Supplementary Materials for

Generalizable neuromarker for autism spectrum disorder across imaging sites and developmental stages: A multi-site study

Takashi Itahashi†, Ayumu Yamashita†, Yuji Takahara, Noriaki Yahata, Yuta Y. Aoki, Junya Fujino, Yujiro Yoshihara, Motoaki Nakamura, Ryuta Aoki, Haruhisa Ohta, Yuki Sakai, Masahiro Takamura, Naho Ichikawa, Go Okada, Naohiro Okada, Kiyoto Kasai, Saori C. Tanaka, Hiroshi Imamizu, Nobumasa Kato, Yasumasa Okamoto, Hidehiko Takahashi, Mitsuo Kawato, Okito Yamashita, Ryu-ichiro Hashimoto*

*Corresponding author. Email: dbridges50@gmail.com (R.H.)

†These authors contributed equally to this work.

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Supplementary Materials

Materials and Methods

Ethics of statement

All participants (if appropriate) and their parent/legal guardian provided written informed consent. The institutional review boards approved recruitment procedures and experimental protocols at the principal investigators' respective institutions. These procedures were conducted in accordance with the Declaration of Helsinki.

Participants

The current study used three adult resting-state fMRI (R-fMRI) datasets for the analyses: one was used as the discovery dataset, and the remaining two were used as independent validation datasets. Tables S1 and S15 show the demographic information and scanning parameters for the three datasets.

Discovery dataset

The discovery dataset contained data of 550 typically developing controls (TDCs) from five scanners at four imaging sites (University of Tokyo [UTO1 and UTO2], Kyoto University [KUT], Center for Innovation in Hiroshima University (COI), and Showa University [SWA1]) and 180 adults with autism spectrum disorder (ASD) from two institutes (SWA1 and UTO2). This dataset consisted of a part of the Strategic Research Program for the Promotion of Brain Science (SRPBS) dataset (https://bicr-resource.atr.jp/srpbsopen/) *(38)*. We also included participants at SWA1 and a part of the dataset used in our prior study *(25)*.

The ABIDE adult validation dataset

The first independent adult validation dataset consisted of participants from the Autism Brain Imaging Data Exchange I (ABIDE-I) *(11)* and -II datasets *(12)*. Since adult participants were limited in both releases, we combined the two datasets. Of note, since some imaging sites participated in both datasets (e.g., New York University Langone Medical Center [NYU] and the University of Utah School of Medicine [USM]), we checked the consistency of the scanning protocols in each imaging site. We used 54 adults with ASD and 67 TDCs that were selected from the following three sites: the University of Leuven (Leuven), NYU, and USM. In this study, we referred this validation dataset to the ABIDE adult dataset.

The Japanese adult validation dataset

To further validate the generalization performance of our classifier, we newly collected R-fMRI data from 22 adults with ASD and 38 controls at Showa University, Karasuyama Hospital (SWA2). The data were collected under the Brain/MINDS Beyond project (BMB; https://brainminds-beyond.jp/). The project details were described elsewhere *(62)*.

Exclusion criteria

We applied the following exclusion criteria for participant selection; 1) participants with no whole-brain coverage were excluded; 2) participants who had less than 4 min of uncontaminated R-fMRI data *(78)*; 3) participants with errors in any preprocessing steps (e.g., segmentation failure and failures in spatial normalization and surface mapping). For the ABIDE adult validation dataset, we excluded imaging sites that contained less than 10 participants per group, according to prior studies *(79)*. We also excluded imaging sites that did not have some missing information about the scanning protocol (e.g., slice acquisition order).

R-fMRI data preprocessing

We preprocessed all the R-fMRI data using fMRIPrep version 1.1.8 *(63)*. The fMRIPrep performs a series of preprocessing steps, including head motion estimation, slice timing correction, co-registration of EPI data to the corresponding T1-weighted anatomical image, distortion correction, and normalization to a standard Montreal Neurological Institute (MNI) space. We used the "fieldmap-less" distortion correction method if the fieldmap data were unavailable. We used the ciftify toolbox version 2.1.1 *(64)* to map the preprocessed data onto the grayordinate *(80)*.

For each vertex, we performed nuisance regression to remove the effects of artifactual and non-neural sources. Nuisance regressors consisted of six head-motion parameters, averaged signals from subject-specific white matter and cerebrospinal fluid masks, global signal, their temporal derivatives, and linear detrending. After nuisance regression, we applied a band-pass filter (0.008–0.1 Hz) to the residuals. We computed frame-wise displacement (FD) *(65)* for each participant to characterize the frame-by-frame head motion during the scans. We used FD as a measure for detecting occasional head movement. To reduce spurious changes in FC due to head motion, we removed volumes with FD > 0.5 mm, as proposed in a previous study *(65)*.

Parcellation and network construction

We used Glasser's 379 surface-based brain parcellations (cortical 360 parcellations and subcortical 19 parcellations) as ROIs *(66)*. We extracted the averaged, denoised signals from these ROIs. We computed the temporal correlations of signals among all possible pairs of ROIs and applied Fisher's *r*-to-*z* transformation, resulting in 71,631 unique FCs for each participant. Because the label of each ROI in Glasser's atlas was not intuitive, we utilized Yeo's resting-

state network (RSN) labels *(67)* to assign important ROIs to the corresponding RSN label. This study added the subcortical network label to the subcortical and cerebellar regions.

Construction of the ASD neuromarker using the discovery dataset

Based on previous studies *(25, 36, 40, 72–74)*, we assumed that psychiatric disorder factors were associated with the limited number of FCs, rather than the whole-brain connections. We, thus, used a logistic regression analysis with least absolute shrinkage and selection operator (LASSO) method that selects an optimal subset of FCs from the whole brain connections *(75)*. The details of our procedures were described elsewhere *(40)*. Briefly, a logistic function is used to define the probability of a participant belonging to the ASD class label as follows:

$$P_i(y_i = 1 \mid x_i;\ w) = \frac{1}{1 + exp\ (-x_i \cdot w)},$$

where y_i and x_i represent the *i*-th participant's class label and FC vector, respectively. The class label was set to 1 if the participant belonged to the ASD group while setting to 0 if the participant belonged to the TDC group. The weight vector was denoted as w. The weight vector was optimized by minimizing the following objective function:

$$L(w) = -\frac{1}{N}\sum_{i=1}^{N} \quad log\left(P_i(y_i = 1 \mid x_i;\ w)\right) + \lambda \cdot ||w||_1,$$

where $||\cdot||_1$ represents L_1-norm and λ stands for a hyperparameter that regulates the sparsity of the weight vector.

We developed the ASD neuromarker using the LASSO method with 10-fold nested cross-validation (CV) and 10 subsampling, yielding 100 trained classifiers (fig. S7). To estimate the optimal weights and tune the hyperparameter, we used a 10-fold nested CV procedure with an undersampling method. In this procedure, we first divided the whole discovery dataset into training (9 folds of 10 folds) and test (1 fold of 10 folds) datasets using the "*cvpartition*"

implemented in MATLAB (R2020b, Mathworks, USA). We then applied an undersampling method to alleviate a bias due to the imbalance in the number of participants between the groups *(81)*. In this undersampling method, we randomly selected participants from the discovery dataset to match the number of participants between the ASD and TDC groups. Similar to our previous study, we matched the mean age between ASD and TDC groups in each subsample. To avoid any subsampling bias, we repeated this undersampling ten times, yielding ten subsampled matched training datasets. For each subsampled dataset, we fitted the logistic regression model while tuning the hyperparameter in the inner loop of the nested CV. For building a logistic regression model, we used the "*lassoglm*" function implemented in MATLAB. The inner CV (i.e., "CV" parameter in the lassoglm function) was set to 10, and "NumLambda" was set to 25. We determined the optimal λ according to the one standard error rule in which we selected the largest λ within the standard deviation of the minimum prediction error among all λ. The mean classifier output value was considered as diagnostic probability, indicating a likelihood of a participant belonging to the ASD class. We considered participants as those with ASD if their diagnostic probability values were higher than 0.5. We calculated the area under the curve (AUC) to assess the classification performance using the "*perfcurve*" implemented in MATLAB. We also computed accuracy, sensitivity, specificity, and the Matthews correlation coefficient (MCC). The MCC is suitable for the imbalanced dataset because this metric takes into account the ratio of the confusion matrix size *(76, 82)*. We used AUC and MCC as performance indices throughout the paper.

The details of the effects of head motion, harmonization, and experimental settings on the generalization performance

To assess the impacts of head motion, harmonization, and experimental factors (i.e., diversity in the characteristics of scanning protocols and choice of atlas), we conducted several control

analyses. We first assessed the association between head motion and classification performance. We calculated the value of the area under the curve (AUC) and the mean frame-wise displacement (FD) value at each imaging site in each validation dataset. We then calculated the Pearson correlation coefficient between the mean FD and AUC values across the validation datasets. A significant positive correlation was not found between the AUC and mean FD (r = -0.56, P = 0.002; fig. S2). This result indicates that the head motion did not artificially improve the generalizability of our neuromarker.

We next assessed the effects of the harmonization method on classification performance in the discovery and adult validation datasets, respectively. We trained an ASD classifier on the discovery dataset without the ComBat harmonization method. The ASD classifier showed better classification performance (accuracy = 77%, AUC = 0.85, and MCC = 0.50) in the discovery dataset (table S5). The ASD classifier, however, exhibited reduced generalizability to the ABIDE adult (accuracy = 60%, AUC = 0.64, and MCC = 0.19) and the Japanese adult (accuracy = 67%, AUC = 0.73, and MCC = 0.23). These results suggest that applying the ComBat harmonization method plays a vital role in improving the generalizability of the ASD classifier to other datasets.

We further investigated the impacts of diversity in imaging sites on the generalization performance since our discovery dataset comprised imbalanced imaging sites (i.e., COI, KUT, and UTO1) and a site with a different scanning protocol (i.e., UTO2). Three imaging sites (i.e., COI, KUT, and UTO1) contained the TDC population only, and thus there is a possibility that the inclusion of imbalanced data might influence the classifier's generalization performance. To test this, we built a neuromarker for the ASD diagnosis using two imaging sites (i.e., SWA1 and UTO2) by removing the three sites. The trained classifier showed a slightly reduced

accuracy of 74%, an AUC of 0.80, and an MCC of 0.47 in the discovery dataset (table S6). The trained classifier did not change the discrimination abilities in the ABIDE adult (accuracy = 58%, AUC = 0.67, and MCC = 0.21) and the Japanese adult (accuracy = 72%, AUC = 0.83, MCC = 0.42). We next investigated the impacts of an imaging site with a different scanning protocol (i.e., UTO2) on the classification and generalization performance. We repeated the same analyses while excluding the UTO2. We did not observe significant changes in the classification and generalization performance (table S7). These results suggest that, at least in our experimental setting, the inclusion of diverse imaging sites does not influence the generalization performance of our ASD neuromarker.

Finally, we assessed whether our generalization performance was not atlas-dependent. To test this, we used Schaefer's cortical atlas *(39)* as an alternative to the Glasser atlas *(66)* because this atlas provided an atlas with multiple levels of resolutions ranging from 100 to 1,000 and thus it is suitable to investigate the effects of ROI resolutions on the generalization performance. Of note, we excluded 1,000 ROIs from analyses because some brain regions could not extract signals reliably. Classifiers with Schaefer's atlas exhibited similar or higher generalization performance in the ABIDE adult and Japanese adult datasets (table S8). These results suggest that our generalization performance was not atlas-dependent.

Consistency of the effect of ASD diagnosis across the datasets

In the mass-univariate analyses, we did not observe a significant positive correlation between the discovery dataset and the child dataset (see **Results** in the main text and fig. S3). We speculated that, instead of the whole-brain pattern, a specific set of important FCs were reproducible between the discovery dataset and the child dataset. To test this, we used a

binomial test, similar to previous studies *(42, 83)*. We calculated a *t*-value as the effect of the ASD diagnosis in each FC of each dataset. We then counted the number of FCs showing the same sign (i.e., the same direction of the effect of diagnosis) within the set of discriminative FCs, *k*, and the whole FCs, *m*, respectively. Since the permutation test identified 141 FCs as important FCs for the ASD diagnosis (see **Results** in the main text) and 98 out of 141 FCs showed the same direction of between-group difference between the discovery dataset and the child dataset (i.e., the same sign of *t*-values between the datasets), we set $n = 141$ (the number of important FCs), $k = 98$ (the number of FCs showing the same sign of *t*-values within the important FCs), and $m = 35{,}443$ (the number of FCs showing the same direction of between-group difference in the whole connections), respectively. The binomial test confirmed that the set of important FCs was reproducible between the discovery dataset and the child dataset ($P < 0.05$). This observation was replicated between the discovery dataset and the adult and adolescent datasets ($k = 94$ and $m = 38{,}969$ for the ABIDE adult; $k = 105$ and $m = 42{,}649$ for the Japanese adult; $k = 98$ and $m = 40{,}124$ for the adolescent dataset; all $P < 0.05$). These results suggest that the reproducible FCs selected by our method might contribute to the generalizability of our neuromarker.

