Supplementary Note 1: HCP-YA data acquisition and preprocessing

Data Acquisition Whole-brain echo-planar imaging acquisitions were measured with a 32 channel head coil on a modified 3T Siemens Skyra (Connectome Skyra) at WashU with time to repetition (TR)=720ms, time to echo (TE)=33.1ms, flip angle=52, bandwidth=2,290 Hz/pixel, in-plane field of view (FOV)=208×180mm, 72 slices, and 2.0mm isotropic voxels, with a multi-band acceleration factor of 8 (Uğurbil et al., 2013). Data were collected over 2 days. On each day 29 min of rest (eyes open with fixation on a cross-hair) BOLD data across two runs were collected (56 min total), followed by 30 min of task fMRI data collection (60 min total). The two 14.5-minute resting-state BOLD runs that were collected on the same day were acquired with opposite phase encoding directions (L/R and R/L). Complete parameters and acquisition details for the HCP dataset were reported by (Smith et al., 2013). Task-based imaging data were not used in this study. Structural scans with the following parameters were also collected: T1-weighted (0.7 mm isotropic resolution, TR=2400ms, TE=2.14ms, flip angle=8, in-plane field of view=224×224) and T2-weighted (0.7 mm isotropic resolution, TR=3200ms, TE=565ms, variable flip angle, in-plane field of view=224×224).

Preprocessing Resting-State fMRI Preprocessing Preprocessing consisted of the following steps, which closely followed the steps advanced by the HCP consortium: i) The 'minimal preprocessing' approach outlined by Glasser and colleagues (Glasser et al., 2013), which involved intensity normalization, phase-encoding direction unwarping, motion correction, and spatial normalization to a standard template (Glasser et al., 2016) MSMAll, Angular Deviation Penalty (ADP) version; (Glasser et al., 2016); ii) High-pass filtering (0.009Hz); iii) ICA-FIX for artifact removal (Salimi-Khorshidi et al., 2014). The final 'minimally preprocessed' BOLD data was represented in the Connectivity Informatics Technology Initiative (CIFTI) file format, which combines surface-based data representation for 1 cortex and volume-based data for subcortex gray matter locations (i.e. 'grayordinates'). The CIFTI grayordinate BOLD time series were in turn used for subsequent analysis. Additional analyses were performed with Workbench v1.2.3 and Matlab 2014b (The Mathworks). To remove any potential artifact at the onset/offset of each new run, the first 100 frames were removed from every BOLD run for each subject. Subsequently, BOLD runs were concatenated in order of acquisition (resting-state fMRI runs 2-1-4-3, R/L first, then L/R) following removal of the mean of each run from each time series.

Visualization All visualizations were produced using Connectome Workbench using the CIFTI format, which combines surface data for cortex with volume data for subcortex. To convert a 360-element partition vector (cortex) into a CIFTI file, the following steps were taken: 1. For each hemisphere, a template 32k vertex CIFTI surface map file was loaded, where each vertex was labeled with its corresponding parcel label from the Glasser parcels. 2. Each parcel label was replaced with its corresponding network label from the 360element partition vector. 3. Step 2 was repeated for the opposite hemisphere. 4. Results were saved as a func.gii file for visualization in Connectome Workbench.

