

## Supplemental Online Content

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### **eMethods.**

**eFigure 1.** Cortical and Subcortical Parcellation Used in the Analysis

**eFigure 2.** The Calinski-Harabasz Index for Each Clustering Solution for the POND (A) and HBN (B) Clustering

**eFigure 3.** POND (A) and HBN (B) Dendrograms

**eFigure 4.** Distributions of Intelligence and Hyperactivity/Impulsivity, Separated for Males and Females, for the Subgroups Showing Replicable Differences

**eTable 1.** MRI Protocols for the T1-Weighted and Resting-State Data Acquired Using the 3 Scanners

**eTable 2.** Normality Test Statistics for the Continuous Measures Describing the POND and HBN Sample Characteristics and the Clinical Behavioural Measures

**eTable 3.** Race and Ethnicity Data for the POND and HBN Data Sets

**eTable 4.** Descriptive Statistics of the Participant Demographics and Clinical Behavioural Measures Comparing the POND and HBN Data Sets, With Corresponding Statistics Identifying Significant ( $p < 0.05$ ) Differences Between the Data Sets, With the Directionality of the Difference Highlighted

**eTable 5.** Descriptive Statistics of the Participant Demographics and Clinical Behavioural Measures for Each Leaf Cluster for Each Layer of the POND Dendrogram

**eTable 6.** Descriptive Statistics of the Participant Demographics and Clinical Behavioural Measures for Each Leaf Cluster for Each Layer of the HBN Dendrogram

**eTable 7.** Statistical Details of the Mann Whitney U and t Tests and  $\chi^2$  Tests Examining Differences in Sample Characteristics Between the Leaf Clusters in Each Layer of the POND Dendrogram

**eTable 8.** Statistical Details of the Mann Whitney U and t Tests and  $\chi^2$  Tests Examining Differences in Sample Characteristics Between the Leaf Clusters in Each Layer of the HBN Dendrogram

**eTable 9.** Descriptive Statistics of the Network-Averaged Measures of Segregation and Integration for Each Leaf Cluster for Each Layer of the POND Dendrogram

**eTable 10.** Descriptive Statistics of the Network-Averaged Measures of Segregation and Integration for Each Leaf Cluster for Each Layer of the HBN Dendrogram

**eTable 11.** Statistical Details of the Tests Examining Differences in the Network-Averaged Measures of Segregation and Integration Between the Leaf Clusters in Each Layer of the POND Dendrogram

**eTable 12.** Statistical Details of the Tests Examining Differences in the Network-Averaged Measures of Segregation and Integration Between the Leaf Clusters in Each Layer of the HBN Dendrogram

**eTable 13.** Statistical Details of the Tests Examining Differences in the Network-Averaged Measures of Segregation and Integration Between the Leaf Clusters From the HBN Dendrogram That Differed in Hyperactivity/Impulsivity Problems (Subgroup d and g)

**eReferences.**

This supplemental material has been provided by the authors to give readers additional information about their work.

## **eMethods.**

### ***Participants***

The POND dataset consists of children and adolescents who are either typically developing (absence of neurodevelopmental, neurological, or neurodevelopmental diagnoses, prematurity, and first-degree family member with a neurodevelopmental condition), or who have a diagnosis of ASD, ADHD, or OCD (confirmed with expert clinical judgement and diagnostic tests<sup>1-4</sup>). Data for the current study was collected at two of the participating institutions: the Hospital for Sick Children (Toronto, Ontario, Canada) and Queen's University (Kingston, Ontario, Canada). The POND study was approved by each participating institution's research ethics boards; written informed consent or assent was obtained from the primary caregiver or participant where appropriate.

For the HBN dataset, data were collected at three of the participating institutions in the New York City area (the CitiGroup Cornell Brain Imaging Center (CBIC), Rutgers University (RU), and a mobile site in Staten Island (SI)). The Child Mind Institute's research ethics board approved the study; informed consent and verbal assent was obtained from the primary caregiver and participant, respectively. The consensus clinical diagnosis using the DSM-5<sup>5</sup> was used to identify individuals with ASD, ADHD, or OCD; those who did not receive a neurodevelopmental diagnosis, nor any other diagnosis, were considered TD.

Race and ethnicity were reported to evaluate the racial and ethnic distribution in both the POND and HBN cohorts, and to identify whether the identified subgroups differed in their distributions. For the POND dataset, self/parent-reported race and ethnicity data was collected on 386 of the participants; categories (Black, East Asian, Indigenous, Latino, Middle Eastern, Other, South Asian, Southeast Asian, and White) were determined according to the Canadian Institute for Health Information (CIHI) standards. Participants were classified into multiple categories if they were of mixed race; those who did not identify as one of the CIHI groups were categorized as "Other". For the HBN dataset, self/parent-reported race and ethnicity data was available for 509 participants, and categories were defined according to the United States census

guidelines (American Indian/Alaskan Native, Asian, Black, Hispanic, Indian, Two or More (Mixed), Native Hawaiian/Other Pacific Islander, Native American Indian, Other, and White). Participants of mixed race were classified as such, and thus participants were only assigned to one category; those who did not identify as one of the census groups were categorized as “Other”. Due to low sample size, categories for both datasets were collapsed into minoritized racial and ethnic group and white for statistical tests, with full details provided in **Supplemental Table 3**; categories with no individuals were excluded from the table.

Socio-economic status (SES) for the POND dataset was determined using the highest level of education achieved by the primary caregiver (323 participants; Level 1: did not complete high school, Level 2: high school education, Level 3: associate degree, Level 4: undergraduate degree, Level 5: graduate/professional degree) and household income (287 participants; Low: <\$74,999, Medium: \$75,000 – \$199,999, High: <\$200,000). For the HBN dataset, Barratt Simplified Measure of Social Status (BSMSS) was obtained on 540 participants.

### ***Clinical behavioural measures***

For the POND and HBN datasets, full-scale IQ (FSIQ) was assessed with Wechsler<sup>6–10</sup> or Stanford-Binet<sup>11</sup> scales (range: 40-160, with higher scores indicating higher intelligence). ASD-like traits were measured using Social Communication Questionnaire<sup>12</sup> (range: 0-39, with higher scores indicating more severe difficulties with social communication), and repetitive behaviours were measured using the Repetitive Behaviours Scale – Revised<sup>13</sup> (range: 0-129, with higher scores indicating more severe difficulties with repetitive behaviours). The Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour<sup>14</sup> rating scale inattention subscale (SWAN-I) was used to measure inattention (range: 0-9, with higher scores indicating more severe difficulties with inattention), while hyperactivity and impulsivity was measured using the SWAN hyperactivity/impulsivity subscale (SWAN-HI) (range: 0-9, with higher scores indicating more severe difficulties with hyperactivity/impulsivity). For the POND dataset, obsessive-compulsive traits were measured using the Toronto Obsessive-Compulsive Scale (TOCS) (range: -63 to 63, with higher scores indicating more severe difficulties

with obsessive-compulsive traits). A direct measure of obsessive-compulsive traits was not obtained on the HBN participants, and thus the obsessive-compulsive subscale of the CBCL (CBCL-OCS<sup>15</sup>) was used (range: 0-16, with higher scores indicating more severe difficulties with obsessive-compulsive traits), which shows moderate correlation with TOCS<sup>16</sup>.

### **Data acquisition**

Neuroimaging data from POND were acquired on one of three Siemens 3T MRI scanners; for each participant, a T1-weighted image and five minutes of resting-state data were obtained while the participant viewed a movie of their choosing or *Inscapes*, a naturalistic movie paradigm<sup>17</sup>. Neuroimaging data from HBN were acquired at one of three sites; for each participant, a T1-weighted image and resting-state data were obtained while the participant was instructed to focus on a fixation cross. Ten minutes of resting-state data were acquired, broken up into two five-minute runs. To best conform with the five-minute POND dataset, for HBN participants with two five-minute runs, a single run was selected by using propensity score matching to minimize the difference in head motion between the two datasets (see section **Propensity score matching** in the eMethods). The MRI protocols for each scanner are summarized in **eTable 1**.

### **Preprocessing**

The neuroimaging data were preprocessed using *fMRIPrep*<sup>18,19</sup>, a preprocessing tool based in Nipype<sup>20,21</sup> that consists of an anatomical and functional pipeline. For the anatomical pipeline, each participant's T1-weighted image was corrected for intensity non-uniformity<sup>22</sup> and skull-stripped using the OASIS template with Advance Normalization Tools (ANTs) to generate a brain mask. FreeSurfer<sup>23</sup> was used to reconstruct brain surfaces, which were used to refine the brain mask using a custom variation of Mindboggle<sup>24</sup>. ANTs nonlinear registration<sup>25</sup> was used to spatially normalize the brain-extracted image to a pediatric template<sup>26,27</sup>. FMRIB's Software Library (FSL) was used to segment the brain-extracted normalized image into cerebrospinal fluid (CSF), white matter (WM), and gray matter<sup>28</sup>.

For the functional pipeline, each participant's data was slice-time and motion corrected using Analysis of Functional NeuroImages (AFNI<sup>29</sup>) and FSL<sup>30</sup> software,

respectively. Fieldmap-less distortion correction was performed by co-registering the data to the corresponding T1-weighted image with intensity inverted<sup>31,32</sup>, constrained with an average fieldmap template<sup>33</sup>, implemented with ANTs. The resulting data were co-registered to the T1-weighted image using boundary-based registration with six degrees of freedom implemented in FreeSurfer<sup>34</sup>. The motion-correcting, functional-to-anatomical, and anatomical-to-template transformations were concatenated and applied in a single step with ANTs using Lanczos interpolation. Framewise displacement (FD<sup>35</sup>) and the standardized derivative of root mean square variance over voxels (DVARs<sup>35</sup>) was computed using the implementation in Nipype; mean FD across all frames was used as a measure of head motion in the analyses. Participants with more than 1/3 of their frames exceeding the recommended threshold (FD: 0.5mm, DVARs: 1.5) were excluded from all subsequent analyses. Following *fMRIPrep*, the functional data was cleaned of nuisance signals. The six motion parameters from motion correction and signal contributions from the white matter and CSF, along with their derivative and quadratic terms, were regressed from the data while simultaneously performing high-pass temporal filtering (0.008Hz) using AFNI<sup>29,36</sup>.

### ***Propensity score matching***

Propensity score matching was used to ensure the two datasets did not differ in age, sex, and motion. Propensity scores were computed as the predicted response of a multiple logistic regression model with age, sex, and motion as independent variables and dataset as the dependent variable. A modified version of nearest-neighbour, one-to-one matching was performed to select a single five-minute run of the HBN data when two were available. For each POND participant that passed quality control ( $N=592$ ), HBN datasets with propensity scores within a pre-specified tolerance (set to a quarter of the standard deviation of the scores<sup>37</sup>) were identified as eligible matches. Nearest-neighbour HBN matches were drawn for each POND participant in a randomized order; once on run of an HBN participant was selected as a match, the remaining run was removed from the list of eligible matches. This procedure was repeated ( $N=100$ ), each time with a new randomized order, and the solution which maximized the final sample size was selected.

