

Table S1. The features and brain areas/cortical structures that show significant differences among the typically developing controls (TDC), attention-deficit/hyperactivity disorder (ADHD) combined type (ADHD-C), and ADHD inattentive type (ADHD-I) groups.

Feature category	Brain area number	Brain area	Feature name	Bonferroni-corrected ANOVA P values	P values in multiple comparison test		
					TDC vs. ADHD-C	TDC vs. ADHD-I	ADHD-C vs. ADHD-I
Surface values	DK-71	Insula	cortical thickness	4.76E-02	7.01E-07	P > 0.05	P > 0.05
Radiomics features	AAL-95	Cerebellum_3_L	IntensityHistogram-20Percentile	6.46E-03	1.60E-07	P > 0.05	P > 0.05
Radiomics features	AAL-95	Cerebellum_3_L	IntensityHistogram-25Percentile	8.02E-03	2.01E-07	P > 0.05	P > 0.05
Radiomics features	AAL-95	Cerebellum_3_L	IntensityHistogram-MedianAbsoluteDeviation	1.06E-02	2.65E-07	P > 0.05	P > 0.05
Radiomics features	AAL-95	Cerebellum_3_L	IntensityHistogram-0.25Quantile	3.75E-02	9.92E-07	P > 0.05	P > 0.05
Radiomics features	AAL-91	Cerebellum_Crus1_L	IntensityDirect-Energy	2.05E-02	4.28E-07	P > 0.05	2.63E-02
Radiomics features	AAL-87	Temporal_Pole_Mid_L	IntensityDirect-LocalEntropyMax	4.72E-03	1.06E-07	P > 0.05	3.44E-02
Radiomics features	AAL-85	Temporal_Mid_L	IntensityHistogram-15Percentile	7.65E-03	1.96E-07	P > 0.05	P > 0.05
Radiomics features	AAL-85	Temporal_Mid_L	IntensityDirect-20Percentile	7.85E-03	1.99E-07	P > 0.05	P > 0.05
Radiomics features	AAL-82	Temporal_Sup_R	IntensityHistogram-30Percentile	5.79E-03	1.45E-07	P > 0.05	P > 0.05
Radiomics features	AAL-82	Temporal_Sup_R	IntensityDirect-45Percentile	9.19E-03	2.35E-07	P > 0.05	P > 0.05
Radiomics features	AAL-82	Temporal_Sup_R	IntensityDirect-40Percentile	2.04E-02	4.98E-07	P > 0.05	P > 0.05
Radiomics features	AAL-81	Temporal_Sup_L	IntensityDirect-10Percentile	3.20E-04	3.31E-09	3.34E-02	1.73E-02
Radiomics features	AAL-81	Temporal_Sup_L	IntensityHistogram-5Percentile	8.86E-03	2.29E-07	P > 0.05	P > 0.05
Radiomics features	AAL-81	Temporal_Sup_L	IntensityDirect-15Percentile	3.23E-02	7.58E-07	P > 0.05	P > 0.05
Radiomics features	AAL-81	Temporal_Sup_L	IntensityHistogram-10Percentile	3.28E-02	7.60E-07	P > 0.05	P > 0.05
Radiomics features	AAL-81	Temporal_Sup_L	IntensityHistogram-15Percentile	3.14E-02	8.98E-07	P > 0.05	P > 0.05
Radiomics features	AAL-81	Temporal_Sup_L	IntensityDirect-20Percentile	4.16E-02	9.70E-07	P > 0.05	P > 0.05
Radiomics features	AAL-80	Heschl_R	IntensityDirect-MedianAbsoluteDeviation	9.87E-03	2.21E-07	P > 0.05	2.73E-03
Radiomics features	AAL-80	Heschl_R	IntensityDirect-40Percentile	2.88E-03	5.88E-08	P > 0.05	2.78E-03
Radiomics features	AAL-80	Heschl_R	IntensityDirect-25Percentile	2.04E-02	4.54E-07	P > 0.05	4.11E-03
Radiomics features	AAL-80	Heschl_R	IntensityDirect-0.25Quantile	4.41E-02	1.06E-06	P > 0.05	4.19E-03
Radiomics features	AAL-80	Heschl_R	IntensityDirect-EnergyNorm	1.07E-02	2.22E-07	P > 0.05	4.71E-03
Radiomics features	AAL-80	Heschl_R	IntensityDirect-RootMeanSquare	4.03E-02	9.02E-07	P > 0.05	5.76E-03
Radiomics features	AAL-80	Heschl_R	IntensityHistogram-5Percentile	4.03E-02	9.02E-07	P > 0.05	5.76E-03
Radiomics features	AAL-80	Heschl_R	IntensityDirect-10Percentile	1.68E-02	3.61E-07	P > 0.05	3.25E-02
Radiomics features	AAL-80	Heschl_R	IntensityDirect-Skewness	1.68E-02	3.61E-07	P > 0.05	3.25E-02
Radiomics features	AAL-80	Heschl_R	IntensityHistogram-10Percentile	4.81E-03	1.07E-07	P > 0.05	3.33E-02
Radiomics features	AAL-80	Heschl_R	IntensityHistogram-30Percentile	2.41E-03	5.97E-08	4.40E-02	4.36E-02
Radiomics features	AAL-80	Heschl_R	IntensityHistogram-20Percentile	1.94E-02	4.40E-07	P > 0.05	4.42E-02
Radiomics features	AAL-80	Heschl_R	IntensityDirect-20Percentile	3.59E-02	8.12E-07	P > 0.05	4.61E-02
Radiomics features	AAL-80	Heschl_R	IntensityHistogram-0.25Quantile	3.56E-03	8.87E-08	4.66E-02	4.78E-02
Radiomics features	AAL-80	Heschl_R	IntensityHistogram-25Percentile	2.42E-03	2.05E-07	3.07E-03	P > 0.05
Radiomics features	AAL-80	Heschl_R	IntensityDirect-30Percentile	3.12E-03	2.05E-07	5.06E-03	P > 0.05
Radiomics features	AAL-80	Heschl_R	IntensityDirect-35Percentile	3.97E-03	2.55E-07	5.62E-03	P > 0.05

