dNNDR: Deep Neural Networks assisted Drug Recommendation system for identifying potential drug-target interactions

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[Additional file 1]

1. Supplementary figures

Figure S1: A general overview of the interface of dNNDR-featx, where it shows the different components of the application. (A) This section lets the user input their drug target pairs in a text file. (B) For protein features, five types of features are available from which the user can choose. The user may also select 'All' to get features corresponding to all the options. (C) Once the features are extracted, the program allows the user to proceed further for model training. (D) This section provides all the information regarding the input file, output file location and progress bar.

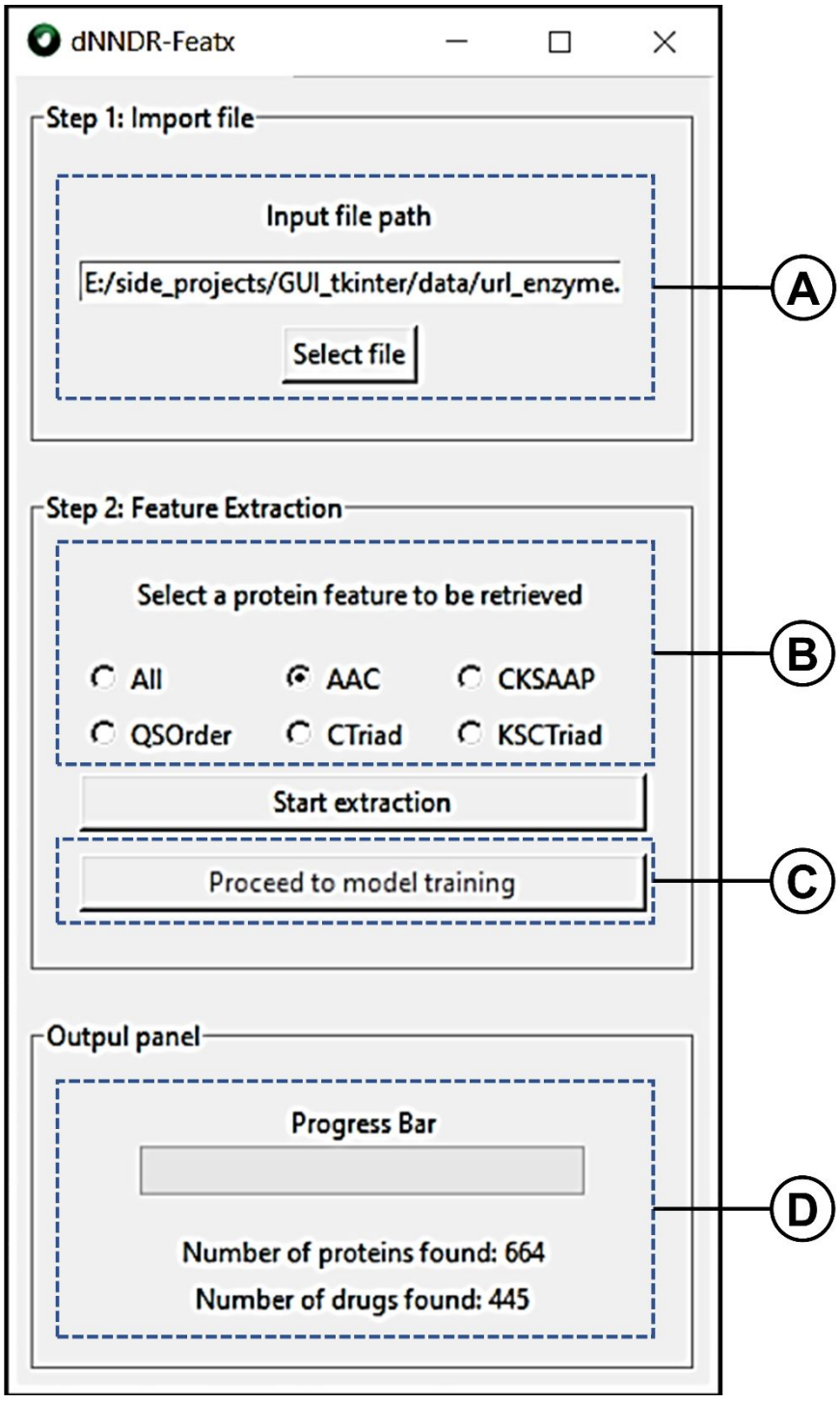


Figure S2: Model architecture of dNNDRa (only att-biLSTM for drug and protein sequences)

