

## Supplementary Figures

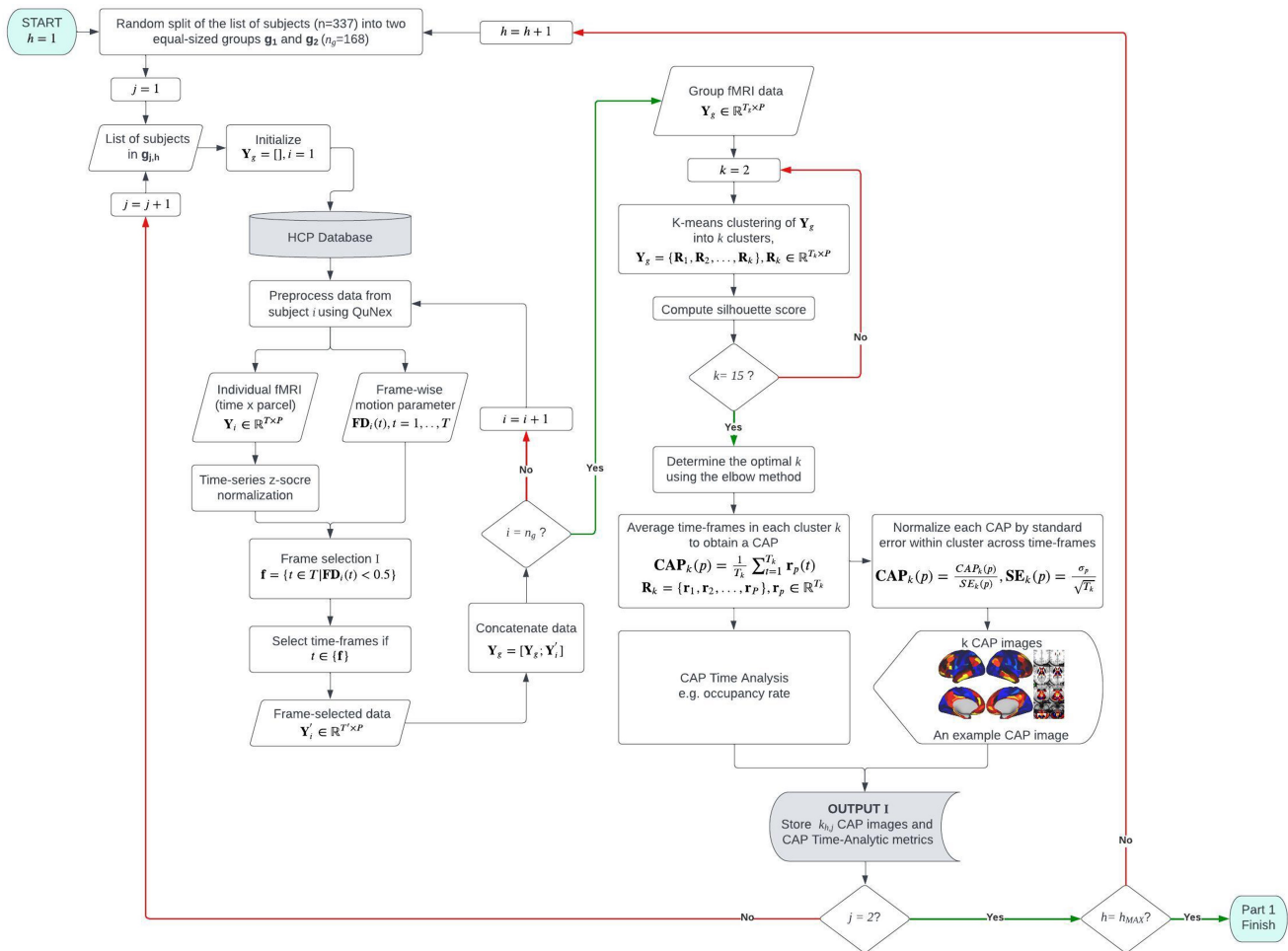
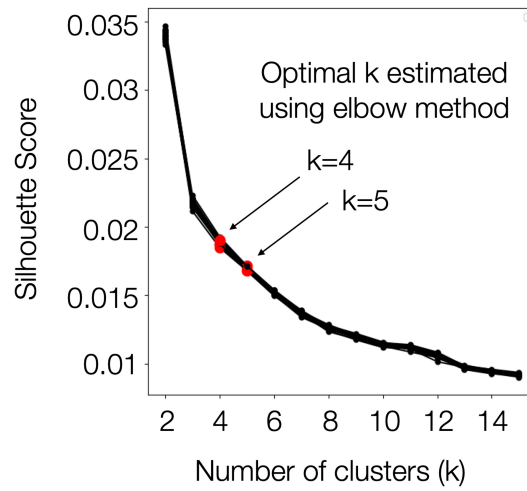
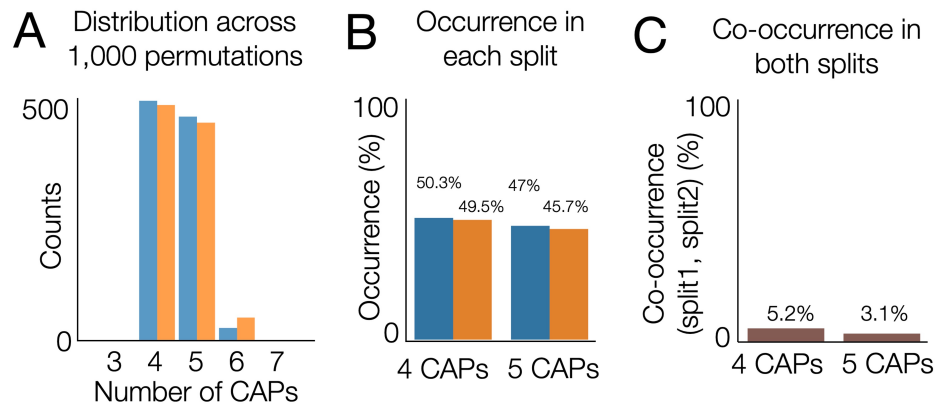