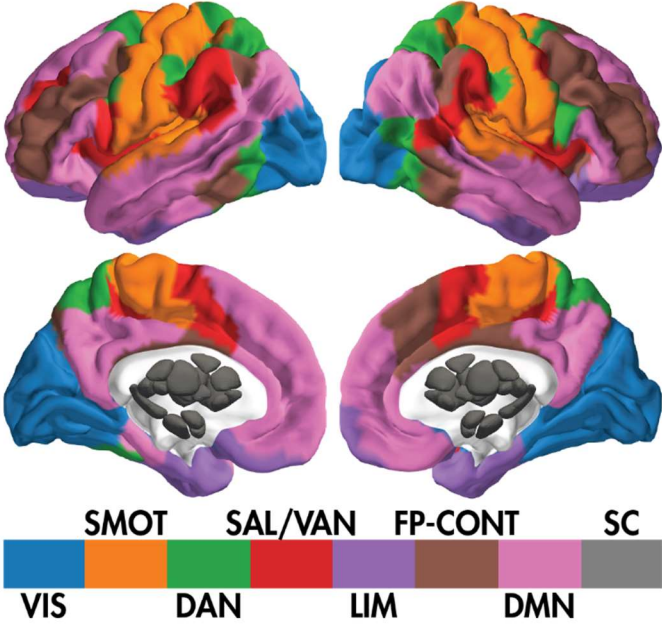
## ***Nuisance covariates***

To account for the influence of scanner, age, and sex, a two-step approach was employed. The first step corrected the connectome data for the different acquisition scanner (see **eTable 1**) using ComBat harmonization<sup>38</sup>. During ComBat, no biological variables were included as fixed effects to preserve, and the default parametric prior method was used in the empirical Bayes procedure. Next, the age and motion variables (linear, quadratic, and cubic to account for nonlinear developmental trajectories<sup>39,40</sup>) along with sex were regressed from each connection. Due to the non-normality of motion, the data were log-transformed prior to the regression. Both steps were applied on the pooled POND and HBN datasets to ensure no biases were introduced if applied separately, and repeated subsampling (randomly selecting 63.2% of the sample for each iteration, performed over 10,000 iterations) was employed to increase robustness<sup>41,42</sup>.

## ***Clustering***

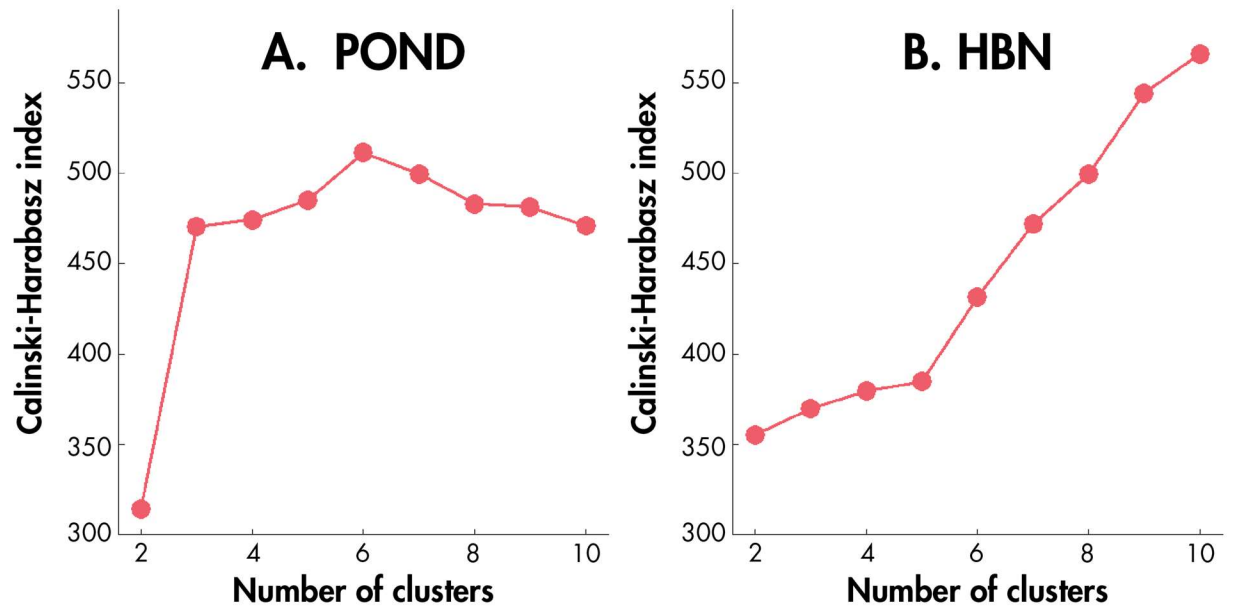
Similarity Network Fusion (SNF) depends on two free hyperparameters which can produce different clustering solutions:  $\mu$ , the scaling parameter in the weighted similarity kernel, and  $K$ , the number of nearest neighbours used in both similarity matrix construction and fusion. Hyperparameters were optimized using the methods described in Markello et al.<sup>44</sup>, exploring the hyperparameter space constructed using 100 logarithmically spaced values of both  $\mu$  and  $K$  between their recommended ranges ( $\mu \in [0.3, 0.8]$ ,  $K \in [10, 30]$ , 10,000 unique combinations). A participant co-assignment matrix was then generated by computing the percentage of times two participants were clustered in the same subgroup across cluster solutions that were stable across the hyperparameter exploration.