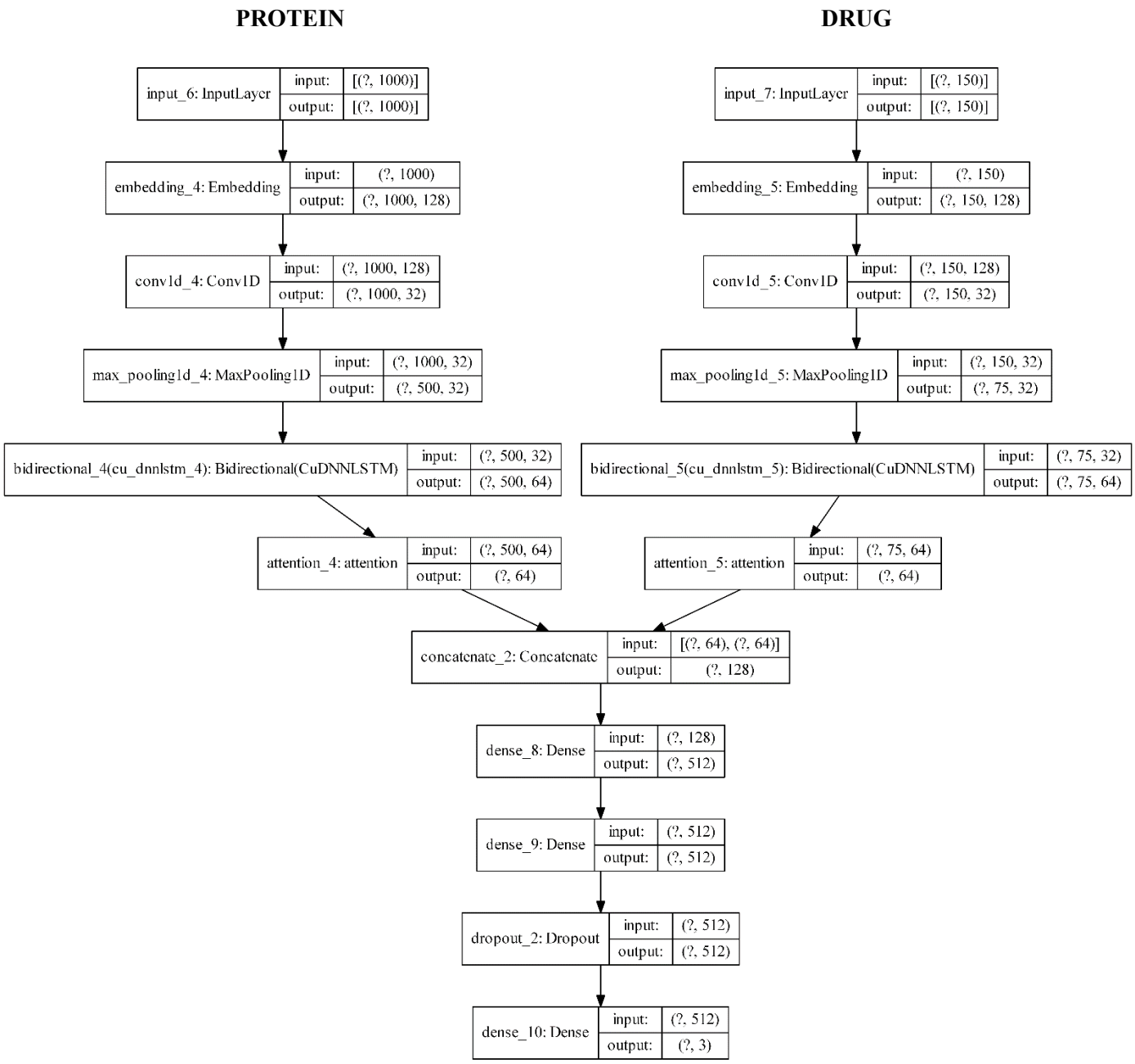


Figure S3: Model architecture of dNNDRa (att-biLSTM for drug and protein sequences along with molecular descriptors)