Fig. S1. Workflow of CAP analysis.



**Fig. S2. Quality of the K means clustering solution in CAP analysis.** Silhouette scores were estimated across different numbers of clusters ( $k$ ) from the K-means clustering solution from a split data. Results from 10 permutations (two split-halves in each permutation) are shown. Optimal  $k$  values were estimated using the elbow method for the Silhouette scores and are highlighted in red.

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**Fig. S3. Occurrence of CAPs across permutations.** (A) The estimated number of CAPs ( $k$ ) in each split across 1,000 permutations. (B) Occurrence rate (%) of  $k=4$  or  $k=5$  solutions in each split. (C) Co-occurrence rate (%) of  $k=4$  or  $k=5$  solutions in both splits.

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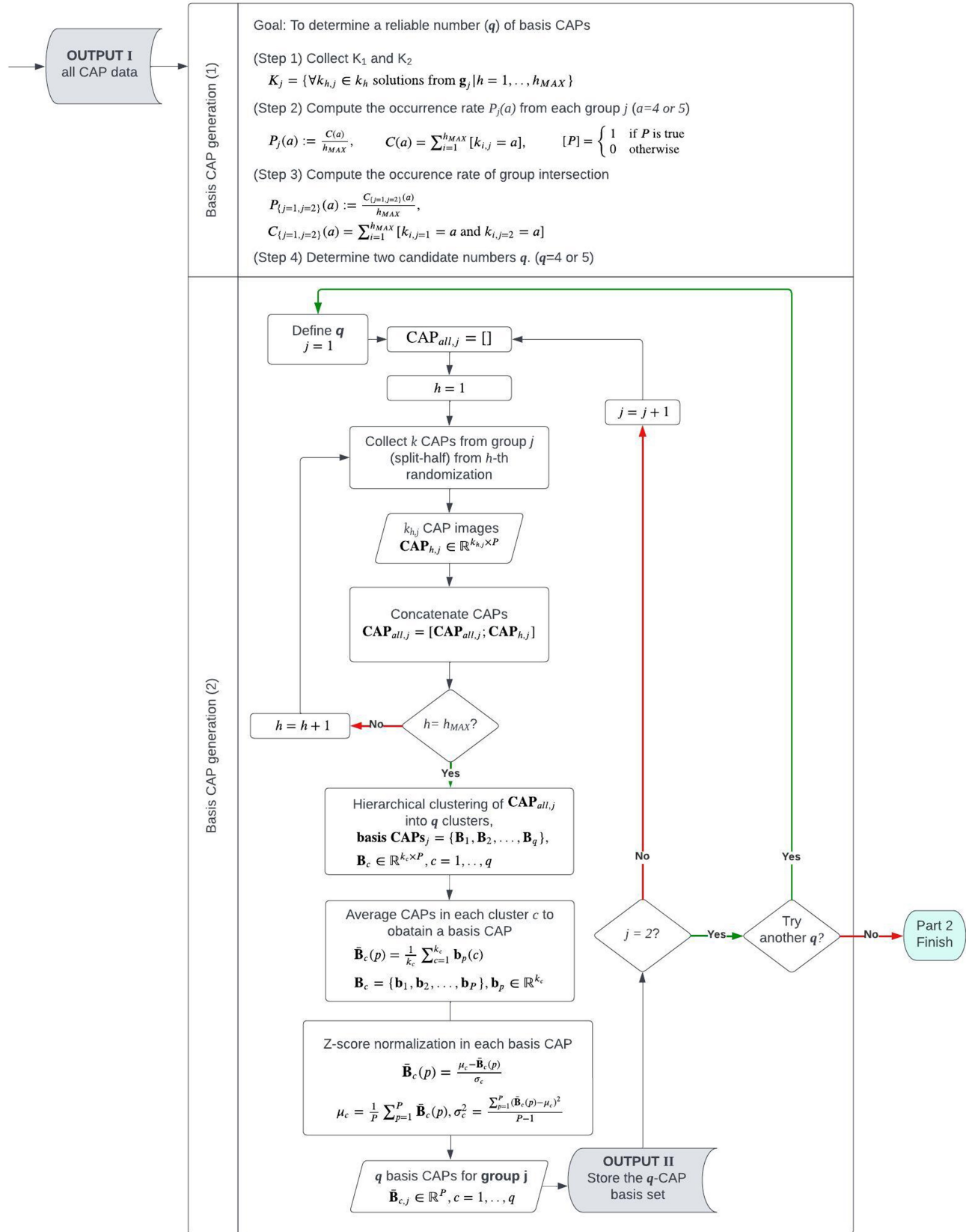
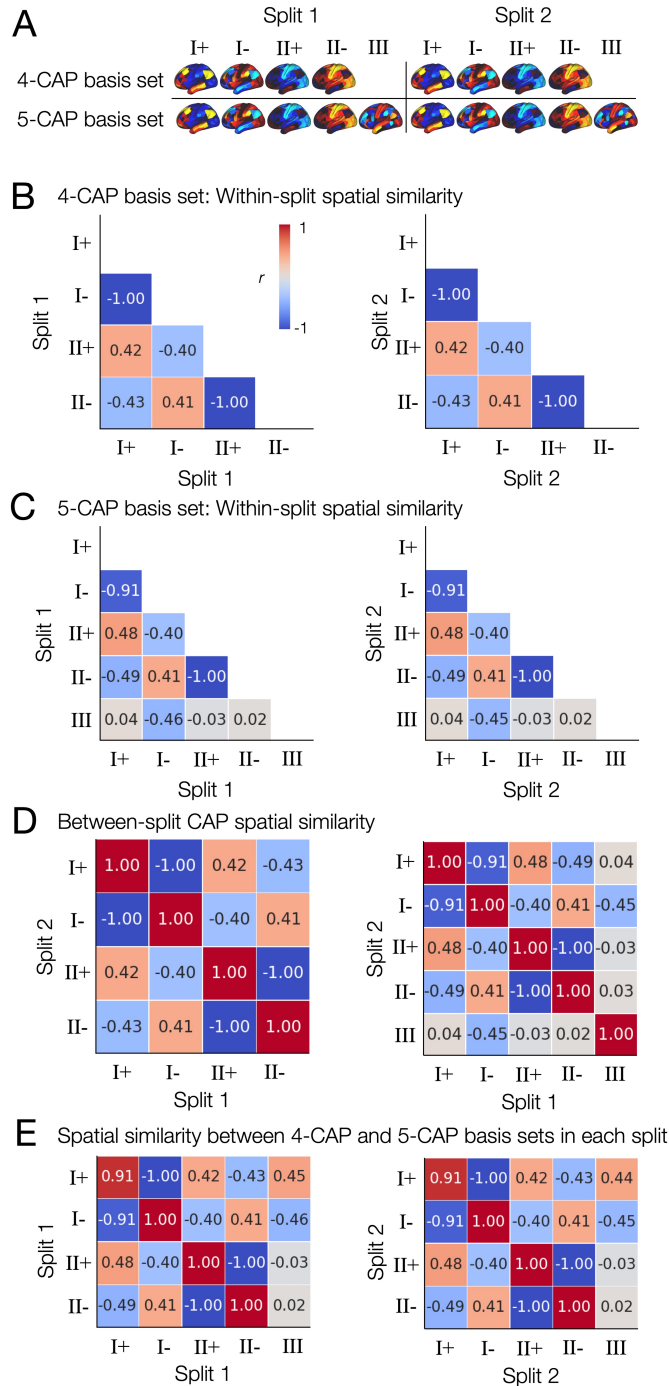


