

# **Supplementary Information: Reproducible comparison and interpretation of machine learning classifiers to predict autism on the ABIDE multimodal dataset**

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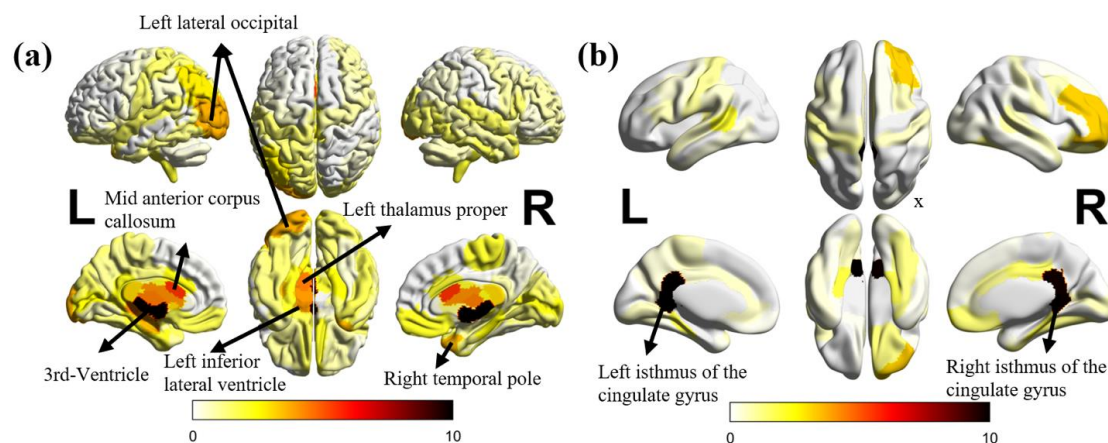
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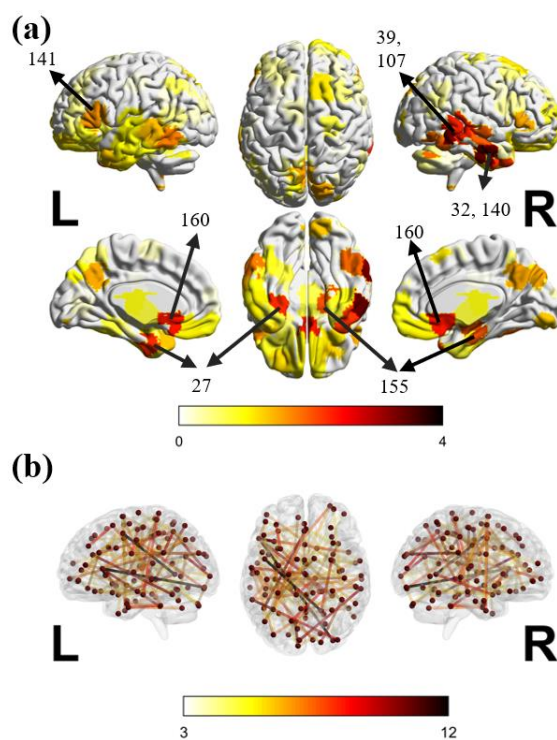
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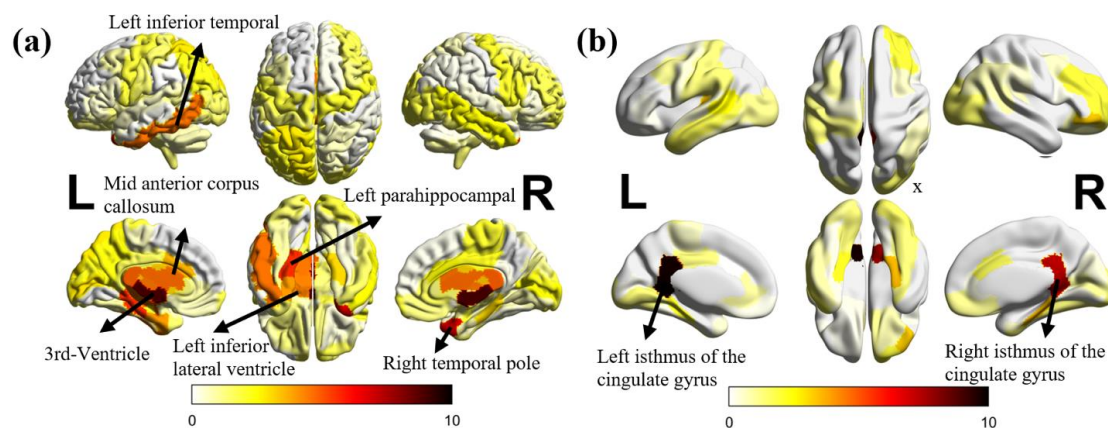
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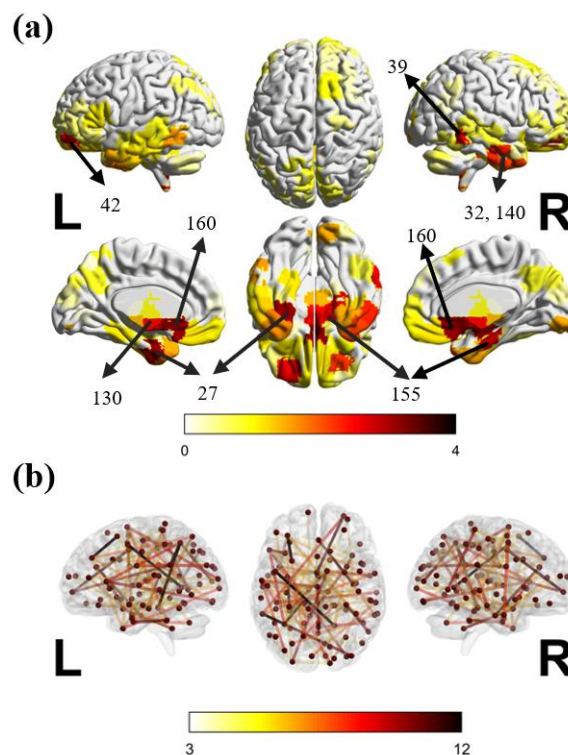
**Supplementary Fig. 1** Important structural brain features identified by GCN model contributing to the autism classification task. (a) Cortical + Subcortical areas. (b) White Matter areas.