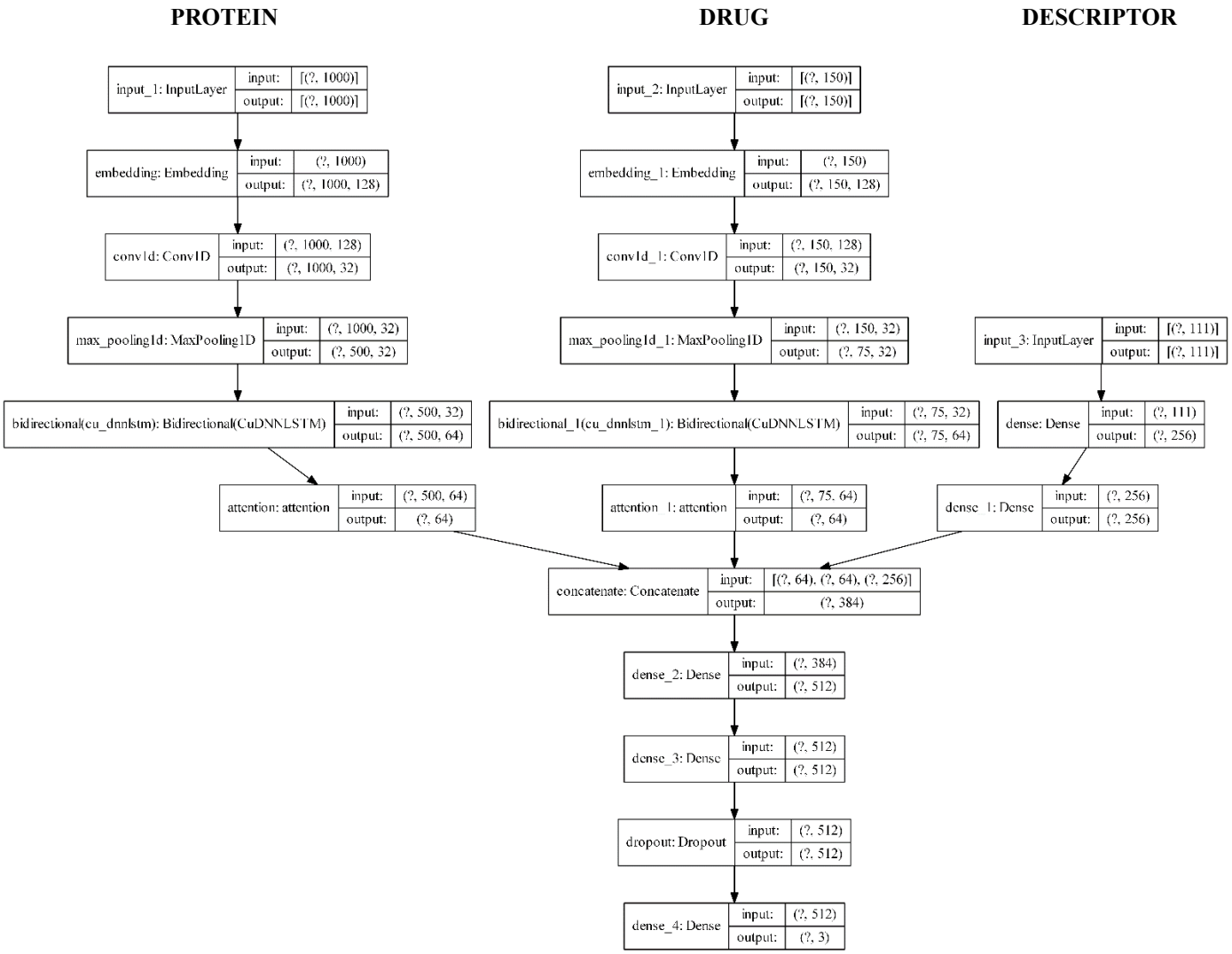


Figure S4: Model architecture of dNNDRa (att-biLSTM and three input gCNN)