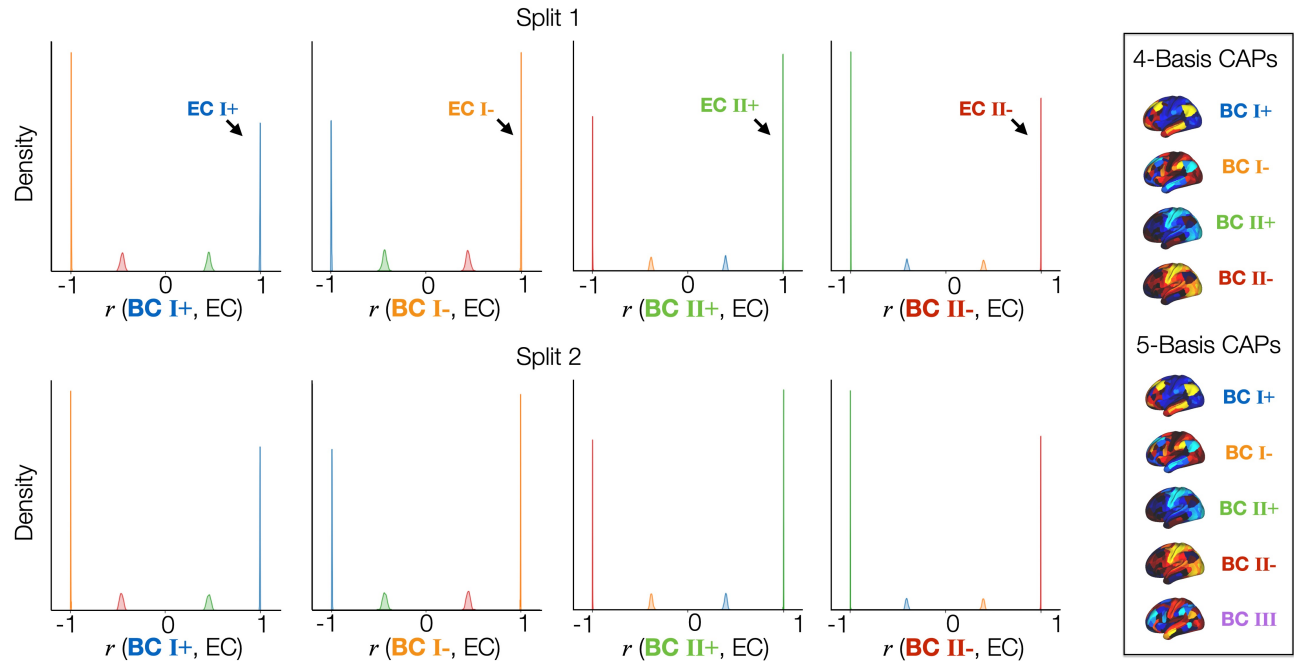
Fig. S4. Generation of basis CAP sets.