Radiomics features	AAL-80	Heschl_R	IntensityHistogram-15Percentile	8.86E-03	2.29E-07	P > 0.05	P > 0.05
Radiomics features	AAL-80	Heschl_R	IntensityDirect-15Percentile	2.91E-02	6.78E-07	P > 0.05	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityDirect-Variance	9.28E-03	5.73E-05	2.29E-05	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityHistogram- 5Percentile	2.59E-03	4.22E-07	1.11E-03	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityDirect-MeanAbsoluteDeviation	1.73E-03	2.67E-08	1.22E-02	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityHistogram-Skewness	9.57E-03	4.22E-07	1.42E-02	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityHistogram-0.025Quantile	2.39E-02	1.05E-06	1.78E-02	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityDirect-MedianAbsoluteDeviation	3.31E-03	1.10E-07	2.08E-02	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityDirect-10Percentile	2.54E-02	9.37E-07	2.63E-02	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityDirect-15Percentile	2.30E-03	6.45E-08	3.03E-02	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityDirect-GlobalStd	4.00E-02	7.73E-07	3.07E-02	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityDirect-InterQuartileRange	4.51E-02	8.90E-07	3.10E-02	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityDirect-20Percentile	4.02E-03	1.16E-07	3.14E-02	P > 0.05
Radiomics features	AAL-79	Heschl_L	IntensityDirect- 5Percentile	4.45E-03	1.12E-07	4.74E-02	P > 0.05
Radiomics features	AAL-63	SupraMarginal_L	IntensityDirect- 15Percentile	3.04E-03	1.23E-07	P > 0.05	2.21E-04
Radiomics features	AAL-63	SupraMarginal_L	IntensityDirect-MedianAbsoluteDeviation	9.35E-03	1.97E-07	P > 0.05	2.45E-04
Radiomics features	AAL-63	SupraMarginal_L	IntensityDirect-InterQuartileRange	1.93E-02	5.89E-07	P > 0.05	1.15E-03
Radiomics features	AAL-63	SupraMarginal_L	IntensityHistogram-10Percentile	5.99E-03	5.47E-08	P > 0.05	8.45E-03
Radiomics features	AAL-63	SupraMarginal_L	IntensityDirect-20Percentile	4.42E-02	5.12E-07	P > 0.05	1.38E-02
Radiomics features	AAL-63	SupraMarginal_L	IntensityHistogram-15Percentile	7.01E-03	6.70E-08	P > 0.05	1.45E-02
Radiomics features	AAL-63	SupraMarginal_L	IntensityDirect-25Percentile	7.01E-03	6.70E-08	P > 0.05	1.45E-02
Radiomics features	AAL-63	SupraMarginal_L	IntensityDirect-30Percentile	2.67E-02	5.52E-07	P > 0.05	2.42E-02
Radiomics features	AAL-63	SupraMarginal_L	IntensityDirect- 0.25Quantile	2.42E-02	7.05E-07	4.56E-02	P > 0.05
Radiomics features	AAL-63	SupraMarginal_L	IntensityHistogram-20Percentile	3.88E-02	1.14E-06	4.98E-02	P > 0.05
Radiomics features	AAL-39	ParaHippocampal_L	IntensityDirect-LocalEntropyMedian	4.07E-03	8.00E-08	P > 0.05	4.64E-03
Radiomics features	AAL-32	Cingulum_Ant_R	IntensityHistogram-40Percentile	1.26E-02	7.01E-07	P > 0.05	2.22E-04
Radiomics features	AAL-32	Cingulum_Ant_R	IntensityHistogram-30Percentile	1.34E-02	5.05E-07	P > 0.05	5.44E-04
Radiomics features	AAL-32	Cingulum_Ant_R	IntensityDirect-RootMeanSquare	4.06E-02	1.02E-06	P > 0.05	3.25E-03
Radiomics features	AAL-32	Cingulum_Ant_R	IntensityDirect-75Percentile	7.39E-03	1.56E-07	P > 0.05	3.39E-03
Radiomics features	AAL-32	Cingulum_Ant_R	IntensityDirect-GlobalMean	3.83E-04	7.74E-09	P > 0.05	3.84E-03
Radiomics features	AAL-32	Cingulum_Ant_R	IntensityDirect- 0.75Quantile	3.97E-04	8.01E-09	P > 0.05	4.56E-03
Radiomics features	AAL-32	Cingulum_Ant_R	IntensityDirect-EnergyNorm	1.91E-04	2.09E-09	P > 0.05	7.52E-03
Radiomics features	AAL-30	Insula_R	IntensityHistogram- 5Percentile	5.30E-03	1.14E-07	P > 0.05	1.53E-04
Radiomics features	AAL-30	Insula_R	IntensityHistogram-10Percentile	6.09E-03	1.32E-07	P > 0.05	1.67E-04
Radiomics features	AAL-30	Insula_R	IntensityDirect-LocalEntropyMean	3.80E-02	1.17E-06	P > 0.05	2.99E-04
Radiomics features	AAL-30	Insula_R	IntensityDirect-GlobalUniformity	4.13E-02	1.09E-06	P > 0.05	4.41E-04
Radiomics features	AAL-30	Insula_R	IntensityDirect-45Percentile	1.02E-02	2.97E-07	P > 0.05	9.59E-04
Radiomics features	AAL-30	Insula_R	IntensityDirect-55Percentile	1.02E-02	2.97E-07	P > 0.05	9.59E-04
Radiomics features	AAL-30	Insula_R	IntensityDirect-30Percentile	1.41E-02	1.86E-07	P > 0.05	1.32E-03
Radiomics features	AAL-30	Insula_R	IntensityDirect-25Percentile	3.60E-03	3.59E-08	P > 0.05	1.34E-03