Dimensional relationships among three psychiatric disorders

We examined the exchangeability among the three psychiatric disorders, constructing classifiers for the SCZ and MDD diagnoses and applying these classifiers to the remaining psychiatric disorders. We used the same analytical procedures, including 10-fold nested CV, 10 subsampling, and parameter settings for the LASSO method. We then calculated AUC, accuracy, sensitivity, specificity, and MCC as performance indices. To test the statistical significance, we constructed null distributions using permutation tests with 100 iterations. We

set iterations to 100 instead of 500 because this procedure was computationally expensive. Statistical significance was set to $P < 0.05$.

We tested the sensitivity of each classifier to the remaining psychiatric disorders by applying each classifier to other psychiatric disorders. Since participants with TDC were identical to those in the discovery dataset, we focused on sensitivity instead of other performance indices. We constructed null distributions of performance indices using a permutation test with 100 iterations and applied a statistical threshold of $P < 0.05$, one-sided.

Cross-validated neuromarkers for schizophrenia and major depressive disorder

Similar to the ASD classifier, we used a 10-fold nested CV with 10 subsamples to determine the weights and hyperparameters. The statistical significance of both classifiers was confirmed by permutation tests with 100 iterations. The SCZ classifier exhibited an accuracy of 82%, AUC of 0.89, and MCC of 0.51 (permutation test, all $P < 0.05$; table S12). The corresponding sensitivity and specificity were 83% and 82%, respectively. On the other hand, the MDD classifier exhibited an accuracy of 68%, AUC of 0.78, and MCC of 0.32 (permutation test, $P < 0.05$; table S12). The corresponding sensitivity and specificity were 75% and 66%, respectively. These results indicate that both classifiers hold acceptable classification performance to the training dataset.

Identification of discriminative FCs for SCZ and MDD

Similar to identifying discriminative FCs for the ASD diagnosis, we used permutation tests with 100 iterations to identify important FCs for schizophrenia (SCZ) and major depressive disorder (MDD), respectively. At each iteration, we shuffled the diagnostic labels to create a permuted dataset and constructed permuted classifiers. We used the number of counts for each FC

selected by the LASSO across 10-fold cross-validation and 10 subsampling (i.e., across 100 classifiers). To control for the multiple comparisons, we only kept the maximum counts among all the connections at each iteration and constructed a null distribution using these maxima. We considered FCs as important contributors to the SCZ or MDD diagnosis if their *P*-values were below 0.05. The list of discriminative FCs and their spatial distributions are provided in fig. S4 and table S13, while those for MDD are in fig. S5 and table S14.

Supplementary Figures

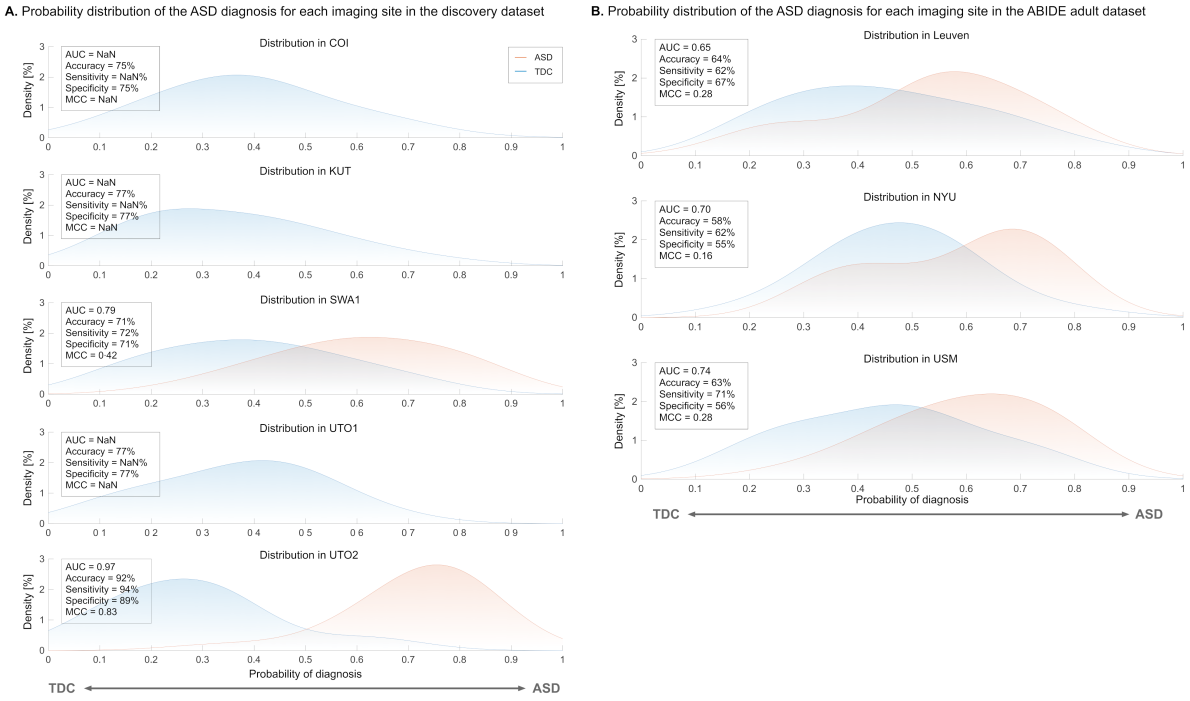

Fig. S1. The distribution of the ASD diagnosis probability in each imaging site in the discovery dataset and the ABIDE adult validation dataset. (A) In the discovery dataset, we visualized the probability distributions in each imaging site. (B) In the ABIDE adult dataset, we visualized the probability distributions in each imaging site. **Abbreviations:** AUC: area under the curve, ASD: autism spectrum disorder, MCC: Matthews correlation coefficient, and TDC: typically developing control.

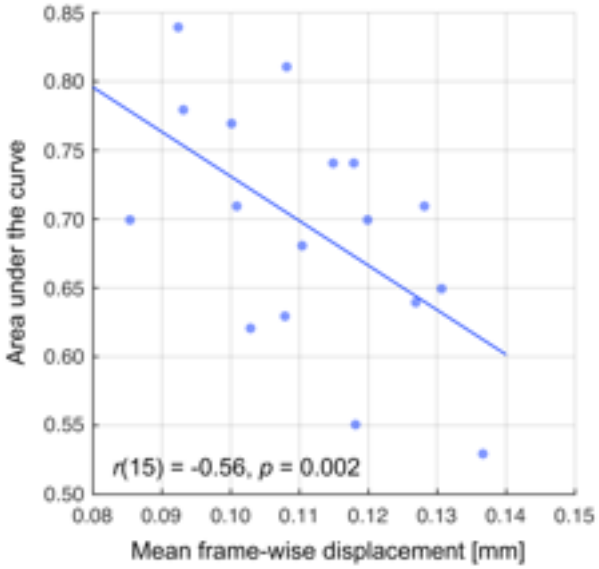

Fig. S2. The relation between the head motion and performance index across the validation datasets. We computed the area under the curve (AUC) and the mean frame-wise displacement (FD) in every imaging site. We then computed the Pearson correlation coefficient between the AUC and mean FD across imaging sites to investigate whether the head motion improved the classification performance.

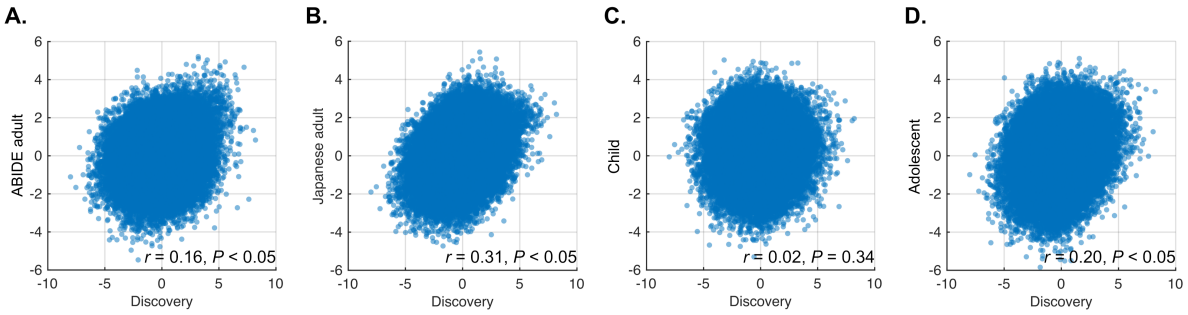

Fig. S3. Results of mass-univariate analyses between the discovery and validation datasets. (A) The relationship between the discovery dataset and the ABIDE adult dataset. (B) The relationship between the discovery dataset and the Japanese adult dataset. (C) The relationship between the discovery dataset and the child dataset. (D) The relationship between the discovery dataset and the adolescent dataset. **Abbreviations:** ABIDE: autism brain imaging data exchange.

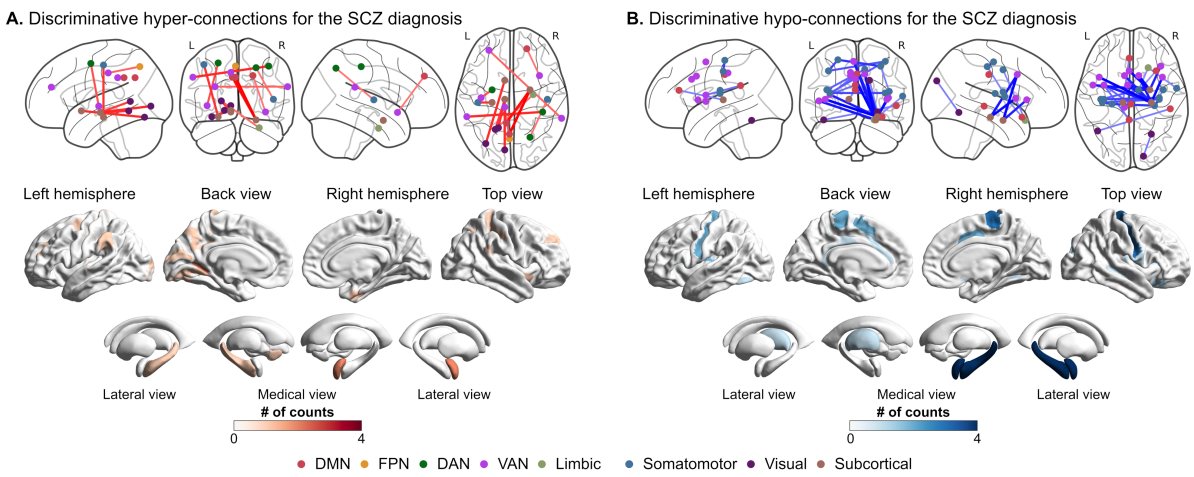

Fig. S4. Discriminative functional connections for the SCZ diagnosis. (A) The spatial distribution of hyper-connections for the diagnosis of schizophrenia (SCZ). (B) The spatial distribution of hypo-connections or the diagnosis of SCZ.

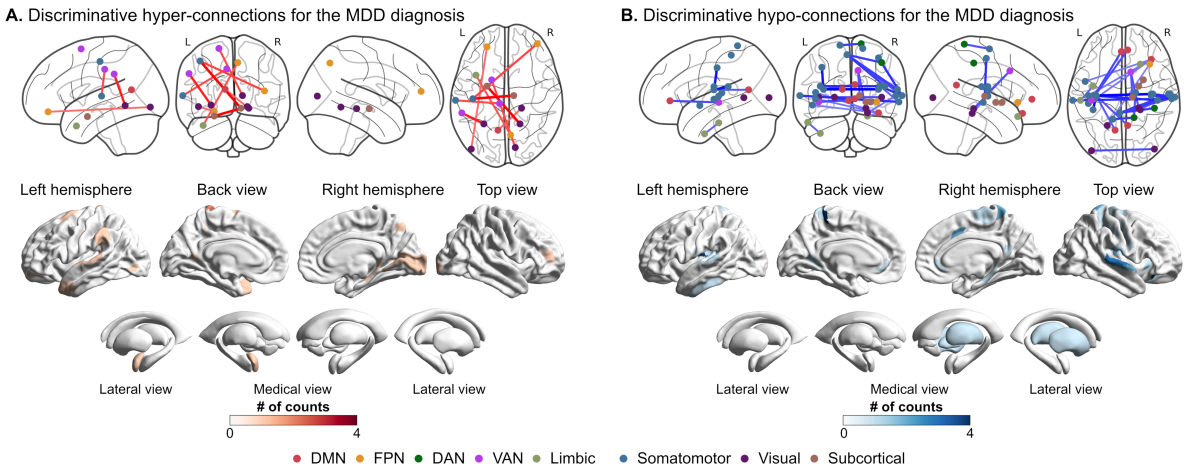

Fig. S5. Discriminative functional connections for the MDD diagnosis. (A) The spatial distribution of hyper-connections for the diagnosis of major depressive disorder (MDD). (B) The spatial distribution of hypo-connections or the diagnosis of MDD.