Supplementary Figures

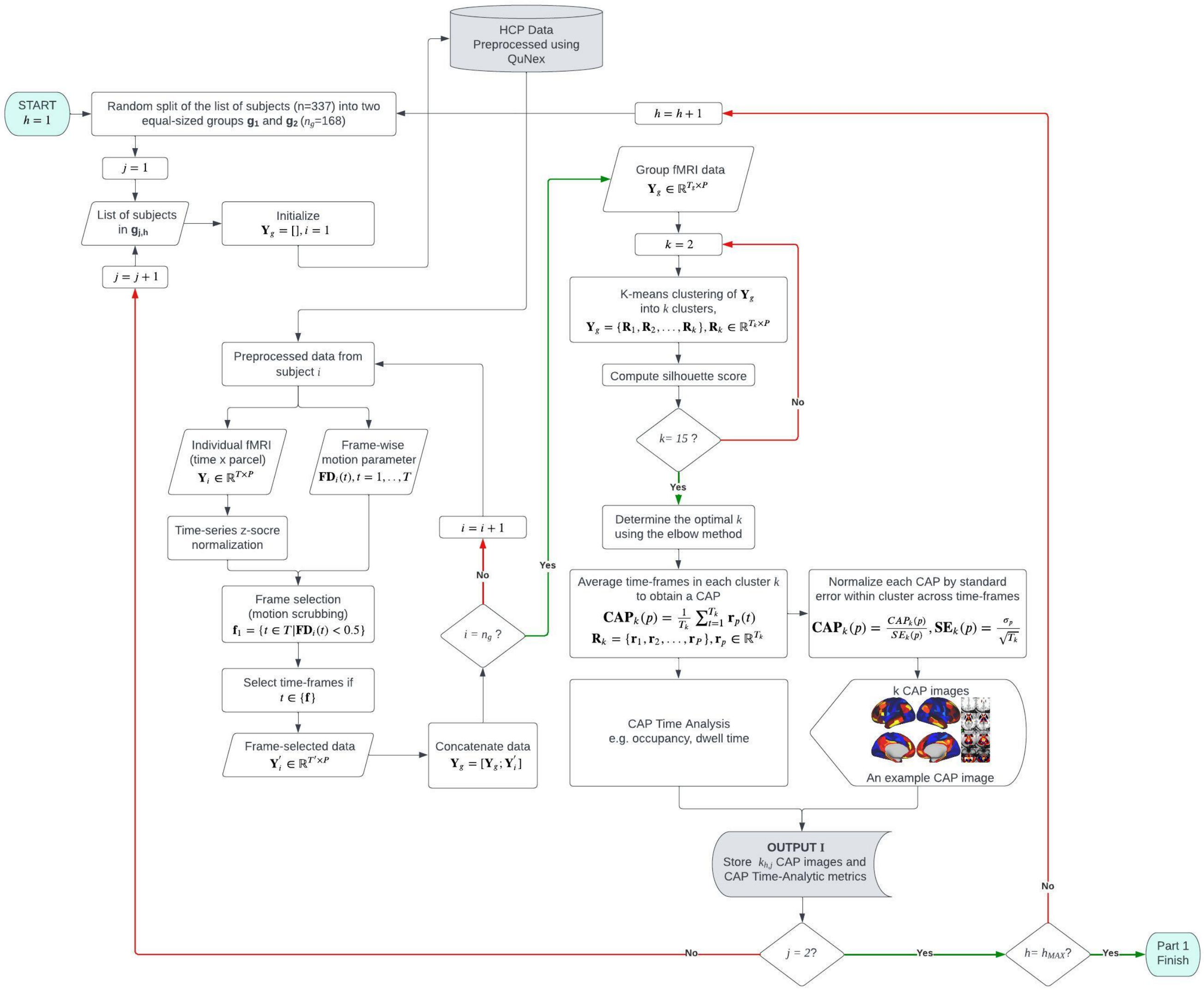

Fig. S1. Workflow of CAP analysis.

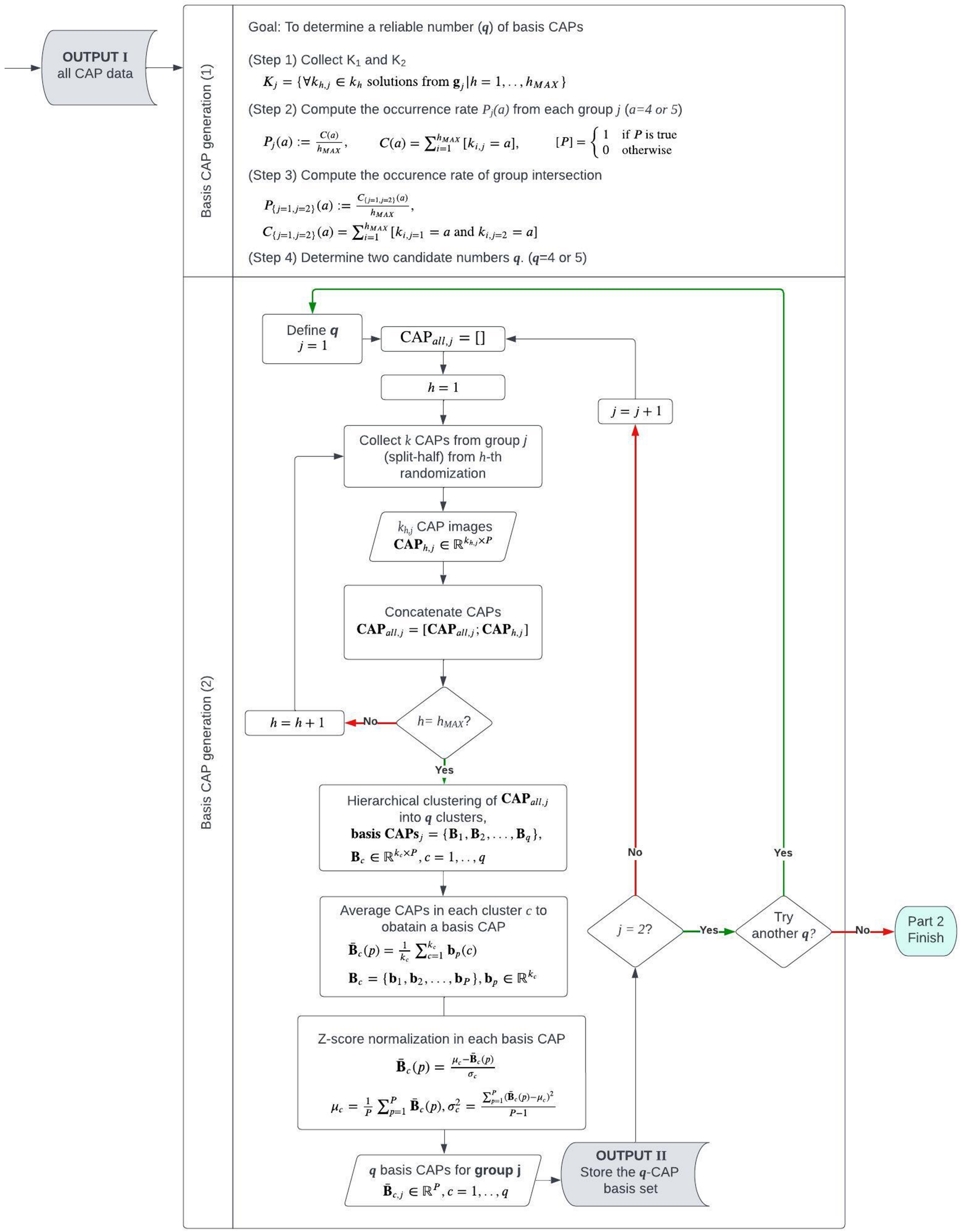

Fig. S2. Generation of basis CAP sets.