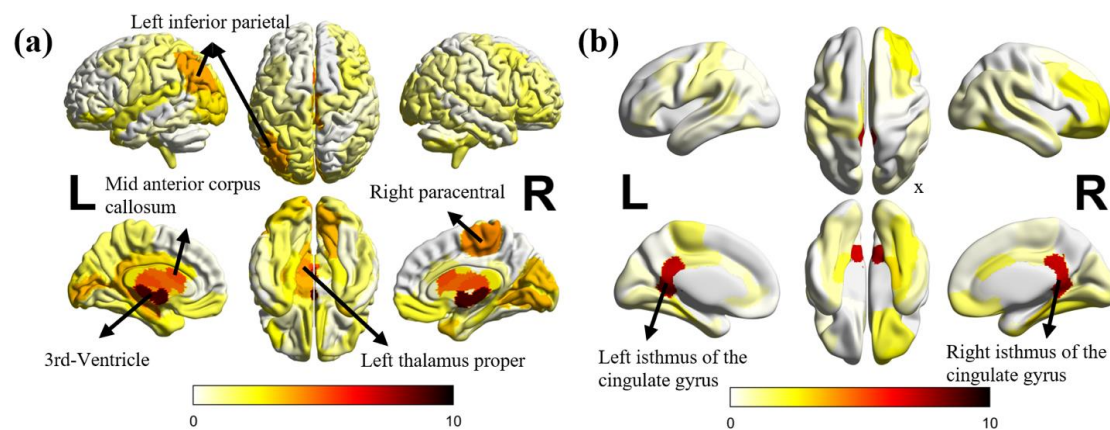
**Supplementary Fig. 2** (a) The important brain regions identified from fMRI features by GCN model, with numbers corresponding to regions in the CC200 atlas. (b) Top 100 connections.



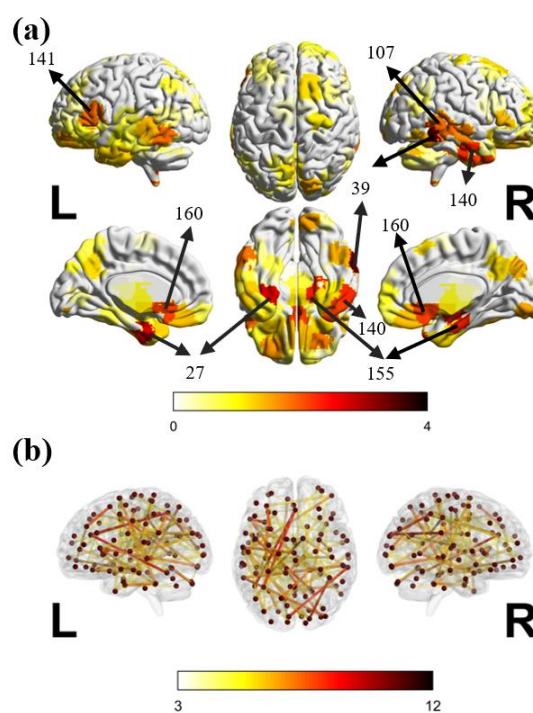
**Supplementary Fig. 3** Important structural brain features identified by AE-FCN model contributing to the autism classification task. (a) Cortical + Subcortical areas. (b) White Matter areas.



**Supplementary Fig. 4** (a) The important brain regions identified from fMRI features by AE-FCN model, with numbers corresponding to regions in the CC200 atlas. (b) Top 100 connections.



**Supplementary Fig. 5** Important structural brain features identified by EV-GCN model contributing to the autism classification task. (a) Cortical + Subcortical areas. (b) White Matter areas.



**Supplementary Fig. 6** (a) The important brain regions identified from fMRI features by EV-GCN model, with numbers corresponding to regions in the CC200 atlas. (b) Top 100 connections.