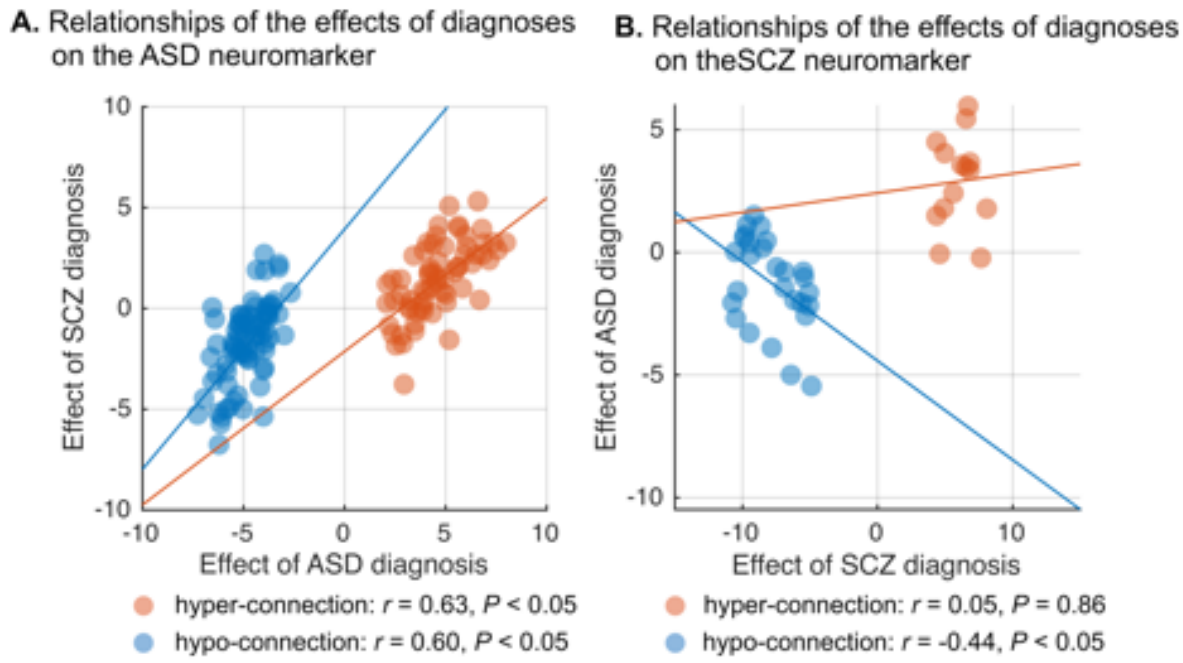

Fig. S6. Relationship of the ASD and SCZ diagnosis on ASD and SCZ neuromarkers. (A)The relationship of both diagnoses on ASD neuromarker. (B) The relationship of both diagnoses on SCZ neuromarker. **Abbreviations:** ASD: autism spectrum disorder, and SCZ: schizophrenia.

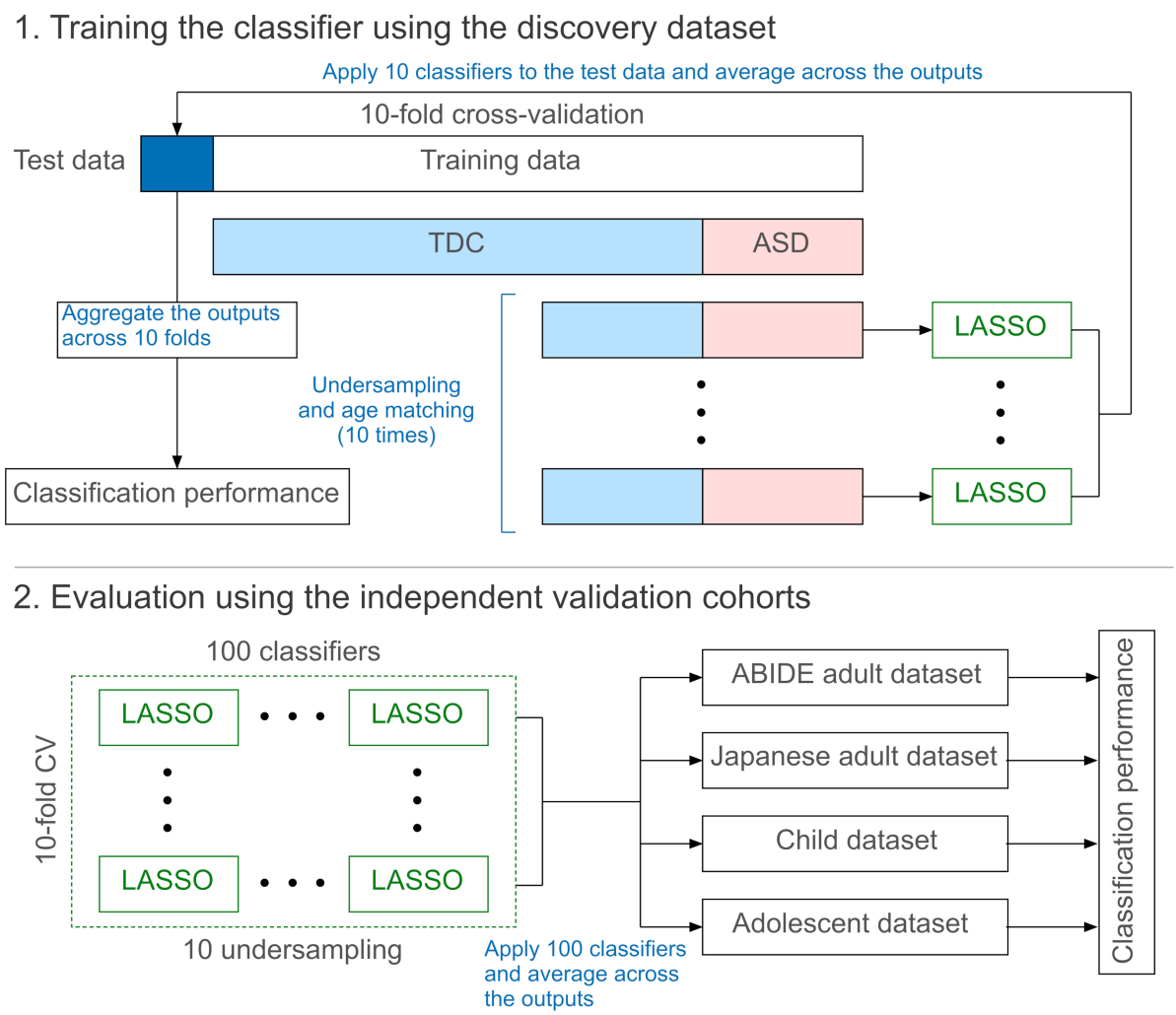

Fig. S7. Schematic representation of training and evaluation procedures of the ASD neuromarker. We built a neuromarker for autism spectrum disorder (ASD) using a 10-fold nested cross-validation (CV) procedure with ten undersamplings. The neuromarker's generalizability was evaluated by applying 100 trained classifiers to the validation datasets. **Abbreviations:** ABIDE: autism brain imaging data exchange, ASD: autism spectrum disorder, and TDC: typically developing control.

Table S1. Demographic information of the discovery and adult validation datasets.

	TDC			ASD		
	N (M/F)	**Age**	**Mean FD (SD) [mm]**	**N (M/F)**	**Age**	**Mean FD (SD) [mm]**
Discovery cohort						
COI	106 (41/65)	50.75 (13.02)	0.18 (0.05)	-	-	-
KUT	148 (85/63)	36.64 (13.41)	0.13 (0.04)	-	-	-
SWA1	174 (151/23)	30.94 (7.64)	0.13 (0.04)	145 (122/23)	31.37 (7.78)	0.14 (0.06)
UTO1	86 (29/57)	44.45 (13.82)	0.11 (0.04)	-	-	-
UTO2	36 (18/18)	35.5 (7.57)	0.16 (0.06)	35 (23/12)	31.94 (8.78)	0.15 (0.04)
Total	550 (324/226)	38.70 (13.65)	0.14 (0.05)	180 (145/35)	31.48 (7.96)	0.14 (0.06)
ABIDE adult validation dataset						
Leuven	15 (15/0)	23.27 (2.91)	0.13 (0.04)	13 (13/0)	21.31 (3.71)	0.13 (0.03)
NYU	20 (15/5)	23.81 (3.78)	0.08 (0.02)	13 (9/4)	24.17 (4.44)	0.08 (0.03)
USM	32 (29/3)	25.79 (6.09)	0.11 (0.04)	28 (26/2)	25.69 (6.37)	0.12 (0.04)
Total	67 (59/8)	24.63 (4.96)	0.11 (0.04)	54 (48/6)	24.27 (5.61)	0.11 (0.04)
Japanese adult validation dataset						
SWA2	38 (27/11)	28.5 (6.83)	0.10 (0.03)	22 (19/3)	25.77 (5.23)	0.12 (0.05)

Abbreviations: ABIDE: autism brain imaging data exchange, ASD: autism spectrum disorder, COI: Center of Innovation, F: female, FD: frame-wise displacement, M: male, NYU: New York University, KUT: Kyoto University TimTrio, SD: standard deviation, SWA: Showa University, TDC: typically developing control, UTO: University of Tokyo, and USM: University of Utah School of Medicine

*The discovery dataset was matched for the mean FD ($p > 0.05$), except for age and sex ($p < 0.05$).

**The US adult validation cohort was matched for age, sex, and mean FD ($p > 0.05$).

***The Japanese adult validation cohort was matched for age and sex ($p > 0.05$) , but not matched for mean FD ($p < 0.05$)

Table S2. The classification performance of the ASD classifier in the discovery and adult validation datasets.

	AUC	Accuracy [%]	Sensitivity [%]	Specificity [%]	MCC	PPV	NPV
Classification performance on the discovery dataset							
All	**0.84**	**75.62**	**76.11**	**75.45**	**0.46**	**0.50**	**0.91**
COI	-	75.47	-	75.47	-	-	-
KUT	-	77.03	-	77.03	-	-	-
SWA1	0.79	71.16	71.72	70.69	0.42	0.67	0.75
UTO1	-	76.74	-	76.74	-	-	-
UTO2	0.97	91.55	94.29	88.89	0.83	0.89	0.94
Generalizability of ASD classifier to the ABIDE adult dataset							
All	**0.70**	**61.98**	**66.67**	**58.21**	**0.25**	**0.56**	**0.68**
Leuven	0.65	64.29	61.54	66.67	0.28	0.62	0.66
NYU	0.70	57.59	61.54	55.00	0.16	0.47	0.69
USM	0.74	63.33	71.43	56.25	0.29	0.59	0.69
Generalizability of ASD classifier to the Japanese adult dataset							
SWA2	**0.81**	**78.33**	**63.64**	**86.84**	**0.52**	**0.74**	**0.80**

Abbreviations: ABIDE: autism brain imaging data exchange, AUC: area under the curve, COI: Center of Innovation, NYU: New York University, KUT: Kyoto University TimTrio, MCC: Matthews correlation coefficient, SWA: Showa University, UTO: University of Tokyo, and USM: University of Utah School of Medicine

Table S3. Demographic information for the child and adolescent validation datasets.

