

Fig 1. The entire process of this experiment

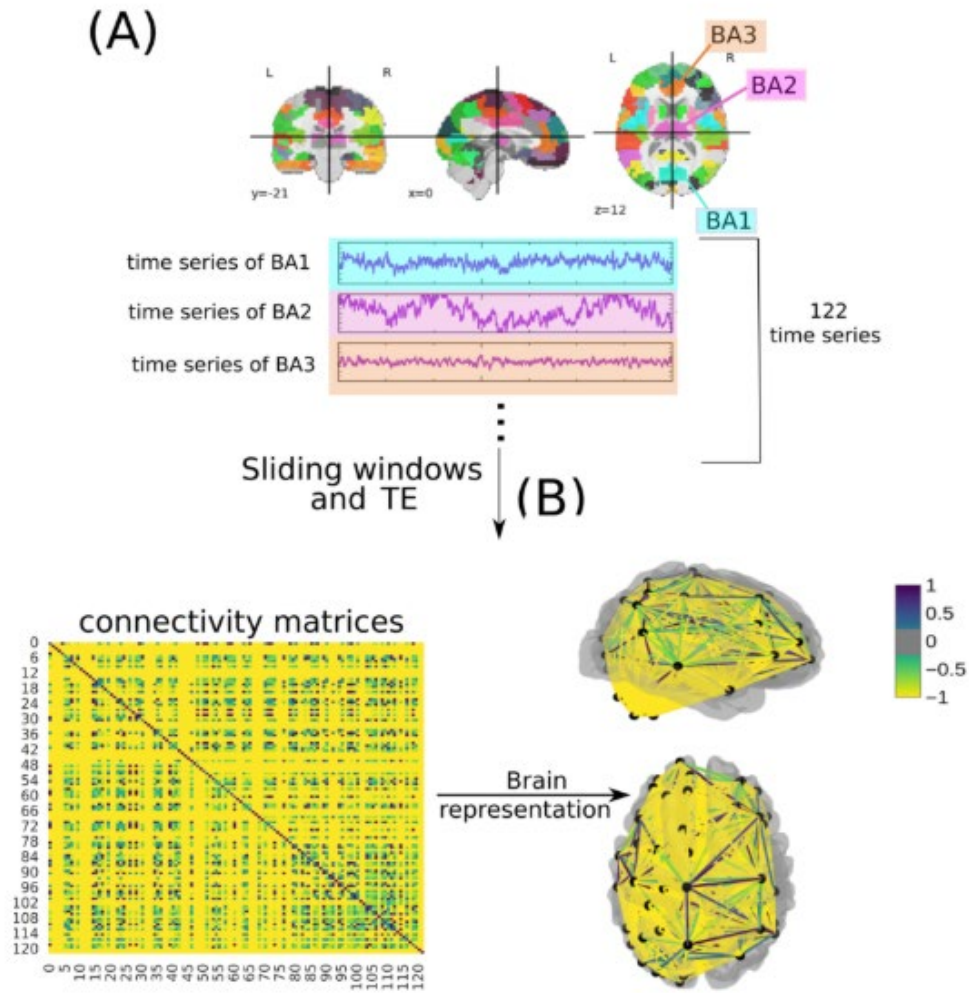


Figure 2: Methodology for Obtaining Connectivity Matrices

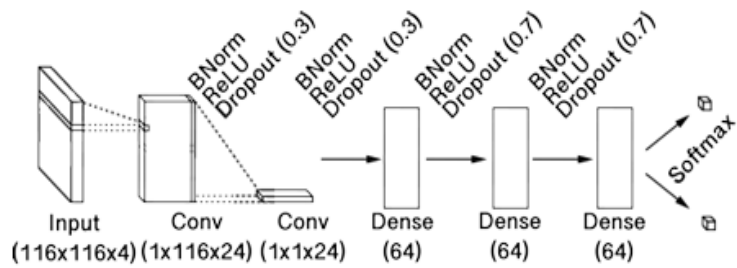


Figure 3. The structure of the neural network. This ensemble model averaged the outputs of 300 independently-trained neural networks within a cross-validation scheme.