Radiomics features	AAL-30	Insula_R	IntensityDirect-50Percentile	4.04E-02	1.32E-06	P > 0.05	1.34E-03
Radiomics features	AAL-30	Insula_R	IntensityHistogram-Kurtosis	2.88E-03	5.88E-08	P > 0.05	2.78E-03
Radiomics features	AAL-30	Insula_R	IntensityDirect-40Percentile	1.09E-02	1.16E-07	P > 0.05	2.91E-03
Radiomics features	AAL-30	Insula_R	IntensityDirect-0.025Quantile	1.07E-02	2.28E-07	P > 0.05	3.79E-03
Radiomics features	AAL-30	Insula_R	IntensityHistogram-50Percentile	9.50E-03	1.95E-07	P > 0.05	4.83E-03
Radiomics features	AAL-30	Insula_R	IntensityDirect-35Percentile	2.69E-03	2.26E-08	P > 0.05	5.00E-03
Radiomics features	AAL-30	Insula_R	IntensityHistogram-Skewness	1.19E-02	2.42E-07	P > 0.05	5.88E-03
Radiomics features	AAL-30	Insula_R	IntensityHistogram-15Percentile	1.59E-02	3.28E-07	P > 0.05	6.49E-03
Radiomics features	AAL-30	Insula_R	IntensityDirect-GlobalMedian	2.06E-02	2.17E-07	P > 0.05	1.02E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-EnergyNorm	3.81E-02	4.36E-07	P > 0.05	1.04E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-GlobalEntropy	3.81E-02	4.36E-07	P > 0.05	1.04E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-GlobalStd	4.46E-02	5.21E-07	P > 0.05	1.05E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram-45Percentile	2.20E-02	4.44E-07	P > 0.05	1.06E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-GlobalMean	2.71E-02	2.96E-07	P > 0.05	1.18E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect- 0.25Quantile	9.18E-03	1.80E-07	P > 0.05	1.20E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram-35Percentile	9.18E-03	1.80E-07	P > 0.05	1.20E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-RootMeanSquare	2.88E-03	5.67E-08	P > 0.05	1.35E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram-20Percentile	1.41E-02	2.81E-07	P > 0.05	1.54E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect- 5Percentile	3.37E-02	6.87E-07	P > 0.05	1.62E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-10Percentile	3.37E-02	6.87E-07	P > 0.05	1.62E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram-40Percentile	4.72E-02	9.75E-07	P > 0.05	1.68E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-LocalEntropyStd	1.70E-02	3.46E-07	P > 0.05	2.03E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect- MeanAbsoluteDeviation	2.65E-02	5.41E-07	P > 0.05	2.07E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram-25Percentile	2.26E-02	4.64E-07	P > 0.05	2.29E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-15Percentile	2.68E-02	5.53E-07	P > 0.05	2.34E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-20Percentile	4.19E-02	8.71E-07	P > 0.05	2.38E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect-Variance	4.46E-03	9.46E-08	P > 0.05	2.57E-02
Radiomics features	AAL-30	Insula_R	IntensityDirect- 0.5Quantile	2.37E-03	5.17E-08	P > 0.05	2.65E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram-60Percentile	9.48E-03	2.00E-07	P > 0.05	2.75E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram-0.025Quantile	8.29E-03	1.81E-07	P > 0.05	3.31E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram- 0.5Quantile	8.29E-03	1.81E-07	P > 0.05	3.31E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram-55Percentile	4.29E-03	1.05E-07	P > 0.05	4.71E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram-30Percentile	4.92E-02	1.12E-06	P > 0.05	4.86E-02
Radiomics features	AAL-30	Insula_R	IntensityHistogram- 0.25Quantile	2.90E-02	6.67E-07	P > 0.05	4.89E-02
Radiomics features	AAL-29	Insula_L	IntensityDirect-LocalEntropyStd	4.79E-02	1.17E-06	P > 0.05	5.84E-04
Radiomics features	AAL-29	Insula_L	IntensityDirect- MeanAbsoluteDeviation	4.79E-02	1.08E-06	P > 0.05	6.94E-04
Radiomics features	AAL-29	Insula_L	IntensityHistogram-Skewness	1.29E-02	2.70E-07	P > 0.05	4.93E-03
Radiomics features	AAL-29	Insula_L	IntensityDirect-0.025Quantile	9.48E-03	1.87E-07	P > 0.05	7.75E-03
Radiomics features	AAL-29	Insula_L	IntensityDirect-LocalEntropyMean	2.46E-02	2.65E-07	P > 0.05	1.12E-02
Radiomics features	AAL-29	Insula_L	IntensityDirect-Variance	3.41E-02	3.83E-07	P > 0.05	1.36E-02
Radiomics features	AAL-29	Insula_L	IntensityDirect-GlobalStd	2.81E-02	5.71E-07	P > 0.05	1.81E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityDirect- 0.25Quantile	2.81E-02	5.71E-07	P > 0.05	1.81E-02