	TDC			ASD		
	N (M/F)	**Age**	**Mean FD (SD) [mm]**	**N (M/F)**	**Age**	**Mean FD (SD) [mm]**
Child dataset						
GU	13 (6/7)	9.46 (1.08)	0.12 (0.03)	19 (16/3)	10.36 (1.12)	0.12 (0.03)
OHSU	35 (16/19)	9.60 (0.98)	0.10 (0.03)	11 (8/3)	9.64 (1.43)	0.12 (0.04)
KKI	105 (61/44)	10.13 (1.01)	0.12 (0.04)	32 (24/8)	9.81 (1.23)	0.14 (0.03)
NYU	33 (28/5)	9.09 (1.62)	0.10 (0.03)	38 (34/4)	8.81 (1.80)	0.11 (0.04)
UCLA	16 (12/4)	10.30 (1.43)	0.10 (0.04)	19 (17/2)	10.69 (0.97)	0.12 (0.04)
Total	202 (123/79)	9.84 (1.22)	0.11 (0.04)	119 (99/20)	9.70 (1.55)	0.12 (0.04)
Adolescent dataset						
OHSU	12 (8/4)	12.58 (0.79)	0.10 (0.03)	18 (15/3)	13.39 (1.09)	0.12 (0.03)
SDSU	10 (9/1)	15.15 (1.97)	0.09 (0.04)	12 (11/1)	15.37 (1.95)	0.09 (0.03)
NYU	33 (24/9)	14.65 (1.49)	0.09 (0.04)	13 (10/3)	14.19 (1.46)	0.11 (0.03)
TRINITY	13 (13/0)	14.81 (1.60)	0.13 (0.02)	12 (12/0)	15.19 (1.37)	0.14 (0.03)
UCLA	30 (24/6)	13.79 (1.47)	0.09 (0.02)	26 (24/2)	14.73 (1.71)	0.10 (0.03)
UM	10 (7/3)	15.82 (1.75)	0.10 (0.03)	12 (10/2)	15.34 (1.55)	0.12 (0.05)
USM	11 (11/0)	14.81 (1.50)	0.12 (0.03)	18 (18/0)	16.30 (1.27)	0.13 (0.04)
YALE	13 (8/5)	14.85 (1.64)	0.11 (0.04)	10 (7/3)	14.54 (1.92)	0.13 (0.03)
Total	132 (104/28)	14.44 (1.69)	0.10 (0.03)	121 (107/14)	14.86 (1.73)	0.12 (0.04)

Abbreviations: ASD: autism spectrum disorder, GU: Georgetown University, KKI: Kennedy Krieger Institute, NYU: New York UniversityOHSU: Oregon Health and Science University, SD: standard deviation, SDSU: San Diego State University, TDC: typically developing control, TRINITY: Trinity Centre for Health Sciences, UCLA: the University of California, Los Angeles, UM: University of Michigan, USM: University of Utah School of Medicine, and YALE: Yale Child Study Center.

*The child cohort was matched for age ($p > 0.05$), but not matched for sex and mean FD ($p < 0.05$).

**The adolescent cohort was matched for age and sex ($p > 0.05$), but not matched for mean FD ($p < 0.05$).

Table S4. The classification performance of the ASD classifier in the child and adolescent datasets.

	AUC	Accuracy [%]	Sensitivity [%]	Specificity [%]	MCC	PPV	NPV
Generalizability of ASD classifier to the child dataset							
All	**0.66**	**60.75**	**75.63**	**51.98**	**0.27**	**0.48**	**0.78**
GU	0.70	68.75	84.21	46.15	0.33	0.70	0.67
OHSU	0.71	65.23	72.73	62.86	0.30	0.38	0.88
KKI	0.64	56.20	75.00	50.48	0.22	0.32	0.87
NYU	0.62	59.15	71.05	45.45	0.17	0.60	0.58
UCLA	0.68	68.57	78.95	56.25	0.36	0.68	0.69
Generalizability of ASD classifier to the adolescent dataset							
All	**0.71**	**65.61**	**71.07**	**60.61**	**0.32**	**0.62**	**0.70**
OHSU	0.55	46.67	55.56	33.33	-0.112	0.56	0.33
SDSU	0.84	68.18	66.67	70.00	0.37	0.73	0.64
NYU	0.77	67.39	76.92	63.64	0.37	0.45	0.88
TRINITY	0.53	56.00	50.00	61.54	0.12	0.55	0.57
UCLA	0.78	69.64	76.92	63.33	0.40	0.65	0.76
UM	0.63	72.73	91.67	50.00	0.47	0.69	0.83
USM	0.71	68.97	77.78	54.55	0.33	0.74	0.60
YALE	0.74	73.91	70.00	76.92	0.47	0.70	0.77

Abbreviations: ASD: autism spectrum disorder, GU: Georgetown University, KKI: Kennedy Krieger Institute, NPV: negative predictive value, NYU: New York UniversityOHSU: Oregon Health and Science University, PPV: positive predictive value, SD: standard deviation, SDSU: San Diego State University, TDC: typically developing control, TRINITY: Trinity Centre for Health Sciences, UCLA: the University of California, Los Angeles, UM: University of Michigan, USM: University of Utah School of Medicine, and YALE: Yale Child Study Center.

Table S5. The classification performance of the ASD classifier on the discovery dataset without ComBat harmonization method.

	AUC	Accuracy [%]	Sensitivity [%]	Specificity [%]	MCC
Classification performance on the discovery dataset without harmonization					
All	**0.85**	**76.71**	**80.56**	**75.45**	**0.50**
COI	-	80.19	-	80.19	-
KUT	-	89.19	-	89.19	-
SWA1	0.75	66.77	0.793103	56.32	0.36
UTO1	-	79.07	-	79.07	-
UTO2	0.90	87.32	0.857143	88.89	0.75
Generalizability of ASD classifier to the ABIDE adult dataset					
All	**0.64**	**59.50**	**59.23**	**59.70**	**0.19**
Leuven	0.60	57.14	38.46	73.33	0.13
NYU	0.62	51.52	69.23	40.00	0.09
USM	0.70	65.00	64.29	65.63	0.30
Generalizability of ASD classifier to the Japanese adult dataset					
SWA2	**0.73**	**66.67**	**36.36**	**84.21**	**0.23**

Abbreviations: AUC: area under the curve, COI: Center of Innovation, NYU: New York University, KUT: Kyoto University TimTrio, MCC: Matthews correlation coefficient, SWA: Showa University, UTO: University of Tokyo, and USM: University of Utah School of Medicine

Table S6. The classification performance of the ASD classifier trained on SWA1 and UTO2 only.

	AUC	Accuracy [%]	Sensitivity [%]	Specificity [%]	MCC
Classification performance on the balanced discovery dataset					
All	**0.80**	**73.85**	**72.22**	**75.24**	**0.47**
SWA1	0.76	71.16	68.28	73.56	0.42
UTO2	0.96	85.92	88.57	83.33	0.72
Generalizability of ASD classifier to the ABIDE adult dataset					
All	**0.67**	**57.85**	**77.78**	**41.79**	**0.21**
Leuven	0.56	57.14	69.23	46.67	0.16
NYU	0.60	48.48	76.92	30.00	0.08
USM	0.72	63.33	82.14	46.88	0.31
Generalizability of ASD classifier to the Japanese adult dataset					
SWA2	**0.83**	**71.67**	**72.73**	**71.05**	**0.42**

Abbreviations: AUC: area under the curve, COI: Center of Innovation, NYU: New York University, KUT: Kyoto University TimTrio, MCC: Matthews correlation coefficient, SWA: Showa University, UTO: University of Tokyo, and USM: University of Utah School of Medicine

Table S7. The classification performance of the ASD classifier trained on the SRPBS dataset only.

	AUC	Accuracy [%]	Sensitivity [%]	Specificity [%]	MCC
Classification performance on the SRPBS dataset					
All	**0.84**	**76.33**	**77.93**	**75.88**	**0.46**
COI	-	77.36	-	77.36	-
KUT	-	78.38	-	78.38	-
SWA1	0.82	75.24	77.93	72.99	0.51
UTO	-	75.58	-	75.58	-
Generalizability of ASD classifier to the ABIDE adult dataset					
All	**0.70**	**62.81**	**59.26**	**65.67**	**0.25**
Leuven	0.65	60.71	53.85	66.67	0.21
NYU	0.68	60.61	53.85	65.00	0.19
USM	0.74	65.00	64.29	65.63	0.30
Generalizability of ASD classifier to the Japanese adult dataset					
SWA2	**0.82**	**73.33**	**63.64**	**78.95**	**0.43**

Abbreviations: AUC: area under the curve, COI: Center of Innovation, NYU: New York University, KUT: Kyoto University TimTrio, MCC: Matthews correlation coefficient, SWA: Showa University, UTO: University of Tokyo, and USM: University of Utah School of Medicine

Table S8. Comparisons of classification and generalization performance between higher/lower resolutions of regions of interest.

Atlas	AUC	Accuracy [%]	Sensitivity [%]	Specificity [%]	MCC
Classification performance on the discovery dataset					
Glasser	0.84	**75.62**	76.11	**75.45**	0.46
Schaefer 100	0.81	71.91	72.78	71.64	0.39
Schaefer 200	**0.85**	75.48	**80.56**	73.82	**0.48**
Schaefer 300	0.82	73.70	75.56	73.09	0.43
Schaefer 400	0.83	74.52	78.89	73.09	0.46
Schaefer 500	0.82	74.52	76.67	73.82	0.45
Schaefer 600	0.83	74.11	77.22	73.09	0.44
Schaefer 700	0.83	74.38	77.78	73.27	0.45
Schaefer 800	0.83	73.42	76.67	72.36	0.43
Schaefer 900	0.83	73.42	75.56	72.73	0.43
Generalizability on the ABIDE adult dataset					
Glasser	0.70	61.98	66.67	58.21	0.25
Schaefer 100	0.70	65.29	64.81	65.67	0.30
Schaefer 200	0.73	65.29	59.26	70.15	0.30
Schaefer 300	0.70	65.29	57.41	**71.64**	0.29
Schaefer 400	0.72	66.12	59.26	**71.64**	0.31
Schaefer 500	**0.75**	**71.07**	74.07	68.66	0.42
Schaefer 600	0.73	69.42	68.52	70.15	0.39
Schaefer 700	0.72	67.77	74.07	62.69	0.37
Schaefer 800	0.72	66.94	64.81	68.66	0.33
Schaefer 900	0.72	**71.07**	**77.78**	65.67	**0.43**
Generalizability on the Japanese adult dataset					
Glasser	0.81	**78.33**	63.64	**86.84**	0.52
Schaefer 100	0.84	76.67	**86.36**	71.05	**0.55**
Schaefer 200	0.83	73.33	68.18	76.32	0.44
Schaefer 300	0.84	71.67	72.73	71.05	0.42
Schaefer 400	0.84	76.67	72.73	78.95	0.51
Schaefer 500	0.84	76.67	72.73	78.95	0.51
Schaefer 600	0.83	73.33	63.64	78.95	0.43
Schaefer 700	0.82	70.00	68.18	71.05	0.38
Schaefer 800	0.82	73.33	72.73	73.68	0.45
Schaefer 900	**0.85**	71.67	77.27	68.42	0.44

Abbreviations: ABIDE: autism brain imaging data exchange, AUC: area under the curve, and MCC: Matthews correlation coefficient.

Table S9. The list of discriminative FCs for the ASD diagnosis.

ROI 1			ROI 2			*z*(ASD)	*z*(TDC)	*t*-value	Mean weight
Glasser's label	**AAL label**	**Network**	**Glasser's label**	**AAL label**	**Network**				
R.Amy	Hippocampus_R	Subcortical	R.A5	Temporal_Sup_R	Somatomotor	0.12	0.01	8.03	1.51
R.PBelt	Temporal_Sup_R	Somatomotor	L.POS2	Precuneus_L	FPN	0.03	-0.08	7.42	0.48
R.25	Olfactory_R	Limbic	L.PHT	Temporal_Mid_L	DAN	0.01	-0.05	4.32	0.41
R.MBelt	Heschl_R	Somatomotor	R.LIPv	Parietal_Inf_R	DAN	-0.02	-0.08	4.51	0.41
R.A5	Temporal_Sup_R	Somatomotor	R.23d	Cingulum_Mid_R	DMN	0.12	0.01	6.73	0.35
R.PBelt	Temporal_Sup_R	Somatomotor	L.IFJp	Frontal_Inf_Oper_L	DAN	0.08	0.03	3.90	0.26
R.p24	Cingulum_Ant_R	FPN	R.A5	Temporal_Sup_R	Somatomotor	0.12	0.01	7.62	0.26
R.MidB	-	Subcortical	R.TGd	Temporal_Pole_Mid_R	Limbic	0.03	-0.06	5.70	0.26
R.VMV2	Lingual_R	Visual	L.STGa	Temporal_Pole_Sup_L	Limbic	0.03	-0.01	3.53	0.25
L.TGd	Temporal_Pole_Mid_L	Limbic	L.FOP1	Rolandic_Oper_L	VAN	-0.10	-0.15	3.28	0.24
R.Amy	Hippocampus_R	Subcortical	L.TGd	Temporal_Pole_Mid_L	Limbic	0.01	-0.04	4.22	0.21
R.Amy	Hippocampus_R	Subcortical	R.6d	Precentral_R	Somatomotor	0.07	-0.04	7.20	0.16
R.PCV	Precuneus_R	FPN	L.a9-46v	Frontal_Mid_L	FPN	-0.01	-0.09	5.00	0.16
R.Pallidum	Pallidum_R	Subcortical	L.MST	Occipital_Mid_L	Visual	0.02	-0.05	5.97	0.15
R.s32	Frontal_Med_Orb_R	DMN	L.MIP	Parietal_Sup_L	DAN	-0.06	-0.11	3.65	0.15

