Figure S1. The classification accuracy of our proposed GIN model with different threshold values.

Table S1. The coordinates of salient ROIs for ASD group in four hidden layers.

NO.	ASD							
	1st layer		2nd layer		3rd layer		4th layer	
	ROI	Coordinates	ROI	Coordinates	ROI	Coordinates	ROI	Coordinates
1	LH_Default_PHC_1	(-26, -32, -18)	LH_Vis_6	(-14, -44, -2)	RH_Cont_PFCl_4	(46, 24, 26)	LH_Vis_6	(-14, -44, -2)
2	RH_Cont_PFCmp_2	(8, 24, 56)	LH_DorsAttn_Post_3	(-26, -70, 38)	RH_Cont_PFCmp_1	(8, 30, 28)	RH_Cont_PFCl_4	(46, 24, 26)
3	LH_Cont_Cing_1	(-4, -28, 28)	LH_Default_PFC_5	(-52, 22, 8)	RH_Cont_Par_1	(62, -38, 36)	LH_Limbic_TempPole_4	(-42, 8, -18)
4	LH_Default_PFC_1	(-34, 20, -14)	LH_Default_pCunPCC_4	(-6, -54, 42)	RH_Default_Par_3	(50, -58, 44)	RH_Vis_9	(8, -76, 8)
5	LH_Default_PFC_4	(-12, 64, -6)	LH_Default_PHC_1	(-26, -32, -18)	RH_Default_Temp_1	(48, 12, -30)	RH_Vis_11	(42, -80, 10)
6	LH_Default_PFC_5	(-52, 22, 8)	RH_SomMot_19	(20, -30, 70)	LH_Vis_6	(-14, -44, -2)	RH_DorsAttn_Post_1	(50, -54, -16)
7	LH_Default_pCunPCC_4	(-6, -54, 42)	RH_Cont_PFCl_4	(46, 24, 26)	LH_Limbic_TempPole_2	(-44, -20, -30)	RH_DorsAttn_Post_2	(52, -60, 10)
8	RH_SomMot_19	(20, -30, 70)	LH_Limbic_TempPole_2	(-44, -20, -30)	LH_Cont_Cing_1	(-4, -28, 28)	RH_SalVentAttn_FrOperIns_1	(40, 6, -16)
9	RH_Default_Par_1	(46, -70, 28)	LH_Cont_Cing_1	(-4, -28, 28)	LH_Default_Temp_2	(-60, -18, -22)	RH_Cont_Par_2	(52, -42, 48)
10	RH_Default_Par_3	(50, -58, 44)	LH_Default_PFC_4	(-12, 64, -6)	LH_Default_PFC_5	(-52, 22, 8)	RH_Cont_PFCl_2	(30, 58, 4)
11	LH_DorsAttn_Post_3	(-26, -70, 38)	RH_Vis_6	(12, -92, -6)	RH_Vis_6	(12, -92, -6)	RH_Default_Par_3	(50, -58, 44)
12	RH_Vis_6	(12, -92, -6)	RH_Default_Par_3	(50, -58, 44)	RH_DorsAttn_Post_2	(52, -60, 10)	RH_Default_Temp_2	(60, -12, -20)
13	RH_Default_PFCv_1	(50, 28, 0)	LH_DorsAttn_Post_2	(-56, -60, -2)	LH_Vis_12	(-12, -72, 22)	LH_Vis_12	(-12, -72, 22)
14	RH_Default_PFCdPFCm_1	(4, 36, -14)	LH_Cont_PFCl_3	(-42, 40, 16)	LH_DorsAttn_Post_3	(-26, -70, 38)	LH_DorsAttn_Post_4	(-54, -26, 42)
15	LH_Vis_10	(-12, -70, 8)	LH_Default_PFC_1	(-34, 20, -14)	LH_SalVentAttn_ParOper_2	(-62, -26, 28)	LH_Limbic_TempPole_2	(-44, -20, -30)
16	LH_Vis_11	(-40, -84, 10)	RH_Vis_9	(8, -76, 8)	LH_Limbic_TempPole_3	(-28, 10, -34)	LH_Limbic_TempPole_3	(-28, 10, -34)
17	LH_Vis_12	(-12, -72, 22)	RH_Vis_12	(20, -90, 22)	LH_Cont_PFCl_3	(-42, 40, 16)	LH_Cont_PFCl_3	(-42, 40, 16)
18	LH_DorsAttn_Post_2	(-56, -60, -2)	RH_Cont_PFCmp_2	(8, 24, 56)	LH_Default_Par_1	(-48, -58, 18)	LH_Cont_Cing_1	(-4, -28, 28)
19	LH_Cont_Cing_2	(-4, 4, 30)	RH_Default_Par_1	(46, -70, 28)	LH_Default_PHC_1	(-26, -32, -18)	LH_Default_Temp_2	(-60, -18, -22)