Radiomics features	AAL-18	Rolandic_Oper_R	IntensityDirect-35Percentile	1.13E-02	2.28E-07	P > 0.05	1.88E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityDirect-40Percentile	1.77E-02	3.59E-07	P > 0.05	1.98E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityHistogram-20Percentile	4.76E-02	9.84E-07	P > 0.05	2.03E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityDirect-30Percentile	6.07E-03	1.24E-07	P > 0.05	2.09E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityHistogram-15Percentile	4.92E-02	1.03E-06	P > 0.05	2.47E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityDirect-25Percentile	5.64E-03	1.18E-07	P > 0.05	2.50E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityHistogram-25Percentile	3.36E-03	7.53E-08	P > 0.05	3.19E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityDirect-InterQuartileRange	9.32E-03	2.03E-07	P > 0.05	3.27E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityHistogram- 0.25Quantile	9.32E-03	2.03E-07	P > 0.05	3.27E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityDirect-EnergyNorm	6.16E-03	1.49E-07	P > 0.05	4.79E-02
Radiomics features	AAL-18	Rolandic_Oper_R	IntensityDirect-RootMeanSquare	1.04E-02	2.48E-07	P > 0.05	4.88E-02
Radiomics features	AAL-17	Rolandic_Oper_L	IntensityDirect-InterQuartileRange	1.60E-02	3.27E-07	P > 0.05	2.17E-02
Radiomics features	AAL-17	Rolandic_Oper_L	IntensityDirect-MedianAbsoluteDeviation	2.05E-02	4.28E-07	P > 0.05	2.63E-02
Radiomics features	AAL-17	Rolandic_Oper_L	IntensityDirect- 0.25Quantile	2.05E-02	4.28E-07	P > 0.05	2.63E-02
Radiomics features	AAL-17	Rolandic_Oper_L	IntensityDirect-15Percentile	3.86E-02	8.06E-07	P > 0.05	2.64E-02
Radiomics features	AAL-17	Rolandic_Oper_L	IntensityDirect-20Percentile	4.33E-03	9.50E-08	P > 0.05	3.05E-02
Radiomics features	AAL-17	Rolandic_Oper_L	IntensityHistogram-10Percentile	4.81E-03	1.07E-07	P > 0.05	3.33E-02
Radiomics features	AAL-17	Rolandic_Oper_L	IntensityDirect-25Percentile	1.08E-02	2.53E-07	P > 0.05	4.52E-02
Radiomics features	AAL-17	Rolandic_Oper_L	IntensityHistogram-15Percentile	7.85E-03	1.88E-07	P > 0.05	4.75E-02
Radiomics features	AAL-12	Frontal_Inf_Oper_R	IntensityHistogram-35Percentile	1.03E-02	2.11E-07	P > 0.05	2.19E-02
Radiomics features	AAL-12	Frontal_Inf_Oper_R	IntensityHistogram-30Percentile	6.48E-03	1.38E-07	P > 0.05	2.77E-02
Radiomics features	AAL-106	Cerebelum_9_R	GrayLevelRunLengthMatrix-90GrayLevelNonuniformity	9.68E-03	2.15E-07	P > 0.05	3.65E-02
Radiomics features	AAL-106	Cerebelum_9_R	GrayLevelRunLengthMatrix--GrayLevelNonuniformity	1.23E-02	2.74E-07	P > 0.05	3.84E-02
Radiomics features	AAL-106	Cerebelum_9_R	GrayLevelRunLengthMatrix-0GrayLevelNonuniformity	1.08E-02	2.53E-07	P > 0.05	4.52E-02
Radiomics features	AAL-105	Cerebelum_9_L	GrayLevelRunLengthMatrix-0LongRunLowGrayLevelEmpha	1.84E-02	4.00E-07	P > 0.05	3.52E-02
Radiomics features	AAL-105	Cerebelum_9_L	GrayLevelRunLengthMatrix--LongRunLowGrayLevelEmpha	7.85E-03	1.88E-07	P > 0.05	4.75E-02