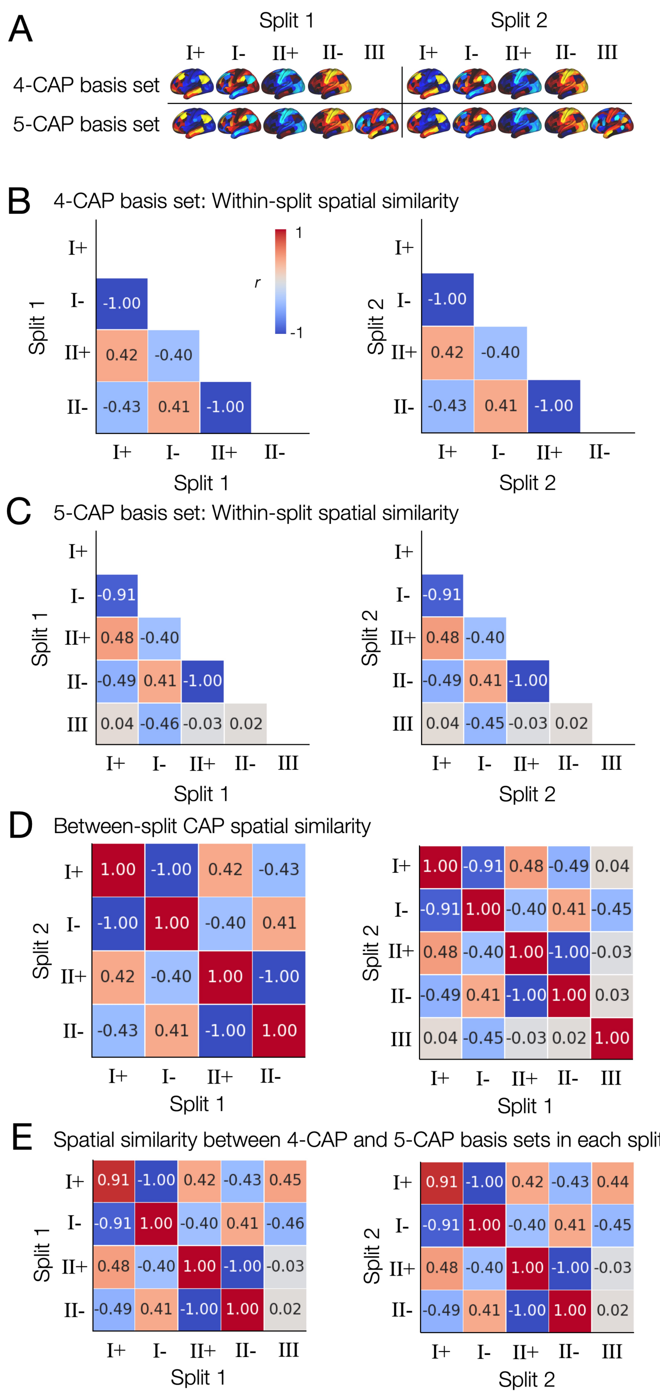

Fig. S3. Spatial patterns of the basis CAPs are distinct to each other and reproducible using the proposed shuffled split-half analysis. (A) Spatial patterns of the basis CAPs in each split-half data. The 4-CAP basis set and the 5-CAP basis set were generated independently from the same split-half data, using the hierarchical clustering across 1,000 shuffled split-half resampling, as described in **Fig. S2**. **(B)** Spatial similarity (r, correlation coefficient) of the 4-CAP basis set within the split 1 data (left) and within the split 2 data (right). r values were rounded to the nearest 2 decimal digits for visualization. **(C)** Spatial similarity of the 5-CAP basis set within the split 1 data (left) and within the split 2 data (right). **(D)** Spatial similarity of the 4-CAP basis set between the split 1 and 2 data (left) and of the 5-CAP basis set between the split 1 and 2 data (right). **(E)** Spatial similarity between the 4-CAP basis set and the 5-CAP basis set within the split 1 data (left) and within the split 2 data (right).