NO	1st layer ROI	Coordinates	2nd layer ROI	Coordinates	3rd layer ROI	Coordinates	4th layer ROI	Coordinates
20	RH_Vis_5	(48, -72, -6)	LH_Vis_10	(-12, -70, 8)	RH_Vis_9	(8, -76, 8)	LH_Default_Par_1	(-48, -58, 18)
21	RH_Vis_11	(42, -80, 10)	LH_Vis_12	(-12, -72, 22)	RH_Vis_12	(20, -90, 22)	LH_Default_PFC_5	(-52, 22, 8)
22	RH_Vis_12	(20, -90, 22)	RH_Vis_5	(48, -72, -6)	RH_SomMot_19	(20, -30, 70)	LH_Default_PFC_7	(-8, 60, 20)
23	RH_SomMot_18	(6, -22, 68)	RH_Vis_11	(42, -80, 10)	RH_DorsAttn_Post_1	(50, -54, -16)	RH_Vis_12	(20, -90, 22)
24	RH_Default_Temp_2	(60, -12, -20)	RH_SomMot_18	(6, -22, 68)	RH_Cont_Par_2	(52, -42, 48)	RH_DorsAttn_Post_8	(26, -62, 58)
25	RH_Default_PFCdPFCm_4	(8, 58, 18)	RH_Cont_Par_1	(62, -38, 36)	RH_Cont_PFCl_5	(30, 48, 28)	RH_Cont_Par_1	(62, -38, 36)
26			RH_Cont_PFCmp_1	(8, 30, 28)	RH_Cont_PFCl_6	(40, 34, 38)	RH_Cont_PFCl_5	(30, 48, 28)
27			RH_Default_PFCv_1	(50, 28, 0)	LH_Vis_8	(-48, -70, 10)	RH_Cont_PFCmp_2	(8, 24, 56)
28			LH_Vis_3	(-46, -70, -8)	LH_Vis_10	(-12, -70, 8)	RH_Default_Par_1	(46, -70, 28)
29			LH_Vis_5	(-26, -96, -12)	LH_DorsAttn_Post_2	(-56, -60, -2)	RH_Default_PFCdPFCm_4	(8, 58, 18)
30			LH_Vis_8	(-48, -70, 10)	LH_Cont_Par_2	(-34, -62, 48)	LH_Vis_10	(-12, -70, 8)
31			LH_Default_Temp_2	(-60, -18, -22)	LH_Cont_PFCl_4	(-44, 20, 28)	LH_DorsAttn_Post_3	(-26, -70, 38)
32			LH_Default_PFC_3	(-46, 30, -8)	LH_Default_Temp_3	(-56, -6, -12)	LH_Default_Temp_4	(-58, -30, -4)
33			RH_Vis_7	(16, -46, -2)	LH_Default_PFC_4	(-12, 64, -6)	RH_Vis_6	(12, -92, -6)
34			RH_Vis_10	(22, -60, 8)	LH_Default_pCunPCC_4	(-6, -54, 42)	RH_Vis_7	(16, -46, -2)
35			RH_Default_Temp_1	(48, 12, -30)	RH_Vis_1	(38, -34, -24)	RH_DorsAttn_PrCv_1	(52, 10, 20)
36			RH_Default_PFCdPFCm_4	(8, 58, 18)	RH_Vis_7	(16, -46, -2)	RH_Cont_PFCmp_1	(8, 30, 28)
37					RH_Vis_11	(42, -80, 10)	RH_Default_Temp_1	(48, 12, -30)
38					RH_DorsAttn_PrCv_1	(52, 10, 20)	RH_Default_PFCdPFCm_2	(8, 42, 4)
39					RH_Cont_PFCl_2	(30, 58, 4)		
40					RH_Cont_PFCmp_2	(8, 24, 56)		
41					RH_Default_Par_1	(46, -70, 28)		
42					RH_Default_Temp_2	(60, -12, -20)		
43					RH_Default_PFCdPFCm_4	(8, 58, 18)		

for each layer, we took the ROIs that selected as the top salient ROIs for more than half of the times in the 10-folds (above 5 times) as the final salient ROIs. So the number of salient ROIs varied for each layer.