**Supplementary Table 1.** The top 100 most important brain connections

| The top 100 connections | Brain regions in CC200 atlas | The corresponding brain regions in AAL atlas                       |
|-------------------------|------------------------------|--------------------------------------------------------------------|
| 1                       | 101                          | Temporal_Inf_L: 0.58, Temporal_Mid_L: 0.38                         |
|                         | 155                          | Hippocampus_R: 0.39, ParaHippocampal_R: 0.37, None: 0.11           |
| 2                       | 53                           | Frontal_Inf_Orb_R: 0.88                                            |
|                         | 127                          | Frontal_Mid_R: 0.70, Frontal_Sup_R: 0.30                           |
| 3                       | 72                           | Temporal_Mid_L: 0.88                                               |
|                         | 104                          | Frontal_Sup_Medial_L: 0.70, Frontal_Sup_L: 0.29                    |
| 4                       | 32                           | Temporal_Pole_Mid_R: 0.59, Temporal_Inf_R: 0.35                    |
|                         | 155                          | Hippocampus_R: 0.39, ParaHippocampal_R: 0.37, None: 0.11           |
| 5                       | 56                           | Parietal_Inf_L: 0.85                                               |
|                         | 144                          | Frontal_Inf_Tri_R: 0.91                                            |
| 6                       | 19                           | Calcarine_L: 0.37, Cuneus_L: 0.36, Precuneus_L: 0.16               |
|                         | 140                          | Temporal_Mid_R: 0.65, Temporal_Inf_R: 0.33                         |
| 7                       | 155                          | Hippocampus_R: 0.39, ParaHippocampal_R: 0.37, None: 0.11           |
|                         |                              | Fusiform_R: 0.41, ParaHippocampal_R: 0.25, Temporal_Pole_Mid_R:    |
|                         | 198                          | 0.15, Temporal_Inf_R: 0.13                                         |
| 8                       |                              | Frontal_Inf_Oper_R: 0.44, Precentral_R: 0.31, Frontal_Mid_R: 0.13, |
|                         | 17                           | Frontal_Inf_Tri_R: 0.13                                            |
|                         | 20                           | Insula_L: 0.76, Frontal_Inf_Tri_L: 0.12                            |
| 9                       | 40                           | Cingulum_Ant_R: 0.44, Cingulum_Ant_L: 0.40                         |
|                         | 140                          | Temporal_Mid_R: 0.65, Temporal_Inf_R: 0.33                         |
| 10                      | 102                          | Occipital_Mid_R: 1.00                                              |
|                         | 160                          | Olfactory_L: 0.27, Olfactory_R: 0.22                               |
|                         |                              | Occipital_Inf_R: 0.55, Temporal_Inf_R: 0.16, Cerebelum_Crus1_R:    |
| 11                      | 26                           | 0.11                                                               |
|                         | 102                          | Occipital_Mid_R: 1.00                                              |
| 12                      | 94                           | Caudate_R: 0.84, Thalamus_R: 0.14                                  |
|                         | 124                          | Frontal_Mid_Orb_R: 0.61, Frontal_Sup_Orb_R: 0.28                   |
| 13                      | 11                           | Temporal_Mid_L: 0.96                                               |
|                         | 32                           | Temporal_Pole_Mid_R: 0.59, Temporal_Inf_R: 0.35                    |
| 14                      | 92                           | Hippocampus_L: 0.41, Amygdala_L: 0.29, ParaHippocampal_L: 0.15     |
|                         | 141                          | Frontal_Inf_Tri_L: 0.96                                            |
| 15                      |                              | Hippocampus_L: 0.38, Fusiform_L: 0.31, ParaHippocampal_L: 0.16,    |
|                         | 145                          | Temporal_Inf_L: 0.15                                               |
|                         |                              | ParaHippocampal_L: 0.38, Cerebelum_4_5_L: 0.34, Cerebelum_3_L:     |
| 16                      | 199                          | 0.18                                                               |
|                         | 140                          | Temporal_Mid_R: 0.65, Temporal_Inf_R: 0.33                         |
|                         | 155                          | Hippocampus_R: 0.39, ParaHippocampal_R: 0.37, None: 0.11           |
| 17                      | 39                           | Temporal_Mid_R: 0.67, Temporal_Inf_R: 0.33                         |
|                         | 155                          | Hippocampus_R: 0.39, ParaHippocampal_R: 0.37, None: 0.11           |
| 18                      | 47                           | Caudate_L: 0.45, Putamen_L: 0.39                                   |
|                         | 135                          | Caudate_R: 0.85, Putamen_R: 0.11                                   |