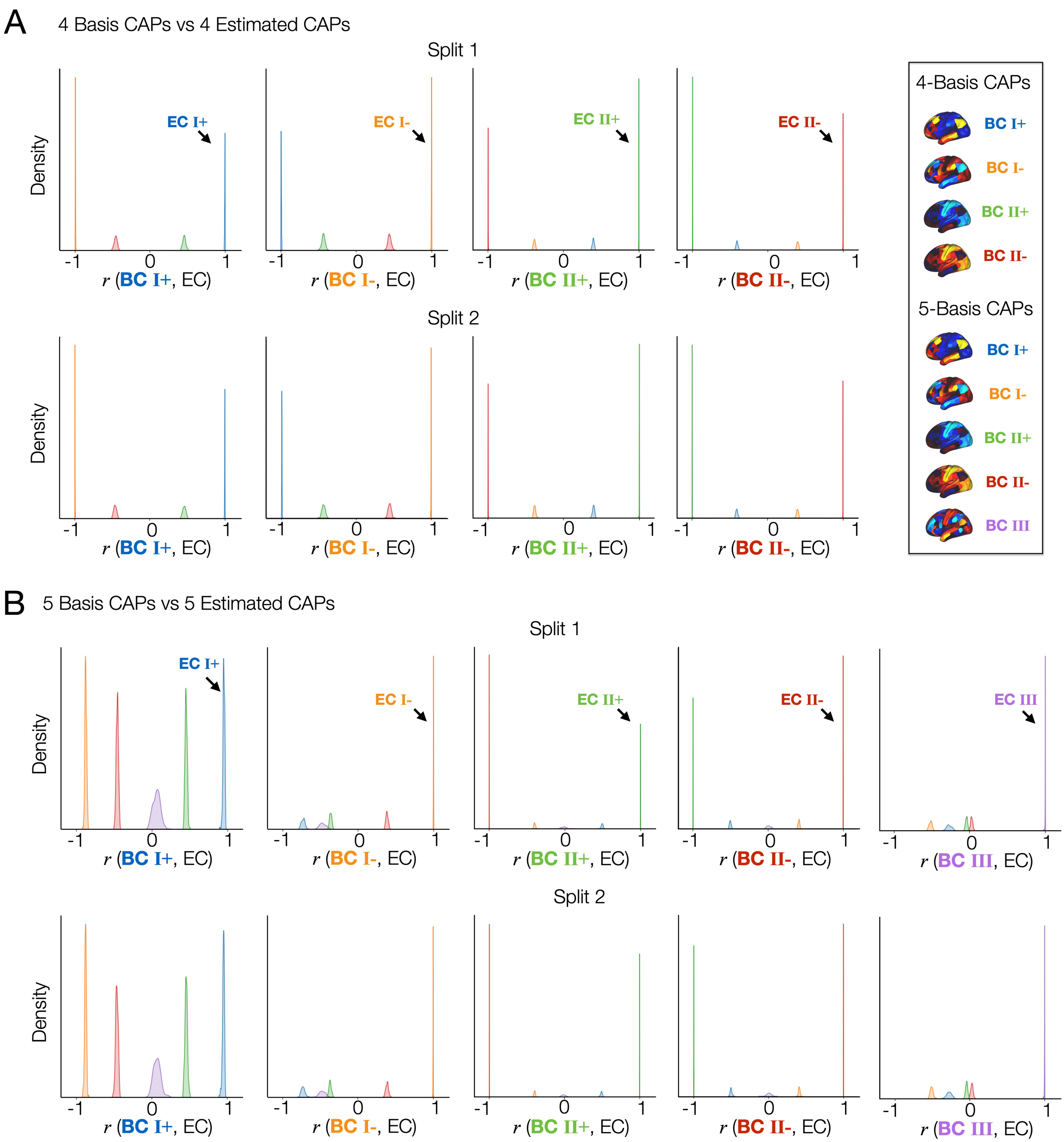

Fig. S4. Spatial patterns of the CAPs estimated from both splits are reproducible and strongly correlated with at least one of the basis CAPs. (A) From left to right, the marginal distributions of r between all estimated CAPs (ECs) and each basis CAP (BC) from the 4-CAP basis set are illustrated using kernel density estimation. Results were obtained from the split 1 data (top) and the split 2 data (bottom). Each r value is color-coded using a sorting algorithm to label the corresponding EC using the maximum spatial correlation with BCs. **(B)** From left to right, the marginal distributions of r between all estimated CAPs and each BC from the 5-CAP basis set are illustrated using kernel density estimation.

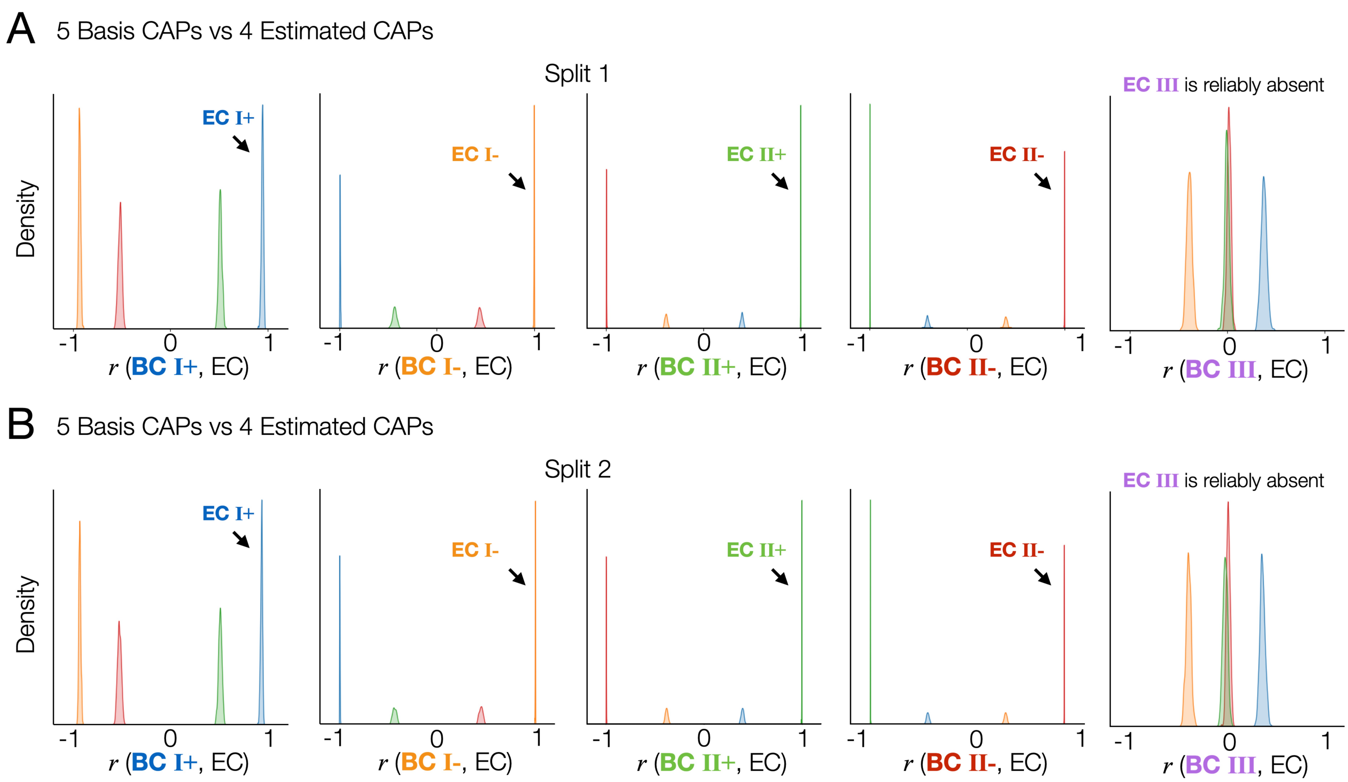

Fig. S5. CAP state III is reproducibly absent across permutations in both splits.