Table S2. The serial numbers and coordinates of salient ROIs for TD group in four hidden layers.

	TD							
NO.	1st layer		2nd layer		3rd layer		4th layer	
	ROI	Coordinates	ROI	Coordinates	ROI	Coordinates	ROI	Coordinates
1	LH_Default_PHC_1	(-26, -32, -18)	LH_Default_pCunPCC_2	(-6, -54, 28)	LH_Default_Temp_4	(-58, -30, -4)	LH_DorsAttn_PrCv_1	(-48, 6, 28)
2	RH_Cont_PFCmp_2	(8, 24, 56)	RH_Default_PFCdPFCm_5	(16, 46, 44)	LH_Default_Par_3	(-58, -54, 28)	LH_SalVentAttn_ParOper_2	(-62, -26, 28)
3	RH_Default_Par_1	(46, -70, 28)	LH_Vis_1	(-24, -54, -10)	LH_Default_Par_4	(-46, -66, 38)	LH_SalVentAttn_FrOperIns_1	(-40, -4, -4)
4	LH_SomMot_5	(-52, -22, 18)	RH_Vis_1	(38, -34, -24)	LH_Default_PFC_6	(-6, 44, 8)	LH_SalVentAttn_FrOperIns_3	(-38, 0, 10)
5	LH_DorsAttn_Post_3	(-26, -70, 38)	LH_Vis_2	(-26, -78, -14)	LH_Default_PFC_7	(-8, 60, 20)	LH_Default_Temp_2	(-60, -18, -22)
6	LH_DorsAttn_Post_7	(-16, -72, 54)	LH_Vis_5	(-26, -96, -12)	LH_Default_pCunPCC_2	(-6, -54, 28)	LH_Default_Temp_4	(-58, -30, -4)