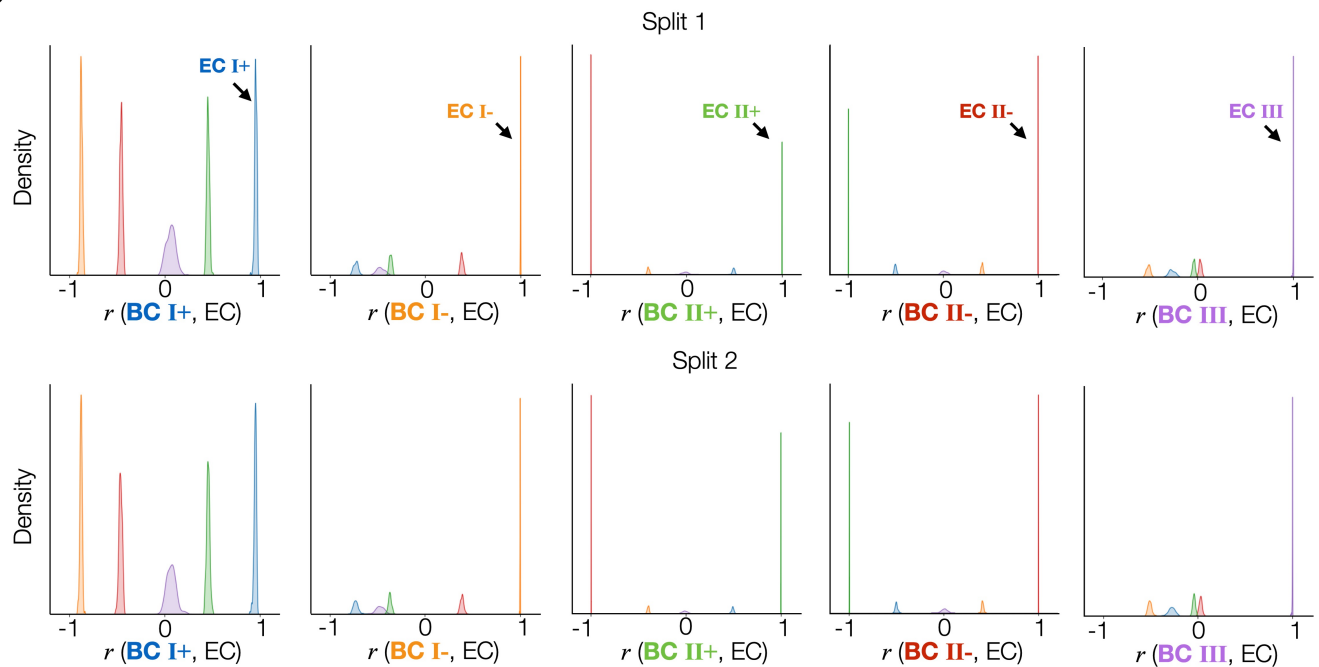


**Fig. S5. Spatial patterns of the basis CAPs are distinct to each other and reproducible using the proposed shuffled split-half analysis.** (A) Spatial patterns of the basis CAPs in each split-half data. The 4-CAP basis set and the 5-CAP basis set were generated independently from the same split-half 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).