R.6v	Precentral_R	Somatomotor	L.MI	Insula_L	VAN	0.21	0.12	6.09	0.14
R.s32	Frontal_Med_Orb_R	DMN	L.V6	Cuneus_L	Visual	-0.07	-0.11	2.42	0.14
L.MidB	-	Subcortical	R.STSda	Temporal_Sup_R	DMN	0.15	0.04	6.85	0.14
R.SFL	Supp_Motor_Area_R	DMN	R.V3A	Occipital_Sup_R	Visual	0.00	-0.09	6.56	0.13
L.MidB	-	Subcortical	R.TPOJ1	Temporal_Mid_R	VAN	0.01	-0.06	5.68	0.12
R.p47r	Frontal_Inf_Tri_R	FPN	L.TPOJ2	Temporal_Mid_L	DAN	-0.07	-0.13	3.51	0.12
R.VIP	Parietal_Sup_R	DAN	L.FEF	Precentral_L	DAN	0.28	0.20	4.43	0.11
L.FFC	Fusiform_L	Visual	L.RSC	-	DMN	-0.08	-0.14	4.59	0.11
R.VMV2	Lingual_R	Visual	R.STGa	Temporal_Pole_Sup_R	DMN	0.02	-0.01	2.87	0.11
R.p24	Cingulum_Ant_R	FPN	R.A4	Temporal_Sup_R	Somatomotor	0.10	0.02	5.49	0.11
L.OFC	Rectus_L	Limbic	L.6r	Frontal_Inf_Oper_L	VAN	-0.03	-0.07	2.92	0.10
R.HC	Hippocampus_R	Subcortical	L.A5	Temporal_Mid_L	DMN	0.12	0.04	6.02	0.10
R.PGp	Occipital_Mid_R	DAN	L.A1	Rolandic_Oper_L	Somatomotor	-0.01	-0.08	5.06	0.10
R.LIPv	Parietal_Inf_R	DAN	L.6v	Precentral_L	Somatomotor	0.28	0.20	4.89	0.10
R.SFL	Supp_Motor_Area_R	DMN	L.V3A	Occipital_Sup_L	Visual	0.02	-0.07	6.92	0.10
L.V7	Occipital_Mid_L	Visual	L.RSC	-	DMN	-0.04	-0.12	5.23	0.10
R.6v	Precentral_R	Somatomotor	L.5mv	Cingulum_Mid_L	VAN	0.15	0.06	5.64	0.10
R.47m	Frontal_Inf_Orb_R	DMN	R.v23ab	Precuneus_R	DMN	0.27	0.16	5.67	0.10
R.LBelt	Temporal_Sup_R	Somatomotor	R.7Pm	Precuneus_R	FPN	-0.04	-0.09	4.28	0.09
R.V3CD	Occipital_Mid_R	Visual	L.MBelt	Temporal_Sup_L	Somatomotor	-0.02	-0.08	4.63	0.09

L.Pallidum	Pallidum_L	Subcortical	L.TE2a	Temporal_Inf_L	Limbic	0.00	-0.06	3.34	0.09
R.VMV2	Lingual_R	Visual	R.TGd	Temporal_Pole_Mid_R	Limbic	0.00	-0.04	2.51	0.09
R.6d	Precentral_R	Somatomotor	L.FEF	Precentral_L	DAN	0.19	0.12	3.47	0.08
R.PFm	Parietal_Inf_R	DMN	R.d32	Cingulum_Ant_R	DMN	0.38	0.29	5.23	0.08
R.PCV	Precuneus_R	FPN	L.AVI	Insula_L	FPN	0.00	-0.05	3.99	0.08
R.MidB	-	Subcortical	R.PBelt	Temporal_Sup_R	Somatomotor	0.17	0.06	6.65	0.08
L.MidB	-	Subcortical	L.PHA2	ParaHippocampal_L	DMN	0.15	0.08	4.99	0.08
R.Putamen	Putamen_R	Subcortical	R.A5	Temporal_Sup_R	Somatomotor	0.05	-0.03	6.36	0.08
R.MidB	-	Subcortical	R.TE1a	Temporal_Mid_R	DMN	-0.02	-0.09	4.71	0.08
L.A5	Temporal_Mid_L	DMN	L.9m	Frontal_Sup_Medial_L	DMN	0.26	0.16	5.88	0.07
R.IP1	Angular_R	DAN	R.PGp	Occipital_Mid_R	DAN	0.26	0.16	4.63	0.07
R.Amy	Hippocampus_R	Subcortical	R.TGd	Temporal_Pole_Mid_R	Limbic	-0.01	-0.07	4.23	0.07
R.PCV	Precuneus_R	FPN	L.a32pr	Cingulum_Ant_L	FPN	0.10	0.03	4.15	0.07
R.6ma	Frontal_Sup_R	DAN	L.PreS	ParaHippocampal_L	DMN	-0.05	-0.08	2.14	0.07
R.25	Olfactory_R	Limbic	R.PHT	Temporal_Inf_R	DAN	0.01	-0.04	3.90	0.06
R.s32	Frontal_Med_Orb_R	DMN	L.7AL	Parietal_Sup_L	DAN	-0.06	-0.10	2.59	0.06
R.PHT	Temporal_Inf_R	DAN	L.a24	Cingulum_Ant_L	DMN	-0.13	-0.16	2.25	0.06
R.SFL	Supp_Motor_Area_R	DMN	L.9-46d	Frontal_Mid_L	VAN	0.14	0.05	4.71	0.06
R.IPS1	Occipital_Sup_R	DAN	L.6v	Precentral_L	Somatomotor	0.20	0.12	4.39	0.06
R.HC	Hippocampus_R	Subcortical	L.V7	Occipital_Mid_L	Visual	-0.02	-0.08	5.10	0.06
R.25	Olfactory_R	Limbic	R.IPS1	Occipital_Sup_R	DAN	-0.04	-0.09	3.94	0.06
R.s6-8	Frontal_Sup_R	FPN	L.a9-46v	Frontal_Mid_L	FPN	0.09	0.04	2.40	0.06

R.VIP	Parietal_Sup_R	DAN	L.LO2	Occipital_Inf_L	Visual	0.22	0.14	4.01	0.06
R.7Pm	Precuneus_R	FPN	L.A1	Rolandic_Oper_L	Somatomotor	-0.05	-0.10	4.05	0.05
R.6v	Precentral_R	Somatomotor	L.PF	SupraMarginal_L	VAN	0.22	0.10	6.88	0.05
L.OFC	Rectus_L	Limbic	L.IFSa	Frontal_Inf_Tri_L	FPN	0.05	0.01	3.21	0.05
R.7PL	Parietal_Sup_R	DAN	R.LO2	Occipital_Inf_R	Visual	0.09	0.04	2.85	0.05
R.6mp	Supp_Motor_Area_R	Somatomotor	R.5L	Postcentral_R	DAN	0.60	0.54	2.99	0.05
R.p32pr	Cingulum_Mid_R	VAN	R.7Pm	Precuneus_R	FPN	-0.03	-0.08	2.84	0.05
L.p47r	Frontal_Inf_Tri_L	FPN	L.10d	Frontal_Sup_Medial_L	DMN	0.10	0.05	2.16	0.05
R.10d	Frontal_Sup_Medial_R	DMN	L.9p	Frontal_Sup_L	DMN	0.25	0.34	-3.93	-0.03
R.46	Frontal_Mid_R	FPN	R.47m	Frontal_Inf_Orb_R	DMN	-0.08	0.01	-5.19	-0.03
R.Ig	Insula_R	Somatomotor	R.FOP2	Rolandic_Oper_R	Somatomotor	0.47	0.54	-3.97	-0.04
L.LBelt	Temporal_Sup_L	Somatomotor	L.Ig	Insula_L	Somatomotor	0.24	0.30	-3.88	-0.04
R.9m	Frontal_Sup_Medial_R	DMN	R.PCV	Precuneus_R	FPN	0.00	0.11	-5.49	-0.04
R.TPOJ1	Temporal_Mid_R	VAN	R.4	Precentral_R	Somatomotor	0.08	0.17	-5.65	-0.04
L.PFcm	Temporal_Sup_L	Somatomotor	L.PSL	Temporal_Sup_L	VAN	0.40	0.45	-2.62	-0.05
L.p10p	Frontal_Sup_L	DMN	L.25	Olfactory_L	Limbic	-0.03	0.03	-3.45	-0.05
R.47l	Frontal_Inf_Orb_R	DMN	L.47l	Frontal_Inf_Orb_L	DMN	0.48	0.56	-4.05	-0.05
L.VMV1	Lingual_L	Visual	L.TPOJ3	Occipital_Mid_L	DAN	0.08	0.16	-4.35	-0.05
R.Pir	Insula_R	Limbic	L.V3	Occipital_Sup_L	Visual	-0.10	-0.05	-3.85	-0.05
R.TPOJ1	Temporal_Mid_R	VAN	L.A5	Temporal_Mid_L	DMN	0.33	0.43	-4.98	-0.05

R.p24	Cingulum_Ant_R	FPN	L.9m	Frontal_Sup_Medial_L	DMN	0.27	0.34	-3.69	-0.05
R.TPOJ1	Temporal_Mid_R	VAN	L.MT	Occipital_Mid_L	Visual	0.05	0.16	-5.72	-0.06
R.STSdp	Temporal_Sup_R	DMN	L.V4t	Occipital_Mid_L	Visual	-0.04	0.01	-3.92	-0.06
R.MidB	-	Subcortical	R.46	Frontal_Mid_R	FPN	-0.01	0.07	-6.02	-0.06
R.8Ad	Frontal_Mid_R	DMN	R.FFC	Fusiform_R	Visual	-0.20	-0.15	-3.76	-0.06
R.5m	Paracentral_Lobule_R	Somatomotor	L.STV	Temporal_Sup_L	DMN	-0.03	0.04	-4.74	-0.06
L.TE2p	Temporal_Inf_L	DAN	L.10d	Frontal_Sup_Medial_L	DMN	-0.18	-0.12	-3.69	-0.06
R.FFC	Fusiform_R	Visual	L.55b	Precentral_L	DAN	-0.07	0.00	-4.34	-0.06
R.5L	Postcentral_R	DAN	L.STV	Temporal_Sup_L	DMN	-0.03	0.04	-5.17	-0.06
R.9m	Frontal_Sup_Medial_R	DMN	L.SFL	Supp_Motor_Area_L	DMN	0.24	0.30	-3.21	-0.06
R.MidB	-	Subcortical	L.a9-46v	Frontal_Mid_L	FPN	0.01	0.10	-6.07	-0.06
R.Cereb	Cerebellum_R	Subcortical	L.44	Frontal_Inf_Oper_L	DMN	-0.03	0.05	-5.80	-0.06
L.Putamen	Putamen_L	Subcortical	R.A4	Temporal_Sup_R	Somatomotor	-0.02	0.06	-6.26	-0.07
R.p32	Frontal_Sup_Medial_R	DMN	L.d23ab	Cingulum_Post_L	DMN	0.16	0.22	-3.66	-0.07
R.A4	Temporal_Sup_R	Somatomotor	R.TE2p	Temporal_Inf_R	DAN	-0.05	0.04	-6.49	-0.07
R.v23ab	Precuneus_R	DMN	L.v23ab	Precuneus_L	DMN	0.96	1.05	-4.49	-0.07
R.RSC	Cingulum_Post_R	DMN	L.RSC	-	DMN	1.03	1.08	-2.94	-0.07
R.PHA2	ParaHippocampal_R	Visual	R.a24	Cingulum_Ant_R	DMN	0.09	0.14	-3.22	-0.07
R.VMV1	Lingual_R	Visual	L.PCV	Precuneus_L	DMN	-0.01	0.08	-5.31	-0.07
L.A5	Temporal_Mid_L	DMN	L.PIT	Fusiform_L	Visual	-0.08	0.00	-5.49	-0.07
L.TPOJ3	Occipital_Mid_L	DAN	L.ProS	Precuneus_L	Visual	0.10	0.17	-3.85	-0.08
R.TPOJ1	Temporal_Mid_R	VAN	L.V4t	Occipital_Mid_L	Visual	0.00	0.11	-6.48	-0.08