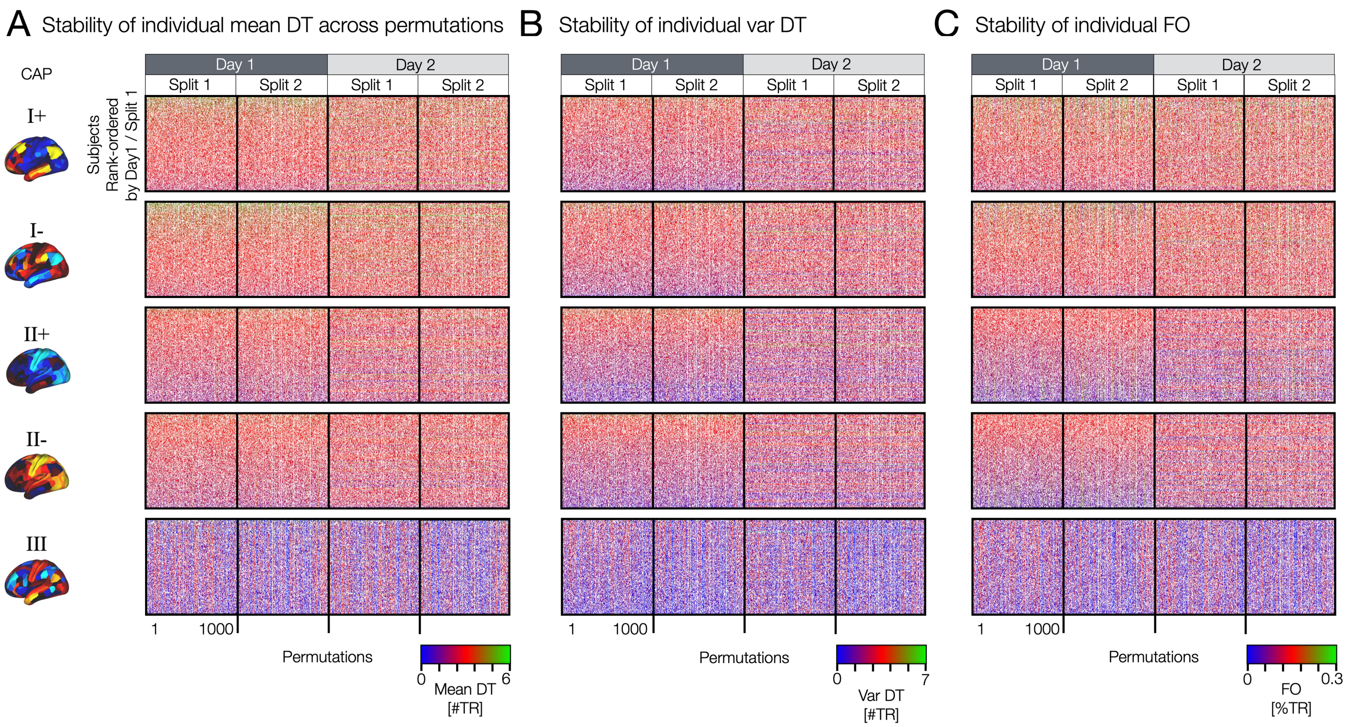

Fig. S6. Stability of individual mean DT, var DT and FO across permutations

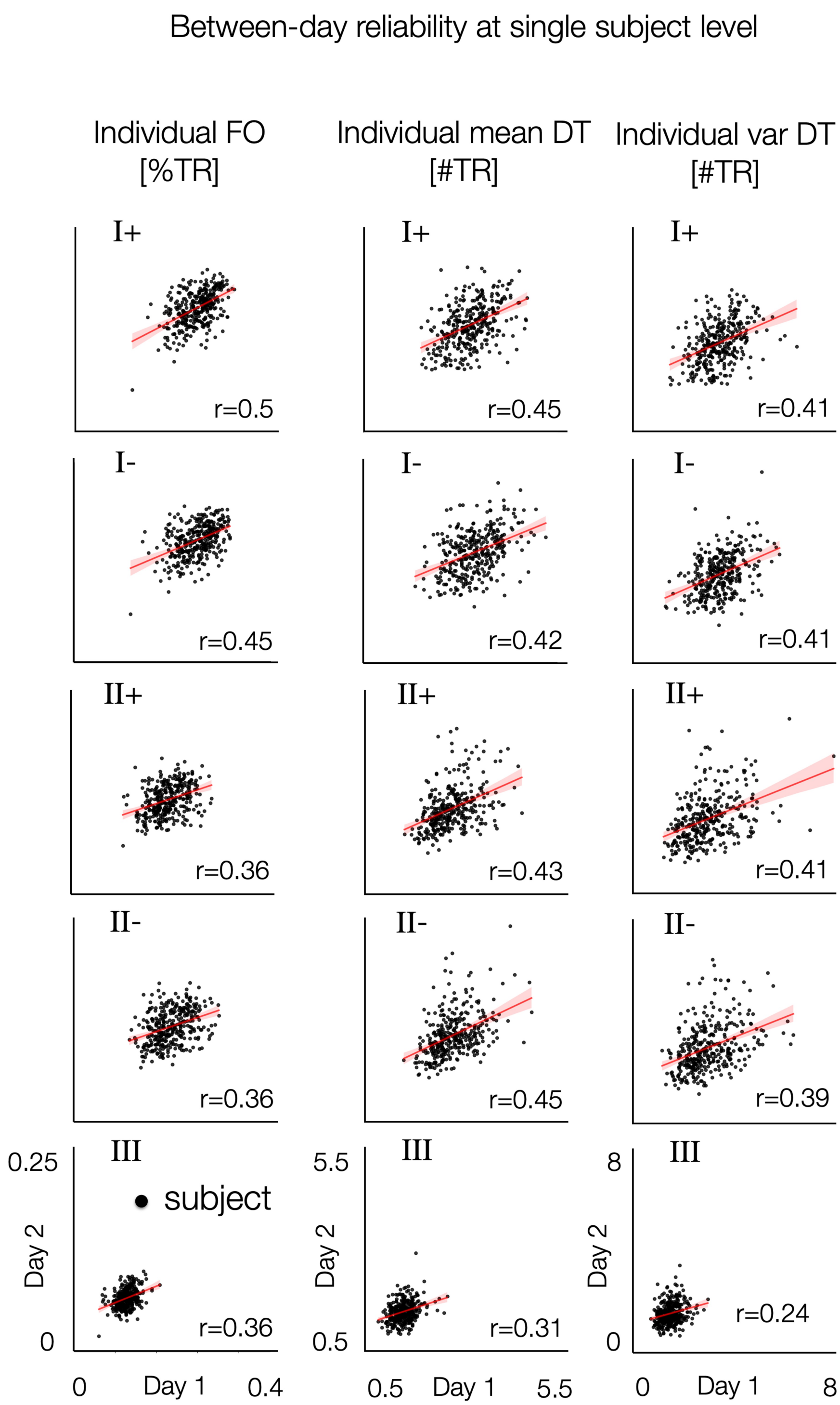

Fig. S7. Between-day reliability of neural measures at single subject level. Each datapoint in the scatter plot is a subject. For each subject, neural measures were averaged across permutations.