### CNN for Static FC

Input:  $116 \times 116 \times 1$  tensor

Conv1: 32 filters,  $1 \times 116$  kernel

Conv2: 64 filters,  $116 \times 1$  kernel

Conv3: 16 filters,  $1 \times 1$  kernel

Batch Norm, ReLU, Dropout (50%)

Attention Mechanism

Final Layer: Static FC Features

### CNN for Dynamic FC

Input:  $116 \times 116 \times 40$  matrix

Similar structure as Static FC

Channel Compression

Final Layer: Dynamic FC Features

Figure 4. CNN Architecture for FC Feature Extraction

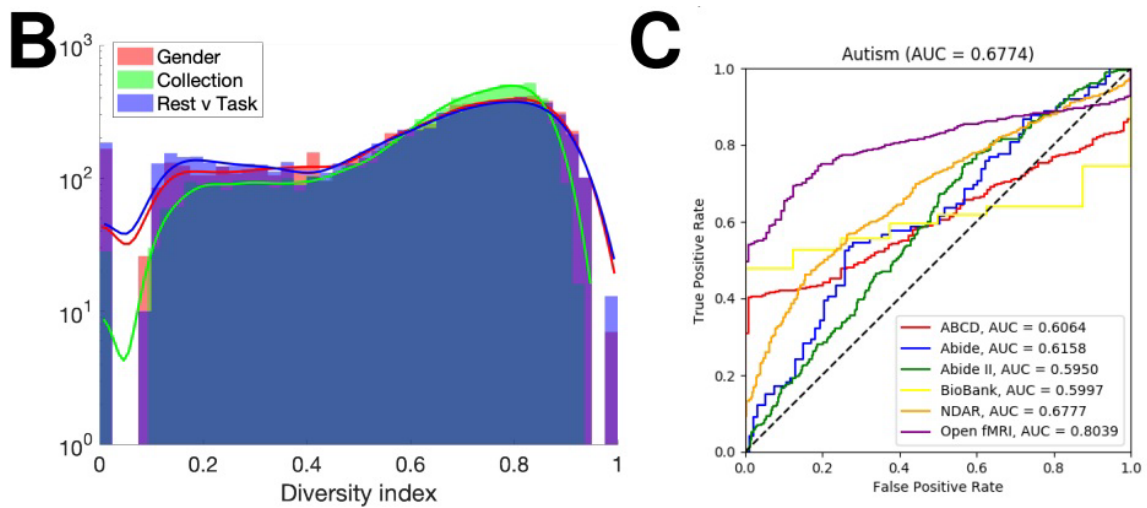


Figure 5. Results for autism classification

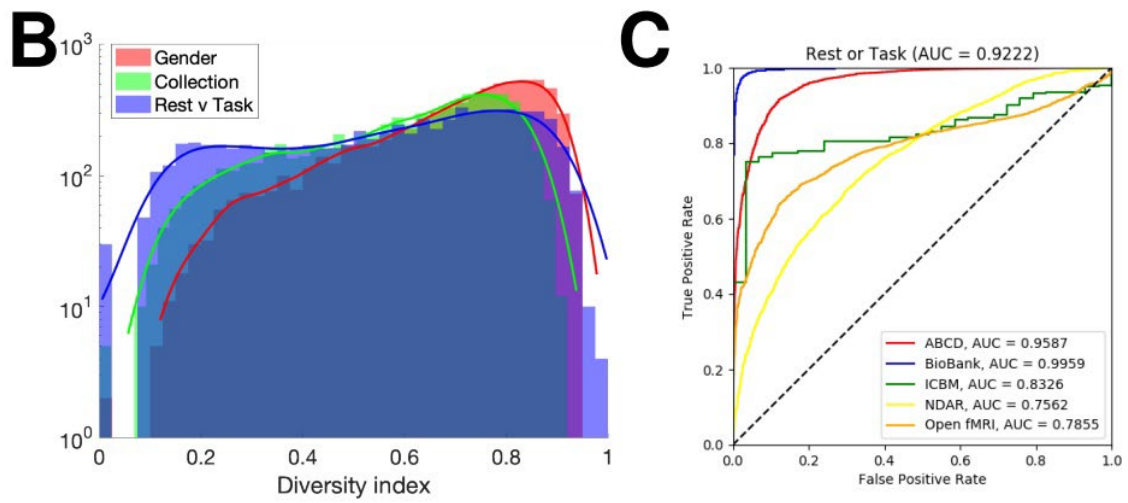


Figure 6. Results for resting-state/task classification

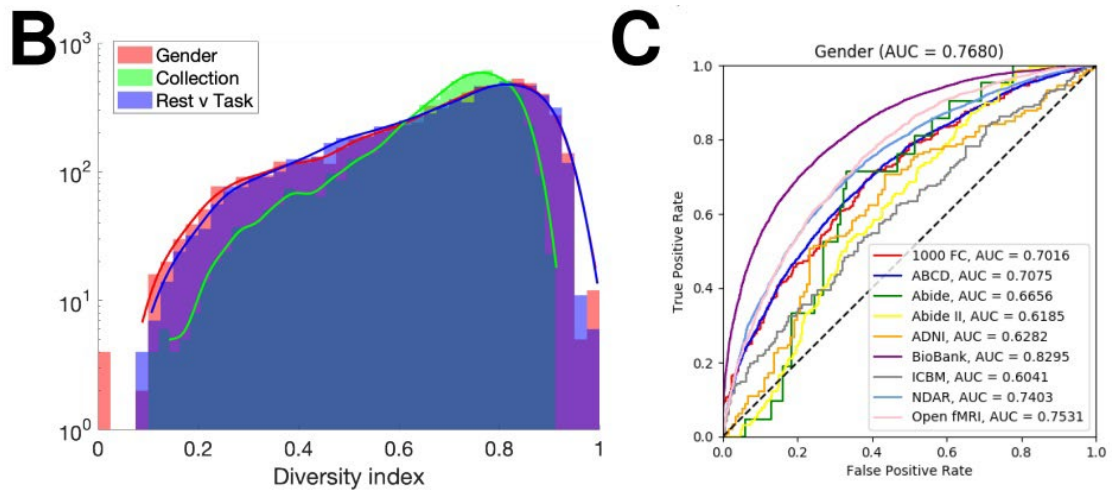


Figure 7. Results for gender classification