**eFigure 1.** Cortical and Subcortical Parcellation Used in the Analysis



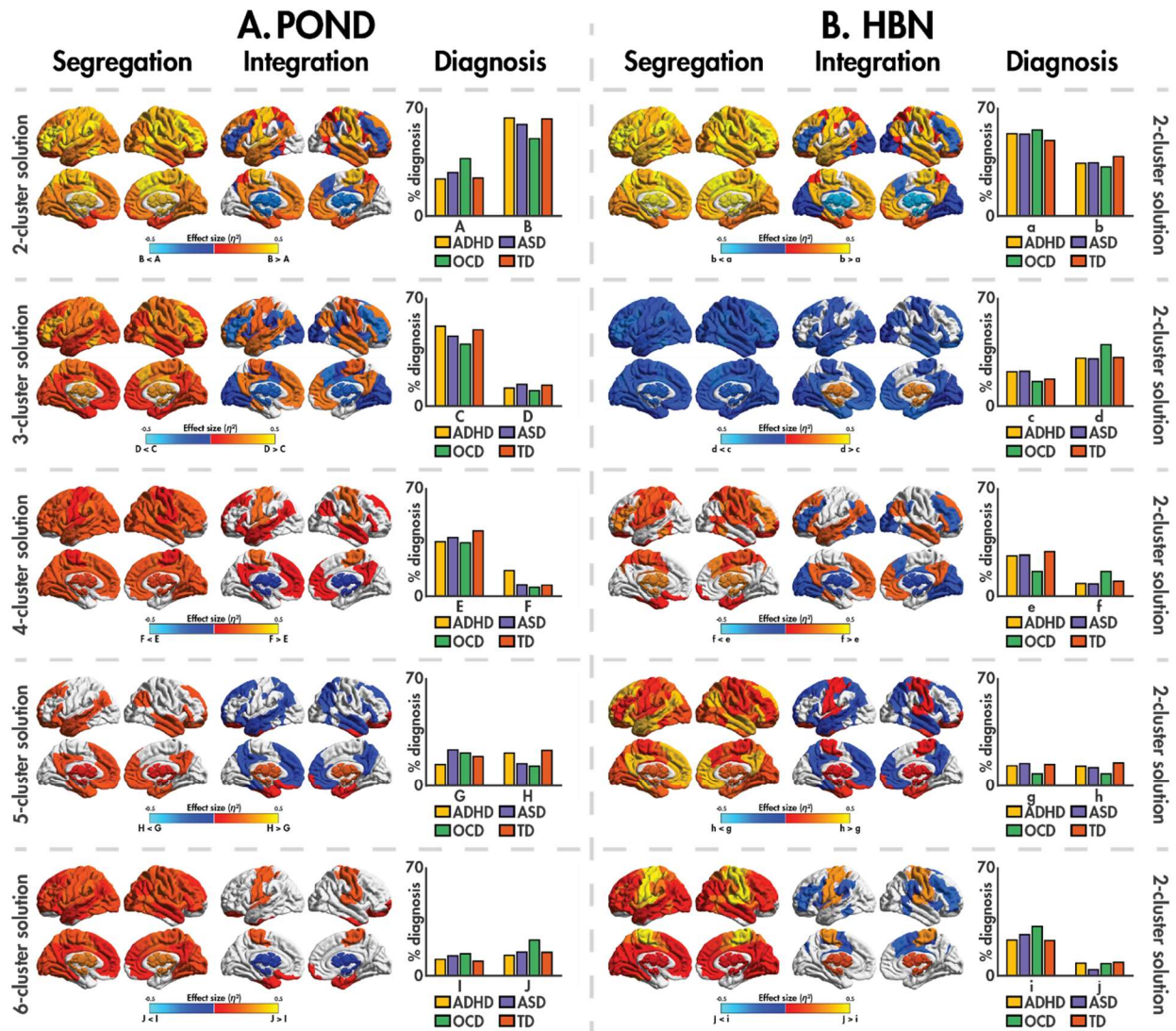


**eFigure 2.** The Calinski-Harabasz Index for Each Clustering Solution for the POND (A) and HBN (B) Clustering



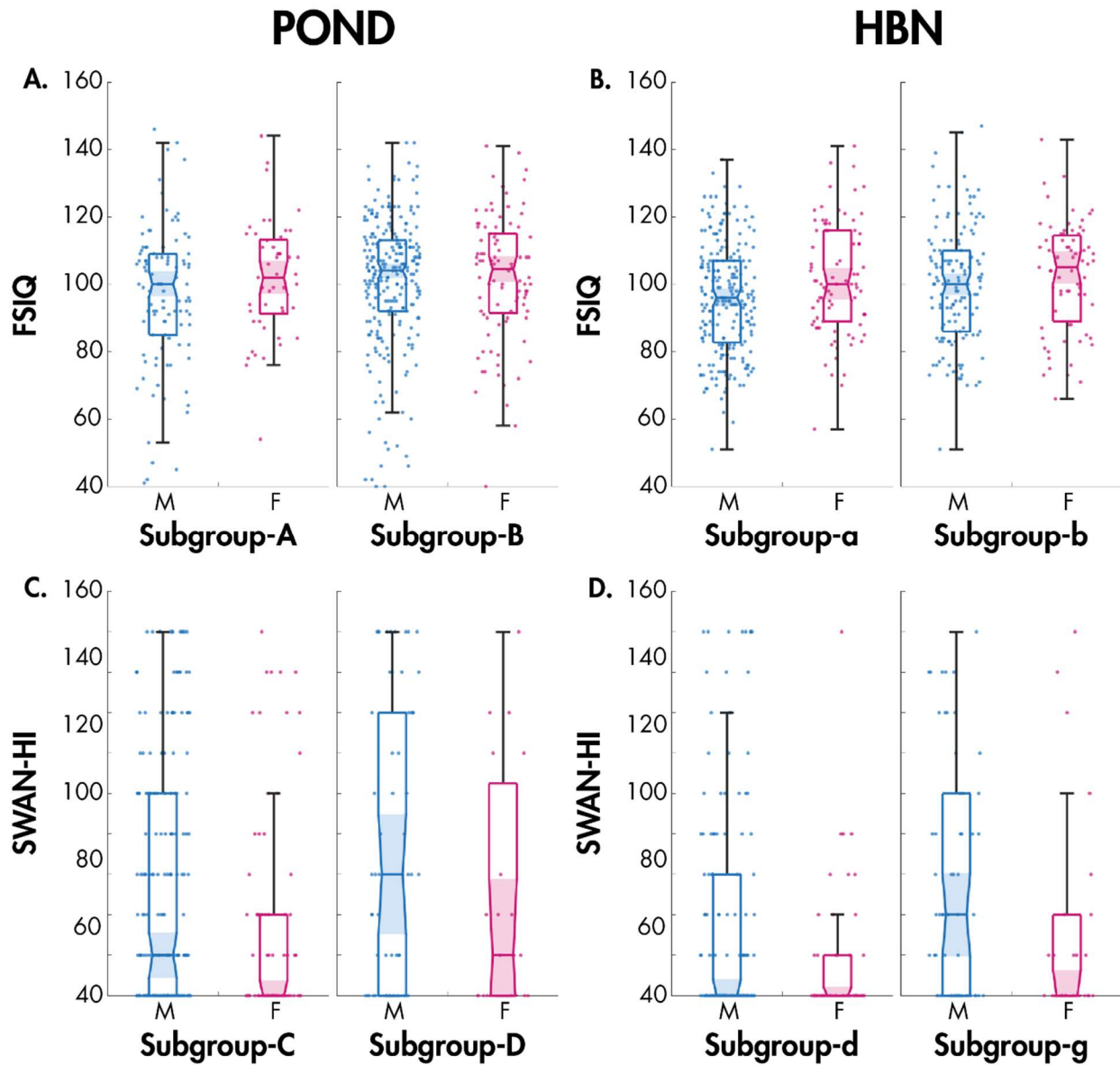
POND: Province of Ontario Neurodevelopmental Network; HBN: Healthy Brain Network.

**eFigure 3. POND (A) and HBN (B) Endrograms**



For each layer of the POND (A) and HBN (B) dendrograms, Mann-U Whitney or t-tests were used to identify pairwise differences in network-averaged measures of segregation and integration between the leaf clusters. The effect size of significant ( $p_{corr} < 0.05$ ) differences between pairs of leaf clusters are presented, showing which networks were driving the split of the root cluster. The percentage distribution of each diagnosis (yellow: ADHD, purple: ASD, green: OCD, red: TD) is shown for each of the leaf clusters. POND: Province of Ontario Neurodevelopmental Network; HBN: Healthy Brain Network; ADHD: attention-deficit/hyperactivity disorder; ASD: autism spectrum disorder; OCD: obsessive-compulsive disorder; TD: typically developing.

**eFigure 4.** Distributions of Intelligence (POND: A, HBN: B) and Hyperactivity/Impulsivity (POND: C, HBN: D), Separated for Males (M; blue) and Females (F; pink), for the Subgroups Showing Replicable Differences



**eFigure 4.** Distributions of Intelligence (POND: A, HBN: B) and Hyperactivity/Impulsivity (POND: C, HBN: D), Separated for Males (M; blue) and Females (F; pink), for the Subgroups Showing Replicable Differences. POND: Province of Ontario Neurodevelopmental Network; HBN: Healthy Brain Network; FSQ: full-scale intelligence quotient; SWAN-HI: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour hyperactivity/impulsivity subscale.

**eTable 1.** MRI Protocols for the T1-Weighted and Resting-State Data Acquired Using the 3 Scanners

| T1-weighted protocols   |                    |           |     |          |         |         |        |             |                 |                 |
|-------------------------|--------------------|-----------|-----|----------|---------|---------|--------|-------------|-----------------|-----------------|
| Dataset                 | Scanner            | Scan Type | N   | Sequence | TR (ms) | TE (ms) | FA (°) | FOV (mm)    | Voxel size (mm) | Scan time (min) |
| POND                    | SK: 3T TimTrio     | -         | 240 | MPRAGE   | 2300    | 2.96    | 9      | 192×240×256 | 1               | 5.0             |
|                         | QU: 3T TimTrio     | -         | 112 | MPRAGE   | 2300    | 3.14    | 9      | 192×240×256 | 0.8             | 6.2             |
|                         | SK: 3T PrismaFIT   | -         | 365 | MPRAGE   | 1870    | 3.14    | 9      | 192×240×256 | 0.8             | 5.0             |
| HBN                     | CBIC: 3T PrismaFIT | -         | 293 | MPRAGE   | 2500    | 3.15    | 8      | 179×256×256 | 0.8             | 7.00            |
|                         | RU: 3T TimTrio     | -         | 477 | MPRAGE   | 2500    | 3.15    | 8      | 179×256×256 | 0.8             | 7.00            |
|                         | SI: 1.5T Avanto    | -         | 188 | MPRAGE   | 2730    | 1.64    | 7      | 176×256×256 | 1               | 6.53            |
| Resting-state protocols |                    |           |     |          |         |         |        |             |                 |                 |
| Dataset                 | Scanner            | Scan Type | N   | Sequence | TR (ms) | TE (ms) | FA (°) | FOV (mm)    | Voxel size (mm) | Scan time (min) |
| POND                    | SK: 3T TimTrio     | Movies    | 240 | EPI      | 2340    | 30      | 70     | 224×224×140 | 3.5             | 5.0             |
|                         | QU: 3T TimTrio     | Inscapes  | 112 | EPI      | 2340    | 30      | 70     | 224×224×140 | 3.5             | 5.0             |
|                         | SK: 3T PrismaFIT   | Inscapes  | 365 | EPI      | 1500    | 30      | 70     | 222×222×150 | 3               | 5.0             |
| HBN                     | CBIC: 3T PrismaFIT | Fixation  | 293 | EPI      | 800     | 30      | 31     | 202×202×144 | 2.4             | 2×5.1           |
|                         | RU: 3T TimTrio     | Fixation  | 477 | EPI      | 800     | 30      | 31     | 202×202×144 | 2.4             | 2×5.1           |
|                         | SI: 1.5T Avanto    | Fixation  | 188 | EPI      | 1450    | 40      | 55     | 195×195×135 | 2.5             | 10.3            |

POND: Province of Ontario Neurodevelopmental network; HBN: Healthy Brain Network; SK: Hospital for Sick Children, QU: Queen's University, CBIC: CitiGroup Cornell Brain Imaging Center, RU: Rutgers University, SI: Staten Island, TR: repetition time, TE: echo time, FA: flip angle, FOV: field of view

**eTable 2.** Normality Test Statistics for the Continuous Measures Describing the POND and HBN Sample Characteristics and the Clinical Behavioural Measures

Degrees of freedom indicate the sample size for each variable; participants with missing data were excluded from the statistical analysis on a case-by-case basis.

| Variable    | Normality test statistics             |  |
|-------------|---------------------------------------|--|
|             | POND                                  | HBN                                    |
| Age         | $W(551)=0.04, p=0.01$                 | $W(551)=0.05, p=1.05 \times 10^{-3}$   |
| Head motion | $W(551)=0.17, p=2.72 \times 10^{-46}$ | $W(551)=0.15, p=7.06 \times 10^{-35}$  |
| FSIQ        | $W(491)=0.08, p=3.43 \times 10^{-8}$  | $W(518)=0.04, p=0.09$                  |
| SCQ         | $W(501)=0.16, p=1.07 \times 10^{-33}$ | $W(546)=0.13, p=5.58 \times 10^{-25}$  |
| RBS-R       | $W(513)=0.16, p=2.90 \times 10^{-34}$ | $W(406)=0.21, p=1.74 \times 10^{-49}$  |
| SWAN-I      | $W(500)=0.18, p=8.51 \times 10^{-47}$ | $W(540)=0.18, p=4.10 \times 10^{-48}$  |
| SWAN-H/I    | $W(500)=0.22, p=1.28 \times 10^{-65}$ | $W(540)=0.28, p=3.73 \times 10^{-116}$ |
| TOCS        | $W(501)=0.10, p=5.44 \times 10^{-14}$ | –                                      |
| CBCL-OCS    | –                                     | $W(534)=0.16, p=3.39 \times 10^{-35}$  |

POND: Province of Ontario Neurodevelopmental network; HBN: Healthy Brain Network; FSIQ: full scale intelligence quotient; SCQ: Social Communication Questionnaire; RBS-R: Repetitive Behaviours Scale – Revised; SWAN-I: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour inattention subscale; SWAN-HI: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour hyperactivity/impulsivity subscale; TOCS: Toronto Obsessive-Compulsive Scale; CBCL-E: Child Behaviour Checklist obsessive-compulsive subscale

**eTable 3.** Race and Ethnicity Data for the POND and HBN Data Sets

|             |                            | <b>ADHD</b> | <b>ASD</b> | <b>OCD</b> | <b>TD</b> |
|-------------|----------------------------|-------------|------------|------------|-----------|
| <b>POND</b> | <b>Black</b>               | 5           | 6          | 1          | 8         |
|             | <b>East Asian</b>          | 6           | 11         | 4          | 7         |
|             | <b>Indigenous</b>          | 10          | 4          | 1          | 7         |
|             | <b>Latino</b>              | 10          | 10         | 1          | 7         |
|             | <b>Middle Eastern</b>      | 1           | 5          | 3          | 1         |
|             | <b>Other</b>               | 12          | 14         | 3          | 6         |
|             | <b>South Asian</b>         | 7           | 6          | 4          | 4         |
|             | <b>Southeast Asian</b>     | 4           | 8          | 1          | 5         |
|             | <b>White</b>               | 95          | 98         | 30         | 76        |
| <b>HBN</b>  | <b>Asian</b>               | 6           | 4          | 1          | 8         |
|             | <b>Black</b>               | 66          | 10         | 0          | 6         |
|             | <b>Hispanic</b>            | 44          | 3          | 0          | 10        |
|             | <b>Two or More (Mixed)</b> | 59          | 9          | 1          | 16        |
|             | <b>Other</b>               | 7           | 0          | 0          | 2         |
|             | <b>White</b>               | 170         | 30         | 8          | 49        |

ADHD: attention-deficit/hyperactivity disorder; ASD: autism spectrum disorder; OCD: obsessive-compulsive disorder; TD: typically developing; IQR: interquartile range; "Other" group: individuals who did not identify as one of the Canadian Institutes of Health Information or US census guideline categories