Supplementary Table 1

|    |     |                                                                  |
|----|-----|------------------------------------------------------------------|
|    |     | Fusiform_R: 0.32, ParaHippocampal_R: 0.23, Temporal_Inf_R: 0.23, |
| 19 | 87  | Hippocampus_R: 0.22                                              |
|    | 96  | Postcentral_L: 0.65, Precentral_L: 0.21, Parietal_Sup_L: 0.12    |
| 20 | 70  | Calcarine_L: 0.51, Lingual_L: 0.49                               |
|    | 81  | Cuneus_R: 0.51, Precuneus_R: 0.31, Occipital_Sup_R: 0.14         |
| 21 | 39  | Temporal_Mid_R: 0.67, Temporal_Inf_R: 0.33                       |
|    | 62  | Fusiform_R: 0.54, Hippocampus_R: 0.21, ParaHippocampal_R: 0.19   |
| 22 | 100 | Temporal_Inf_R: 0.66, Fusiform_R: 0.26                           |
|    | 189 | Fusiform_L: 0.51, Cerebelum_6_L: 0.29, Lingual_L: 0.17           |
| 23 | 95  | Frontal_Mid_L: 0.72, Frontal_Sup_L: 0.28                         |
|    | 147 | Precuneus_L: 0.54, Cuneus_L: 0.33                                |
| 24 | 56  | Parietal_Inf_L: 0.85                                             |
|    | 107 | Temporal_Sup_R: 0.50, Temporal_Mid_R: 0.49                       |
| 25 | 107 | Temporal_Sup_R: 0.50, Temporal_Mid_R: 0.49                       |
|    | 153 | Temporal_Sup_R: 0.64, Temporal_Mid_R: 0.33                       |
| 26 | 81  | Cuneus_R: 0.51, Precuneus_R: 0.31, Occipital_Sup_R: 0.14         |
|    | 105 | Lingual_R: 0.53, Calcarine_R: 0.31                               |
| 27 | 99  | Temporal_Mid_L: 0.60, Temporal_Inf_L: 0.40                       |
|    | 151 | Frontal_Inf_Tri_L: 0.73, Frontal_Mid_L: 0.20                     |
|    |     | Occipital_Inf_R: 0.55, Temporal_Inf_R: 0.16, Cerebelum_Crus1_R:  |
| 28 | 26  | 0.11                                                             |
|    |     | Occipital_Inf_R: 0.52, Fusiform_R: 0.15, Lingual_R: 0.14,        |
|    | 175 | Cerebelum_Crus1_R: 0.14                                          |
| 29 | 63  | Temporal_Inf_L: 0.45, Fusiform_L: 0.36, Cerebelum_Crus1_L: 0.13  |
|    | 197 | Precuneus_L: 0.92                                                |
|    |     | Hippocampus_R: 0.28, Lingual_R: 0.21, Thalamus_R: 0.20,          |
| 30 | 48  | ParaHippocampal_R: 0.15                                          |
|    |     | ParaHippocampal_L: 0.38, Cerebelum_4_5_L: 0.34, Cerebelum_3_L:   |
|    | 199 | 0.18                                                             |
| 31 | 128 | SupraMarginal_R: 0.82, Temporal_Sup_R: 0.17                      |
|    | 188 | Parietal_Sup_L: 0.61, Precuneus_L: 0.37                          |
| 32 | 40  | Cingulum_Ant_R: 0.44, Cingulum_Ant_L: 0.40                       |
|    | 72  | Temporal_Mid_L: 0.88                                             |
| 33 | 104 | Frontal_Sup_Medial_L: 0.70, Frontal_Sup_L: 0.29                  |
|    | 109 | Frontal_Med_Orb_L: 0.37, Frontal_Med_Orb_R: 0.35                 |
| 34 | 107 | Temporal_Sup_R: 0.50, Temporal_Mid_R: 0.49                       |
|    | 150 | Occipital_Mid_L: 0.54, Temporal_Mid_L: 0.46                      |
| 35 | 20  | Insula_L: 0.76, Frontal_Inf_Tri_L: 0.12                          |
|    | 144 | Frontal_Inf_Tri_R: 0.91                                          |
| 36 | 32  | Temporal_Pole_Mid_R: 0.59, Temporal_Inf_R: 0.35                  |
|    |     | Lingual_L: 0.48, Cerebelum_4_5_L: 0.21, Calcarine_L: 0.14,       |
|    | 179 | Precuneus_L: 0.12                                                |
|    |     | Fusiform_R: 0.32, ParaHippocampal_R: 0.23, Temporal_Inf_R: 0.23, |
| 37 | 87  | Hippocampus_R: 0.22                                              |

Supplementary Table 1

|    |     |                                                                 |
|----|-----|-----------------------------------------------------------------|
|    | 122 | Fusiform_L: 0.47, ParaHippocampal_L: 0.23, Hippocampus_L: 0.21  |
| 38 | 140 | Temporal_Mid_R: 0.65, Temporal_Inf_R: 0.33                      |
|    | 174 | Precuneus_L: 0.46, Precuneus_R: 0.36                            |
| 39 | 160 | Olfactory_L: 0.27, Olfactory_R: 0.22                            |
|    | 170 | Occipital_Mid_R: 0.70, Occipital_Sup_R: 0.30                    |
| 40 | 74  | Frontal_Inf_Orb_L: 0.90                                         |
|    | 92  | Hippocampus_L: 0.41, Amygdala_L: 0.29, ParaHippocampal_L: 0.15  |
| 41 | 81  | Cuneus_R: 0.51, Precuneus_R: 0.31, Occipital_Sup_R: 0.14        |
|    | 95  | Frontal_Mid_L: 0.72, Frontal_Sup_L: 0.28                        |
| 42 | 47  | Caudate_L: 0.45, Putamen_L: 0.39                                |
|    | 94  | Caudate_R: 0.84, Thalamus_R: 0.14                               |
| 43 | 42  | Frontal_Mid_Orb_L: 0.78, Frontal_Inf_Orb_L: 0.14                |
|    | 78  | Temporal_Pole_Mid_L: 0.54, Temporal_Pole_Sup_L: 0.40            |
| 44 | 141 | Frontal_Inf_Tri_L: 0.96                                         |
|    | 155 | Hippocampus_R: 0.39, ParaHippocampal_R: 0.37, None: 0.11        |
| 45 | 39  | Temporal_Mid_R: 0.67, Temporal_Inf_R: 0.33                      |
|    | 86  | Cerebelum_9_R: 0.48, None: 0.29, Vermis_10: 0.14                |
| 46 | 59  | Insula_R: 0.61, Putamen_R: 0.20, Frontal_Inf_Tri_R: 0.11        |
|    | 144 | Frontal_Inf_Tri_R: 0.91                                         |
| 47 | 75  | Frontal_Mid_R: 0.58, Frontal_Sup_R: 0.42                        |
|    |     | Temporal_Pole_Sup_L: 0.62, Frontal_Inf_Orb_L: 0.22, Insula_L:   |
|    | 196 | 0.11                                                            |
| 48 | 63  | Temporal_Inf_L: 0.45, Fusiform_L: 0.36, Cerebelum_Crus1_L: 0.13 |
|    | 136 | Parietal_Sup_L: 0.50, Precuneus_L: 0.50                         |
| 49 | 50  | Precentral_L: 0.64, Frontal_Sup_L: 0.27                         |
|    | 150 | Occipital_Mid_L: 0.54, Temporal_Mid_L: 0.46                     |
| 50 | 141 | Frontal_Inf_Tri_L: 0.96                                         |
|    |     | Hippocampus_L: 0.38, Fusiform_L: 0.31, ParaHippocampal_L: 0.16, |
|    | 145 | Temporal_Inf_L: 0.15                                            |
| 51 | 49  | Temporal_Mid_R: 0.64, Temporal_Inf_R: 0.34                      |
|    | 62  | Fusiform_R: 0.54, Hippocampus_R: 0.21, ParaHippocampal_R: 0.19  |
| 52 | 81  | Cuneus_R: 0.51, Precuneus_R: 0.31, Occipital_Sup_R: 0.14        |
|    | 89  | Calcarine_R: 0.43, Lingual_R: 0.35                              |
| 53 | 100 | Temporal_Inf_R: 0.66, Fusiform_R: 0.26                          |
|    | 102 | Occipital_Mid_R: 1.00                                           |
|    |     | Occipital_Inf_R: 0.55, Temporal_Inf_R: 0.16, Cerebelum_Crus1_R: |
| 54 | 26  | 0.11                                                            |
|    | 160 | Olfactory_L: 0.27, Olfactory_R: 0.22                            |
| 55 | 4   | Temporal_Sup_L: 0.33, Putamen_L: 0.28, Insula_L: 0.25           |
|    |     | Fusiform_R: 0.41, ParaHippocampal_R: 0.25, Temporal_Pole_Mid_R: |
|    | 198 | 0.15, Temporal_Inf_R: 0.13                                      |
| 56 | 6   | Cingulum_Mid_R: 0.60, Precuneus_R: 0.21                         |
|    | 147 | Precuneus_L: 0.54, Cuneus_L: 0.33                               |
| 57 | 63  | Temporal_Inf_L: 0.45, Fusiform_L: 0.36, Cerebelum_Crus1_L: 0.13 |