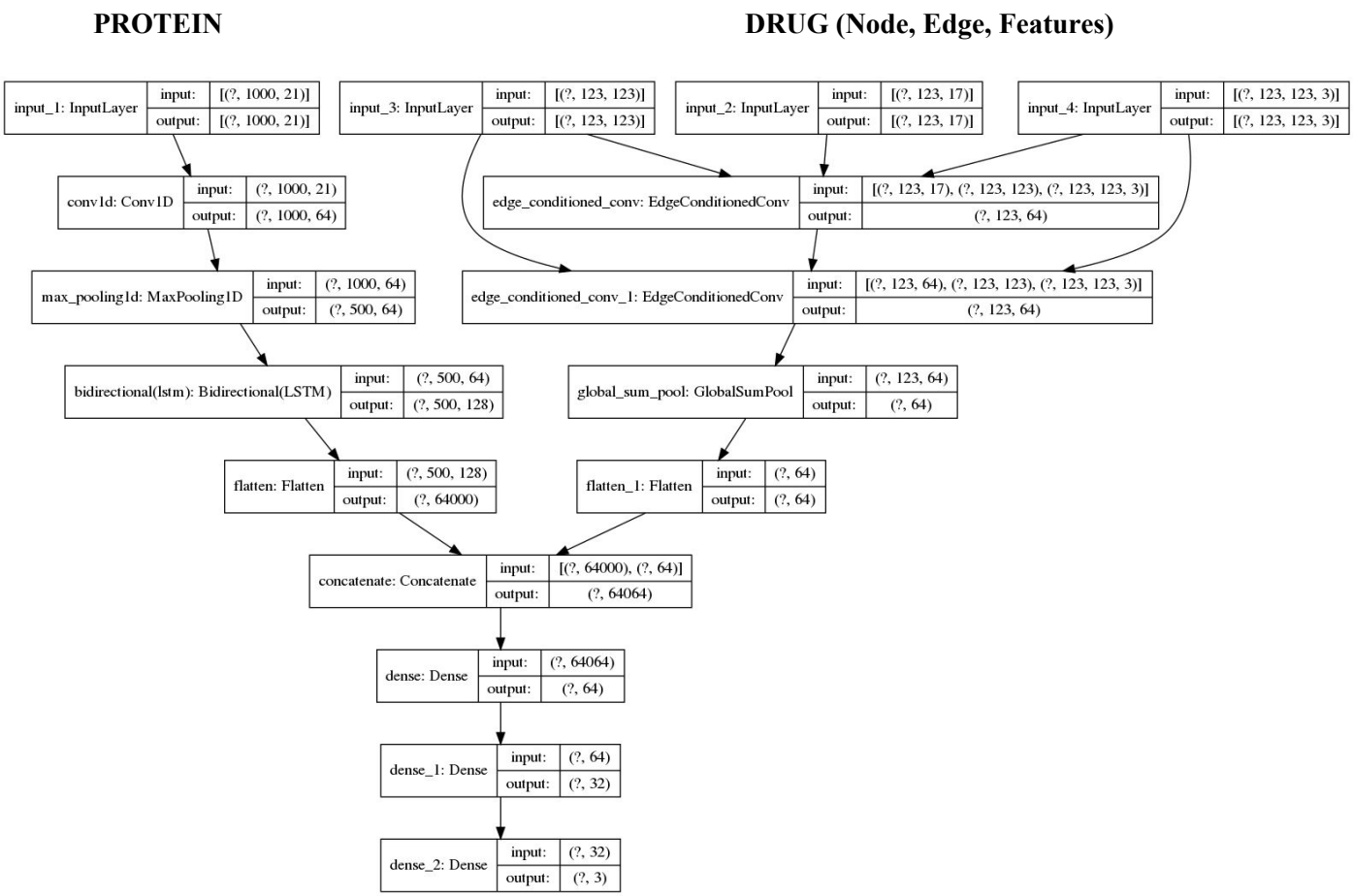


Figure S5: Model architecture of first baseline method (Sequence and CTD features)