**eTable 4.** Descriptive Statistics of the Participant Demographics and Clinical Behavioural Measures Comparing the POND and HBN Data Sets, With Corresponding Statistics Identifying Significant ( $p < 0.05$ ) Differences Between the Data Sets, With the Directionality of the Difference Highlighted

| Measure                                     | Median (IQR)   |               | Statistics                  |                        |                          |  |
|---|----------------|---------------|-----------------------------|------------------------|--------------------------|--|
|   | POND           | HBN           | Test statistic <sup>a</sup> | <i>p</i> -value        | Effect size <sup>b</sup> | Directionality                           |
| <b>N</b>                                    | 551            | 551           | –                           | –                      | –                        | –  |
| <b>Dx (ADHD:ASD:OCD:TD)</b>                 | 164:217:110:61 | 374:66:100:11 | 197.7                       | $1.30 \times 10^{-42}$ | 0.42                     | ADHD: HBN > POND<br>ASD, OCD: POND > HBN |
| <b>Age (years)</b>                          | 11.87 (5.25)   | 11.50 (4.98)  | $1.43 \times 10^5$          | 0.07                   | $2.88 \times 10^{-3}$    | –  |
| <b>Sex (M:F)</b>                            | 394:158        | 390:161       | 0.05                        | 0.83                   | 0.01                     | –  |
| <b>Race and ethnicity (Non-White:White)</b> | 158:228        | 252:257       | 6.50                        | 0.01                   | 0.09                     | Non-White: HBN > POND                    |
| <b>Head motion (mm)</b>                     | 0.16 (0.13)    | 0.17 (0.13)   | $1.60 \times 10^5$          | 0.11                   | $2.27 \times 10^{-3}$    | –  |
| <b>FSIQ</b>                                 | 103.00 (22.50) | 99.00 (24.00) | $1.15 \times 10^5$          | 0.01                   | $7.44 \times 10^{-3}$    | POND > HBN                               |
| <b>SCQ</b>                                  | 8.00 (15.00)   | 7.00 (6.00)   | $1.26 \times 10^5$          | 0.03                   | $4.71 \times 10^{-3}$    | POND > HBN                               |
| <b>RBS-R</b>                                | 14.00 (25.00)  | 12.00 (37.00) | $1.07 \times 10^5$          | 0.42                   | $7.13 \times 10^{-4}$    | –  |
| <b>SWAN-I</b>                               | 4.00 (7.00)    | 3.00 (6.00)   | $1.27 \times 10^5$          | 0.07                   | $3.06 \times 10^{-3}$    | –  |
| <b>SWAN-H/I</b>                             | 1.00 (5.00)    | 0.00 (3.00)   | $1.09 \times 10^5$          | $2.21 \times 10^{-8}$  | 0.03                     | POND > HBN                               |

ADHD: attention-deficit/hyperactivity disorder; ASD: autism spectrum disorder; OCD: obsessive-compulsive disorder; TD: typically developing; IQR: interquartile range; SD: standard deviation; M: male; F: female; FD: framewise displacement; FSIQ: full scale intelligence quotient; SCQ: Social Communication Questionnaire; RBS-R: Repetitive Behaviours Scale – Revised; SWAN-I: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour inattention subscale; SWAN-HI: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour hyperactivity/impulsivity subscale; <sup>a</sup>Test statistic: Mann-Whitney *U*-statistic for non-normally distributed continuous variables, *t*-statistic for normally distributed continuous variables, and chi-squared  $X^2$  for categorical variables; <sup>b</sup>Effect size: eta-squared ( $\eta^2$ ) for continuous variables and Cramer's *V* for categorical variables

**eTable 5.** Descriptive Statistics of the Participant Demographics and Clinical Behavioural Measures for Each Leaf Cluster for Each Layer of the POND Dendrogram

| Dendrogram layer<br>Leaf cluster                             | Median (IQR)       |                   |                    |                   |                    |                   |                    |                   |                    |                  |
|--|--------------------|-------------------|--------------------|-------------------|--------------------|-------------------|--------------------|-------------------|--------------------|------------------|
|  | 2-cluster solution |                   | 3-cluster solution |                   | 4-cluster solution |                   | 5-cluster solution |                   | 6-cluster solution |                  |
|  | A                  | B                 | C                  | D                 | E                  | F                 | G                  | H                 | I                  | J                |
| <b>Dx<br/>(ADHD:ASD:OCD:TD)</b>                              | 45:70:26:31        | 119:147:35:79     | 97:112:28:62       | 22:35:7:17        | 66:94:24:53        | 31:18:4:9         | 26:58:15:24        | 40:36:9:29        | 20:32:10:12        | 25:38:16:19      |
| <b>Age (years)</b>   | 11.77<br>(5.51)    | 11.91<br>(5.15)   | 12.24<br>(5.02)    | 11.09<br>(4.69)   | 12.12<br>(5.38)    | 12.55<br>(4.53)   | 12.57<br>(4.92)    | 11.31<br>(5.10)   | 11.44<br>(5.48)    | 12.01<br>(5.67)  |
| <b>Sex<br/>(M:F)</b>   | 118:54             | 276:104           | 216:83             | 60:21             | 171:66             | 45:17             | 89:34              | 82:32             | 47:27              | 71:27            |
| <b>Primary caregiver<br/>education<br/>(Level 1:2:3:4:5)</b> | 0:17:22:34:28      | 5:26:51:81:58     | 3:23:38:59:49      | 2:3:13:22:9       | 1:16:30:51:42      | 2:7:8:8:7         | 1:8:16:21:22       | 0:8:14:30:20      | 0:7:11:19:11       | 0:10:11:15:17    |
| <b>Household income<br/>(Low:Medium:High)</b>                | 20:43:24           | 40:97:62          | 27:80:46           | 13:17:16          | 19:63:39           | 8:17:7            | 7:28:30            | 12:35:19          | 9:22:12            | 11:21:12         |
| <b>Race and ethnicity<br/>(Non-White:White)</b>              | 49:66              | 109:162           | 84:125             | 25:37             | 72:95              | 12:30             | 36:47              | 36:48             | 24:27              | 25:39            |
| <b>Scanner<br/>(SK-TT:QU-TT:SK-PF)</b>                       | 91:60:21           | 196:125:59        | 153:101:45         | 43:24:14          | 125:78:34          | 28:23:11          | 64:47:12           | 61:31:22          | 41:25:8            | 50:35:13         |
| <b>Head motion (mm)</b>                                      | 0.15<br>(0.16)     | 0.16<br>(0.13)    | 0.15<br>(0.14)     | 0.17<br>(0.10)    | 0.15<br>(0.14)     | 0.14<br>(0.10)    | 0.14<br>(0.08)     | 0.18<br>(0.19)    | 0.18<br>(0.16)     | 0.14<br>(0.13)   |
| <b>FSIQ</b>  | 100.00<br>(22.00)  | 104.00<br>(22.00) | 105.00<br>(20.25)  | 102.50<br>(27.50) | 104.00<br>(21.00)  | 108.00<br>(18.75) | 104.00<br>(26.00)  | 104.00<br>(15.75) | 100.00<br>(22.00)  | 99.00<br>(23.00) |
| <b>SCQ</b>   | 9.00<br>(15.00)    | 6.50<br>(15.00)   | 6.00<br>(14.50)    | 7.50<br>(16.00)   | 6.00<br>(16.00)    | 6.00<br>(9.50)    | 10.00<br>(19.00)   | 5.00<br>(10.00)   | 11.00<br>(15.00)   | 9.00<br>(14.00)  |
| <b>RBS-R</b>   | 17.00<br>(26.25)   | 13.00<br>(24.00)  | 11.00<br>(25.00)   | 17.00<br>(27.50)  | 13.00<br>(25.00)   | 10.50<br>(19.00)  | 14.00<br>(27.75)   | 9.00<br>(22.50)   | 17.00<br>(21.50)   | 15.00<br>(27.50) |
| <b>SWAN-I</b>  | 4.00<br>(7.00)     | 3.50<br>(7.00)    | 3.50<br>(7.00)     | 3.50<br>(6.00)    | 3.00<br>(7.00)     | 5.00<br>(6.00)    | 3.00<br>(6.75)     | 3.50<br>(7.00)    | 4.00<br>(7.00)     | 5.00<br>(7.00)   |
| <b>SWAN-H/I</b>  | 2.00<br>(5.00)     | 1.00<br>(5.00)    | 1.00<br>(5.00)     | 2.50<br>(7.00)    | 1.00<br>(4.00)     | 2.00<br>(6.00)    | 1.00<br>(3.00)     | 1.00<br>(5.00)    | 2.00<br>(5.00)     | 2.00<br>(4.00)   |
| <b>TOCS</b>  | -5.00<br>(44.00)   | -15.00<br>(51.00) | -17.00<br>(51.75)  | -1.50<br>(46.00)  | -16.00<br>(48.00)  | -33.00<br>(48.75) | -12.50<br>(55.50)  | -21.00<br>(45.00) | -5.00<br>(49.50)   | -5.00<br>(40.50) |

Dx: Diagnosis; ADHD: attention-deficit/hyperactivity disorder; ASD: autism spectrum disorder; OCD: obsessive-compulsive disorder; TD: typically developing; IQR: interquartile range; M: male; F: female; SK-TT: SickKids TimTrio; QU-TT: Queen's University TimTrio; SK-PF: SickKids PrismaFIT; FSIQ: full scale intelligence quotient; SCQ: Social Communication Questionnaire; RBS-R: Repetitive Behaviours Scale – Revised; SWAN-I: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour inattention subscale; SWAN-HI: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour hyperactivity/impulsivity subscale; TOCS: Toronto Obsessive-Compulsive Scale