R.VMV2	Lingual_R	Visual	L.PCV	Precuneus_L	DMN	0.04	0.12	-4.36	-0.08
R.a10p	Frontal_Sup_Orb_R	FPN	L.47m	Frontal_Inf_Orb_L	DMN	-0.09	0.01	-4.66	-0.08
R.MidB	-	Subcortical	B.Stem	-	Subcortical	0.23	0.31	-5.40	-0.08
R.TGv	Temporal_Inf_R	Limbic	R.TGd	Temporal_Pole_Mid_R	Limbic	0.49	0.58	-3.73	-0.08
R.8Av	Frontal_Mid_R	FPN	L.V3B	Occipital_Mid_L	Visual	-0.23	-0.17	-3.89	-0.08
R.25	Olfactory_R	Limbic	R.SCEF	Supp_Motor_Area_R	VAN	-0.15	-0.08	-5.38	-0.08
R.VMV2	Lingual_R	Visual	R.7Am	Precuneus_R	DAN	0.08	0.14	-3.79	-0.08
R.10pp	Frontal_Sup_Orb_R	Limbic	L.47m	Frontal_Inf_Orb_L	DMN	-0.09	0.01	-4.50	-0.09
R.VMV2	Lingual_R	Visual	R.DVT	Cuneus_R	DMN	0.29	0.38	-4.71	-0.09
R.Cereb	Cerebellum_R	Subcortical	R.LIPd	Angular_R	DAN	-0.12	-0.06	-5.12	-0.09
L.SFL	Supp_Motor_Area_L	DMN	L.POS2	Precuneus_L	FPN	-0.08	0.00	-5.44	-0.09
R.V6A	Occipital_Sup_R	Visual	L.9-46d	Frontal_Mid_L	VAN	-0.12	-0.07	-3.21	-0.10
R.23c	Cingulum_Mid_R	VAN	L.STSdp	Temporal_Mid_L	DMN	-0.09	-0.03	-4.05	-0.10
L.Pallidum	Pallidum_L	Subcortical	L.Thalamus	Thalamus_L	Subcortical	-0.02	0.05	-5.07	-0.10
R.PGi	Angular_R	DMN	R.6v	Precentral_R	Somatomotor	-0.18	-0.08	-6.36	-0.10
L.HP	Hippocampus_L	Subcortical	B.Stem	-	Subcortical	0.87	0.96	-4.96	-0.10
R.RSC	Cingulum_Post_R	DMN	L.SFL	Supp_Motor_Area_L	DMN	-0.09	-0.01	-5.22	-0.10
R.A4	Temporal_Sup_R	Somatomotor	L.A5	Temporal_Mid_L	DMN	0.37	0.51	-6.16	-0.10
R.SFL	Supp_Motor_Area_R	DMN	L.POS1	Precuneus_L	DMN	-0.18	-0.08	-6.57	-0.10
R.47s	Insula_R	DMN	L.a10p	Frontal_Sup_Orb_L	DMN	-0.01	0.08	-4.94	-0.10
R.RSC	Cingulum_Post_R	DMN	L.10pp	Frontal_Sup_Orb_L	Limbic	0.00	0.05	-3.88	-0.10
R.pOFC	Olfactory_R	Limbic	L.TGv	Temporal_Inf_L	Limbic	0.07	0.16	-4.90	-0.11
R.HC	Hippocampus_R	Subcortical	R.46	Frontal_Mid_R	FPN	0.07	0.15	-6.21	-0.11

L.VMV1	Lingual_L	Visual	L.STV	Temporal_Sup_L	DMN	0.01	0.09	-5.18	-0.12
R.A5	Temporal_Sup_R	Somatomotor	R.PBelt	Temporal_Sup_R	Somatomotor	0.15	0.29	-5.83	-0.12
R.Pir	Insula_R	Limbic	L.a10p	Frontal_Sup_Orb_L	DMN	-0.08	-0.02	-4.15	-0.12
L.LBelt	Temporal_Sup_L	Somatomotor	L.RI	Rolandic_Oper_L	Somatomotor	0.57	0.65	-3.96	-0.13
L.PFop	SupraMarginal_L	VAN	L.9m	Frontal_Sup_Medial_L	DMN	-0.30	-0.19	-5.77	-0.13
R.ProS	Lingual_R	Visual	L.TPOJ1	Temporal_Mid_L	DMN	-0.02	0.06	-4.96	-0.15
R.ProS	Lingual_R	Visual	L.TPOJ2	Temporal_Mid_L	DAN	0.00	0.07	-4.70	-0.15
R.Amy	Hippocampus_R	Subcortical	L.IFSa	Frontal_Inf_Tri_L	FPN	0.09	0.19	-7.22	-0.17
R.25	Olfactory_R	Limbic	R.24dd	Cingulum_Mid_R	Somatomotor	-0.11	-0.04	-4.77	-0.17
L.STSda	Temporal_Mid_L	DMN	L.MST	Occipital_Mid_L	Visual	-0.05	0.04	-6.27	-0.18
R.PGi	Angular_R	DMN	R.SFL	Supp_Motor_Area_R	DMN	0.16	0.24	-4.44	-0.18
R.24dv	Cingulum_Mid_R	Somatomotor	L.PI	Temporal_Sup_L	VAN	0.02	0.10	-5.18	-0.22
R.p32	Frontal_Sup_Medial_R	DMN	L.31a	Cingulum_Mid_L	DMN	0.08	0.15	-4.29	-0.22
R.s32	Frontal_Med_Orb_R	DMN	R.PHA2	ParaHippocampal_R	Visual	0.11	0.16	-3.52	-0.22
R.TE2p	Temporal_Inf_R	DAN	L.55b	Precentral_L	DAN	-0.12	-0.05	-4.40	-0.22
R.SFL	Supp_Motor_Area_R	DMN	L.IP1	Occipital_Mid_L	DAN	-0.19	-0.09	-6.90	-0.29
R.Pallidum	Pallidum_R	Subcortical	R.Putamen	Putamen_R	Subcortical	0.27	0.33	-4.12	-0.31
R.pOFC	Olfactory_R	Limbic	R.10pp	Frontal_Sup_Orb_R	Limbic	0.09	0.19	-5.11	-0.34
R.s32	Frontal_Med_Orb_R	DMN	R.H	Hippocampus_R	DMN	0.12	0.20	-4.76	-0.81

Abbreviations: ASD: autism spectrum disorder, DAN: dorsal attention network, DMN: default mode network, FP: fronto-parietal, TDC: typically developing control, and VAN: ventral attention network.

Table S10. The list of discriminative FCs reproducible across the five datasets.

ROI 1			ROI 2			Discovery dataset			Child cohort			Adolescent cohort			US adult cohort			Japanese adult cohort		
Glasser	**AAL label**	**Network**	**Glasser**	**AAL label**	**Network**	***z*(ASD)**	***z*(TDC)**	***t*-value**	***z*(ASD)**	***z*(TDC)**	***t*-value**	***z*(ASD)**	***z*(TDC)**	***t*-value**	***z*(ASD)**	***z*(TDC)**	***t*-value**	***z*(ASD)**	***z*(TDC)**	***t*-value**
R.Amy	Hippocampus_R	Subcortical	R.A5	Temporal_Sup_R	Somatomotor	0.12	0.01	8.03	0.15	0.11	1.84	0.10	0.06	1.26	-0.02	-0.06	1.33	0.10	0.00	2.77
R.PBelt	Temporal_Sup_R	Somatomotor	L.POS2	Precuneus_L	FPN	0.03	-0.08	7.42	-0.03	-0.09	2.88	0.01	-0.06	3.49	-0.02	-0.06	1.50	0.08	0.01	2.00
R.Amy	Hippocampus_R	Subcortical	R.6d	Precentral_R	Somatomotor	0.07	-0.04	7.20	0.05	0.05	0.32	0.07	0.05	0.85	0.06	-0.09	4.65	0.13	0.01	3.21
L.MidB	-	Subcortical	R.STSda	Temporal_Sup_R	DMN	0.15	0.04	6.85	0.07	0.04	1.54	0.10	0.05	2.27	0.07	0.00	2.38	0.09	0.02	1.68
R.MidB	-	Subcortical	R.PBelt	Temporal_Sup_R	Somatomotor	0.17	0.06	6.65	0.13	0.12	0.66	0.09	0.06	1.50	0.06	-0.02	2.44	0.14	0.07	1.60
R.Putamen	Putamen_R	Subcortical	R.A5	Temporal_Sup_R	Somatomotor	0.05	-0.03	6.36	0.04	0.03	0.81	0.05	0.02	1.36	0.00	-0.06	1.91	0.04	-0.01	1.70
R.HC	Hippocampus_R	Subcortical	L.A5	Temporal_Mid_L	DMN	0.12	0.04	6.02	0.13	0.13	0.12	0.09	0.07	1.07	0.02	-0.03	1.56	0.11	0.03	2.09
R.Pallidum	Pallidum_R	Subcortical	L.MST	Occipital_Mid_L	Visual	0.02	-0.05	5.97	0.04	0.01	1.53	0.04	0.00	2.46	0.00	-0.02	0.43	0.00	-0.05	2.26

R.MidB	-	Subcortical	R.TGd	Temporal_Pole_Mid_R	Limbic	0.03	-0.06	5.70	0.00	-0.05	2.34	-0.02	-0.05	1.25	0.03	-0.05	2.60	-0.05	-0.08	0.82
L.MidB	-	Subcortical	R.TPOJ1	Temporal_Mid_R	DAN	0.01	-0.06	5.68	0.04	-0.01	2.29	0.02	-0.02	1.63	-0.01	-0.10	2.82	0.03	-0.05	2.23
L.V7	Occipital_Mid_L	Visual	L.RSC	-	DMN	-0.04	-0.12	5.23	-0.01	-0.06	2.57	-0.03	-0.05	1.31	-0.04	-0.07	1.02	-0.09	-0.15	1.88
R.PFm	Parietal_Inf_R	DMN	R.d32	Cingulum_Ant_R	DMN	0.38	0.29	5.23	0.34	0.31	1.44	0.35	0.32	1.31	0.33	0.29	0.96	0.34	0.31	0.58
R.MidB	-	Subcortical	R.TE1a	Temporal_Mid_R	DMN	-0.02	-0.09	4.71	-0.05	-0.12	3.33	-0.09	-0.14	2.03	-0.04	-0.09	1.72	-0.06	-0.10	1.12
R.SFL	Supp_Motor_Area_R	DMN	L.9-46d	Frontal_Mid_L	DAN	0.14	0.05	4.71	0.13	0.09	1.88	0.12	0.03	3.66	0.10	0.06	0.85	0.12	0.07	0.73
R.Amy	Hippocampus_R	Subcortical	R.TGd	Temporal_Pole_Mid_R	Limbic	-0.01	-0.07	4.23	-0.02	-0.04	0.80	0.01	-0.02	1.40	0.04	-0.02	1.82	-0.02	-0.05	0.69
R.7Pm	Precuneus_R	FPN	L.A1	Rolandic_Oper_L	Somatomotor	-0.05	-0.10	4.05	-0.11	-0.12	0.66	-0.08	-0.10	0.55	-0.08	-0.08	0.09	-0.03	-0.07	1.63
R.PCV	Precuneus_R	FPN	L.AVI	Insula_L	FPN	0.00	-0.05	3.99	-0.03	-0.04	0.76	-0.02	-0.11	3.73	-0.06	-0.08	0.78	0.06	-0.04	2.63
R.25	Olfactory_R	Limbic	R.IPS1	Occipital_Sup_R	DAN	-0.04	-0.09	3.94	-0.05	-0.11	3.00	-0.07	-0.08	0.19	-0.01	-0.03	0.62	-0.06	-0.09	1.09
R.25	Olfactory_R	Limbic	R.PHT	Temporal_Inf_R	DAN	0.01	-0.04	3.90	-0.02	-0.06	1.76	-0.03	-0.04	0.07	-0.02	-0.05	1.04	-0.05	-0.11	1.46