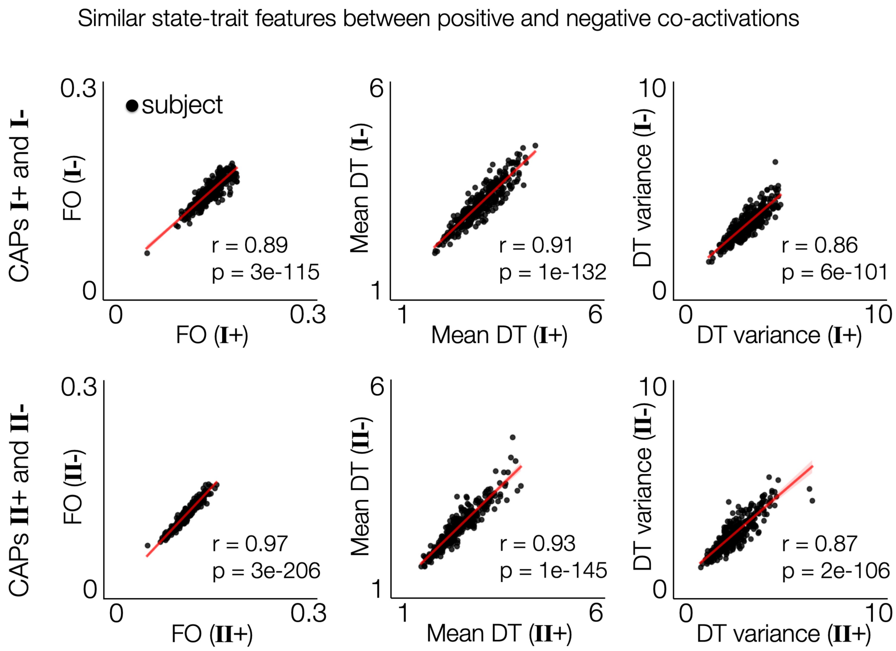

Fig. S8. Similarity of temporal organizations between positive and negative co-activation patterns. CAP states I and II have similar FO, mean DT and DT variance across the positive and negative co-activation states (I+ vs I- and II+ vs II-). Each data-point indicate a subject. The temporal metric values across all permutations and two days were averaged within each subject.

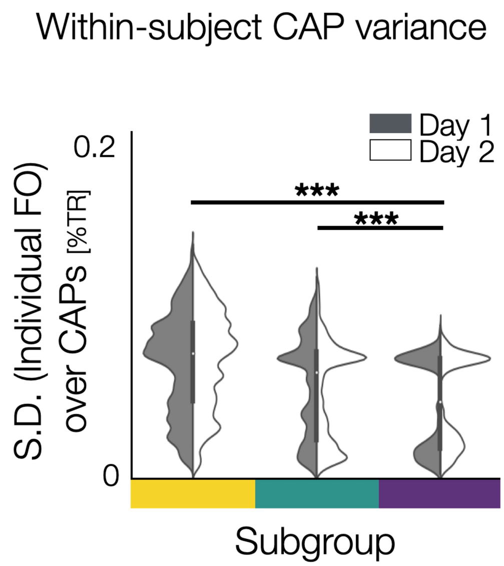

Fig. S9. Within-subject variance of FO across 5 CAPs across permutations.