Supplementary Table 1

|    |     |                                                                     |
|----|-----|---------------------------------------------------------------------|
|    | 168 | Frontal_Mid_R: 0.96                                                 |
| 58 | 58  | Precuneus_L: 0.31, Precuneus_R: 0.28, Vermis_4_5: 0.14              |
|    | 109 | Frontal_Med_Orb_L: 0.37, Frontal_Med_Orb_R: 0.35                    |
| 59 | 76  | Cingulum_Mid_L: 0.86                                                |
|    | 107 | Temporal_Sup_R: 0.50, Temporal_Mid_R: 0.49                          |
|    |     | Rolandic_Oper_R: 0.42, Frontal_Inf_Oper_R: 0.23,                    |
| 60 | 119 | Temporal_Sup_R: 0.19                                                |
|    | 188 | Parietal_Sup_L: 0.61, Precuneus_L: 0.37                             |
| 61 | 14  | Angular_R: 0.46, Temporal_Mid_R: 0.36                               |
|    | 81  | Cuneus_R: 0.51, Precuneus_R: 0.31, Occipital_Sup_R: 0.14            |
| 62 | 11  | Temporal_Mid_L: 0.96                                                |
|    | 78  | Temporal_Pole_Mid_L: 0.54, Temporal_Pole_Sup_L: 0.40                |
|    |     | Postcentral_R: 0.33, Paracentral_Lobule_R: 0.26, Precuneus_R: 0.22, |
| 63 | 65  | Parietal_Sup_R: 0.19                                                |
|    | 96  | Postcentral_L: 0.65, Precentral_L: 0.21, Parietal_Sup_L: 0.12       |
| 64 | 57  | Frontal_Inf_Orb_L: 0.72, Frontal_Mid_Orb_L: 0.25                    |
|    | 127 | Frontal_Mid_R: 0.70, Frontal_Sup_R: 0.30                            |
| 65 | 25  | Frontal_Mid_R: 0.69, Frontal_Inf_Tri_R: 0.31                        |
|    | 183 | Frontal_Mid_L: 0.43, Frontal_Sup_L: 0.42                            |
| 66 | 39  | Temporal_Mid_R: 0.67, Temporal_Inf_R: 0.33                          |
|    | 58  | Precuneus_L: 0.31, Precuneus_R: 0.28, Vermis_4_5: 0.14              |
| 67 | 71  | Frontal_Inf_Orb_R: 0.55, Insula_R: 0.30                             |
|    |     | Insula_L: 0.34, Frontal_Inf_Orb_L: 0.29, Temporal_Pole_Sup_L:       |
|    | 112 | 0.26                                                                |
| 68 | 153 | Temporal_Sup_R: 0.64, Temporal_Mid_R: 0.33                          |
|    | 194 | None: 0.71, Vermis_3: 0.14                                          |
| 69 | 38  | Frontal_Mid_R: 0.77, Frontal_Inf_Tri_R: 0.14                        |
|    |     | Frontal_Mid_Orb_R: 0.42, Frontal_Mid_R: 0.28, Frontal_Inf_Orb_R:    |
|    | 113 | 0.25                                                                |
| 70 | 160 | Olfactory_L: 0.27, Olfactory_R: 0.22                                |
|    |     | Occipital_Inf_R: 0.52, Fusiform_R: 0.15, Lingual_R: 0.14,           |
|    | 175 | Cerebelum_Crus1_R: 0.14                                             |
| 71 | 32  | Temporal_Pole_Mid_R: 0.59, Temporal_Inf_R: 0.35                     |
|    | 97  | Occipital_Mid_L: 0.87, Occipital_Sup_L: 0.11                        |
| 72 | 144 | Frontal_Inf_Tri_R: 0.91                                             |
|    | 153 | Temporal_Sup_R: 0.64, Temporal_Mid_R: 0.33                          |
| 73 | 27  | Fusiform_L: 0.45, Temporal_Inf_L: 0.21, ParaHippocampal_L: 0.13     |
|    | 57  | Frontal_Inf_Orb_L: 0.72, Frontal_Mid_Orb_L: 0.25                    |
| 74 | 19  | Calcarine_L: 0.37, Cuneus_L: 0.36, Precuneus_L: 0.16                |
|    | 147 | Precuneus_L: 0.54, Cuneus_L: 0.33                                   |
|    |     | Frontal_Med_Orb_L: 0.27, Rectus_L: 0.23, Frontal_Med_Orb_R:         |
| 75 | 51  | 0.21, Rectus_R: 0.18                                                |
|    | 103 | Cerebelum_6_L: 0.46, Cerebelum_4_5_L: 0.32                          |
| 76 | 10  | Cerebelum_Crus1_R: 0.77, Cerebelum_6_R: 0.11                        |