## A 4 Basis CAPs vs 4 Estimated CAPs

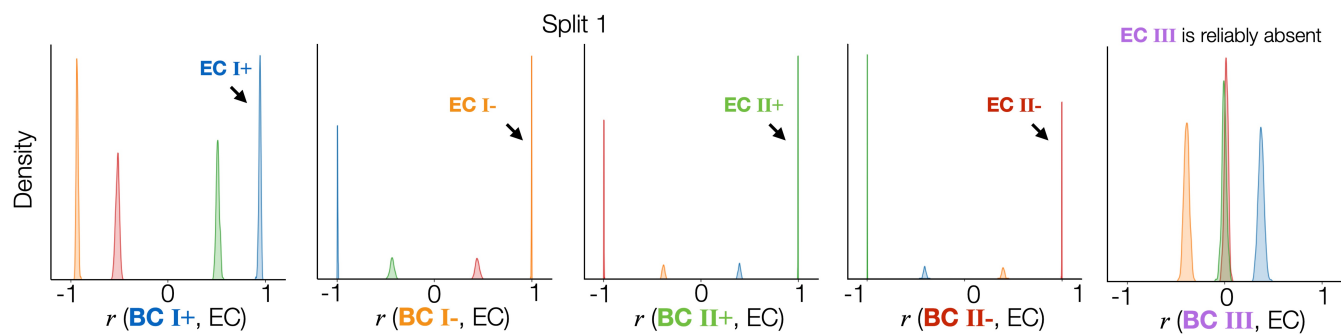


## B 5 Basis CAPs vs 5 Estimated CAPs

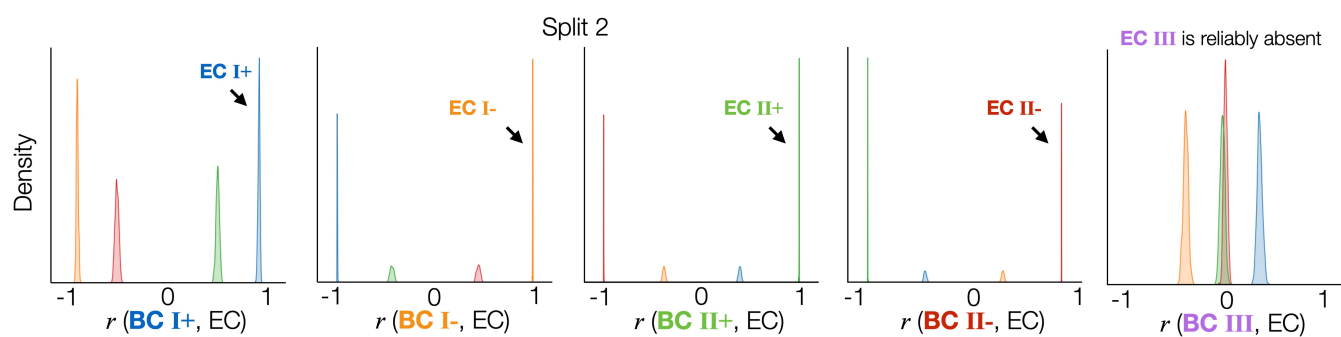


**Fig. S6. Spatial patterns of the CAPs estimated from both splits are reproducible and strongly correlated with at least one of the basis CAPs. (A)** From left to right, the marginal distributions of  $r$  between all estimated CAPs (ECs) and each basis CAP (BC) from the 4-CAP basis set are illustrated 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.