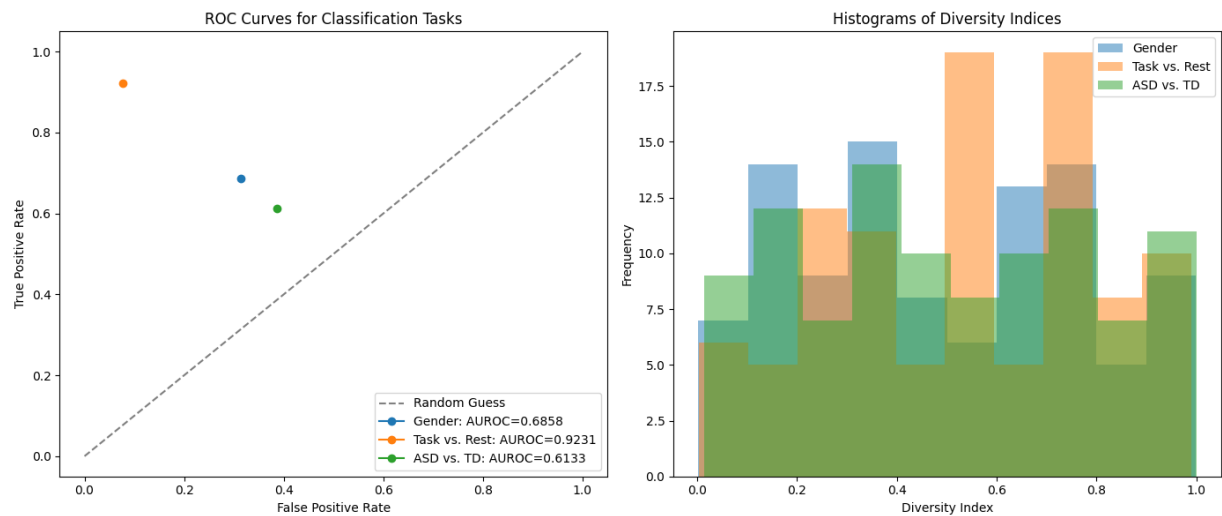


Figure8: ROC Curves and Diversity Indices

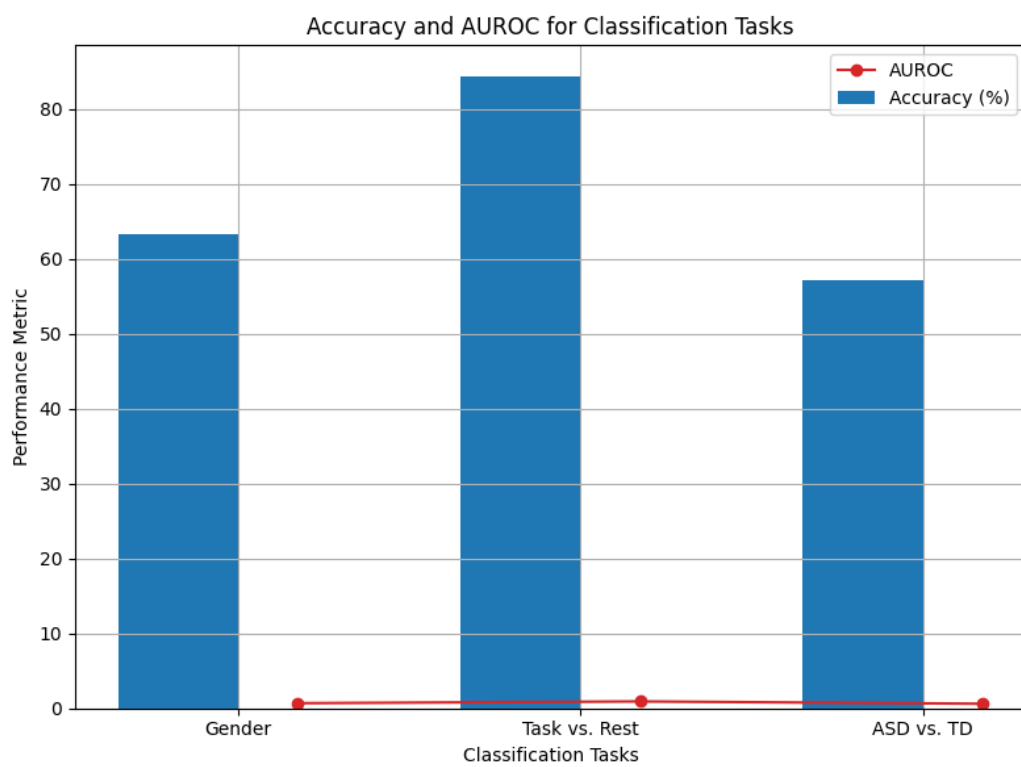


Figure9: Performance Metrics

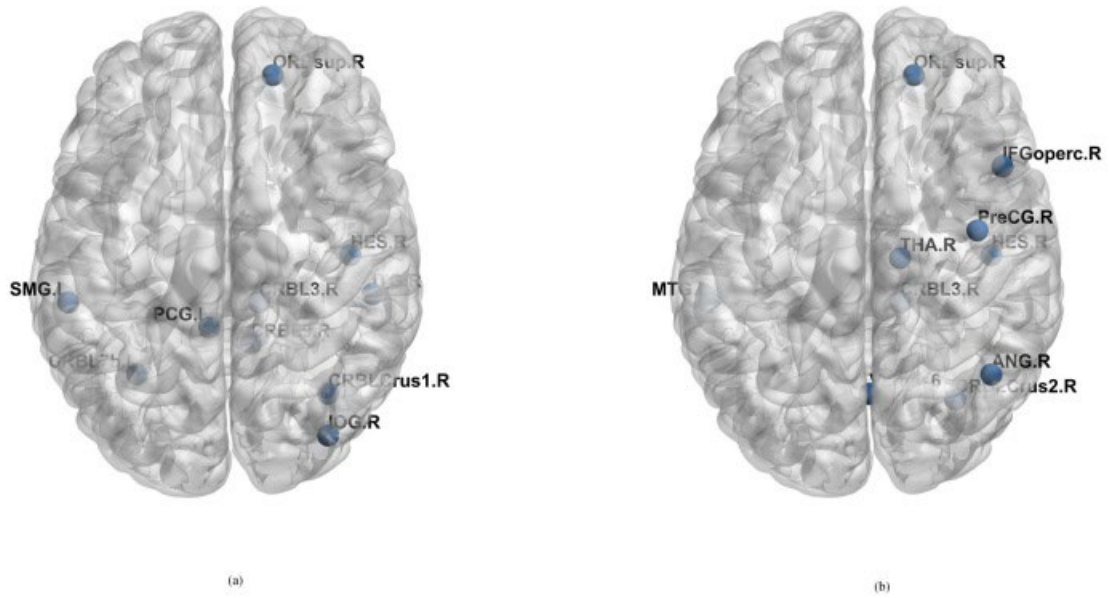


Fig 10. The most discriminating brain areas related to ASD.

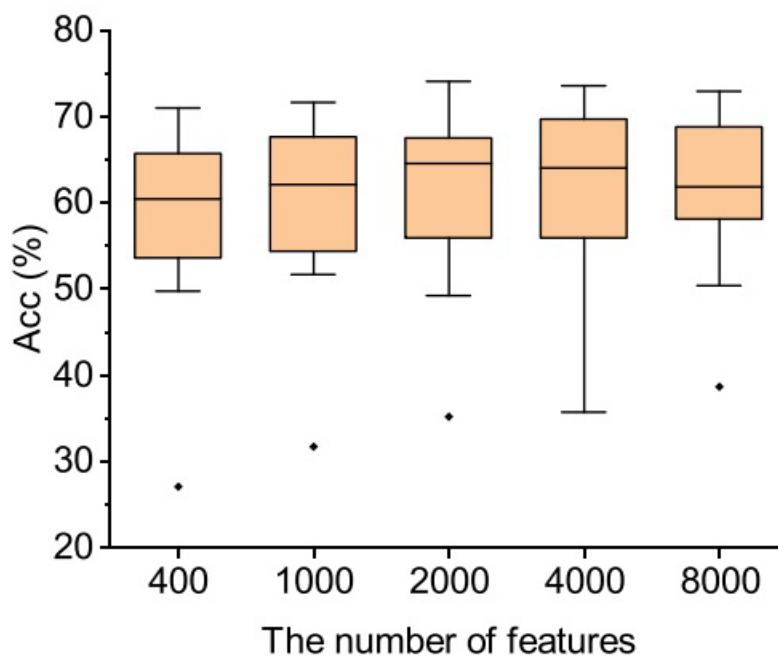


Fig. 11. The accuracy results with different number of features among all