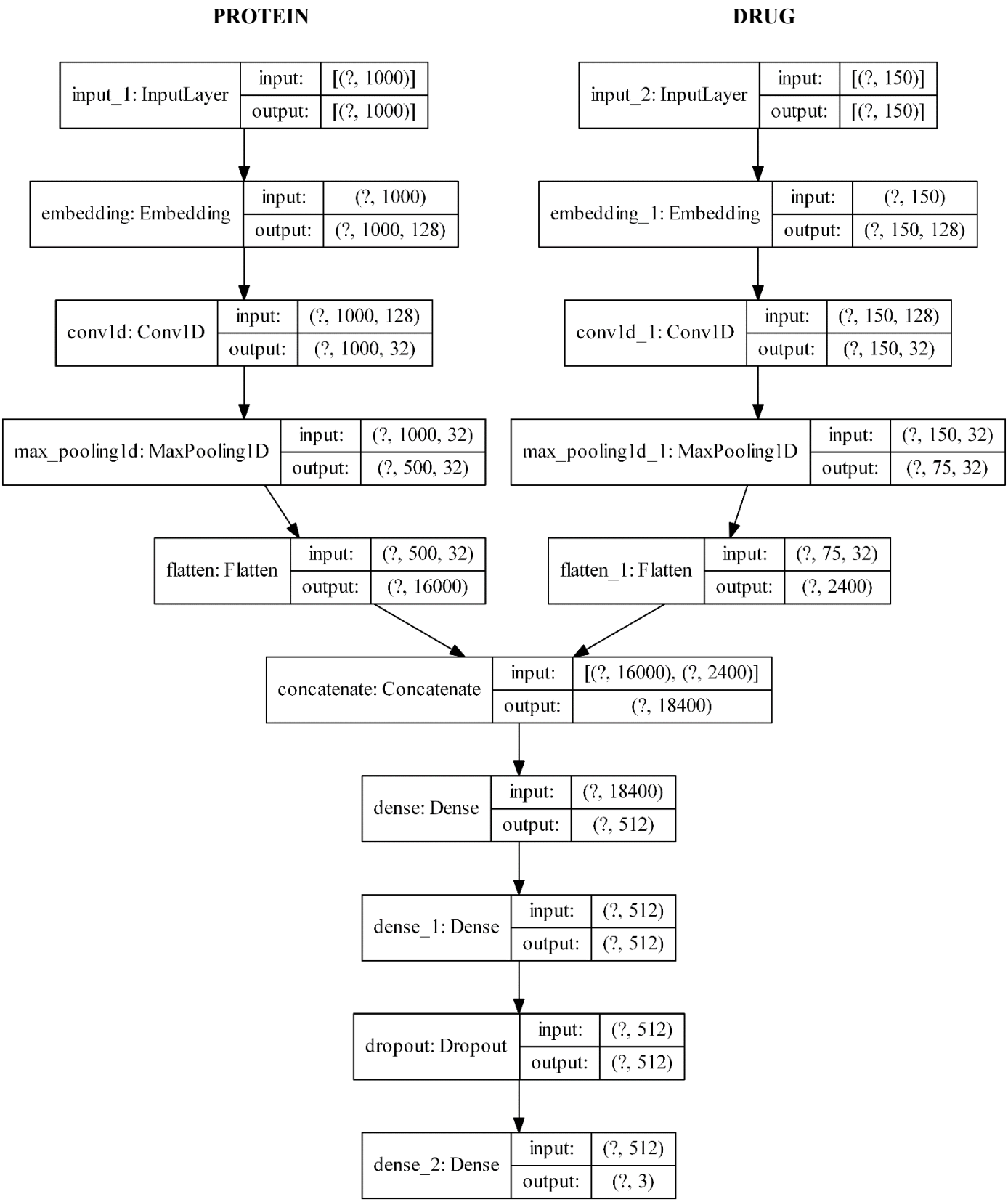
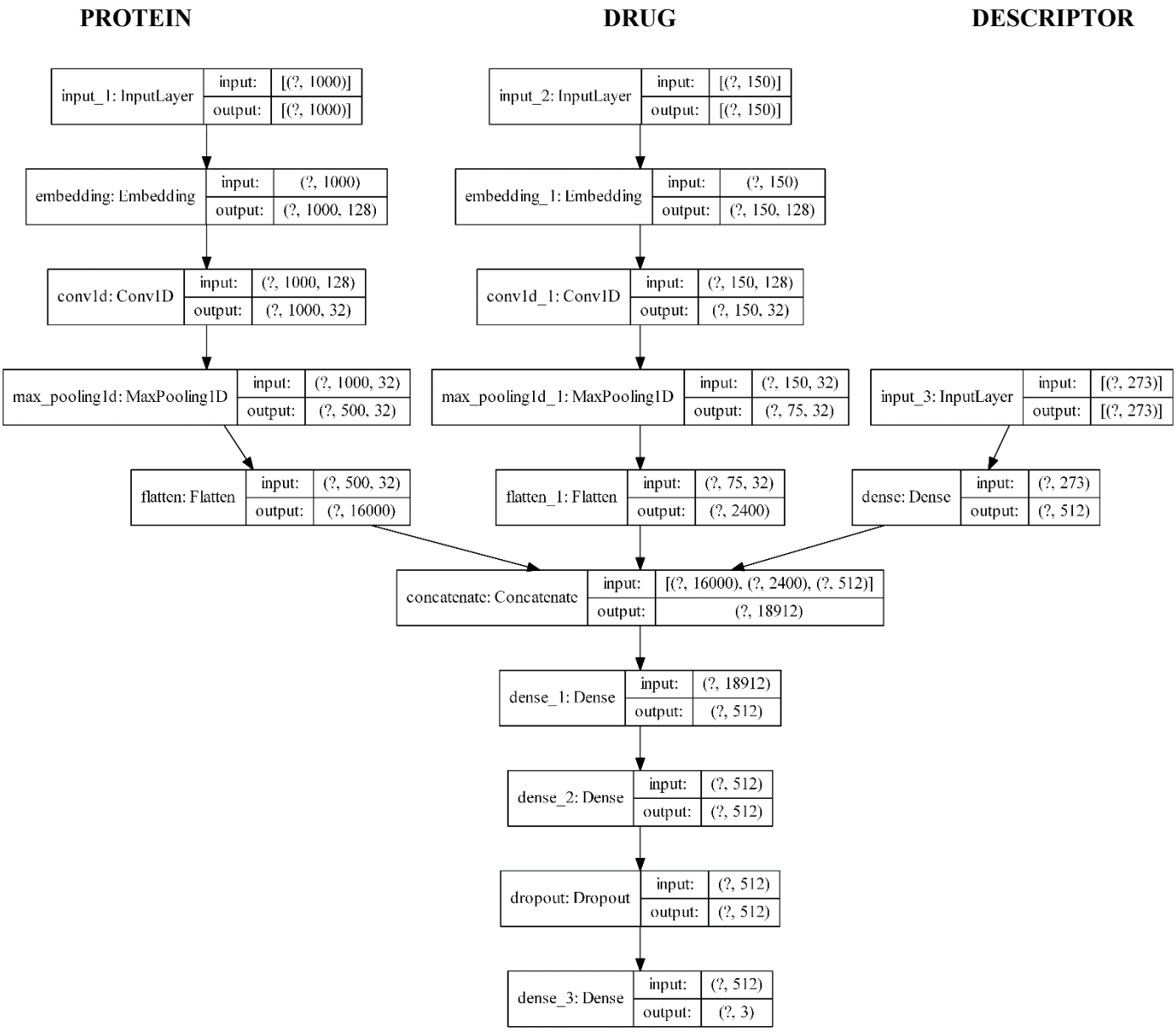