Table S2. The features that showed significant differences in the association of brain and age between typically developing controls (TDC) and patients with attention-deficit/hyperactivity disorder (ADHD).

Feature categories	Feature names	Corrected P values
Volumetric measurements	Gray matter volume	4.36×10^{-13}
	White matter volume	9.12×10^{-23}
Surface values	Sqrtsulc	0.01
	Cortical thickness	4.49×10^{-8}
Radiomics features	First-order-EnergyNorm	7.17×10^{-5}
	First-order-GlobalEntropy	1.79×10^{-3}
	First-order-GlobalMean	8.83×10^{-3}
	First-order-LocalEntropyMax	1.64×10^{-6}
	First-order-LocalEntropyMean	1.73×10^{-5}
	First-order-LocalEntropyStd	1.59×10^{-4}
	First-order-LocalRangeMax	0.01
	First-order-LocalRangeMedian	1.11×10^{-4}
	First-order-LocalRangeStd	4.00×10^{-3}
	First-order-LocalStdMedian	9.10×10^{-6}
	First-order-65Percentile	0.04
	First-order-70Percentile	7.78×10^{-3}
	First-order-75Percentile	1.63×10^{-3}
	First-order-80Percentile	4.59×10^{-4}
	First-order-85Percentile	1.15×10^{-4}
	First-order-90Percentile	1.21×10^{-4}
	First-order-95Percentile	7.22×10^{-4}
	First-order-0.75Quantile	1.63×10^{-3}
	First-order-0.975Quantile	6.60×10^{-3}
	First-order-RootMeanSquare	7.17×10^{-5}
First-order-70PercentileArea	0.02	

	First-order-75PercentileArea	8.68×10^{-3}
	First-order-80PercentileArea	1.44×10^{-3}
	First-order-85PercentileArea	7.83×10^{-4}
	First-order-90PercentileArea	2.34×10^{-3}
	First-order-95PercentileArea	1.62×10^{-4}
	First-order-0.975Quantile	0.03
	First-order-Range	5.02×10^{-12}
	Texture-GLRLM- 90LongRunLowGrayLevelEmpha	7.52×10^{-3}
	Texture-GLRLM- 90LowGrayLevelRunEmpha	8.48×10^{-3}

Table S3. The classification results of typically developing controls (TDC) and patients with attention-deficit/hyperactivity disorder (ADHD).