sites. The smaller the IQR, the more stable the method is. Thus, we set  $k = 2000$  when evaluating the accuracy on whole dataset

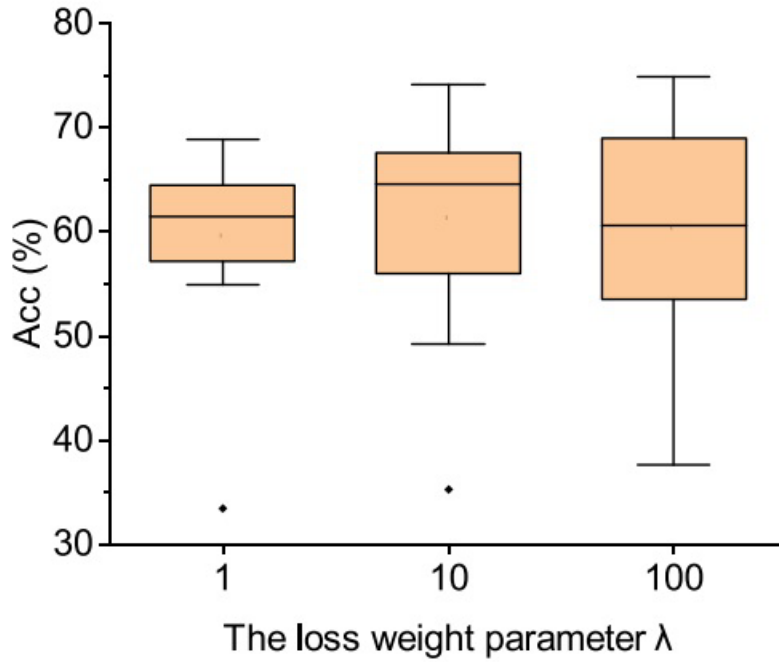


Fig. 12. The accuracy results with different values of the loss balance parameter among all sites. Based on the results, the loss balance parameter  $\lambda$  was set to 10 when evaluating the whole dataset