Supplementary Table 1

|    |     |                                                                  |
|----|-----|------------------------------------------------------------------|
|    | 117 | Temporal_Mid_L: 0.82, Temporal_Sup_L: 0.18                       |
| 77 | 23  | Frontal_Inf_Tri_L: 0.57, Frontal_Mid_L: 0.42                     |
|    | 42  | Frontal_Mid_Orb_L: 0.78, Frontal_Inf_Orb_L: 0.14                 |
| 78 | 39  | Temporal_Mid_R: 0.67, Temporal_Inf_R: 0.33                       |
|    | 99  | Temporal_Mid_L: 0.60, Temporal_Inf_L: 0.40                       |
| 79 | 23  | Frontal_Inf_Tri_L: 0.57, Frontal_Mid_L: 0.42                     |
|    | 91  | Frontal_Sup_Medial_L: 0.56, Frontal_Sup_Medial_R: 0.34           |
| 80 | 39  | Temporal_Mid_R: 0.67, Temporal_Inf_R: 0.33                       |
|    | 97  | Occipital_Mid_L: 0.87, Occipital_Sup_L: 0.11                     |
| 81 | 70  | Calcarine_L: 0.51, Lingual_L: 0.49                               |
|    | 164 | Frontal_Inf_Tri_R: 0.62, Frontal_Inf_Oper_R: 0.36                |
| 82 | 42  | Frontal_Mid_Orb_L: 0.78, Frontal_Inf_Orb_L: 0.14                 |
|    | 43  | Temporal_Inf_L: 0.50, Temporal_Pole_Mid_L: 0.26, None: 0.16      |
| 83 | 18  | Thalamus_R: 0.99                                                 |
|    | 107 | Temporal_Sup_R: 0.50, Temporal_Mid_R: 0.49                       |
| 84 | 20  | Insula_L: 0.76, Frontal_Inf_Tri_L: 0.12                          |
|    | 39  | Temporal_Mid_R: 0.67, Temporal_Inf_R: 0.33                       |
| 85 | 155 | Hippocampus_R: 0.39, ParaHippocampal_R: 0.37, None: 0.11         |
|    | 193 | Frontal_Sup_R: 0.50, Frontal_Sup_Medial_R: 0.42                  |
| 86 | 133 | Frontal_Sup_Medial_L: 0.62, Frontal_Sup_L: 0.36                  |
|    | 155 | Hippocampus_R: 0.39, ParaHippocampal_R: 0.37, None: 0.11         |
| 87 | 54  | Cuneus_L: 0.62, Occipital_Sup_L: 0.20                            |
|    |     | Temporal_Sup_L: 0.34, Temporal_Mid_L: 0.26,                      |
|    | 129 | Temporal_Pole_Sup_L: 0.17                                        |
|    |     | Fusiform_R: 0.32, ParaHippocampal_R: 0.23, Temporal_Inf_R: 0.23, |
| 88 | 87  | Hippocampus_R: 0.22                                              |
|    |     | Lingual_L: 0.48, Cerebelum_4_5_L: 0.21, Calcarine_L: 0.14,       |
|    | 179 | Precuneus_L: 0.12                                                |
|    |     | Temporal_Sup_L: 0.34, Temporal_Mid_L: 0.26,                      |
| 89 | 129 | Temporal_Pole_Sup_L: 0.17                                        |
|    | 140 | Temporal_Mid_R: 0.65, Temporal_Inf_R: 0.33                       |
| 90 | 118 | Cerebelum_6_R: 0.70, Cerebelum_4_5_R: 0.18                       |
|    | 166 | Angular_R: 0.85, Occipital_Mid_R: 0.13                           |
| 91 | 75  | Frontal_Mid_R: 0.58, Frontal_Sup_R: 0.42                         |
|    | 106 | Frontal_Mid_R: 0.72, Frontal_Sup_R: 0.28                         |
| 92 | 20  | Insula_L: 0.76, Frontal_Inf_Tri_L: 0.12                          |
|    | 115 | Precentral_R: 0.56, Frontal_Mid_R: 0.44                          |
| 93 | 6   | Cingulum_Mid_R: 0.60, Precuneus_R: 0.21                          |
|    | 81  | Cuneus_R: 0.51, Precuneus_R: 0.31, Occipital_Sup_R: 0.14         |
| 94 | 11  | Temporal_Mid_L: 0.96                                             |
|    |     | Frontal_Med_Orb_L: 0.27, Rectus_L: 0.23, Frontal_Med_Orb_R:      |
|    | 51  | 0.21, Rectus_R: 0.18                                             |
| 95 | 27  | Fusiform_L: 0.45, Temporal_Inf_L: 0.21, ParaHippocampal_L: 0.13  |