**eTable 6.** Descriptive Statistics of the Participant Demographics and Clinical Behavioural Measures for Each Leaf Cluster for Each Layer of the HBN Dendrogram

| Dendrogram layer                                | Median (IQR)       |                   |                    |                  |                    |                  |                    |                   |                    |                  |
|---|--------------------|-------------------|--------------------|------------------|--------------------|------------------|--------------------|-------------------|--------------------|------------------|
|   | 2-cluster solution |                   | 3-cluster solution |                  | 4-cluster solution |                  | 5-cluster solution |                   | 6-cluster solution |                  |
| Leaf cluster                                    | a                  | b                 | c                  | d                | e                  | f                | g                  | h                 | i                  | j                |
| <b>Dx<br/>(ADHD:ASD:OCD:TD)</b>                 | 228:40:7:56        | 146:26:4:44       | 95:17:2:20         | 133:23:5:36      | 111:20:2:33        | 35:6:2:11        | 56:11:1:16         | 55:9:1:17         | 98:20:4:26         | 35:3:1:10        |
| <b>Age (years)</b>                              | 11.58<br>(5.09)    | 11.39<br>(4.86)   | 11.25<br>(4.92)    | 11.73<br>(5.26)  | 11.35<br>(4.87)    | 11.90<br>(4.90)  | 11.49<br>(4.82)    | 11.33<br>(4.81)   | 11.74<br>(4.91)    | 11.64<br>(5.60)  |
| <b>Sex<br/>(M:F)</b>                            | 242:89             | 148:72            | 103:31             | 139:58           | 115:51             | 33:21            | 59:25              | 56:26             | 101:47             | 38:11            |
| <b>BSMSS</b>                                    | 51.25<br>(20.25)   | 50.00<br>(16.50)  | 53.00<br>(14.12)   | 50.00<br>(21.25) | 50.00<br>(16.50)   | 50.75<br>(15.50) | 49.75<br>(18.50)   | 51.50<br>(16.00)  | 50.00<br>(19.00)   | 46.25<br>(29.00) |
| <b>Race and ethnicity<br/>(Non-White:White)</b> | 155:150            | 97:107            | 59:65              | 96:85            | 80:79              | 17:28            | 43:40              | 37:39             | 65:71              | 31:14            |
| <b>Scanner<br/>(CBIC:RU:SI)</b>                 | 124:156:51         | 79:104:37         | 48:71:15           | 76:85:36         | 61:78:27           | 18:26:10         | 29:39:16           | 32:39:11          | 56:64:28           | 20:21:8          |
| <b>Mean head motion<br/>(mm)</b>                | 0.16<br>(0.11)     | 0.17<br>(0.14)    | 0.15<br>(0.10)     | 0.17<br>(0.12)   | 0.17<br>(0.15)     | 0.17<br>(0.11)   | 0.17<br>(0.15)     | 0.18<br>(0.18)    | 0.17<br>(0.12)     | 0.18<br>(0.11)   |
| <b>Mean FSIQ (SD)</b>                           | 97.08<br>(16.55)   | 100.63<br>(16.98) | 96.44<br>(16.13)   | 97.51<br>(16.86) | 101.57<br>(17.43)  | 97.51<br>(15.14) | 101.28<br>(18.65)  | 101.86<br>(16.20) | 98.75<br>(17.53)   | 93.71<br>(14.10) |
| <b>SCQ</b>                                      | 7.00<br>(7.00)     | 7.00<br>(6.00)    | 7.00<br>(6.00)     | 7.00<br>(7.00)   | 7.00<br>(7.00)     | 7.00<br>(5.50)   | 7.00<br>(7.00)     | 6.00<br>(6.00)    | 7.00<br>(7.00)     | 7.00<br>(5.25)   |
| <b>RBS-R</b>                                    | 11.00<br>(37.00)   | 12.00<br>(44.00)  | 15.00<br>(40.00)   | 10.00<br>(29.25) | 13.00<br>(44.00)   | 8.00<br>(38.50)  | 24.00<br>(54.50)   | 8.00<br>(27.50)   | 7.00<br>(27.75)    | 11.50<br>(35.00) |
| <b>SWAN-I</b>                                   | 3.00<br>(6.00)     | 3.00<br>(6.00)    | 3.00<br>(5.00)     | 3.00<br>(6.00)   | 3.00<br>(6.00)     | 3.00<br>(5.00)   | 4.00<br>(7.00)     | 2.00<br>(4.25)    | 2.50<br>(6.00)     | 3.00<br>(5.00)   |
| <b>SWAN-H/I</b>                                 | 0.00<br>(2.00)     | 1.00<br>(3.00)    | 1.00<br>(3.00)     | 0.00<br>(2.00)   | 1.00<br>(3.00)     | 0.00<br>(2.00)   | 1.00<br>(4.00)     | 0.00<br>(2.00)    | 0.00<br>(2.00)     | 0.00<br>(3.00)   |
| <b>CBCL-OCS</b>                                 | 3.00<br>(2.00)     | 3.00<br>(3.00)    | 3.00<br>(3.00)     | 2.00<br>(2.00)   | 3.00<br>(3.00)     | 3.00<br>(3.00)   | 3.00<br>(4.00)     | 2.00<br>(2.25)    | 2.50<br>(2.00)     | 2.00<br>(2.00)   |

Dx: Diagnosis; ADHD: attention-deficit/hyperactivity disorder; ASD: autism spectrum disorder; OCD: obsessive-compulsive disorder; TD: typically developing; IQR: interquartile range; SD: standard deviation; M: male; F: female; CBIC: CitiGroup Cornell Brain Imaging Center; RU: Rutgers University; SI: Staten Island; FSIQ: full scale intelligence quotient; SCQ: Social Communication Questionnaire; RBS-R: Repetitive Behaviours Scale – Revised; SWAN-I: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour inattention subscale; SWAN-HI: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour hyperactivity/impulsivity subscale; CBCL-OCS: Child Behaviour Checklist obsessive-compulsive subscale

**eTable 7.** Statistical Details of the Mann Whitney U and *t* Tests and  $\chi^2$  Tests Examining Differences in Sample Characteristics Between the Leaf Clusters in Each Layer of the POND Dendrogram

| Dendrogram layer           | Test statistic <sup>a</sup> |      |       |      |      | <i>p</i> -value |      |      |                       |      | Effect size <sup>b</sup> |      |      |      |      |
|----------------------------|-----------------------------|------|-------|------|------|-----------------|------|------|-----------------------|------|--------------------------|------|------|------|------|
|                            | 2                           | 3    | 4     | 5    | 6    | 2               | 3    | 4    | 5                     | 6    | 2                        | 3    | 4    | 5    | 6    |
| <b>Dx</b>                  | 5.37                        | 1.15 | 11.08 | 9.76 | 0.70 | 0.15            | 0.76 | 0.01 | 0.02                  | 0.87 | 0.10                     | 0.06 | 0.19 | 0.20 | 0.06 |
| <b>Age</b>                 | 3.17                        | 1.08 | 0.76  | 0.58 | 0.38 | 0.58            | 0.15 | 0.64 | 0.02                  | 0.49 | 0.00                     | 0.01 | 0.00 | 0.02 | 0.00 |
| <b>Sex</b>                 | 0.94                        | 0.11 | 0.00  | 0.01 | 1.56 | 0.33            | 0.74 | 0.95 | 0.94                  | 0.21 | 0.04                     | 0.02 | 0.00 | 0.00 | 0.10 |
| <b>Caregiver education</b> | 0.01                        | 0.26 | 4.67  | 0.02 | 0.06 | 0.92            | 0.61 | 0.03 | 0.88                  | 0.80 | 0.00                     | 0.00 | 0.03 | 0.00 | 0.00 |
| <b>Household income</b>    | 0.50                        | 0.17 | 2.11  | 1.12 | 0.09 | 0.48            | 0.68 | 0.15 | 0.29                  | 0.76 | 0.00                     | 0.00 | 0.01 | 0.01 | 0.00 |
| <b>Race and ethnicity</b>  | 0.19                        | 0.00 | 2.95  | 0.00 | 0.74 | 0.66            | 0.99 | 0.09 | 0.95                  | 0.39 | 0.02                     | 0.00 | 0.12 | 0.01 | 0.08 |
| <b>Scanner</b>             | 1.08                        | 0.58 | 1.18  | 5.96 | 0.41 | 0.58            | 0.75 | 0.55 | 0.05                  | 0.82 | 0.04                     | 0.04 | 0.06 | 0.16 | 0.05 |
| <b>Head motion</b>         | 3.18                        | 1.29 | 0.72  | 0.91 | 0.30 | 0.60            | 0.37 | 0.84 | 7.97×10 <sup>-5</sup> | 0.05 | 0.00                     | 0.00 | 0.00 | 0.07 | 0.02 |
| <b>FSIQ</b>                | 2.86                        | 0.90 | 0.66  | 0.58 | 0.28 | 0.04            | 0.35 | 0.03 | 0.78                  | 0.89 | 0.01                     | 0.00 | 0.02 | 0.00 | 0.00 |
| <b>SCQ</b>                 | 2.49                        | 1.05 | 0.57  | 0.45 | 0.30 | 0.17            | 0.32 | 0.47 | 3.05×10 <sup>-3</sup> | 0.90 | 0.00                     | 0.00 | 0.00 | 0.04 | 0.00 |
| <b>RBS-R</b>               | 2.70                        | 1.18 | 0.56  | 0.53 | 0.29 | 0.41            | 0.06 | 0.44 | 0.06                  | 0.42 | 0.00                     | 0.01 | 0.00 | 0.02 | 0.00 |
| <b>SWAN-I</b>              | 2.51                        | 0.99 | 0.66  | 0.62 | 0.29 | 0.29            | 0.88 | 0.22 | 0.42                  | 0.94 | 0.00                     | 0.00 | 0.01 | 0.00 | 0.00 |
| <b>SWAN-H/I</b>            | 2.59                        | 1.19 | 0.65  | 0.62 | 0.26 | 0.59            | 0.01 | 0.28 | 0.46                  | 0.27 | 0.00                     | 0.02 | 0.00 | 0.00 | 0.01 |
| <b>TOCS</b>                | 2.46                        | 1.20 | 0.51  | 0.51 | 0.30 | 0.13            | 0.01 | 0.21 | 0.10                  | 0.93 | 0.00                     | 0.02 | 0.01 | 0.01 | 0.00 |

Dx: Diagnosis; FSIQ: full scale intelligence quotient; SCQ: Social Communication Questionnaire; RBS-R: Repetitive Behaviours Scale – Revised; SWAN-I: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour inattention subscale; SWAN-HI: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour hyperactivity/impulsivity subscale; TOCS: Toronto Obsessive-Compulsive Scale; <sup>a</sup>Test statistic: Mann-Whitney *U*-statistic (×10<sup>4</sup>) for non-normally distributed continuous variables, *t*-statistic for normally distributed continuous variables, and chi-squared  $\chi^2$  for categorical variables; <sup>b</sup>Effect size: eta-squared ( $\eta^2$ ) for continuous variables and Cramer's *V* for categorical variables

