

Description of Additional Supplementary Files

Supplementary Dataset 1: Contain the experiments and results of the neural network without knowledge enhancement (Feed-Forward Neural Network) with Intermediate Fusion for DTI. It is comma-separated and contains the following columns: Molecular modalities; DG; Davis drug; Davis target; Davis random; Kiba drug; Kiba target; Kiba random

Supplementary Dataset 2: Contain the experiments and results of the neural network without knowledge enhancement (Feed-Forward Neural Network) with Late Fusion for DTI. It is comma-separated and contains the following columns: Molecular modalities; DG; Davis drug; Davis target; Davis random; Kiba drug; Kiba target; Kiba random

Supplementary Dataset 3: Contain the experiments and results of the knowledge-enhanced neural network (Otter-Knowledge) with Intermediate Fusion for DTI. It also contains the experiments for modality selection (i.e. the experiments with IM and ESM-2). It is comma-separated and contains the following columns: Molecular modalities; Protein modalities; DG; Davis drug; Davis target; Davis random; Kiba drug; Kiba target; Kiba random

Supplementary Dataset 4: Contain the experiments and results of the knowledge-enhanced neural network (Otter-Knowledge) with Late Fusion for DTI. It is comma-separated and contains the following columns: Molecular modalities; DG; Davis drug; Davis target; Davis random; Kiba drug; Kiba target; Kiba random

Supplementary Dataset 5: Contain the experiments and results of the neural network without knowledge enhance (Feed-Forward Neural Network) with Intermediate Fusion for ADMET. It is comma-separated and contains the following columns: Molecular modalities; Ames; Bbb martins; Bioavailability ma; Caco2 wang; Clearance hepatocyte az; Clearance microsome az; Cyp2c9 substrate carbonmangels; Cyp2c9 veith; Cyp2d6 substrate carbonmangels; Cyp2d6 veith; Cyp3a4 substrate carbonmangels; Cyp3a4 veith; Dili; Half life obach; Herg; Hia hou; Ld50 zhu; Lipophilicity astrazeneca; Pgp broccatelli; Ppbr az; Solubility aqsolddb; Vdss lombardo

Supplementary Dataset 6: Contain the experiments and results of the neural network without knowledge enhancement (Feed-Forward Neural Network) with Late Fusion for ADMET. It is comma-separated and contains the following columns: Molecular modalities; Ames; Bbb martins; Bioavailability ma; Caco2 wang; Clearance hepatocyte az; Clearance microsome az; Cyp2c9 substrate carbonmangels; Cyp2c9 veith; Cyp2d6 substrate carbonmangels; Cyp2d6 veith; Cyp3a4 substrate carbonmangels; Cyp3a4 veith; Dili; Half life obach; Herg; Hia hou; Ld50 zhu; Lipophilicity astrazeneca; Pgp broccatelli; Ppbr az; Solubility aqsolddb; Vdss lombardo