7	LH_DorsAttn_Post_8	(-30, -60, 60)	LH_Vis_11	(-40, -84, 10)	RH_SalVentAttn_PrC_1	(50, 4, 40)	LH_Default_Par_1	(-48, -58, 18)
8	LH_Cont_Cing_1	(-4, -28, 28)	LH_Default_Temp_5	(-58, -42, 8)	RH_Limbic_OFC_1	(12, 38, -22)	LH_Default_Par_3	(-58, -54, 28)
9	LH_Default_PFC_5	(-52, 22, 8)	LH_Default_Par_3	(-58, -54, 28)	RH_Default_Temp_3	(54, -6, -10)	LH_Default_PFC_6	(-6, 44, 8)
10	RH_SomMot_7	(58, -4, 30)	LH_Default_Par_4	(-46, -66, 38)	RH_Default_Temp_5	(52, -32, 2)	LH_Default_PFC_7	(-8, 60, 20)
11	RH_SomMot_8	(10, -16, 42)	LH_Default_PFC_6	(-6, 44, 8)	LH_SalVentAttn_FrOperIns_4	(-52, 8, 10)	RH_DorsAttn_Post_1	(50, -54, -16)
12	LH_SomMot_3	(-36, -22, 16)	RH_Vis_5	(48, -72, -6)	LH_Default_Temp_2	(-60, -18, -22)	RH_DorsAttn_FEF_2	(26, 8, 58)
13	LH_SomMot_6	(-56, -8, 30)	RH_Vis_8	(30, -94, -4)	LH_Default_Temp_5	(-58, -42, 8)	RH_SalVentAttn_PrC_1	(50, 4, 40)
14	LH_DorsAttn_Post_9	(-6, -60, 56)	RH_SalVentAttn_PrC_1	(50, 4, 40)	LH_Default_Par_1	(-48, -58, 18)	RH_SalVentAttn_Med_1	(8, 10, 42)
15	RH_Vis_11	(42, -80, 10)	RH_Limbic_OFC_1	(12, 38, -22)	LH_Default_Par_2	(-38, -80, 32)	RH_Cont_PFCl_2	(30, 58, 4)
16	RH_SomMot_4	(44, -28, 18)	RH_Default_Temp_3	(54, -6, -10)	RH_Vis_1	(38, -34, -24)	RH_Default_Temp_2	(60, -12, -20)
17	RH_SomMot_6	(56, -12, 14)	LH_Vis_7	(-6, -92, -4)	RH_Cont_PFCl_2	(30, 58, 4)	RH_Default_Temp_5	(52, -32, 2)
18	RH_DorsAttn_Post_2	(52, -60, 10)	LH_Vis_9	(-22, -96, 6)	RH_Default_Temp_2	(60, -12, -20)	LH_SomMot_7	(-48, -8, 46)
19	RH_DorsAttn_Post_6	(14, -74, 52)	LH_SalVentAttn_ParOper_1	(-56, -40, 20)	RH_Default_PFCdPFCm_5	(16, 46, 44)	LH_SomMot_10	(-40, -26, 56)
20			LH_Default_Par_2	(-38, -80, 32)	LH_Vis_5	(-26, -96, -12)	LH_DorsAttn_Post_10	(-18, -54, 68)
21			RH_SomMot_18	(6, -22, 68)	LH_Vis_7	(-6, -92, -4)	LH_DorsAttn_FEF_1	(-32, -4, 54)
22			LH_Vis_4	(-10, -68, -4)	LH_Cont_Par_2	(-34, -62, 48)	LH_Default_Temp_5	(-58, -42, 8)
23			LH_Vis_6	(-14, -44, -2)	RH_Vis_5	(48, -72, -6)	LH_Default_Par_2	(-38, -80, 32)
24			LH_SalVentAttn_FrOperIns_1	(-40, -4, -4)	RH_Vis_7	(16, -46, -2)	LH_Default_Par_4	(-46, -66, 38)
25			LH_Cont_Par_2	(-34, -62, 48)	RH_Vis_8	(30, -94, -4)	LH_Default_pCunPCC_2	(-6, -54, 28)
26			LH_Default_PFC_1	(-34, 20, -14)	RH_DorsAttn_Post_1	(50, -54, -16)	RH_Vis_1	(38, -34, -24)
27			RH_Vis_4	(12, -64, -4)	RH_DorsAttn_Post_2	(52, -60, 10)	RH_DorsAttn_Post_8	(26, -62, 58)
28			RH_Vis_7	(16, -46, -2)	RH_DorsAttn_FEF_2	(26, 8, 58)	RH_DorsAttn_FEF_1	(34, -4, 52)
29			RH_Vis_10	(22, -60, 8)	RH_SalVentAttn_TempOccPar_2	(60, -38, 16)	RH_DorsAttn_PrCv_1	(52, 10, 20)
30			RH_Vis_11	(42, -80, 10)	RH_SalVentAttn_FrOperIns_1	(40, 6, -16)	RH_SalVentAttn_TempOccPar_2	(60, -38, 16)
31			RH_DorsAttn_Post_2	(52, -60, 10)	RH_SalVentAttn_FrOperIns_4	(44, 6, 4)	RH_SalVentAttn_FrOperIns_4	(44, 6, 4)
32			RH_SalVentAttn_TempOccPar_2	(60, -38, 16)	RH_Cont_Temp_1	(62, -42, -12)	RH_Limbic_OFC_1	(12, 38, -22)
33			RH_SalVentAttn_FrOperIns_4	(44, 6, 4)	RH_Cont_PFCl_5	(30, 48, 28)	RH_Cont_Par_2	(52, -42, 48)
34			RH_Default_Par_2	(54, -50, 28)	RH_Default_Par_1	(46, -70, 28)	RH_Cont_Temp_1	(62, -42, -12)
35			RH_Default_Temp_5	(52, -32, 2)	LH_Vis_1	(-24, -54, -10)	RH_Cont_PFCl_5	(30, 48, 28)
36			RH_Default_PFCdPFCm_1	(4, 36, -14)	LH_Vis_8	(-48, -70, 10)		
37					LH_Vis_11	(-40, -84, 10)		

