

**Table S1** The impact of AAL atlas on the performance of existing methods on the ABIDE dataset

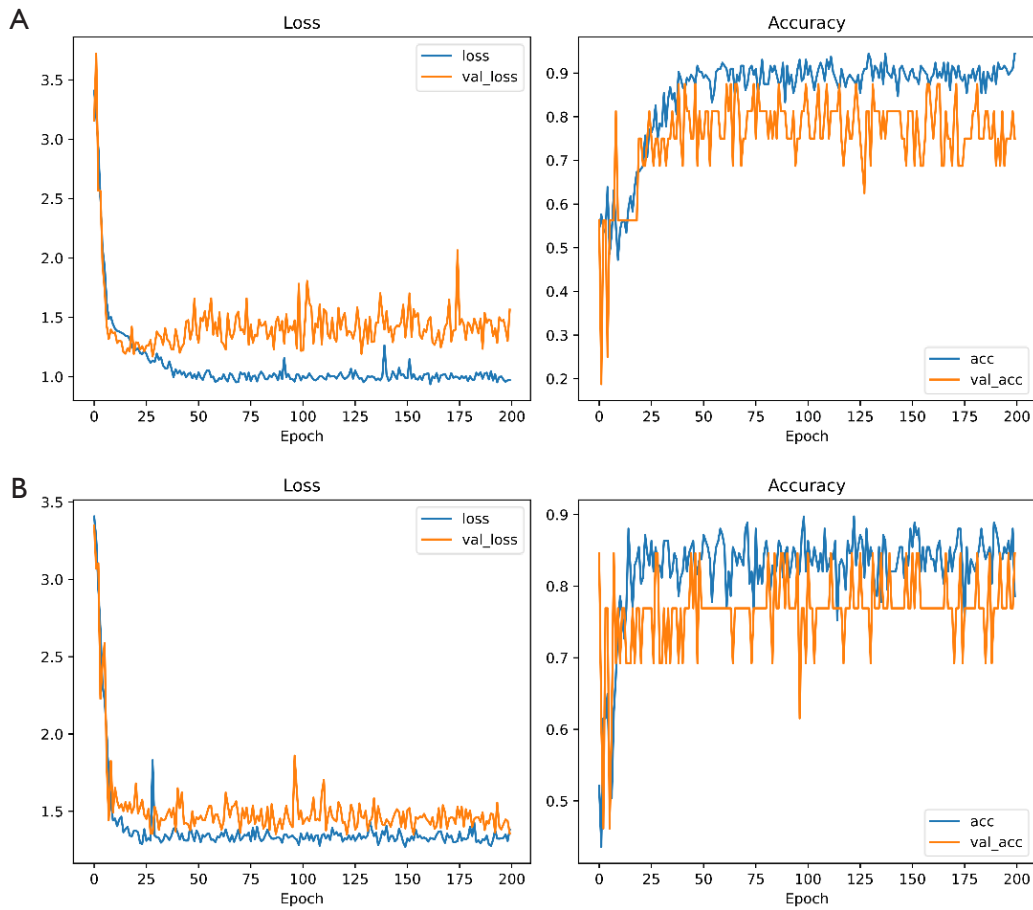
Method	Smith atlas				AAL atlas			
	ACC (%)	SEN (%)	SPE (%)	AUC (%)	ACC (%)	SEN (%)	SPE (%)	AUC (%)
SVM	63.82	56.61	69.44	66.40	64.51	52.32	73.56	71.34
LSTM	67.58	37.32	90.67	60.67	66.31	36.96	87.56	53.09
GCN	68.01	36.96	92.00	59.12	69.87	35.36	95.78	65.35
EDGE-CONV	71.01	59.82	79.33	65.62	69.84	50.18	83.33	64.84
DiffPool-GCN	71.01	61.25	78.67	62.57	68.14	45.71	84.67	60.04
GraphSAGE	67.48	37.32	90.89	71.26	67.52	50.71	80.78	69.14
Our method	74.48	57.68	88.00	72.34	72.75	48.93	90.89	64.00

AAL, automated anatomical labeling; ABIDE, Autism Brain Imaging Data Exchange; ACC, accuracy; SEN, sensitivity; SPE, specificity; AUC, area under the receiver operating characteristic curve; SVM, support vector machine; LSTM, long short-term memory; GCN, graph convolutional network; EDGE-CONV, dynamic graph convolutional neural network; DiffPool-GCN, hierarchical graph representation learning with differentiable pooling; GraphSAGE, inductive representation learning on large graphs.

**Table S2** The impact of AAL atlas on the performance of existing methods on the SUDMEX CONN dataset

Method	Smith atlas				AAL atlas			
	ACC (%)	SEN (%)	SPE (%)	AUC (%)	ACC (%)	SEN (%)	SPE (%)	AUC (%)
SVM	65.49	71.61	58.57	64.24	63.13	65.89	59.52	65.82
LSTM	71.70	77.32	65.71	64.72	69.40	80.36	57.62	58.89
GCN	68.74	83.57	51.90	60.00	70.88	70.54	71.43	67.27
EDGE-CONV	69.40	81.61	54.52	59.73	67.91	87.68	45.71	59.78
DiffPool-GCN	73.96	87.14	58.10	66.39	73.13	74.46	70.48	66.86
GraphSAGE	68.02	87.14	45.71	62.42	70.93	83.39	57.62	66.04
Our method	76.15	86.07	64.76	68.60	71.59	77.68	64.76	63.46

AAL, automated anatomical labeling; SUDMEX CONN, Mexican Cocaine Use Disorders; ACC, accuracy; SEN, sensitivity; SPE, specificity; AUC, area under the receiver operating characteristic curve; SVM, support vector machine; LSTM, long short-term memory; GCN, graph convolutional network; EDGE-CONV, dynamic graph convolutional neural network; DiffPool-GCN, hierarchical graph representation learning with differentiable pooling; GraphSAGE, inductive representation learning on large graphs.



**Figure S1** An illustration of loss and accuracy during training epochs. (A) ABIDE dataset. (B) SUDMEX CONN dataset. It is worth noting that due to the small dataset used in this study, the normal fluctuations in validation accuracy will appear as spikes when the model converges. ABIDE, Autism Brain Imaging Data Exchange; SUDMEX CONN, Mexican Cocaine Use Disorders; ACC, accuracy; Val\_ACC, validation accuracy.