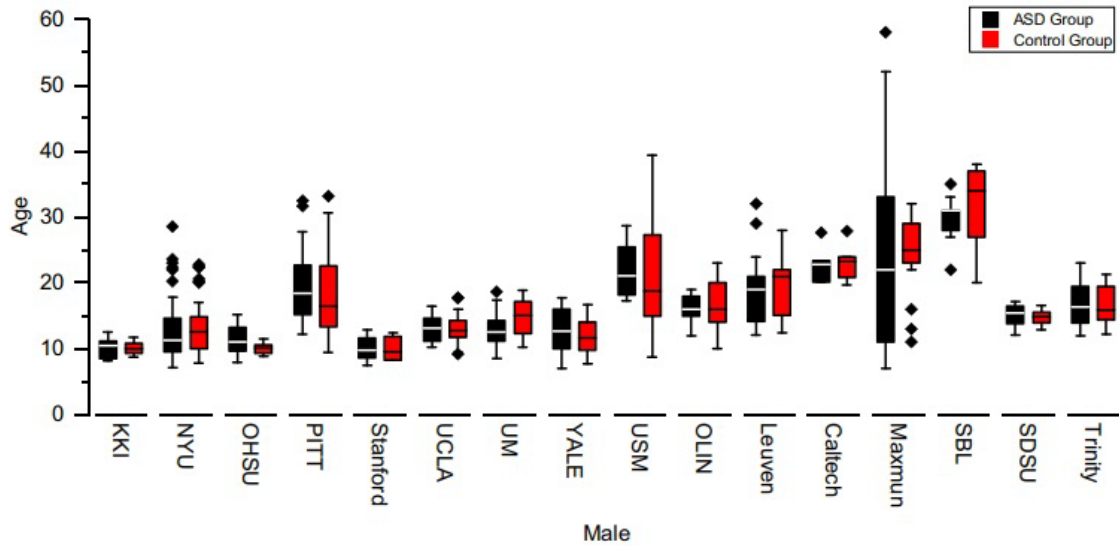


Fig. 13. There was no significant difference between ASD and control group in terms of age for each site. Error bars represent the standard error. The independent t test (Fisher LSD) is used to determine the significant difference between the two groups and marked with asterisks (\*  $p \leq 0.05$ , \*\*  $p \leq 0.01$ , \*\*\*  $p \leq 0.001$ ). The outliers are represented as black diamonds