**A** 5 Basis CAPs vs 4 Estimated CAPs

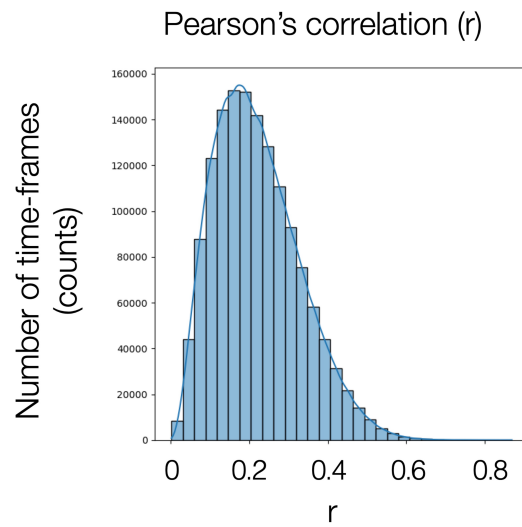


**B** 5 Basis CAPs vs 4 Estimated CAPs



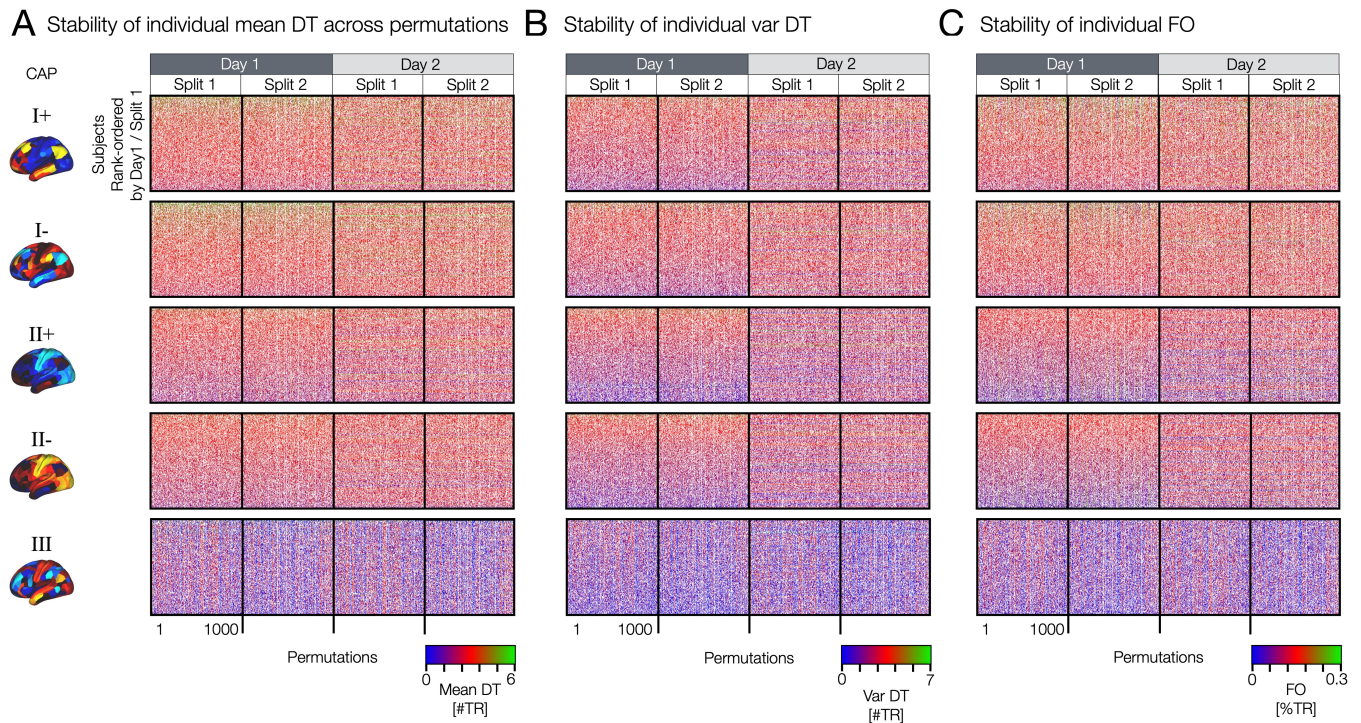
**Fig. S7.** The spatial topography of CAP state III is reproducible when it is found in one split and not in another across permutations.

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**Fig. S8.