Supplementary Table 1

|     |     |                                                                                             |
|-----|-----|---------------------------------------------------------------------------------------------|
|     | 114 | Occipital_Mid_L: 0.32, Occipital_Sup_L: 0.27, Parietal_Sup_L: 0.26,<br>Parietal_Inf_L: 0.15 |
| 96  | 114 | Occipital_Mid_L: 0.32, Occipital_Sup_L: 0.27, Parietal_Sup_L: 0.26,<br>Parietal_Inf_L: 0.15 |
|     | 160 | Olfactory_L: 0.27, Olfactory_R: 0.22                                                        |
| 97  | 32  | Temporal_Pole_Mid_R: 0.59, Temporal_Inf_R: 0.35                                             |
|     | 178 | Putamen_R: 0.69, Pallidum_R: 0.21                                                           |
| 98  | 140 | Temporal_Mid_R: 0.65, Temporal_Inf_R: 0.33                                                  |
|     | 178 | Putamen_R: 0.69, Pallidum_R: 0.21                                                           |
| 99  | 57  | Frontal_Inf_Orb_L: 0.72, Frontal_Mid_Orb_L: 0.25                                            |
|     | 122 | Fusiform_L: 0.47, ParaHippocampal_L: 0.23, Hippocampus_L: 0.21                              |
| 100 | 32  | Temporal_Pole_Mid_R: 0.59, Temporal_Inf_R: 0.35                                             |
|     | 106 | Frontal_Mid_R: 0.72, Frontal_Sup_R: 0.28                                                    |

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**Supplementary Table 2.** The top 100 most important structural volumetric features

| The top 100 structural features | Desikan-Killiany atlas regions | feature names        |
|---------------------------------|--------------------------------|----------------------|
| 1                               | 3rd-Ventricle                  | Volume               |
| 2                               | wm-lh-isthmuscingulate         | Intensity normMin    |
| 3                               | Left-Inf-Lat-Vent              | Volume               |
| 4                               | 3rd-Ventricle                  | Number of Voxels     |
| 5                               | wm-rh-isthmuscingulate         | Intensity normRange  |
| 6                               | ctx-rh-temporalpole            | CurvInd              |
| 7                               | wm-rh-isthmuscingulate         | Intensity normMin    |
| 8                               | CC_Mid_Anterior                | Intensity normMin    |
| 9                               | wm-lh-isthmuscingulate         | Intensity normRange  |
| 10                              | wm-lh-isthmuscingulate         | Intensity normStdDev |
| 11                              | Left-VentralDC                 | Volume               |
| 12                              | Left-Thalamus                  | Intensity normMax    |
| 13                              | Left-Inf-Lat-Vent              | Number of Voxels     |
| 14                              | 4th-Ventricle                  | Intensity normStdDev |
| 15                              | wm-rh-parahippocampal          | Volume               |
| 16                              | CSF                            | Volume               |
| 17                              | ctx-rh-paracentral             | ThickAvg             |
| 18                              | Left-VentralDC                 | Number of Voxels     |
| 19                              | Left-choroid-plexus            | Intensity normMean   |
| 20                              | non-WM-hypointensities         | Intensity normStdDev |
| 21                              | Left-Lateral-Ventricle         | Intensity normStdDev |
| 22                              | ctx-lh-pericalcarine           | MeanCurv             |
| 23                              | CC_Mid_Anterior                | Intensity normRange  |
| 24                              | ctx-rh-parahippocampal         | NumVert              |
| 25                              | Left-Caudate                   | Intensity normMax    |
| 26                              | CSF                            | Number of Voxels     |
| 27                              | CC_Posterior                   | Intensity normMin    |
| 28                              | ctx-rh-pericalcarine           | MeanCurv             |
| 29                              | Left-Pallidum                  | Intensity normMax    |
| 30                              | ctx-lh-isthmuscingulate        | MeanCurv             |
| 31                              | ctx-lh-cuneus                  | GausCurv             |
| 32                              | wm-rh-parahippocampal          | Number of Voxels     |
| 33                              | Left-Hippocampus               | Intensity normStdDev |
| 34                              | ctx-lh-inferiorparietal        | FoldInd              |
| 35                              | ctx-lh-entorhinal              | FoldInd              |
| 36                              | ctx-lh-pericalcarine           | GausCurv             |
| 37                              | ctx-rh-parahippocampal         | GrayVol              |
| 38                              | CC_Central                     | Volume               |
| 39                              | ctx-lh-pericalcarine           | CurvInd              |
| 40                              | ctx-rh-pericalcarine           | ThickStd             |
| 41                              | wm-rh-rostralmiddlefrontal     | Intensity normMin    |