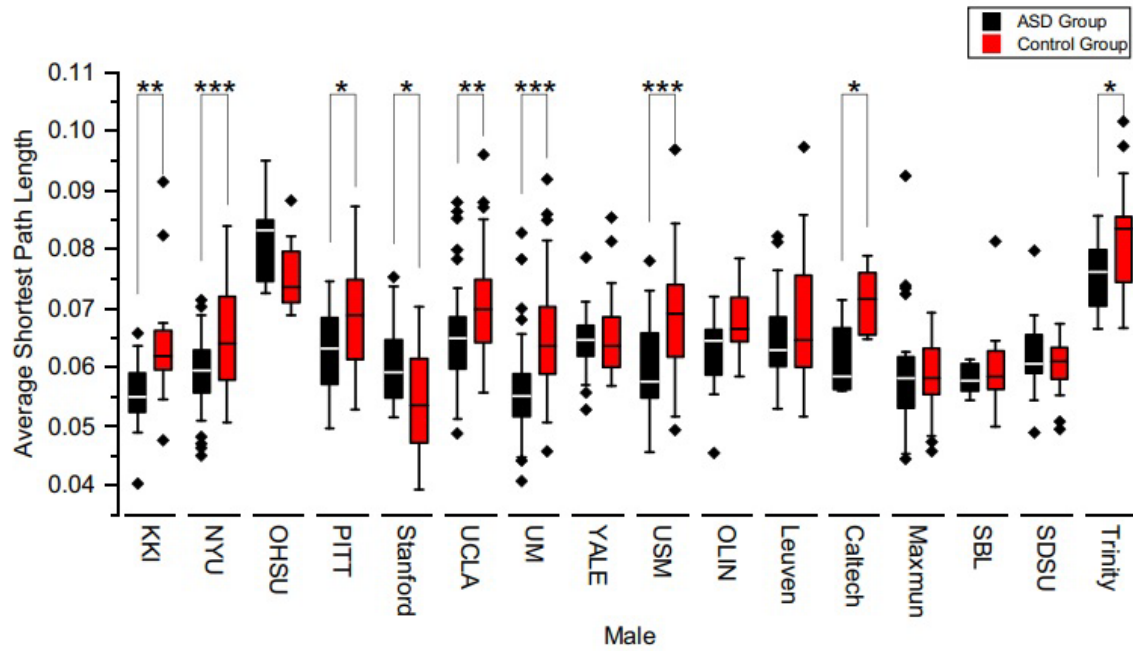


Fig. 14. The cluster coefficients for the males in ASD (black) and TD (red) groups for each site. Error bars represent the standard error. Significant differences identified by an independent t test (\*  $p \leq 0.05$ , \*\*  $p \leq 0.01$ , \*\*\*  $p \leq 0.001$ ) between the two groups are marked by asterisks (Fisher LSD). The outliers are represented as black diamonds



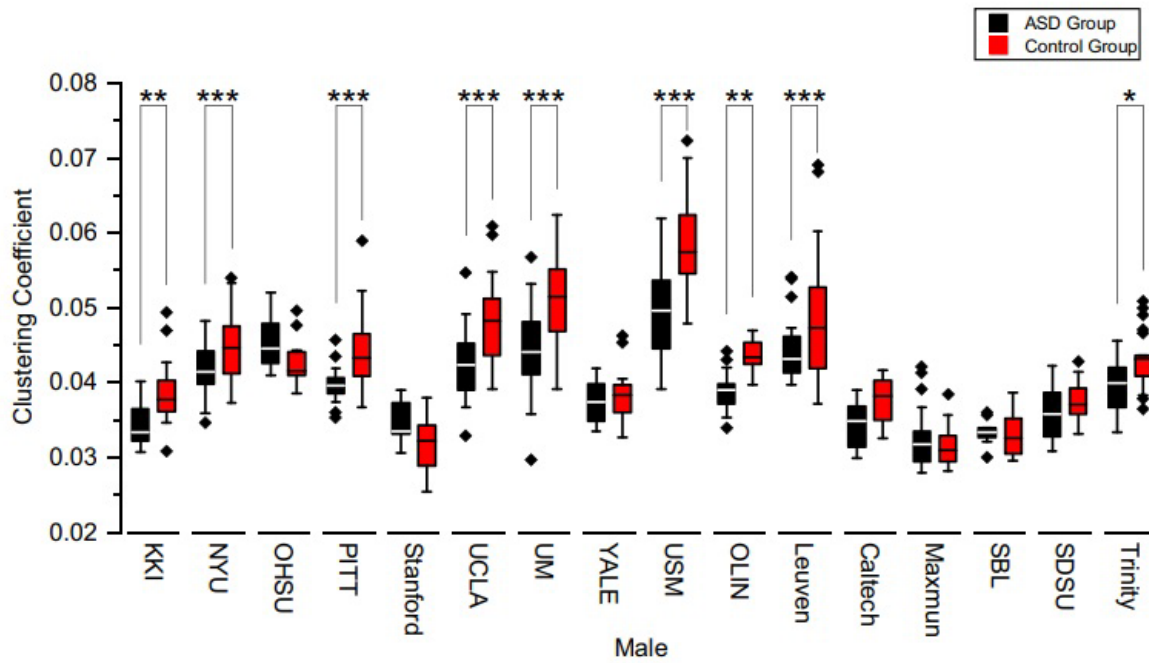


Fig. 15. The average shortest path lengths for males in the ASD (black) and TD (red) groups for each site. Error bars are the standard error. Significant differences with independent t test ( $* p \leq 0.05$ ,  $** p \leq 0.01$ ,  $*** p \leq 0.001$ ) between the two groups are marked by asterisks (Fisher LSD). The outliers are represented as black diamonds