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*Research article*

## **A model for predicting drug-disease associations based on dense convolutional attention network**

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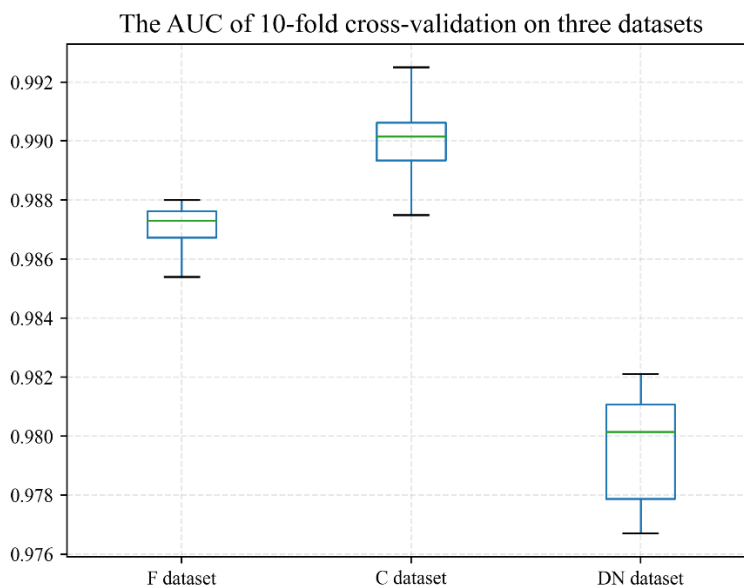
### **Supplementary**

**Table S1.** The AUC values of the DCNN model in the parameters selection process.

AUC	Layer = 2	Layer = 3	Layer = 4	Layer = 5
dense block = 2	97.89	98.11	98.23	98.56
dense block = 3	98.96	98.70	<b>99.04</b>	98.73
dense block = 4	98.68	98.65	98.72	99.01
dense block = 5	97.71	98.12	98.29	98.52

**Table S2.** The AUC values of ten times ten-fold cross-validation of the DCNN model on the F, C and DN datasets.

AUC	F	C	DN
1st	0.9880	0.9904	0.9807
2nd	0.9778	0.9904	0.9813
3rd	0.9854	0.9907	0.9821
4th	0.9867	0.9892	0.9768
5th	0.9855	0.9925	0.9790
6th	0.9872	0.9910	0.9806
7th	0.9874	0.9899	0.9775
8th	0.9873	0.9875	0.9767
9th	0.9868	0.9882	0.9797
10th	0.9877	0.9898	0.9812



**Figure S1.** The Box plot of ten times ten-fold cross-validation of the DCNN model on the F, C and DN datasets.

**Table S3.** The ten-fold cross-validation performance with different similarity combinations. Similarity R\_str means the structural similarity of drugs. Similarity R\_Jac means the Jaccard similarity of drugs. Similarity R\_Mut means the Mutual Information of drugs. Similarity R\_Gau means the Gaussian interaction profile kernel similarity of drugs. Similarity D\_sem means the semantic similarity of diseases. Similarity D\_Jac means the Jaccard similarity of diseases. Similarity D\_Mut means the Mutual Information of diseases. Similarity D\_Gau means the Gaussian interaction profile kernel similarity of diseases.

Information	Dataset	Accuracy (%)	Precision (%)	Recall (%)	F1-score (%)	AUC
R_str + R_Jac;	F	92.13	92.17	92.16	92.16	96.98
D_sem + D_Jac;	C	93.31	93.24	93.23	93.22	97.70
	DN	82.73	83.06	82.74	82.73	88.86
R_str + R_Mut;	F	88.49	88.53	88.48	88.47	92.86
D_sem + D_Mut;	C	90.58	90.61	90.58	90.57	95.48
	DN	88.74	88.87	87.74	87.75	91.95
R_str + R_Gau;	F	95.16	94.46	96.16	95.19	98.77
D_sem + D_Gau;	C	95.51	95.62	95.42	95.51	99.04
	DN	94.59	94.52	94.64	94.88	98.07

**Table S4.** The ten-fold cross-validation performance of verification experiment on the effectiveness of data fusion. Similarity R\_str means the structural similarity of drugs. Similarity R\_Gau means the Gaussian interaction profile kernel similarity of drugs. Similarity D\_sem means the semantic similarity of diseases. Similarity D\_Gau means the Gaussian interaction profile kernel similarity of diseases.

Similarity	Dataset	Accuracy (%)	Precision (%)	Recall (%)	F1-score (%)	AUC
R_str;	F	87.79	87.84	87.80	87.81	92.69
D_sem;	C	89.41	89.44	89.42	89.42	94.26
	DN	87.75	87.83	87.76	87.75	92.38
R_Gau;	F	94.82	94.54	94.82	94.81	98.51
D_Gau;	C	94.93	95.01	95.29	95.28	98.53
	DN	93.60	93.67	94.12	94.54	97.86
R_str + R_Gau;	F	95.16	94.46	96.16	95.15	98.77
D_sem + D_Gau;	C	95.51	95.62	95.42	95.52	99.04
	DN	94.59	94.52	94.64	94.88	98.07

**Table S5.** Top 20 drug candidates for the treatment of Breast cancer.

Drug name	Evidence	Drug name	Evidence
Pyridoxine	Marker	Moxifloxacin	Marker
Nateglinide	Marker	Bexarotene	Therapeutic
Nisoldipine	Marker	Flutamide	Marker
Dextromethorphan	Marker	Promethazine	Marker
Vorinostat	Therapeutic	Penbutolol	Marker
Triamcinolone	Marker	Buclizine	Not confirmed
Tretinoin	Therapeutic	Brimonidine	Not confirmed
Risedronic acid	Marker	Flurbiprofen	Marker
Alitretinoin	Marker	Anisindione	Not confirmed
Lithium cation	Marker	Olanzapine	Marker

**Table S6.** Top 20 drug candidates for the treatment of Alzheimer disease.

Drug name	Evidence	Drug name	Evidence
Methadone	Marker	Ergocalciferol	Marker
Zoledronic acid	Marker	Pyridoxine	Marker
Vincristine	Marker	Quinapril	Marker
Paroxetine	Therapeutic	Pravastatin	Marker
Pralidoxime	Marker	Dihydrocodeine	Not confirmed
Galantamine	Therapeutic	Venlafaxine	Marker
Glipizide	Not confirmed	Prazosin	Marker
Clonazepam	Marker	Fluphenazine	Not confirmed
Promethazine	Marker	Praziquantel	Marker
Decitabine	Marker	Methyclothiazide	Not confirmed



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