1 – MMSE_Score
2 – PSQI_Score
3 – PicSeq_AgeAdj
4 – CardSort_AgeAdj
5 – Flanker_AgeAdj
6 – PMAT24_A_CR
7 – PMAT24_A_SI
8 – PMAT24_A_RTCR
9 – ReadEng_AgeAdj
10 – PicVocab_AgeAdj
11 – ProcSpeed_AgeAdj
12 – DDisc_SV_1mo_200
13 – DDisc_SV_6mo_200
14 – DDisc_SV_1yr_200
15 – DDisc_SV_3yr_200
16 – DDisc_SV_5yr_200
17 – DDisc_SV_10yr_200
18 – DDisc_SV_1mo_40K
19 – DDisc_SV_6mo_40K
20 – DDisc_SV_1yr_40K
21 – DDisc_SV_3yr_40K
22 – DDisc_SV_5yr_40K
23 – DDisc_SV_10yr_40K
24 – DDisc_AUC_200
25 – DDisc_AUC_40K
26 – VSPLOT_TC
27 – VSPLOT_CRTE
28 – VSPLOT_OFF
29 – SCPT_TP
30 – SCPT_TN
31 – SCPT_FP
32 – SCPT_FN
33 – SCPT_TPRT
34 – SCPT_SEN
35 – SCPT_SPEC
36 – SCPT_LRNR
37 – IWRD_TOT
38 – IWRD_RTC
39 – ListSort_AgeAdj
40 – ER40_CR
41 – ER40_CRT
42 – ER40ANG
43 – ER40FEAR
44 – ER40HAP
45 – ER40NOE
46 – ER40SAD
47 – AngAffect_Unadj
48 – AngHostil_Unadj
49 – AngAggr_Unadj
50 – FearAffect_Unadj
51 – FearSomat_Unadj
52 – Sadness_Unadj
53 – LifeSatisf_Unadj
54 – MeanPurp_Unadj
55 – PosAffect_Unadj
56 – Friendship_Unadj
57 – Loneliness_Unadj
58 – PercHostil_Unadj
59 – PercReject_Unadj
60 – EmotSupp_Unadj
61 – InstruSupp_Unadj
62 – PercStress_Unadj
63 – SelfEff_Unadj
64 – NEOFAC_A
65 – NEOFAC_O
66 – NEOFAC_C
67 – NEOFAC_N
68 – NEOFAC_E
69 – Emotion_Task_Acc
70 – Emotion_Task_Median_RT
71 – Emotion_Task_Face_Acc
72 – Emotion_Task_Face_Median_RT
73 – Emotion_Task_Shape_Acc
74 – Emotion_Task_Shape_Median_RT
75 – Gambling_Task_Perc_Larger
76 – Gambling_Task_Perc_Smaller
77 – Gambling_Task_Median_RT_Larger
78 – Gambling_Task_Median_RT_Smaller
79 – Gambling_Task_Reward_Perc_Larger
80 – Gambling_Task_Reward_Median_RT_Larger
81 – Gambling_Task_Reward_Perc_Smaller
82 – Gambling_Task_Reward_Median_RT_Smaller
83 – Gambling_Task_Punish_Perc_Larger
84 – Gambling_Task_Punish_Median_RT_Larger
85 – Gambling_Task_Punish_Perc_Smaller
86 – Gambling_Task_Punish_Median_RT_Smaller
87 – Language_Task_Acc
88 – Language_Task_Median_RT
89 – Language_Task_Story_Acc
90 – Language_Task_Story_Median_RT
91 – Language_Task_Story_Avg_Difficulty_Level
92 – Language_Task_Math_Acc
93 – Language_Task_Math_Median_RT
94 – Language_Task_Math_Avg_Difficulty_Level
95 – Relational_Task_Acc
96 – Relational_Task_Median_RT
97 – Relational_Task_Match_Acc
98 – Relational_Task_Match_Median_RT
99 – Relational_Task_Rel_Acc
100 – Relational_Task_Rel_Median_RT
101 – Social_Task_Perc_Random
102 – Social_Task_Perc_TOM
103 – Social_Task_Perc_Unsure
104 – Social_Task_Median_RT_Random
105 – Social_Task_Median_RT_TOM
106 – Social_Task_Median_RT_Unsure
107 – Social_Task_Random_Perc_Random
108 – Social_Task_Random_Median_RT_Random
109 – Social_Task_Random_Perc_TOM
110 – Social_Task_Random_Perc_Unsure
111 – Social_Task_TOM_Perc_TOM
112 – Social_Task_TOM_Median_RT_TOM
113 – Social_Task_TOM_Perc_Unsure
114 – WM_Task_Acc
115 – WM_Task_Median_RT
116 – WM_Task_2bk_Acc
117 – WM_Task_2bk_Median_RT
118 – WM_Task_0bk_Acc
119 – WM_Task_0bk_Median_RT
120 – WM_Task_0bk_Body_Acc
121 – WM_Task_0bk_Body_Acc_Target
122 – WM_Task_0bk_Body_Acc_Nontarget
123 – WM_Task_0bk_Face_Acc
124 – WM_Task_0bk_Face_Acc_Target
125 – WM_Task_0bk_Face_ACC_Nontarget
126 – WM_Task_0bk_Place_Acc
127 – WM_Task_0bk_Place_Acc_Target
128 – WM_Task_0bk_Place_Acc_Nontarget
129 – WM_Task_0bk_Tool_Acc
130 – WM_Task_0bk_Tool_Acc_Target
131 – WM_Task_0bk_Tool_Acc_Nontarget
132 – WM_Task_2bk_Body_Acc
133 – WM_Task_2bk_Body_Acc_Target
134 – WM_Task_2bk_Body_Acc_Nontarget
135 – WM_Task_2bk_Face_Acc
136 – WM_Task_2bk_Face_Acc_Target
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140 – WM_Task_2bk_Place_Acc_Nontarget
141 – WM_Task_2bk_Tool_Acc
142 – WM_Task_2bk_Tool_Acc_Target
143 – WM_Task_2bk_Tool_Acc_Nontarget
144 – WM_Task_0bk_Body_Median_RT
145 – WM_Task_0bk_Body_Median_RT_Target
146 – WM_Task_0bk_Body_Median_RT_Nontarget
147 – WM_Task_0bk_Face_Median_RT
148 – WM_Task_0bk_Face_Median_RT_Target
149 – WM_Task_0bk_Face_Median_RT_Nontarget
150 – WM_Task_0bk_Place_Median_RT
151 – WM_Task_0bk_Place_Median_RT_Target
152 – WM_Task_0bk_Place_Median_RT_Nontarget
153 – WM_Task_0bk_Tool_Median_RT
154 – WM_Task_0bk_Tool_Median_RT_Target
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156 – WM_Task_2bk_Body_Median_RT
157 – WM_Task_2bk_Body_Median_RT_Target
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163 – WM_Task_2bk_Place_Median_RT_Target
164 – WM_Task_2bk_Place_Median_RT_Nontarget
165 – WM_Task_2bk_Tool_Median_RT
166 – WM_Task_2bk_Tool_Median_RT_Target
167 – WM_Task_2bk_Tool_Median_RT_Nontarget
168 – ASR_Anxd_Pct
169 – ASR_Witd_T
170 – ASR_Soma_T
171 – ASR_Thot_T
172 – ASR_Attn_T
173 – ASR_Aggr_T
174 – ASR_Rule_T
175 – ASR_Intr_T
176 – ASR_Intn_T
177 – ASR_Extn_T
178 – ASR_Totp_T
179 – DSM_Depr_T
180 – DSM_Anxi_T
181 – DSM_Somp_T
182 – DSM_Avoid_T
183 – DSM_Adh_T
184 – DSM_Antis_T
185 – SSAGA_ChildhoodConduct
186 – SSAGA_PanicDisorder
187 – SSAGA_Agoraphobia
188 – SSAGA_Depressive_Ep
189 – SSAGA_Depressive_Sx
190 – Total_Drinks_7days
191 – Num_Days_Drank_7days
192 – Avg_Weekday_Drinks_7days
193 – Avg_Weekend_Drinks_7days
194 – Total_Beer_Wine_Cooler_7days
195 – Avg_Weekday_Beer_Wine_Cooler_7days
196 – Avg_Weekend_Beer_Wine_Cooler_7days
197 – Total_Malt_Liquor_7days
198 – Avg_Weekday_Malt_Liquor_7days
199 – Avg_Weekend_Malt_Liquor_7days
200 – Total_Wine_7days
201 – Avg_Weekday_Wine_7days
202 – Avg_Weekend_Wine_7days
203 – Total_Hard_Liquor_7days
204 – Avg_Weekday_Hard_Liquor_7days
205 – Avg_Weekend_Hard_Liquor_7days
206 – Total_Other_Alc_7days
207 – Avg_Weekend_Other_Alc_7days
208 – SSAGA_Alc_D4_Dp_Sx
209 – SSAGA_Alc_D4_Ab_Dx
210 – SSAGA_Alc_D4_Ab_Sx
211 – SSAGA_Alc_D4_Dp_Dx
212 – SSAGA_Alc_12_Drinks_Per_Day
213 – SSAGA_Alc_12_Frq
214 – SSAGA_Alc_12_Frq_5plus
215 – SSAGA_Alc_12_Frq_Drk
216 – SSAGA_Alc_12_Max_Drinks
217 – SSAGA_Alc_Age_1st_Use
218 – SSAGA_Alc_Hvy_Drinks_Per_Day
219 – SSAGA_Alc_Hvy_Frq
220 – SSAGA_Alc_Hvy_Frq_5plus
221 – SSAGA_Alc_Hvy_Frq_Drk
222 – SSAGA_Alc_Hvy_Max_Drinks
223 – Total_Any_Tobacco_7days
224 – Times_Used_Any_Tobacco_Today
225 – Num_Days_Used_Any_Tobacco_7days
226 – Avg_Weekday_Any_Tobacco_7days
227 – Avg_Weekend_Any_Tobacco_7days
228 – Total_Cigarettes_7days
229 – Avg_Weekday_Cigarettes_7days
230 – Avg_Weekend_Cigarettes_7days
231 – Total_Cigars_7days
232 – Avg_Weekday_Cigars_7days
233 – Avg_Weekend_Cigars_7days
234 – Total_Chew_7days
235 – Avg_Weekday_Chew_7days
236 – Avg_Weekend_Chew_7days
237 – Total_Other_Tobacco_7days
238 – Avg_Weekday_Other_Tobacco_7days
239 – Avg_Weekend_Other_Tobacco_7days
240 – SSAGA_FTND_Score
241 – SSAGA_HSI_Score
242 – SSAGA_TB_Age_1st_Cig
243 – SSAGA_TB_DSM_Difficulty_Quitting
244 – SSAGA_TB_DSM_Tolerance
245 – SSAGA_TB_DSM_Withdrawal
246 – SSAGA_TB_Hvy_CPD
247 – SSAGA_TB_Max_Cigs
248 – SSAGA_TB_Reg_CPD
249 – SSAGA_TB_Smoking_History
250 – SSAGA_TB_Still_Smoking
251 – SSAGA_TB_Yrs_Since_Quit
252 – SSAGA_TB_Yrs_Smoked
253 – SSAGA_Times_Used_Illicits
254 – SSAGA_Times_Used_Cocaine
255 – SSAGA_Times_Used_Hallucinogens
256 – SSAGA_Times_Used_Opiates
257 – SSAGA_Times_Used_Sedatives
258 – SSAGA_Times_Used_Stimulants
259 – SSAGA_Mj_Use
260 – SSAGA_Mj_Ab_Dep
261 – SSAGA_Mj_Age_1st_Use
262 – SSAGA_Mj_Times_Used