Feature Category	Training set				Testing set			
	AUC (95% CI)	sen (%)	spe (%)	acc (%)	AUC (95% CI)	sen (%)	spe (%)	acc (%)
Clinical factors	0.75 (95% CI:0.69-0.81)	62.10	79.20	70.95	0.74 (95% CI:0.63-0.86)	57.14	86.67	73.75
Gray matter volume	0.71 (95% CI:0.64-0.77)	64.66	70.40	67.64	0.63 (95% CI:0.50-.076)	57.14	73.33	66.25
White matter volume	0.76 (95% CI:0.70-0.82)	76.72	66.40	71.37	0.66 (95% CI:0.54-0.78)	88.57	46.67	65.00
Surface values	0.80 (95% CI:0.75-0.86)	83.62	63.20	73.02	0.72 (95% CI:0.61-0.84)	68.57	71.11	70.00
Radiomics features	0.78 (95% CI:0.73-0.84)	83.62	56.00	69.29	0.79 (95% CI:0.69-0.90)	82.85	71.11	76.25
<i>Combination</i>	<i>0.82 (95% CI: 0.77-0.87)</i>	<i>61.21</i>	<i>89.60</i>	<i>75.93</i>	<i>0.83 (95% CI: 0.73-0.92)</i>	<i>68.57</i>	<i>93.33</i>	<i>82.50</i>

95% CI: 95% confidence intervals; acc: accuracy; AUC: area under curve; sen: sensitivity; spe: specificity.

Table S4. The features that were selected by Lasso method for the classification of typically developing controls (TDC) and patients with attention-deficit/hyperactivity disorder (ADHD).

Models	Brain area numbers	Brain area names	Feature names
<i>Clinical model</i>	--	--	Gender
	--	--	Age
	--	--	Verbal IQ
	--	--	Performance IQ
<i>Gray matter model</i>	AAL: 41, 58, 79	Amygdala_L, Postcentral_R, Heschl_L	Gray matter volume
<i>White matter model</i>	AAL: 1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 37, 38, 39, 40, 41, 44, 45, 46, 48, 50, 51, 52, 54, 55, 56,	Precentral_L, Precentral_R, Frontal_Sup_L, Frontal_Sup_R, Frontal_Sup_Orb_L, Frontal_Mid_L, Frontal_Mid_R, Frontal_Mid_Orb_L, Frontal_Mid_Orb_R, Frontal_Inf_Oper_L, Frontal_Inf_Oper_R, Frontal_Inf_Tri_L, Frontal_Inf_Tri_R, Frontal_Inf_Orb_R, Rolandic_Oper_L, Rolandic_Oper_R, Supp_Motor_Area_L, Supp_Motor_Area_R, Olfactory_L, Olfactory_R, Frontal_Sup_Medial_L, Frontal_Sup_Medial_R, Frontal_Med_Orb_L, Frontal_Med_Orb_R, Rectus_L, Rectus_R,	White matter volume

	<p>57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 69, 70, 71, 72, 74, 75, 76, 77, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116</p>	<p>Insula_L, Insula_R, Cingulum_Ant_L, Cingulum_Ant_R, Cingulum_Mid_L, Cingulum_Mid_R, Cingulum_Post_L, Hippocampus_L, Hippocampus_R, ParaHippocampal_L, ParaHippocampal_R, Amygdala_L, Calcarine_R, Cuneus_L, Cuneus_R, Lingual_R, Occipital_Sup_R, Occipital_Mid_L, Occipital_Mid_R, Occipital_Inf_R, Fusiform_L, Fusiform_R, Postcentral_L, Postcentral_R, Parietal_Sup_L, Parietal_Sup_R, Parietal_Inf_L, Parietal_Inf_R, SupraMarginal_L, SupraMarginal_R, Angular_L, Angular_R, Precuneus_L, Paracentral_Lobule_L, Paracentral_Lobule_R, Caudate_L, Caudate_RPutamen_R, Pallidum_L, Pallidum_R, Thalamus_L, Heschl_L, Heschl_R, Temporal_Sup_L, Temporal_Sup_R, Temporal_Pole_Sup_L, Temporal_Pole_Sup_R, Temporal_Mid_L, Temporal_Mid_R, Temporal_Pole_Mid_L, Temporal_Pole_Mid_R, Temporal_Inf_L, Temporal_Inf_R, Cerebelum_Crus1_L, Cerebelum_Crus1_R, Cerebelum_Crus2_L, Cerebelum_Crus2_R, Cerebelum_3_L, Cerebelum_3_R,</p>	
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		Cerebelum_4_5_L, Cerebelum_4_5_R, Cerebelum_6_L, Cerebelum_6_R, Cerebelum_7b_L, Cerebelum_7b_R, Cerebelum_8_R, Cerebelum_9_L, Cerebelum_9_R, Cerebelum_10_L, Cerebelum_10_R, Vermis_1_2, Vermis_3, Vermis_4_5, Vermis_6, Vermis_7, Vermis_8, Vermis_9, Vermis_10	
Surface value model	DK40: 23, 32, 36	Llateraloccipital, rmiddletemporal, rparacentral	Fractal dimension
	DK40: 6, 16, 21, 56, 62	Rcaudalanteriorcingulate, rfusiform, listhmuscingulate, rrostralmiddlefrontal, rsuperiortemporal	Gyrification
	DK40: 20, 29, 52, 58	Rinferiortemporal, lmedialorbitofrontal, rprecuneus, rsuperiorfrontal	sqrtsulc
	DK40: 21, 46, 71	Listhmuscingulate, rpostcentral, linsula	Cortical thickness
Radiomics model	AAL-020	Supp_Motor_Area_R	First-order-LocalRangeMax
	AAL_021	Olfactory_L	First-order-80Percentile
	AAL_030	Insula_R	First-order-GlobalUniformity
	AAL_087	Temporal_Pole_Mid_L	First-order-LocalEntropyMax
	AAL_088	Temporal_Pole_Mid_R	First-order-LocalStdMean