**eTable 8.** Statistical Details of the Mann Whitney U and *t* Tests and  $\chi^2$  Tests Examining Differences in Sample Characteristics Between the Leaf Clusters in Each Layer of the HBN Dendrogram

| Dendrogram layer          | Test statistic <sup>a</sup> |      |      |      |      | <i>p</i> -value |      |      |                       |      | Effect size <sup>b</sup> |      |      |      |      |
|---------------------------|-----------------------------|------|------|------|------|-----------------|------|------|-----------------------|------|--------------------------|------|------|------|------|
|                           | 2                           | 3    | 4    | 5    | 6    | 2               | 3    | 4    | 5                     | 6    | 2                        | 3    | 4    | 5    | 6    |
| <b>Dx</b>                 | 0.88                        | 1.14 | 1.46 | 0.22 | 2.10 | 0.83            | 0.77 | 0.69 | 0.98                  | 0.55 | 0.04                     | 0.06 | 0.08 | 0.04 | 0.10 |
| <b>Age</b>                | 3.59                        | 1.37 | 0.52 | 0.35 | 0.34 | 0.80            | 0.53 | 0.07 | 0.94                  | 0.62 | 0.00                     | 0.00 | 0.02 | 0.00 | 0.00 |
| <b>Sex</b>                | 2.18                        | 1.61 | 1.23 | 0.07 | 1.54 | 0.14            | 0.20 | 0.27 | 0.79                  | 0.22 | 0.06                     | 0.07 | 0.07 | 0.02 | 0.09 |
| <b>BSMSS</b>              | 3.41                        | 1.15 | 4.21 | 0.39 | 0.30 | 0.60            | 0.14 | 0.88 | 0.10                  | 0.15 | 0.00                     | 0.01 | 0.00 | 0.02 | 0.01 |
| <b>Race and ethnicity</b> | 0.52                        | 0.88 | 2.21 | 0.15 | 6.04 | 0.47            | 0.35 | 0.14 | 0.69                  | 0.01 | 0.03                     | 0.05 | 0.10 | 0.03 | 0.18 |
| <b>Scanner</b>            | 0.25                        | 4.39 | 0.27 | 1.05 | 0.22 | 0.88            | 0.11 | 0.88 | 0.59                  | 0.90 | 0.02                     | 0.12 | 0.03 | 0.08 | 0.03 |
| <b>Head motion</b>        | 3.89                        | 1.44 | 0.43 | 0.37 | 0.41 | 0.18            | 0.15 | 0.59 | 0.35                  | 0.18 | 0.00                     | 0.01 | 0.00 | 0.01 | 0.01 |
| <b>FSIQ</b>               | 2.37                        | 0.56 | 1.47 | 0.21 | 1.75 | 0.02            | 0.58 | 0.14 | 0.83                  | 0.08 | 0.01                     | 0.00 | 0.01 | 0.00 | 0.02 |
| <b>SCQ</b>                | 3.37                        | 1.34 | 0.42 | 0.33 | 0.37 | 0.28            | 0.65 | 0.75 | 0.82                  | 0.90 | 0.00                     | 0.00 | 0.00 | 0.00 | 0.00 |
| <b>RBS-R</b>              | 2.04                        | 0.69 | 0.22 | 0.15 | 0.23 | 0.44            | 0.19 | 0.85 | 0.15                  | 0.16 | 0.00                     | 0.01 | 0.00 | 0.01 | 0.01 |
| <b>SWAN-I</b>             | 3.48                        | 1.19 | 0.40 | 0.25 | 0.36 | 0.92            | 0.32 | 0.74 | 4.76×10 <sup>-3</sup> | 0.62 | 0.00                     | 0.00 | 0.00 | 0.05 | 0.00 |
| <b>SWAN-H/I</b>           | 3.68                        | 1.13 | 0.38 | 0.27 | 0.38 | 0.27            | 0.06 | 0.35 | 0.02                  | 0.18 | 0.00                     | 0.01 | 0.00 | 0.03 | 0.01 |
| <b>CBCL-OCS</b>           | 3.31                        | 1.19 | 0.39 | 0.31 | 0.33 | 0.50            | 0.59 | 0.65 | 0.33                  | 0.68 | 0.00                     | 0.00 | 0.00 | 0.01 | 0.00 |

Dx: Diagnosis; FSIQ: full scale intelligence quotient; SCQ: Social Communication Questionnaire; RBS-R: Repetitive Behaviours Scale – Revised; SWAN-I: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour inattention subscale; SWAN-HI: Strengths and Weaknesses of ADHD-symptoms and Normal Behaviour hyperactivity/impulsivity subscale; CBCL-E: Child Behaviour Checklist obsessive-compulsive subscale; <sup>a</sup>Test statistic: Mann-Whitney *U*-statistic (×10<sup>4</sup>) for non-normally distributed continuous variables, *t*-statistic for normally distributed continuous variables, and chi-squared  $\chi^2$  for categorical variables; <sup>b</sup>Effect size: eta-squared ( $\eta^2$ ) for continuous variables and Cramer's *V* for categorical variables

**eTable 9.** Descriptive Statistics of the Network-Averaged Measures of Segregation and Integration for Each Leaf Cluster for Each Layer of the POND Dendrogram

| Median segregation ×10 (IQR)              |              |             |                |              |             |             |             |               |              |
|---|--------------|-------------|----------------|--------------|-------------|-------------|-------------|---------------|--------------|
| Dendrogram layer                          | Leaf cluster | VIS         | Mean SMOT (SD) | DAN          | SAL/VAN     | LIM         | FP-CONT     | Mean DMN (SD) | SC           |
| 2-cluster solution                        | A            | 1.52 (0.59) | 2.08 (0.54)    | 1.27 (0.39)  | 1.01 (0.36) | 1.05 (0.47) | 1.06 (0.32) | 1.10 (0.34)   | 0.90 (0.30)  |
|   | B            | 2.20 (0.73) | 2.75 (0.59)    | 1.80 (0.51)  | 1.64 (0.63) | 1.37 (0.53) | 1.66 (0.56) | 1.43 (0.37)   | 1.44 (0.53)  |
| 3-cluster solution                        | C            | 2.10 (0.69) | 2.67 (0.47)    | 1.74 (0.40)  | 1.54 (0.47) | 1.33 (0.50) | 1.56 (0.40) | 1.38 (0.35)   | 1.31 (0.45)  |
|   | D            | 2.62 (0.57) | 3.16 (0.38)    | 2.28 (0.47)  | 2.17 (0.45) | 1.59 (0.53) | 2.24 (0.40) | 1.61 (0.31)   | 1.96 (0.53)  |
| 4-cluster solution                        | E            | 2.00 (0.57) | 2.60 (0.46)    | 1.69 (0.34)  | 1.46 (0.42) | 1.28 (0.51) | 1.51 (0.32) | 1.32 (0.29)   | 1.24 (0.39)  |
|   | F            | 2.50 (0.53) | 2.80 (0.33)    | 1.97 (0.37)  | 1.88 (0.46) | 1.36 (0.38) | 1.86 (0.43) | 1.63 (0.26)   | 1.62 (0.36)  |
| 5-cluster solution                        | G            | 2.07 (0.71) | 2.58 (0.44)    | 1.68 (0.31)  | 1.40 (0.44) | 1.16 (0.37) | 1.48 (0.31) | 1.26 (0.24)   | 1.19 (0.33)  |
|   | H            | 1.95 (0.48) | 2.65 (0.51)    | 1.69 (0.38)  | 1.50 (0.37) | 1.48 (0.55) | 1.53 (0.34) | 1.41 (0.33)   | 1.37 (0.37)  |
| 6-cluster solution                        | I            | 1.38 (0.43) | 1.93 (0.56)    | 1.11 (0.42)  | 0.86 (0.33) | 1.04 (0.48) | 0.97 (0.24) | 1.01 (0.32)   | 0.79 (0.24)  |
|   | J            | 1.73 (0.52) | 2.21 (0.53)    | 1.36 (0.34)  | 1.12 (0.27) | 1.06 (0.44) | 1.15 (0.32) | 1.15 (0.29)   | 1.01 (0.28)  |
| Median integration ×10 <sup>3</sup> (IQR) |              |             |                |              |             |             |             |               |              |
| Dendrogram layer                          | Leaf cluster | VIS         | SMOT           | DAN          | SAL/VAN     | LIM         | FP-CONT     | DMN           | SC           |
| 2-cluster solution                        | A            | 7.51 (2.41) | 5.53 (2.09)    | 7.75 (3.60)  | 7.26 (3.25) | 2.73 (1.52) | 8.12 (4.31) | 7.34 (2.70)   | 9.28 (4.57)  |
|   | B            | 7.76 (2.36) | 8.86 (3.37)    | 9.20 (3.26)  | 7.04 (2.63) | 4.06 (2.01) | 6.19 (2.64) | 10.34 (3.17)  | 5.64 (2.66)  |
| 3-cluster solution                        | C            | 7.92 (2.34) | 8.27 (2.55)    | 9.00 (3.23)  | 7.23 (2.78) | 4.13 (1.98) | 6.64 (2.46) | 9.60 (2.51)   | 6.15 (2.47)  |
|   | D            | 6.69 (2.76) | 11.81 (3.97)   | 10.24 (4.06) | 6.26 (2.37) | 3.59 (2.20) | 4.27 (1.70) | 12.68 (3.07)  | 4.25 (1.40)  |
| 4-cluster solution                        | E            | 7.92 (2.40) | 7.87 (2.38)    | 9.08 (2.90)  | 7.25 (2.67) | 4.05 (1.72) | 6.74 (2.39) | 9.40 (2.86)   | 6.40 (2.89)  |
|   | F            | 7.91 (1.83) | 10.74 (3.17)   | 8.47 (3.28)  | 7.14 (2.92) | 4.76 (2.78) | 6.24 (1.98) | 10.37 (2.01)  | 5.58 (1.59)  |
| 5-cluster solution                        | G            | 7.88 (2.20) | 7.98 (2.14)    | 9.79 (2.79)  | 7.32 (2.89) | 3.71 (1.47) | 6.54 (2.48) | 10.07 (2.61)  | 5.43 (2.62)  |
|   | H            | 7.96 (2.59) | 7.72 (2.70)    | 8.52 (2.66)  | 7.01 (2.53) | 4.35 (2.49) | 6.93 (2.43) | 8.80 (2.70)   | 7.05 (3.20)  |
| 6-cluster solution                        | I            | 7.31 (2.58) | 4.69 (1.62)    | 7.80 (3.73)  | 7.13 (4.26) | 2.22 (1.42) | 8.87 (4.86) | 6.91 (2.38)   | 11.02 (5.02) |
|   | J            | 7.64 (2.49) | 6.11 (1.82)    | 7.67 (3.34)  | 7.27 (2.95) | 3.00 (1.41) | 7.88 (3.64) | 7.78 (2.69)   | 8.69 (3.29)  |

IQR: interquartile range; SD: standard deviation; VIS: visual network; SMOT: somatomotor network; DAN: dorsal attention network; SAL/VAN: salience/ventral attention network; LIM: limbic network; FP-CONT: frontoparietal control network; DMN: default mode network; SC: subcortical regions