Fig. S10. List of behavioral variables. Behavioral variable names are identical to the variable names provided by the HCP data dictionary for the S1200 data release: `HCP_S1200_DataDictionary_April_20_2018.csv`. Check https://wiki.humanconnectome.org/display/PublicData/HCP-YA+Data+Dictionary-+Updated+for+the+1200+Subject+Release for details.

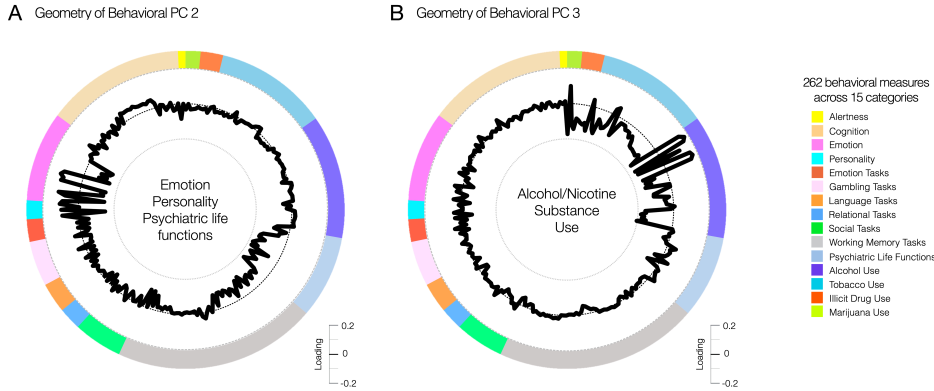

Fig. S11. The geometry of behavioral PCs 2 and 3. PC 3 has a relationship with sex.

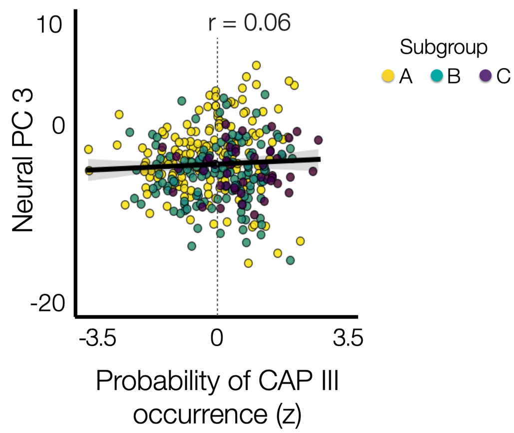

Fig. S12. There is no relationship between individual's preference to CAP III and the individual scores on neural PC 3.