** The distribution of correlations between individual fMRI time-frames and the estimated basis CAPs (cluster centroid), to which individual time-frames were assigned by K-means clustering.

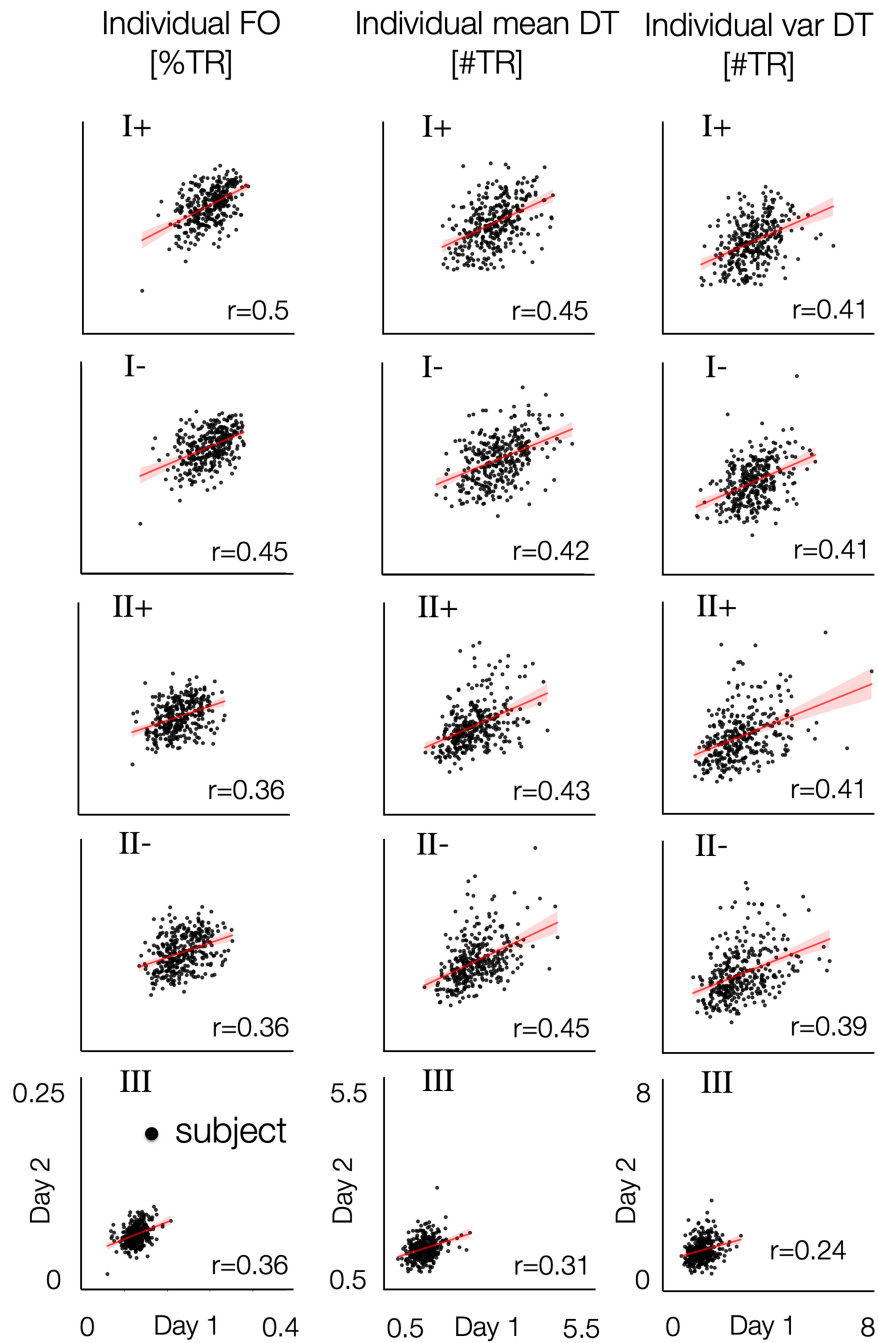
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**Fig. S9. Stability of individual mean DT, var DT and FO across permutations**