	AAL_091	Cerebelum_Crus1_L	First-order-Energy
	AAL_097	Cerebelum_4_5_L	First-order-10Percentile
	AAL_106	Cerebelum_9_R	Texture-GLCM- GrayLevelNonuniformity
	AAL_106	Cerebelum_9_R	Texture-GLRLM- 0GrayLevelNonuniformity
Combined model Radiomics features	AAL_020	Supp_Motor_Area_R	First-order-LocalRangeMax
	AAL_030	Insula_R	First-order-GlobalUniformity
	AAL_032	Cingulum_Ant_R	First-order- LocalEntropyMedian
	AAL_081	Temporal_Sup_L	First-order-5Percentile
	AAL_087	Temporal_Pole_Mid_L	First-order-LocalEntropyMax
	AAL_091	Cerebelum_Crus1_L	First-order-Energy
	AAL_097	Cerebelum_4_5_L	First-order-GlobalMax
	AAL_097	Cerebelum_4_5_L	First-order-10Percentile
	AAL_106	Cerebelum_9_R	Texture-GLRLM-

			GrayLevelNonuniformity
	AAL_106	Cerebelum_9_R	Texture-GLRLM- 0GrayLevelNonuniformity
Surface values	DK40_32	Rmiddletemporal	Fractal dimension
	DK40_62	Rsuperiortemporal	Gyrification
	DK40_71	linsula	Cortical thickness
Gray matter volume	AAL_58	Postcentral_R	Gray matter volume
Clinical factors	--	--	Gender
	--	--	Performance IQ

AAL: automated anatomical labeling; DK: Desikan-Killiany; GLCM: gray-level co-occurrence matrix; GLRLM: gray-level run length matrix; IQ: intelligence quotient.

Table S5. The classification results of patients with attention-deficit/hyperactivity disorder (ADHD) inattentive type (ADHD-I) and patients with ADHD combined type (ADHD-C).

Feature Category	Training set				Testing set			
	AUC (95% CI)	sen (%)	spe (%)	acc (%)	AUC (95% CI)	sen (%)	spe (%)	acc (%)
Clinical factors	0.69 (95% CI:0.58-0.79)	56.52	79.41	70.18	0.65 (95% CI:0.46-0.84)	84.21	55.56	70.27
Gray matter volume	0.75 (95% CI:0.66-0.85)	86.96	54.41	67.54	0.66 (95% CI:0.47-0.85)	94.74	50.00	72.97
White matter volume	0.69 (95% CI:0.58-0.79)	67.39	69.12	68.42	0.61 (95% CI:0.42-0.79)	57.90	66.67	62.16
Surface values	0.73 (95% CI:0.63-0.83)	45.65	95.59	75.44	0.60 (95% CI:0.40-0.79)	57.90	72.22	64.87
Radiomics features	0.94 (95% CI:0.91-0.99)	95.65	85.29	89.47	0.85 (95% CI:0.72-0.98)	84.21	83.33	83.78
<i>Combination</i>	<i>0.94 (95% CI: 0.90-0.98)</i>	<i>89.13</i>	<i>85.29</i>	<i>86.84</i>	<i>0.83 (95% CI: 0.69-0.97)</i>	<i>94.74</i>	<i>66.67</i>	<i>81.08</i>

95% CI: 95% confidence intervals; acc: accuracy; AUC: area under curve; sen: sensitivity; spe: specificity.