L.Pallidum	Pallidum_L	Subcortical	L.TE2a	Temporal_Inf_L	Limbic	0.00	-0.06	3.34	-0.03	-0.06	1.38	0.02	0.01	0.50	0.03	0.00	0.87	-0.03	-0.04	0.54
R.s6-8	Frontal_Sup_R	FPN	L.a9-46v	Frontal_Mid_L	FPN	0.09	0.04	2.40	0.03	0.02	0.48	0.07	0.02	2.02	0.11	0.05	1.72	0.10	0.06	0.75
L.p47r	Frontal_Inf_Tri_L	FPN	L.10d	Frontal_Sup_Medial_L	DMN	0.10	0.05	2.16	0.15	0.06	2.99	0.17	0.06	3.24	0.05	-0.03	1.56	0.04	0.02	0.21
R.RSC	Cingulum_Post_R	DMN	L.RSC	-	DMN	1.03	1.08	-2.94	1.02	1.08	-2.14	1.03	1.09	-2.05	0.92	0.96	-0.94	1.06	1.11	-1.08
L.LBelt	Temporal_Sup_L	Somatomotor	L.Ig	Insula_L	Somatomotor	0.24	0.30	-3.88	0.27	0.33	-2.59	0.31	0.39	-2.98	0.26	0.28	-0.51	0.40	0.41	-0.22
R.STSdp	Temporal_Sup_R	DMN	L.V4t	Occipital_Mid_L	Visual	-0.04	0.01	-3.92	0.02	0.05	-1.52	-0.02	0.05	-3.01	0.00	0.03	-1.04	-0.04	0.04	-2.08
R.47l	Frontal_Inf_Orb_R	DMN	L.47l	Frontal_Inf_Orb_L	DMN	0.48	0.56	-4.05	0.53	0.55	-0.71	0.52	0.59	-2.56	0.54	0.58	-1.06	0.61	0.62	-0.01
R.23c	Cingulum_Mid_R	VAN	L.STSdp	Temporal_Mid_L	DMN	-0.09	-0.03	-4.05	-0.05	-0.02	-1.55	-0.10	-0.03	-3.38	-0.07	-0.02	-1.40	-0.16	-0.05	-2.46
R.FFC	Fusiform_R	Visual	L.55b	Precentral_L	DAN	-0.07	0.00	-4.34	0.03	0.05	-0.58	0.00	0.06	-2.26	0.03	0.03	-0.09	0.01	0.03	-0.68
R.ProS	Lingual_R	Visual	L.TPOJ2	Temporal_Mid_L	DAN	0.00	0.07	-4.70	0.00	0.04	-1.70	0.01	0.03	-0.68	-0.02	0.03	-1.41	0.04	0.07	-0.82

L.HP	Hippocampus_L	Subcortical	B.Stem	-	Subcortical	0.87	0.96	-4.96	0.82	0.86	-1.82	0.91	0.94	-1.46	0.82	0.84	-0.47	1.06	1.13	-1.55
R.PrOS	Lingual_R	Visual	L.TPOJ1	Temporal_Mid_L	DMN	-0.02	0.06	-4.96	-0.01	0.03	-1.67	-0.05	0.02	-2.72	-0.02	0.04	-1.77	-0.03	0.04	-2.26
R.24dv	Cingulum_Mid_R	Somatomotor	L.PI	Temporal_Sup_L	DAN	0.02	0.10	-5.18	0.06	0.10	-2.63	0.08	0.08	-0.20	0.05	0.08	-1.01	0.15	0.19	-0.82
R.MidB	-	Subcortical	B.Stem	-	Subcortical	0.23	0.31	-5.40	0.25	0.30	-2.30	0.22	0.27	-1.95	0.23	0.26	-0.81	0.22	0.33	-3.07
R.9m	Frontal_Sup_Medial_R	DMN	R.PCV	Precuneus_R	FPN	0.00	0.11	-5.49	0.07	0.09	-1.06	0.04	0.07	-1.20	-0.02	0.05	-1.53	0.05	0.12	-1.13
R.TPOJ1	Temporal_Mid_R	VAN	R.4	Precentral_R	Somatomotor	0.08	0.17	-5.65	0.07	0.10	-1.47	0.10	0.12	-0.75	0.11	0.13	-0.59	0.13	0.16	-0.72
R.TPOJ1	Temporal_Mid_R	VAN	L.MT	Occipital_Mid_L	Visual	0.05	0.16	-5.72	0.10	0.12	-0.81	0.09	0.13	-1.66	0.10	0.14	-1.07	0.08	0.15	-1.29
R.A5	Temporal_Sup_R	Somatomotor	R.PBelt	Temporal_Sup_R	Somatomotor	0.15	0.29	-5.83	0.16	0.17	-0.72	0.16	0.22	-2.05	0.15	0.22	-2.03	0.20	0.35	-2.26
R.MidB	-	Subcortical	R.46	Frontal_Mid_R	FPN	-0.01	0.07	-6.02	0.00	0.03	-1.67	-0.01	0.06	-3.49	-0.02	0.01	-0.94	-0.01	0.03	-1.16
R.MidB	-	Subcortical	L.a9-46v	Frontal_Mid_L	FPN	0.01	0.10	-6.07	0.04	0.05	-0.37	0.03	0.08	-2.43	0.03	0.09	-2.10	0.03	0.08	-1.30

R.A4	Temporal_Sup_R	Somatomotor	L.A5	Temporal_Mid_L	DMN	0.37	0.51	-6.16	0.39	0.44	-1.88	0.34	0.47	-4.56	0.35	0.44	-2.08	0.67	0.70	-0.35
R.HC	Hippocampus_R	Subcortical	R.A6	Frontal_Mid_R	FPN	0.07	0.15	-6.21	0.06	0.08	-1.33	0.07	0.10	-1.53	0.03	0.08	-1.72	0.07	0.12	-1.14
L.Putamen	Putamen_L	Subcortical	R.A4	Temporal_Sup_R	Somatomotor	-0.02	0.06	-6.26	0.06	0.06	-0.31	0.05	0.07	-1.06	0.03	0.12	-2.81	0.09	0.10	-0.43

Abbreviations: ASD: autism spectrum disorder, FP: fronto-parietal, DAN: dorsal attention network, DMN: default mode network, HP: hippocampus, MOG: middle occpital gyrus, MTG: middle temporal gyrus, MFG: middle frontal gyrus, SFG: superior frontal gyrus, FUS: fusiform gyrus, IFG: inferior frontal gyrus, Precent: Precentral gyrus, ITG: inferior temporal gyrus, IPL: inferior parietal lobule, ROI: region of interest, STG: superior temporal gyrus, TDC: typically developing control, VAN: ventral attention network

Table S11. Demographic information of SCZ and MDD datasets.

	SCZ			**MDD**		
	N (M/F)	**Age**	**Mean FD [mm]**	**N (M/F)**	**Age**	**Mean FD [mm]**
COI	-	-	-	52 (23/29)	45.23 (12.64)	0.16 (0.06)
KUT	42/ (20/22)	41.90 (10.43)	0.14 (0.06)	15 (9/6)	43.93 (11.60)	0.10 (0.04)
SWA1	18 (14/4)	42.83 (8.65)	0.19 (0.06)	-	-	-
UTO1	34 (24/10)	30.91 (10.42)	0.11 (0.03)	59 (35/24)	38.19 (11.44)	0.10 (0.04)
UTO2	-	-	-	-	-	-
Total	94 (58/36)	38.11 (11.40)	0.14 (0.06)	126 (67/59)	41.78 (12.35)	0.13 (0.06)

Abbreviations: ASD: autism spectrum disorder, COI: Center of Innovation, F: female, KUT: Kyoto University TimTrio, M: male, MDD: major depressive disorder, SCZ: schizophrenia, SD: standard deviation, SWA: Showa University, TDC: typically developing control, and UTO: University of Tokyo.

Table S12. The classification performance of the SCZ and MDD neuromarkers.

	AUC	Accuracy [%]	Sensitivity [%]	Specificity [%]	MCC
Classification performance of SCZ neuromarker					
All	**0.89**	**81.99**	**82.98**	**81.82**	**0.51**
COI	-	65.09	-	65.09	-
KUT	0.91	84.74	83.33	85.14	0.62
SWA1	0.96	85.94	88.89	85.63	0.53
UTO1	0.82	82.50	79.41	83.72	0.60
UTO2	-	94.44	-	94.44	-
Classification performance of MDD neuromarker					
All	**0.78**	**67.60**	**74.60**	**66.00**	**0.32**
COI	0.65	56.96	71.15	50.00	0.20
KUT	0.85	73.01	80.00	72.30	0.32
SWA1	-	69.54	-	69.54	-
UTO1	0.75	68.28	76.27	62.79	0.38
UTO2	-	77.78	-	77.78	-

Abbreviations: AUC: area under the curve, COI: Center of Innovation, KUT: Kyoto University TimTrio, MCC: Matthews correlation coefficient, SWA: Showa University, UTO: University of Tokyo,

Table S13. The list of discriminative FCs for SCZ.

ROI 1			ROI 2			*z*(SCZ)	*z*(TDC)	*t*-value	Mean weight
Glasser's label	**AAL label**	**Network**	**Glasser's label**	**AAL label**	**Network**				
L.MidB	-	Subcortical	L.V2	Lingual_L	Visual	0.00	-0.12	6.90	0.20
L.MidB	-	Subcortical	L.ProS	Precuneus_L	Visual	0.11	-0.01	6.29	0.17
L.23c	Cingulum_Mid_L	VAN	L.7Pm	Precuneus_L	Frontoparietal	0.34	0.21	5.04	0.13
R.PeEc	ParaHippocampal_R	Limbic	L.ProS	Precuneus_L	Visual	0.04	-0.03	4.68	0.12
L.HP	Hippocampus_L	Subcortical	L.3b	Postcentral_L	Somatomotor	0.01	-0.13	6.62	0.11
R.Amy	Hippocampus_R	Subcortical	L.31pv	Cingulum_Post_L	DMN	0.03	-0.09	7.73	0.11
L.PoI1	Insula_L	VAN	L.6a	Frontal_Sup_L	DAN	0.16	0.05	5.69	0.10
R.AAIC	Insula_R	VAN	R.9p	Frontal_Sup_R	DMN	0.15	0.07	4.44	0.10
R.PSL	Temporal_Sup_R	VAN	L.9-46d	Frontal_Mid_L	VAN	0.22	0.10	4.99	0.09
R.Amy	Hippocampus_R	Subcortical	L.7m	Precuneus_L	DMN	0.00	-0.13	8.16	0.09
R.2	Postcentral_R	DAN	L.PF	SupraMarginal_L	VAN	0.24	0.04	6.91	0.08
R.MBelt	Heschl_R	Somatomotor	R.MIP	Occipital_Sup_R	DAN	-0.04	-0.11	4.44	0.08
L.MidB	-	Subcortical	L.VMV1	Lingual_L	Visual	0.11	-0.02	6.63	0.07
L.NAcc	Caudate_L	Subcortical	L.V8	Fusiform_L	Visual	0.04	-0.11	6.77	0.06
R.VMV3	Lingual_R	Visual	R.V3A	Occipital_Sup_R	Visual	0.34	0.48	-5.42	-0.05
R.Ig	Insula_R	Somatomotor	L.Ig	Insula_L	Somatomotor	0.45	0.66	-7.75	-0.05
R.FOP2	Rolandic_Oper_R	Somatomotor	R.3a	Precentral_R	Somatomotor	0.19	0.31	-5.24	-0.07
R.43	Rolandic_Oper_R	Somatomotor	R.13l	Frontal_Inf_Orb_R	Limbic	-0.14	-0.05	-5.00	-0.07

L.3a	Postcentral_L	Somatomotor	L.4	Precentral_L	Somatomotor	0.76	1.03	-8.14	-0.07
R.13l	Frontal_Inf_Orb_R	Limbic	R.24dv	Cingulum_Mid_R	Somatomotor	-0.13	-0.05	-5.00	-0.08
R.4	Precentral_R	Somatomotor	L.3a	Postcentral_L	Somatomotor	0.68	0.92	-7.40	-0.08
R.47s	Insula_R	DMN	L.23c	Cingulum_Mid_L	VAN	-0.26	-0.17	-4.82	-0.09
R.STSdp	Temporal_Sup_R	DMN	L.FFC	Fusiform_L	Visual	-0.10	0.01	-5.56	-0.09
L.Thalamus	Thalamus_L	Subcortical	L.p24	Cingulum_Ant_L	DMN	0.07	0.17	-5.37	-0.10
R.4	Precentral_R	Somatomotor	L.Ig	Insula_L	Somatomotor	0.31	0.48	-6.84	-0.10
R.3a	Precentral_R	Somatomotor	L.4	Precentral_L	Somatomotor	0.60	0.87	-8.57	-0.12
R.HC	Hippocampus_R	Subcortical	R.FOP4	Insula_R	VAN	0.14	0.33	-10.30	-0.13
L.FOP3	Insula_L	VAN	L.23d	Cingulum_Mid_L	DMN	-0.17	-0.05	-6.33	-0.15
R.HC	Hippocampus_R	Subcortical	L.FOP3	Insula_L	VAN	0.10	0.25	-9.41	-0.15
R.Amy	Hippocampus_R	Subcortical	R.FOP5	Insula_R	VAN	0.07	0.23	-9.40	-0.15
R.3a	Precentral_R	Somatomotor	R.4	Precentral_R	Somatomotor	0.72	1.00	-8.44	-0.16
R.HC	Hippocampus_R	Subcortical	L.p32pr	Cingulum_Mid_L	VAN	0.10	0.26	-9.32	-0.16
L.FOP3	Insula_L	VAN	L.RSC	-	DMN	-0.13	-0.02	-6.08	-0.18
R.24dv	Cingulum_Mid_R	Somatomotor	L.OP2-3	Rolandic_Oper_L	Somatomotor	0.29	0.43	-6.81	-0.19
R.HC	Hippocampus_R	Subcortical	R.p32pr	Cingulum_Mid_R	VAN	0.09	0.26	-9.80	-0.21
R.HC	Hippocampus_R	Subcortical	L.FOP4	Insula_L	VAN	0.10	0.28	-10.66	-0.24
R.HC	Hippocampus_R	Subcortical	L.SCEF	Supp_Motor_Area_L	VAN	0.06	0.22	-9.07	-0.27
R.Amy	Hippocampus_R	Subcortical	L.SCEF	Supp_Motor_Area_L	VAN	0.06	0.24	-9.60	-0.35
R.Amy	Hippocampus_R	Subcortical	R.p32pr	Cingulum_Mid_R	VAN	0.08	0.26	-10.45	-0.42
R.Amy	Hippocampus_R	Subcortical	L.FOP1	Rolandic_Oper_L	VAN	0.13	0.30	-9.74	-0.44

R.Amy	Hippocampus_R	Subcortical	L.a24pr	Cingulum_Mid_L	VAN	0.08	0.27	-10.41	-1.31

Abbreviations: AAL: automated anatomical labelling, DAN: dorsal attention network, DMN: default mode network, FP: fronto-parietal, ROI: region of interest, SCZ: schizophrenia, TDC: typically developing control, and VAN: ventral attention network.

