73.1) |

**Supplementary Table 3:** The precisions of DeepTMP on extracellular, cytoplasmic and transmembrane segments for top 1, 10, 25, 50, L/10, L/5, and L predicted contacts on the test set of 52 transmembrane protein complexes when the experimental monomer structures (predicted monomer structures by AlphaFold2) are used as input

| Regions | Top 1 | Top 10 | Top 25 | Top 50 | Top L/10 | Top L/5 | Top L |
|---|---|---|---|---|---|---|---|
| extracellular | 75.0 (66.7) | 73.2 (78.0) | 80.3 (71.9) | 77.7 (67.0) | 78.6 (71.7) | 73.5 (72.1) | 61.7 (57.7) |
| cytoplasmic | 100 (90.0) | 97.6 (74.7) | 84.5 (73.7) | 84.2 (68.7) | 88.1 (71.1) | 84.6 (67.0) | 72.1 (60.8) |
| transmembrane | 84.6 (83.3) | 82.5 (70.9) | 81.5 (72.2) | 80.1 (71.6) | 86.1 (74.9) | 78.2 (73.2) | 66.0 (60.2) |