**eTable 10.** Descriptive Statistics of the Network-Averaged Measures of Segregation and Integration for Each Leaf Cluster for Each Layer of the HBN Dendrogram

| Median segregation ×10 (IQR)              |              |               |                |               |             |             |             |               |              |
|---|--------------|---------------|----------------|---------------|-------------|-------------|-------------|---------------|--------------|
| Dendrogram layer                          | Leaf cluster | Mean VIS (SD) | Mean SMOT (SD) | Mean DAN (SD) | SAL/VAN     | LIM         | FP-CONT     | Mean DMN (SD) | SC           |
| 2-cluster solution                        | a            | 1.85 (0.76)   | 2.30 (0.69)    | 1.42 (0.51)   | 1.09 (0.51) | 0.99 (0.40) | 1.20 (0.49) | 1.14 (0.33)   | 0.85 (0.30)  |
|   | b            | 2.53 (0.57)   | 2.98 (0.49)    | 2.12 (0.44)   | 1.83 (0.50) | 1.44 (0.60) | 1.98 (0.52) | 1.53 (0.30)   | 1.38 (0.63)  |
| 3-cluster solution                        | c            | 2.06 (0.53)   | 2.47 (0.40)    | 1.62 (0.40)   | 1.26 (0.34) | 1.08 (0.40) | 1.41 (0.35) | 1.26 (0.25)   | 0.98 (0.25)  |
|   | d            | 1.63 (0.66)   | 2.06 (0.73)    | 1.27 (0.46)   | 0.91 (0.47) | 0.91 (0.40) | 1.02 (0.37) | 1.05 (0.30)   | 0.77 (0.24)  |
| 4-cluster solution                        | e            | 2.49 (0.56)   | 2.87 (0.47)    | 2.08 (0.47)   | 1.76 (0.48) | 1.37 (0.59) | 1.87 (0.41) | 1.51 (0.32)   | 1.27 (0.42)  |
|   | f            | 2.65 (0.67)   | 3.18 (0.50)    | 2.28 (0.59)   | 2.02 (0.45) | 1.59 (0.41) | 2.30 (0.34) | 1.58 (0.22)   | 1.88 (0.54)  |
| 5-cluster solution                        | g            | 2.34 (0.52)   | 2.74 (0.54)    | 1.92 (0.39)   | 1.60 (0.40) | 1.19 (0.52) | 1.77 (0.34) | 1.37 (0.21)   | 1.12 (0.32)  |
|   | h            | 2.65 (0.54)   | 2.98 (0.49)    | 2.22 (0.35)   | 1.94 (0.43) | 1.59 (0.59) | 1.95 (0.42) | 1.65 (0.26)   | 1.44 (0.48)  |
| 6-cluster solution                        | i            | 1.55 (0.63)   | 1.92 (0.60)    | 1.21 (0.44)   | 0.84 (0.33) | 0.91 (0.37) | 1.00 (0.28) | 1.04 (0.27)   | 0.75 (0.24)  |
|   | j            | 1.80 (0.98)   | 2.81 (0.52)    | 1.58 (0.78)   | 1.26 (0.60) | 1.01 (0.48) | 1.27 (0.77) | 1.12 (0.41)   | 0.81 (0.28)  |
| Median integration ×10 <sup>3</sup> (IQR) |              |               |                |               |             |             |             |               |              |
| Dendrogram layer                          | Leaf cluster | VIS           | SMOT           | DAN           | SAL/VAN     | LIM         | FP-CONT     | DMN           | SC           |
| 2-cluster solution                        | a            | 7.88 (2.84)   | 6.34 (2.80)    | 8.20 (3.67)   | 7.07 (3.20) | 2.69 (1.84) | 7.93 (3.87) | 8.02 (2.72)   | 8.52 (5.27)  |
|   | b            | 7.27 (2.96)   | 10.11 (3.07)   | 9.38 (3.52)   | 7.25 (2.66) | 4.25 (2.64) | 5.28 (2.27) | 11.60 (3.12)  | 4.69 (1.95)  |
| 3-cluster solution                        | c            | 8.42 (2.69)   | 6.94 (2.03)    | 8.65 (3.28)   | 7.44 (2.63) | 3.55 (2.05) | 7.69 (3.16) | 9.21 (2.70)   | 6.33 (2.79)  |
|   | d            | 7.53 (2.86)   | 5.71 (2.83)    | 7.85 (3.74)   | 6.70 (3.12) | 2.17 (1.27) | 8.48 (4.42) | 7.33 (2.30)   | 10.41 (5.34) |
| 4-cluster solution                        | e            | 7.96 (2.69)   | 10.04 (3.34)   | 9.33 (3.61)   | 7.15 (2.61) | 4.36 (2.44) | 5.65 (2.11) | 10.84 (3.00)  | 4.95 (2.05)  |
|   | f            | 5.98 (1.85)   | 10.19 (1.61)   | 9.46 (2.94)   | 7.86 (2.62) | 3.71 (2.45) | 4.03 (1.68) | 13.15 (2.07)  | 3.90 (1.46)  |
| 5-cluster solution                        | g            | 8.41 (2.34)   | 9.35 (2.94)    | 10.75 (4.04)  | 7.09 (3.10) | 4.04 (2.13) | 5.14 (1.61) | 11.39 (2.61)  | 5.18 (1.87)  |
|   | h            | 7.22 (2.78)   | 10.38 (4.05)   | 8.58 (3.05)   | 7.29 (2.54) | 5.21 (3.17) | 6.30 (2.10) | 10.36 (2.67)  | 4.94 (2.09)  |
| 6-cluster solution                        | i            | 7.60 (2.88)   | 4.86 (2.20)    | 8.19 (3.56)   | 7.16 (3.23) | 2.15 (1.28) | 9.00 (4.22) | 7.37 (2.18)   | 9.51 (4.62)  |
|   | j            | 7.24 (2.66)   | 7.82 (2.83)    | 6.95 (3.65)   | 5.23 (2.14) | 2.23 (1.24) | 5.46 (3.97) | 6.89 (2.88)   | 14.10 (5.79) |

IQR: interquartile range; SD: standard deviation; VIS: visual network; SMOT: somatomotor network; DAN: dorsal attention network; SAL/VAN: salience/ventral attention network; LIM: limbic network; FP-CONT: frontoparietal control network; DMN: default mode network; SC: subcortical regions

**eTable 11.** Statistical Details of the Tests Examining Differences in the Network-Averaged Measures of Segregation and Integration Between the Leaf Clusters in Each Layer of the POND Dendrogram

| Dendrogram layer |         | Test statistic |      |      |      |      | p-value                |                        |                        |                       |                       | Effect size ( $\eta^2$ ) |      |      |      |      |
|------------------|---------|----------------|------|------|------|------|------------------------|------------------------|------------------------|-----------------------|-----------------------|--------------------------|------|------|------|------|
|                  |         | 2              | 3    | 4    | 5    | 6    | 2                      | 3                      | 4                      | 5                     | 6                     | 2                        | 3    | 4    | 5    | 6    |
| Segregation      | VIS     | 0.62           | 0.50 | 0.49 | 0.08 | 0.33 | $4.99 \times 10^{-17}$ | $6.89 \times 10^{-9}$  | $4.91 \times 10^{-9}$  | 1.00                  | $8.33 \times 10^{-5}$ | 0.28                     | 0.16 | 0.17 | 0.01 | 0.15 |
|                  | SMOT    | 0.68           | 0.48 | 0.19 | 0.07 | 0.35 | $1.30 \times 10^{-21}$ | $6.36 \times 10^{-14}$ | 0.01                   | 1.00                  | $8.50 \times 10^{-6}$ | 0.37                     | 0.23 | 0.04 | 0.01 | 0.17 |
|                  | DAN     | 0.60           | 0.55 | 0.34 | 0.04 | 0.26 | $2.46 \times 10^{-23}$ | $2.55 \times 10^{-19}$ | $8.43 \times 10^{-10}$ | 1.00                  | $2.14 \times 10^{-6}$ | 0.40                     | 0.29 | 0.18 | 0.00 | 0.19 |
|                  | SAL/VAN | 0.69           | 0.56 | 0.44 | 0.11 | 0.23 | $5.72 \times 10^{-22}$ | $1.17 \times 10^{-14}$ | $1.93 \times 10^{-11}$ | 0.20                  | $9.04 \times 10^{-7}$ | 0.46                     | 0.26 | 0.22 | 0.03 | 0.21 |
|                  | LIM     | 0.29           | 0.24 | 0.07 | 0.31 | 0.08 | $1.96 \times 10^{-10}$ | $9.84 \times 10^{-6}$  | 1.00                   | $5.96 \times 10^{-8}$ | 1.00                  | 0.13                     | 0.07 | 0.01 | 0.18 | 0.01 |
|                  | FP-CONT | 0.64           | 0.62 | 0.34 | 0.07 | 0.18 | $3.97 \times 10^{-22}$ | $9.08 \times 10^{-17}$ | $8.04 \times 10^{-10}$ | 0.83                  | $1.92 \times 10^{-5}$ | 0.47                     | 0.37 | 0.18 | 0.01 | 0.15 |
|                  | DMN     | 0.32           | 0.21 | 0.26 | 0.18 | 0.13 | $2.34 \times 10^{-17}$ | $8.81 \times 10^{-8}$  | $6.55 \times 10^{-10}$ | $4.08 \times 10^{-7}$ | $4.93 \times 10^{-3}$ | 0.27                     | 0.11 | 0.19 | 0.16 | 0.08 |
|                  | SC      | 0.55           | 0.60 | 0.28 | 0.15 | 0.25 | $1.95 \times 10^{-20}$ | $1.84 \times 10^{-16}$ | $3.99 \times 10^{-7}$  | $1.13 \times 10^{-3}$ | $3.49 \times 10^{-8}$ | 0.40                     | 0.32 | 0.15 | 0.08 | 0.28 |
| Integration      | VIS     | 0.05           | 1.35 | 0.27 | 0.14 | 0.48 | 1.00                   | $1.46 \times 10^{-6}$  | 1.00                   | 1.00                  | 1.00                  | 0.00                     | 0.08 | 0.00 | 0.00 | 0.01 |
|                  | SMOT    | 3.47           | 3.22 | 2.59 | 0.39 | 1.30 | $3.46 \times 10^{-19}$ | $1.23 \times 10^{-12}$ | $2.95 \times 10^{-11}$ | 1.00                  | $8.63 \times 10^{-6}$ | 0.39                     | 0.21 | 0.22 | 0.02 | 0.19 |
|                  | DAN     | 1.29           | 0.79 | 0.66 | 1.58 | 0.14 | $3.44 \times 10^{-6}$  | 0.24                   | 1.00                   | $1.18 \times 10^{-4}$ | 1.00                  | 0.06                     | 0.02 | 0.01 | 0.12 | 0.00 |
|                  | SAL/VAN | 0.33           | 0.90 | 0.44 | 0.36 | 0.04 | 1.00                   | 0.02                   | 1.00                   | 1.00                  | 1.00                  | 0.00                     | 0.03 | 0.00 | 0.00 | 0.00 |
|                  | LIM     | 1.42           | 0.49 | 0.70 | 0.92 | 0.61 | $1.14 \times 10^{-10}$ | 0.36                   | 0.08                   | $3.67 \times 10^{-4}$ | 0.04                  | 0.18                     | 0.01 | 0.02 | 0.06 | 0.07 |
|                  | FP-CONT | 2.26           | 2.38 | 0.69 | 0.37 | 0.53 | $8.17 \times 10^{-15}$ | $2.25 \times 10^{-11}$ | 0.26                   | 1.00                  | 1.00                  | 0.15                     | 0.26 | 0.02 | 0.01 | 0.01 |
|                  | DMN     | 2.85           | 2.97 | 0.95 | 1.24 | 0.70 | $1.01 \times 10^{-16}$ | $7.32 \times 10^{-16}$ | 0.02                   | $4.39 \times 10^{-4}$ | 0.33                  | 0.28                     | 0.26 | 0.05 | 0.09 | 0.03 |
|                  | SC      | 3.71           | 2.35 | 1.16 | 2.36 | 1.73 | $1.12 \times 10^{-18}$ | $1.38 \times 10^{-10}$ | 0.02                   | $6.03 \times 10^{-8}$ | 0.02                  | 0.27                     | 0.22 | 0.03 | 0.20 | 0.07 |