Table S14. The list of discriminative FCs for MDD.

ROI 1			ROI 2			*z*(MDD)	*z*(TDC)	*t*-value	Mean weight
Glasser's label	**AAL label**	**Network**	**Glasser's label**	**AAL label**	**Network**				
L.Amy	Amygdala_L	Subcortical	R.VMV1	Lingual_R	Visual	-0.03	-0.16	6.69	6.69
R.MidB	-	Subcortical	L.3b	Postcentral_L	Somatomotor	0.07	-0.09	6.68	6.68
L.VMV2	Lingual_L	Visual	L.PF	SupraMarginal_L	VAN	0.13	0.02	5.89	5.89
R.a9-46v	Frontal_Mid_R	FPN	L.3b	Postcentral_L	Somatomotor	-0.02	-0.11	4.98	4.98
R.V1	Calcarine_R	Visual	L.6ma	Frontal_Sup_L	VAN	0.06	-0.02	4.81	4.81
L.A4	Temporal_Sup_L	Somatomotor	L.23c	Cingulum_Mid_L	VAN	0.20	0.11	4.75	4.75
R.7Pm	Precuneus_R	FPN	L.TGd	Temporal_Pole_Mid_L	Limbic	-0.09	-0.16	4.52	4.52
R.PreS	Hippocampus_R	Visual	L.POS1	Precuneus_L	DMN	0.37	0.29	4.02	4.02
L.11l	Frontal_Sup_Orb_L	FPN	L.LO2	Occipital_Inf_L	Visual	-0.02	-0.08	3.87	3.87
R.13l	Frontal_Inf_Orb_R	Limbic	R.47m	Frontal_Inf_Orb_R	DMN	0.26	0.36	-4.03	-4.03
R.AVI	Insula_R	FPN	L.ProS	Precuneus_L	Visual	-0.05	0.01	-4.07	-4.07
R.47m	Frontal_Inf_Orb_R	DMN	L.TA2	Temporal_Sup_L	Somatomotor	0.01	0.08	-4.34	-4.34
R.47m	Frontal_Inf_Orb_R	DMN	L.MBelt	Temporal_Sup_L	Somatomotor	0.00	0.07	-4.47	-4.47
R.47m	Frontal_Inf_Orb_R	DMN	L.A1	Rolandic_Oper_L	Somatomotor	-0.01	0.06	-4.50	-4.50
R.PHA1	Fusiform_R	Visual	R.PBelt	Temporal_Sup_R	Somatomotor	-0.04	0.03	-4.57	-4.57
L.TGv	Temporal_Inf_L	Limbic	L.TE2a	Temporal_Inf_L	Limbic	0.16	0.28	-5.10	-5.10

R.A5	Temporal_Sup_R	Somatomotor	R.OP2-3	Rolandic_Oper_R	Somatomotor	0.11	0.21	-5.24	-5.24
R.Thalamus	Thalamus_R	Subcortical	R.p32pr	Cingulum_Mid_R	VAN	-0.19	-0.10	-5.37	-5.37
L.Ig	Insula_L	Somatomotor	L.POS1	Precuneus_L	DMN	0.04	0.13	-5.38	-5.38
R.v23ab	Precuneus_R	DMN	L.Ig	Insula_L	Somatomotor	-0.03	0.06	-5.61	-5.61
R.PreS	Hippocampus_R	Visual	R.p32pr	Cingulum_Mid_R	VAN	-0.10	-0.01	-5.69	-5.69
R.6mp	Supp_Motor_Area_R	Somatomotor	R.5L	Postcentral_R	DAN	0.41	0.54	-5.80	-5.80
R.a24	Cingulum_Ant_R	DMN	L.52	Temporal_Sup_L	VAN	-0.03	0.07	-5.83	-5.83
R.LO1	Occipital_Mid_R	Visual	L.LO1	Occipital_Mid_L	Visual	0.57	0.72	-5.83	-5.83
L.52	Temporal_Sup_L	VAN	L.a24	Cingulum_Ant_L	DMN	0.00	0.10	-5.94	-5.94
R.A4	Temporal_Sup_R	Somatomotor	L.5m	Precuneus_L	Somatomotor	0.04	0.15	-5.94	-5.94
R.Pallidum	Pallidum_R	Subcortical	R.Putamen	Putamen_R	Subcortical	0.23	0.33	-6.01	-6.01
R.OP4	Rolandic_Oper_R	Somatomotor	L.5m	Precuneus_L	Somatomotor	0.11	0.22	-6.30	-6.30
R.OP1	Rolandic_Oper_R	Somatomotor	L.5m	Precuneus_L	Somatomotor	0.20	0.33	-6.38	-6.38
R.5L	Postcentral_R	DAN	L.5L	Precuneus_L	Somatomotor	0.71	0.87	-6.40	-6.40
R.2	Postcentral_R	DAN	L.5m	Precuneus_L	Somatomotor	0.32	0.47	-6.41	-6.41
R.A5	Temporal_Sup_R	Somatomotor	L.A4	Temporal_Sup_L	Somatomotor	0.20	0.37	-6.80	-6.80
R.A4	Temporal_Sup_R	Somatomotor	R.4	Precentral_R	Somatomotor	0.13	0.27	-6.81	-6.81
R.A4	Temporal_Sup_R	Somatomotor	R.OP2-3	Rolandic_Oper_R	Somatomotor	0.17	0.31	-6.87	-6.87
R.OP1	Rolandic_Oper_R	Somatomotor	L.OP2-3	Rolandic_Oper_L	Somatomotor	0.40	0.55	-6.90	-6.90

L.Ig	Insula_L	Somatomotor	L.3a	Postcentral_L	Somatomotor	0.44	0.61	-7.76	-7.76
L.Ig	Insula_L	Somatomotor	L.RI	Rolandic_Oper_L	Somatomotor	0.42	0.58	-7.86	-7.86
R.Ig	Insula_R	Somatomotor	L.Ig	Insula_L	Somatomotor	0.46	0.66	-8.25	-8.25

Abbreviations: AAL: automated anatomical labelling, DAN: dorsal attention network, DMN: default mode network, FP: fronto-parietal, ROI: region of interest, MDD: major depressive disorder, TDC: typically developing control, and VAN: ventral attention network.

Table S15. Imaging scanning protocols for R-fMRI data in the discovery dataset.

Imaging site	Center of Innovation in Hiroshima University	Kyoto University	Showa University	University of Tokyo	University of Tokyo
Abbreviation	COI	KUT	SWA1	UTO1	UTO2
Data resource	SRPBS	SRPBS	SRPBS	SRPBS	-
Data category	Discovery				
MRI scanner	*Siemens Verio*	*Siemens TimTrio*	*Siemens Verio*	*GE MR750w*	*Philips Achieva*
Magnetic field strength	3.0 T				
Head coil	12	32	12	24	8
Field-of-view [mm]	212 × 212				224 × 224, 220 × 220
Matrix size	64 × 64				64 × 64, 80 × 80
in-plane resolution [mm]	3.3125 × 3.3125				3.5 × 3.5, 2.75 × 2.75
Slice thickness [mm]	3.2				3.5, 5.0
Slice gap [mm]	0.8				0.0
Number of slices	40				45, 34
Multi-band factor	-				
Number of volumes	240				200
Number of runs	1				
Repetition time [ms]	2,500				
Echo time [ms]	30				
Flip angle [degree]	80				75
Slice acquisition order	Ascending				
Phase encoding	AP		PA		
Eye-status	Fixate				Mixed

Table S16. Image scanning protocols for R-fMRI data in the validation datasets.

Imaging site	Showa University	University of Leuven	New York University Langone Medical Center	University of Utah, School of Medicine	Georgetown University	Oregon Health and Science University	Kennedy Krieger Institute	University of California, Los Angeles	San Diego State University	Trinity Centre for Health Sciences	University of Michigan	Yale School of Medicine
Abbreviation	SWA2	Leuven	NYU	USM	GU	OHSU	KKI	UCLA	SDSU	TRINITY	UM	YALE
Data resource	BMB	ABIDE-I	ADBIE-I/ABIDE-II	ABIDE-I/ABIDE-II	ABIDE-II	ABIDE-II	ABIDE-I/ABIDE-II	ABIDE-I/ABIDE-II	ABIDE-II	ABIDE-I	ABIDE-I	ABIDE-I
Data category	Japanese Adult	ABIDE Adult	ABIDE Adult/Child/Adolescent	ABIDEAdult/Adolescent	Child	Child/Adolescent	Child	Child/Adolescent	Adolescent	Adolescent	Adolescent	Adolescent
MRI scanner	*Siemens Skyra fit*	*Philips Intera*	*Siemens Allegra*	*Siemens TrioTim*	*Siemens TrioTim*	*Siemens TrioTim*	*Philips Achieva*	*Siemens TrioTim*	*GE MR750*	*Philips Achieva*	*GE Signa*	*Siemens TimTrio*
Magnetic field strength	3.0 T	3.0 T										
Head coil	32	8	NA	NA	12	12	8	NA	8	8	NA	NA
Field-of-view [mm]	206 × 206	230 × 230	240 × 192	220 × 220	192 × 192	240 × 240	256 × 256	192 × 192	220 × 220	240 × 240	220 × 220	220 × 220
Matrix size	86 × 86	64 × 64	80 × 64	64 × 64	64 × 64	64 × 64	84 × 84	64 × 64	64 × 64	80 × 80	64 × 64	64 × 64
in-plane resoluti	2.4 × 2.4	3.59 × 3.59	3.0 × 3.0	3.4 × 3.4	3.0 × 3.0	3.8 × 3.8	3.0 × 3.0	3.0 × 3.0	3.4 × 3.4	3.0 × 3.0	3.4 × 3.4	3.4 × 3.4

on [mm]												
Slice thickness [mm]	2.4	4.0	4.0	3.0	2.5	3.8	3.0	4.0	3.4	3.5	3.0	4.0
Slice gap [mm]	0.0	0.0	0.0	0.3	0.5	0.0	0.0	0.0	0.0	0.35	0.0	0.0
Number of slices	60	32	33	40	43	36	47	34	42	38	40	34
Multi-band factor	6					-						
Number of volumes	375	250	180	240	154	120	156	120	180	150	300	200
Number of runs	AP: 2, PA: 2	1	1	1	1	3	1	1	1	1	1	1
Repetition time [ms]	800	1,667	2,000	2,000	2,000	2,500	2,500	3,000	2,000	2,000	2,000	2,000
Echo time [ms]	34.4	33	15	28	30	30	30	28	30	28	30	25
Flip angle [degree]	52	90	90	90	90	90	75	90	90	98	90	60
Slice acquisition order	Interleaved	Ascending	Interleaved	Interleaved	Interleaved	Interleaved	Ascending	Interleaved	Interleaved	Ascending	Interleaved	Interleaved

Phase encoding	AP, PA	AP	RL	AP	AP	AP	AP	AP	RL	AP	AP	AP
Eye-status	Fixate	Fixate	Mixed	Eye-open	Eye-open	Fixate	Fixate	Fixate	Fixate	Eye-closed	Fixate	Eye-open