Supplementary Table 1

|    |                                |                      |
|----|--------------------------------|----------------------|
| 42 | ctx-lh-superiortemporal        | ThickAvg             |
| 43 | ctx-lh-caudalanteriorcingulate | FoldInd              |
| 44 | ctx-lh-superiorparietal        | CurvInd              |
| 45 | ctx-lh-parahippocampal         | NumVert              |
| 46 | ctx-rh-temporalpole            | FoldInd              |
| 47 | ctx-lh-entorhinal              | ThickStd             |
| 48 | ctx-lh-temporalpole            | ThickStd             |
| 49 | ctx-lh-lateraloccipital        | ThickAvg             |
| 50 | Left-Lateral-Ventricle         | Volume               |
| 51 | ctx-lh-parahippocampal         | CurvInd              |
| 52 | CC_Mid_Posterior               | Intensity normMin    |
| 53 | wm-lh-isthmuscingulate         | Number of Voxels     |
| 54 | wm-lh-parahippocampal          | Volume               |
| 55 | Left-Lateral-Ventricle         | Number of Voxels     |
| 56 | ctx-lh-entorhinal              | CurvInd              |
| 57 | ctx-rh-caudalanteriorcingulate | GausCurv             |
| 58 | WM-hypointensities             | Intensity normMean   |
| 59 | Right-Inf-Lat-Vent             | Intensity normStdDev |
| 60 | ctx-lh-posteriorcingulate      | MeanCurv             |
| 61 | ctx-lh-parahippocampal         | SurfArea             |
| 62 | wm-lh-bankssts                 | Volume               |
| 63 | Left-Hippocampus               | Intensity normMax    |
| 64 | wm-lh-bankssts                 | Intensity normStdDev |
| 65 | Right-UnsegmentedWhiteMatter   | Intensity normStdDev |
| 66 | ctx-rh-parahippocampal         | SurfArea             |
| 67 | wm-rh-rostralmiddlefrontal     | Intensity normRange  |
| 68 | CC_Central                     | Number of Voxels     |
| 69 | ctx-rh-parsopercularis         | MeanCurv             |
| 70 | ctx-lh-precuneus               | MeanCurv             |
| 71 | CC_Mid_Anterior                | Intensity normStdDev |
| 72 | ctx-rh-medialorbitofrontal     | ThickStd             |
| 73 | ctx-lh-precuneus               | GausCurv             |
| 74 | wm-rh-lateraloccipital         | Intensity normMax    |
| 75 | ctx-lh-parahippocampal         | ThickStd             |
| 76 | wm-lh-parahippocampal          | Number of Voxels     |
| 77 | Right-Lateral-Ventricle        | Intensity normStdDev |
| 78 | ctx-rh-medialorbitofrontal     | MeanCurv             |
| 79 | Left-Amygdala                  | Volume               |
| 80 | ctx-lh-parahippocampal         | GrayVol              |
| 81 | Right-UnsegmentedWhiteMatter   | Intensity normMean   |
| 82 | wm-rh-entorhinal               | Intensity normStdDev |
| 83 | ctx-rh-pericalcarine           | FoldInd              |
| 84 | wm-lh-isthmuscingulate         | Volume               |

Supplementary Table 1

|     |                           |                      |
|-----|---------------------------|----------------------|
| 85  | wm-lh-transversetemporal  | Number of Voxels     |
| 86  | Left-Hippocampus          | Intensity normRange  |
| 87  | ctx-lh-paracentral        | NumVert              |
| 88  | ctx-lh-precuneus          | CurvInd              |
| 89  | Brain-Stem                | Intensity normStdDev |
| 90  | ctx-rh-entorhinal         | ThickStd             |
| 91  | ctx-rh-inferiortemporal   | CurvInd              |
| 92  | ctx-rh-lateraloccipital   | ThickAvg             |
| 93  | ctx-rh-cuneus             | GrayVol              |
| 94  | ctx-rh-frontalpole        | ThickAvg             |
| 95  | ctx-rh-superiortemporal   | GrayVol              |
| 96  | ctx-lh-inferiorparietal   | CurvInd              |
| 97  | ctx-lh-transversetemporal | GrayVol              |
| 98  | wm-lh-middletemporal      | Intensity normMax    |
| 99  | wm-lh-bankssts            | Number of Voxels     |
| 100 | ctx-lh-bankssts           | MeanCurv             |

**Supplementary Table 3.** Experiment results of the SVM model with a ‘linear’ kernel using six different feature sets

| SVM ‘linear’          | No ensemble |        |       | Max voting |       |
|-----------------------|-------------|--------|-------|------------|-------|
|                       | Validation  | Test   | AUC   | Test       | AUC   |
| sMRI                  | 62.64%      | 59.77% | 0.618 | 62.53%     | 0.66  |
| sMRI+non-imaging      | 64.02%      | 61.15% | 0.638 | 63.91%     | 0.679 |
| fMRI                  | 68.05%      | 66.32% | 0.711 | 68.74%     | 0.74  |
| fMRI+non-imaging      | 68.05%      | 66.09% | 0.712 | 68.97%     | 0.742 |
| sMRI+fMRI             | 69.66%      | 66.55% | 0.724 | 68.62%     | 0.756 |
| sMRI+fMRI+non-imaging | 69.54%      | 66.67% | 0.725 | 69.31%     | 0.757 |