Supplementary Table 1. Average training time and average testing time of our prediction method and the compared methods.

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| Method | DNDTI | NGDTP | GANDTI | GRMF | DTINet | DDR | Lee’s method | AEFS |
| Average training time  (minutes per fold cross-validation) | 15.5 | 17.8 | 1.4 | 0.9 | 2.5 | 0.5 | 0.4 | 13.1 |
| Average testing time  (microseconds per drug-protein pair) | 97.3 | 1024.8 | 50.9 | 1.0 | 0.9 | 197.1 | 24.3 | 1.3 |