Figure S6: Model architecture of second baseline method (Sequence, CTD features and molecular descriptors)



2. Supplementary Table

Table S1: Benchmarking study to compare the performance of LSTM and gNN based methods in predicting molecular properties of the qm9 dataset.

	MAE		**R^2**	
	LSTM	*gNN*	*LSTM*	*gNN*
U_0 (eV)	0.052	0.040	0.971	0.973
U (eV)	0.021	0.084	0.973	0.963
H (eV)	0.198	0.093	0.964	0.968
G (eV)	0.025	0.057	0.978	0.972
C_v (cal mol K^{-1})	0.174	0.163	0.961	0.963
μ (Debye)	0.022	0.016	0.974	0.975
α (a_0^3)	0.069	0.052	0.969	0.972
$\in_{HOMO}$ (eV)	0.193	0.112	0.966	0.980

MAE: Mean absolute error (Lower the better); R^2: coefficient of determination (Higher the better); LSTM: Long short term memory; gNN: graph Neural network

U_0 (eV): Internal energy of atomization at 0 K; U: Internal energy of atomization at 298.15 K; H: Enthalpy of atomization; G: Free energy of atomization; C_v: Heat capacity; μ: Dipole moment; α: Eelectronic polarizability; $\in_{HOMO}$:HOMO energies