**Supplemental Table 1.** The performances of DeepHomo, GLINTER, DRN-1D2D\_Inter, DeepHomo2, CDPred and PLMGraph-Inter on HomoPDB and HeteroPDB after the removal of targets which GLINTER failed to make the prediction using experimental structures (AlphaFold2 predicted structures)

|  |  |  |
| --- | --- | --- |
| Methods | HomoPDB (precision %) | HeteroPDB (precision %) |
| L/5 | L/10 | 50 | 10 | 5 | L/5 | L/10 | 50 | 10 | 5 |
| DeepHomo | 40.8(36.8) | 44.0(39.5) | 40.2(36.1) | 45.7(41.6) | 46.6(42.6) |  |
| GLINTER | 42.6(45.5) | 44.7(48.2) | 41.8(44.2) | 46.1(50.1) | 48.2(51.5) | 24.3(24.6) | 25.2(26.6) | 21.3(21.8) | 25.9(25.3) | 27.1(25.8) |
| DRN-1D2D\_Inter | 50.2 | 52.8 | 49.1 | 53.9 | 54.8 | 33.9 | 36.0 | 31.7 | 36.5 | 37.3 |
| DeepHomo2 | 53.5(49.8) | 56.0(51.3) | 52.9(49.2) | 57.3(53.4) | 59.2(54.1) |  |
| CDPred | 56.3(51.5) | 58.4(52.9) | 55.4(50.9) | 59.7(53.9) | 60.3(54.2) | 30.6(30.7) | 31.5(32.3) | 28.1(27.7) | 32.6(32.8) | 32.4(33.2) |
| PLMGraph-Inter | **66.3****(59.1)** | **68.4****(61.0)** | **65.2****(58.4)** | **69.7****(62.4)** | **70.1****(62.5)** | **45.8****(41.9)** | **48.7****(43.5)** | **41.2****(37.7)** | **49.2****(44.3)** | **52.0****(45.2)** |

Note: The highest mean precision (%) in each column is highlighted in bold.