**Table S2.** The prediction performance of the DNN-based DTI model using 5-fold cross-validation (early stopping at epoch 74).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Validation Loss | Validation Accuracy | Testing Loss | Testing Accuracy |
| 1 | 0.206419 | 0.933903 | 0.193231 | 0.932994 |
| 2 | 0.196016 | 0.929988 | 0.201543 | 0.931002 |
| 3 | 0.192233 | 0.933321 | 0.189356 | 0.933036 |
| 4 | 0.217242 | 0.924825 | 0.205083 | 0.930503 |
| 5 | 0.234524 | 0.927316 | 0.225880 | 0.930441 |
| Average | 0.209287 | 0.929871 | 0.203019 | 0.931595 |
| Standard deviation | 0.015332 | 0.003469 | 0.012740 | 0.001176 |