VIS: visual network; SMOT: somatomotor network; DAN: dorsal attention network; SAL/VAN: salience/ventral attention network; LIM: limbic network; FP-CONT: frontoparietal control network; DMN: default mode network; SC: subcortical regions

**eTable 12.** Statistical Details of the Tests Examining Differences in the Network-Averaged Measures of Segregation and Integration Between the Leaf Clusters in Each Layer of the HBN Dendrogram

| Dendrogram layer |         | Test statistic <sup>a</sup> |      |      |      |                        | p-value                |                        |                        |                        |                        | Effect size <sup>b</sup> |      |      |      |      |
|------------------|---------|-----------------------------|------|------|------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|--------------------------|------|------|------|------|
|                  |         | 2                           | 3    | 4    | 5    | 6                      | 2                      | 3                      | 4                      | 5                      | 6                      | 2                        | 3    | 4    | 5    | 6    |
| Segregation      | VIS     | 0.68                        | 0.44 | 0.17 | 0.37 | 0.31                   | 5.42×10 <sup>-18</sup> | 7.07×10 <sup>-9</sup>  | 0.39                   | 1.41×10 <sup>-5</sup>  | 0.01                   | 0.30                     | 0.16 | 0.02 | 0.16 | 0.06 |
|                  | SMOT    | 0.70                        | 0.33 | 0.38 | 0.20 | 0.86                   | 1.22×10 <sup>-25</sup> | 8.00×10 <sup>-7</sup>  | 2.92×10 <sup>-7</sup>  | 0.01                   | 5.35×10 <sup>-14</sup> | 0.35                     | 0.10 | 0.18 | 0.08 | 0.47 |
|                  | DAN     | 0.70                        | 0.30 | 0.29 | 0.32 | 0.43                   | 7.10×10 <sup>-26</sup> | 9.15×10 <sup>-8</sup>  | 4.64×10 <sup>-5</sup>  | 2.20×10 <sup>-6</sup>  | 2.63×10 <sup>-8</sup>  | 0.46                     | 0.15 | 0.11 | 0.22 | 0.23 |
|                  | SAL/VAN | 0.72                        | 0.30 | 0.31 | 0.30 | 0.48                   | 7.28×10 <sup>-27</sup> | 4.98×10 <sup>-9</sup>  | 3.96×10 <sup>-7</sup>  | 1.57×10 <sup>-6</sup>  | 4.57×10 <sup>-9</sup>  | 0.49                     | 0.20 | 0.12 | 0.19 | 0.25 |
|                  | LIM     | 0.42                        | 0.14 | 0.20 | 0.39 | 0.05                   | 5.41×10 <sup>-15</sup> | 3.04×10 <sup>-3</sup>  | 0.04                   | 1.38×10 <sup>-6</sup>  | 1.00                   | 0.24                     | 0.06 | 0.06 | 0.20 | 0.00 |
|                  | FP-CONT | 0.77                        | 0.31 | 0.44 | 0.15 | 0.33                   | 8.36×10 <sup>-26</sup> | 7.84×10 <sup>-10</sup> | 7.95×10 <sup>-11</sup> | 0.03                   | 2.97×10 <sup>-8</sup>  | 0.56                     | 0.25 | 0.28 | 0.07 | 0.10 |
|                  | DMN     | 0.39                        | 0.20 | 0.08 | 0.29 | 0.13                   | 1.73×10 <sup>-19</sup> | 5.44×10 <sup>-9</sup>  | 0.35                   | 6.48×10 <sup>-11</sup> | 0.02                   | 0.39                     | 0.16 | 0.02 | 0.39 | 0.06 |
| SC               | 0.59    | 0.20                        | 0.55 | 0.30 | 0.07 | 2.08×10 <sup>-25</sup> | 8.67×10 <sup>-12</sup> | 4.97×10 <sup>-12</sup> | 2.51×10 <sup>-6</sup>  | 0.50                   | 0.48                   | 0.21                     | 0.29 | 0.21 | 0.01 |      |
| Integration      | VIS     | 0.72                        | 0.83 | 1.75 | 0.61 | 0.64                   | 0.01                   | 0.03                   | 2.48×10 <sup>-5</sup>  | 1.00                   | 1.00                   | 0.02                     | 0.04 | 0.14 | 0.06 | 0.01 |
|                  | SMOT    | 3.69                        | 1.39 | 0.16 | 1.14 | 3.19                   | 3.40×10 <sup>-20</sup> | 2.60×10 <sup>-7</sup>  | 1.00                   | 4.85×10 <sup>-2</sup>  | 5.92×10 <sup>-11</sup> | 0.42                     | 0.13 | 0.00 | 0.04 | 0.30 |
|                  | DAN     | 1.31                        | 0.63 | 0.08 | 2.10 | 0.96                   | 7.90×10 <sup>-7</sup>  | 0.50                   | 1.00                   | 3.81×10 <sup>-5</sup>  | 0.47                   | 0.06                     | 0.02 | 0.00 | 0.14 | 0.03 |
|                  | SAL/VAN | 0.19                        | 0.85 | 0.28 | 0.40 | 1.92                   | 1.00                   | 0.05                   | 1.00                   | 1.00                   | 1.66×10 <sup>-4</sup>  | 0.00                     | 0.04 | 0.01 | 0.01 | 0.13 |
|                  | LIM     | 1.67                        | 1.36 | 0.78 | 1.70 | 0.27                   | 1.12×10 <sup>-10</sup> | 7.17×10 <sup>-8</sup>  | 0.69                   | 6.18×10 <sup>-4</sup>  | 1.00                   | 0.18                     | 0.24 | 0.03 | 0.10 | 0.00 |
|                  | FP-CONT | 2.56                        | 0.28 | 1.74 | 0.92 | 3.23                   | 1.21×10 <sup>-14</sup> | 1.00                   | 3.31×10 <sup>-8</sup>  | 0.06                   | 1.11×10 <sup>-8</sup>  | 0.23                     | 0.00 | 0.19 | 0.08 | 0.22 |
|                  | DMN     | 3.42                        | 1.91 | 2.23 | 1.19 | 0.24                   | 1.76×10 <sup>-20</sup> | 1.80×10 <sup>-8</sup>  | 2.03×10 <sup>-7</sup>  | 4.64×10 <sup>-3</sup>  | 1.00                   | 0.37                     | 0.18 | 0.21 | 0.08 | 0.00 |
| SC               | 4.16    | 3.98                        | 1.27 | 0.07 | 4.00 | 1.30×10 <sup>-18</sup> | 1.06×10 <sup>-12</sup> | 6.19×10 <sup>-4</sup>  | 1.00                   | 1.92×10 <sup>-7</sup>  | 0.38                   | 0.29                     | 0.12 | 0.00 | 0.17 |      |

VIS: visual network; SMOT: somatomotor network; DAN: dorsal attention network; SAL/VAN: salience/ventral attention network; LIM: limbic network; FP-CONT: frontoparietal control network; DMN: default mode network; SC: subcortical region

**eTable 13.** Statistical Details of the Tests Examining Differences in the Network-Averaged Measures of Segregation and Integration Between the Leaf Clusters From the HBN Dendrogram That Differed in Hyperactivity/Impulsivity Problems (Subgroup d and g)

|                          |                | Subgroup-d   | Subgroup-g   | Statistics                  |                        |                          |
|--------------------------|----------------|--------------|--------------|-----------------------------|------------------------|--------------------------|
|                          |                |              |              | Test statistic <sup>a</sup> | p-value                | Effect size <sup>b</sup> |
| Median segregation (IQR) | Mean VIS (SD)  | 1.67 (0.54)  | 2.30 (0.41)  | 0.63                        | 3.74×10 <sup>-9</sup>  | 0.25                     |
|                          | Mean SMOT (SD) | 2.14 (0.55)  | 2.78 (0.36)  | 0.64                        | 1.62×10 <sup>-10</sup> | 0.26                     |
|                          | Mean DAN (SD)  | 1.31 (0.39)  | 1.90 (0.30)  | 0.60                        | 3.33×10 <sup>-17</sup> | 0.36                     |
|                          | SAL/VAN        | 0.91 (0.47)  | 1.60 (0.40)  | 0.62                        | 9.43×10 <sup>-14</sup> | 0.58                     |
|                          | LIM            | 0.91 (0.40)  | 1.19 (0.52)  | 0.24                        | 2.11×10 <sup>-5</sup>  | 0.12                     |
|                          | FP-CONT        | 1.02 (0.37)  | 1.77 (0.34)  | 0.72                        | 1.51×10 <sup>-15</sup> | 0.70                     |
|                          | Mean DMN (SD)  | 1.07 (0.25)  | 1.38 (0.18)  | 0.31                        | 1.11×10 <sup>-13</sup> | 0.28                     |
|                          | SC             | 0.77 (0.24)  | 1.12 (0.32)  | 0.38                        | 3.32×10 <sup>-14</sup> | 0.54                     |
| Median integration (IQR) | VIS            | 7.53 (2.86)  | 8.41 (2.34)  | 0.35                        | 1.00                   | 0.03                     |
|                          | SMOT           | 5.71 (2.83)  | 9.35 (2.94)  | 3.65                        | 1.46×10 <sup>-12</sup> | 0.54                     |
|                          | DAN            | 7.85 (3.74)  | 10.75 (4.04) | 2.58                        | 4.10×10 <sup>-8</sup>  | 0.25                     |
|                          | SAL/VAN        | 6.70 (3.12)  | 7.09 (3.10)  | 0.27                        | 1.00                   | 0.01                     |
|                          | LIM            | 2.17 (1.27)  | 4.04 (2.13)  | 1.58                        | 1.49×10 <sup>-8</sup>  | 0.39                     |
|                          | FP-CONT        | 8.48 (4.42)  | 5.14 (1.61)  | 2.70                        | 2.02×10 <sup>-9</sup>  | 0.26                     |
|                          | DMN            | 7.33 (2.30)  | 11.39 (2.61) | 4.23                        | 8.85×10 <sup>-18</sup> | 0.66                     |
|                          | SC             | 10.41 (5.34) | 5.18 (1.87)  | 5.42                        | 2.60×10 <sup>-11</sup> | 0.61                     |

VIS: visual network; SMOT: somatomotor network; DAN: dorsal attention network; SAL/VAN: salience/ventral attention network; LIM: limbic network; FP-CONT: frontoparietal control network; DMN: default mode network; SC: subcortical regions; <sup>a</sup>Test statistic: Mann-Whitney *U*-statistic for non-normally distributed continuous variables, and *t*-statistic for normally distributed continuous variables; <sup>b</sup>Effect size: eta-squared ( $\eta^2$ ) for continuous variables



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