38					LH_DorsAttn_Post_2	(-56, -60, -2)		
39					LH_DorsAttn_Post_4	(-54, -26, 42)		
40					LH_DorsAttn_PrCv_1	(-48, 6, 28)		
41					LH_SalVentAttn_FrOperIns_1	(-40, -4, -4)		
42					LH_SalVentAttn_FrOperIns_3	(-38, 0, 10)		
43					RH_Vis_11	(42, -80, 10)		
44					RH_DorsAttn_PrCv_1	(52, 10, 20)		
45					RH_SalVentAttn_Med_1	(8, 10, 42)		
46					RH_Cont_Par_2	(52, -42, 48)		
47					RH_Cont_Par_3	(38, -62, 48)		
48					RH_Default_PFCdPFCm_4	(8, 58, 18)		

for each layer, we took the ROIs that selected as the top salient ROIs for more than half of the times in the 10-folds (above 5 times) as the final salient ROIs. So the number of salient ROIs varied for each layer.

Table S3. Description of ROI's abbreviation.

ROI name	Network name	Full component name
LH_Vis	visual	visual
LH_SomMot	somatomotor	somatomotor
LH_DorsAttn_Post	dorsal attention	posterior
LH_DorsAttn_FEF	dorsal attention	frontal eye fields
LH_DorsAttn_PrCv	dorsal attention	precentral ventral
LH_SalVentAttn_ParOper	salience/ventral attention	parietal operculum
LH_SalVentAttn_TempOcc	salience/ventral attention	temporal occipital
LH_SalVentAttn_FrOperIns	salience/ventral attention	frontal operculum insula
LH_SalVentAttn_PFCl	salience/ventral attention	lateral prefrontal cortex
LH_SalVentAttn_Med	salience/ventral attention	medial
LH_Limbic_OFC	limbic	orbital frontal cortex
LH_Limbic_TempPole	limbic	temporal pole
LH_Cont_Par	control	parietal
LH_Cont_Temp	control	temporal
LH_Cont_PFCd	control	dorsal prefrontal cortex
LH_Cont_PFCl	control	lateral prefrontal cortex
LH_Cont_OFC	control	orbital frontal cortex
LH_Cont_PFCv	control	ventral prefrontal cortex
LH_Cont_pCun	control	precuneus
LH_Cont_Cing	control	cingulate
LH_Cont_PFCmp	control	medial posterior prefrontal cortex
LH_Default_Par	default	parietal
LH_Default_Temp	default	temporal
LH_Default_PFC	default	prefrontal cortex
LH_Default_pCunPCC	default	precuneus posterior cingulate cortex

LH_Default_PHC	default	parahippocampal cortex
RH_Vis	visual	visual
RH_SomMot	somatomotor	somatomotor
RH_DorsAttn_Post	dorsal attention	posterior
RH_DorsAttn_FEF	dorsal attention	frontal eye fields
RH_DorsAttn_PrCv	dorsal attention	precentral ventral
RH_SalVentAttn_TempOccPar	salience/ventral attention	temporal occipital parietal
RH_SalVentAttn_PrC	salience/ventral attention	precentral
RH_SalVentAttn_FrOperIns	salience/ventral attention	frontal operculum insula
RH_SalVentAttn_PFCv	salience/ventral attention	ventral prefrontal cortex
RH_SalVentAttn_PFCl	salience/ventral attention	lateral prefrontal cortex
RH_SalVentAttn_Med	salience/ventral attention	medial
RH_Limbic_OFC	limbic	orbital frontal cortex
RH_Limbic_TempPole	limbic	temporal pole
RH_Cont_Par	control	parietal
RH_Cont_Temp	control	temporal
RH_Cont_PFCv	control	ventral prefrontal cortex
RH_Cont_PFCl	control	lateral prefrontal cortex
RH_Cont_pCun	control	precuneus
RH_Cont_Cing	control	cingulate
RH_Cont_PFCmp	control	medial posterior prefrontal cortex
RH_Default_Par	default	parietal
RH_Default_Temp	default	temporal
RH_Default_PFCv	default	ventral prefrontal cortex
RH_Default_PFCdPFCm	default	dorsal prefrontal cortex medial prefrontal cortex
RH_Default_pCunPCC	default	precuneus posterior cingulate cortex

LH represents the left hemisphere and RH represents the right hemisphere of the brain.