Table S6. The features that were selected by Lasso method for the classification of patients with attention-deficit/hyperactivity disorder (ADHD) inattentive type (ADHD-I) and patients with ADHD combined type (ADHD-C).

Models	Brain area numbers	Brain area names	Feature names
<i>Clinical model</i>	--	--	Gender
	--	--	Age
	--	--	Verbal IQ
<i>Gray matter model</i>	AAL: 20, 33, 42, 72, 80, 101, 116	Supp_Motor_Area_R, Cingulum_Mid_L, Amygdala_R, Caudate_R, Heschl_R, Cerebellum_7b_L, Vermis_10	Gray matter volume
<i>White matter model</i>	AAL: 65, 81	Angular_L, Temporal_Sup_L	White matter volume
<i>Surface value model</i>	DK40: 6	Rcaudalanteriorcingulate	sqrtsulc
	DK40: 4, 12	Rbankssts, rcuneus	Cortical thickness
<i>Radiomics model</i>	AAL-006	Frontal_Sup_Orb_R	Texture-GLCM-7InformationMeasureCorr1
	AAL_010	Frontal_Mid_Orb_R	Texture-GLRLM-90ShortRunEmphasis
	AAL_010	Frontal_Mid_Orb_R	Texture-GLRLM-ShortRunLowGrayLevelEmphasis

	AAL_014	Frontal_Inf_Tri_R	First-order-GlobalMax
	AAL_014	Frontal_Inf_Tri_R	First-order-Range
	AAL_035	Cingulum_Post_L	First-order-35Percentile
	AAL_035	Cingulum_Post_L	First-order-InterQuartileRange
	AAL_037	Hippocampus_L	Texture-NIDM- Busyness
	AAL_041	Amygdala_L	First-order-75Percentile
	AAL_041	Amygdala_L	First-order-0.75Quantile
	AAL-042	Amygdala_R	First-order-GlobalMax
	AAL_044	Calcarine_R	First-order-LocalRangeMin
	AAL_048	Lingual_R	First-order-80Percentile
	AAL_049	Occipital_Sup_L	First-order-Energy
	AAL_049	Occipital_Sup_L	First-order-LocalRangeMean
	AAL_049	Occipital_Sup_L	First-order-70Percentile
	AAL_051	Occipital_Mid_L	Texture-NIDM-Busyness
	AAL_063	SupraMarginal_L	First-order-MedianAbsoluteDeviation

	AAL_069	Paracentral_Lobule_L	First-order-0.975Quantile
	AAL_071	Caudate_L	First-order-LocalStdMin
	AAL_095	Cerebellum_3_L	First-order-0.975Quantile
	AAL_109	Vermis_1_2	First-order-Skewness
	AAL_113	Vermis_7	First-order-0.025Quantile
<i>Combined model</i> Radiomics features	AAL-006	Frontal_Sup_Orb_R	Texture-GLCM-7InformationMeasureCorr1
	AAL_010	Frontal_Mid_Orb_R	Texture-GLRLM-90ShortRunEmphasis
	AAL_010	Frontal_Mid_Orb_R	Texture-GLRLM- ShortRunLowGrayLevelEmpha
	AAL_014	Frontal_Inf_Tri_R	First-order-GlobalMax
	AAL_014	Frontal_Inf_Tri_R	First-order-Range
	AAL_035	Cingulum_Post_L	First-order-35Percentile
	AAL_035	Cingulum_Post_L	First-order-InterQuartileRange
	AAL_037	Hippocampus_L	Texture-NIDM-Busyness
	AAL_041	Amygdala_L	First-order-75Percentile
	AAL_041	Amygdala_L	First-order-0.75Quantile

Clinical factors	AAL-044	Calcarine_R	First-order-LocalRangeMin
	AAL_048	Lingual_R	First-order-80Percentile
	AAL_049	Occipital_Sup_L	First-order-Energy
	AAL_049	Occipital_Sup_L	First-order-LocalRangeMean
	AAL_049	Occipital_Sup_L	First-order-70Percentile
	AAL_051	Occipital_Mid_L	Texture-NIDM-Busyness
	AAL_063	SupraMarginal_L	MedianAbsoluteDeviation
	AAL_069	Paracentral_Lobule_L	First-order-0.975Quantile
	AAL_071	Caudate_L	First-order-LocalStdMin
	AAL_095	Cerebellum_3_L	First-order-0.975Quantile
	AAL_109	Vermis_1_2	First-order-Skewness
	--	--	Gender

AAL: automated anatomical labeling; DK: Desikan-Killiany; GLCM: gray-level co-occurrence matrix; GLRLM: gray-level run length matrix; IQ: intelligence quotient; NIDM: Neighbor Intensity Difference Matrix.