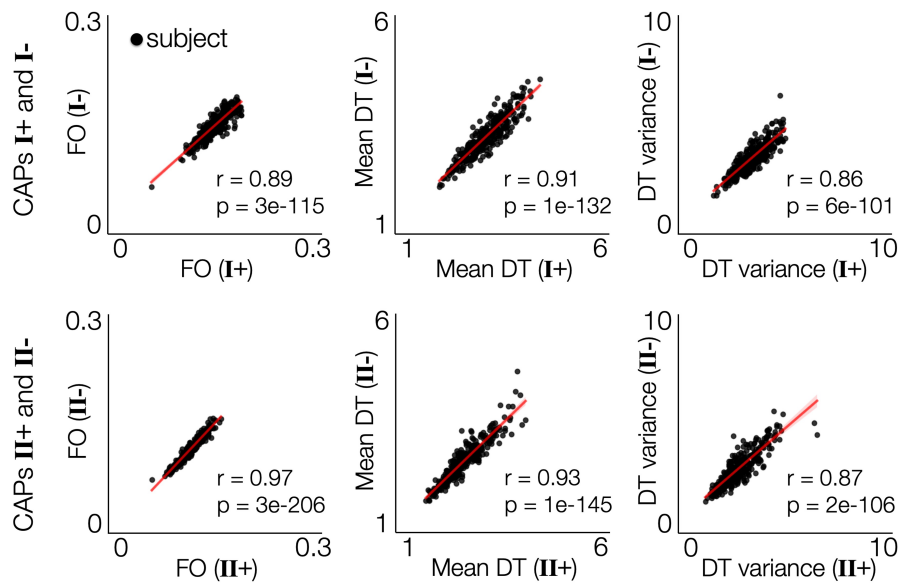
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Between-day reliability at single subject level



**Fig. S10. 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.**

Similar state-trait features between positive and negative co-activations



**Fig. S11. 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.

### Within-subject CAP variance

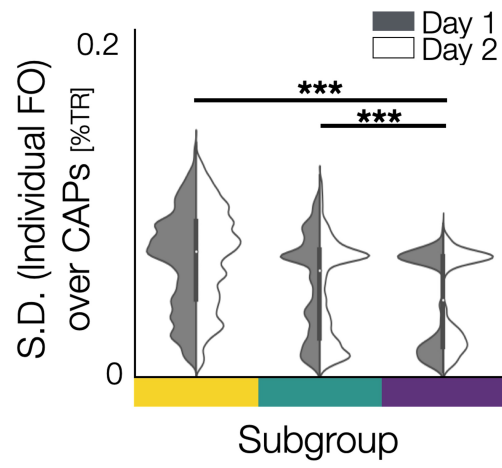
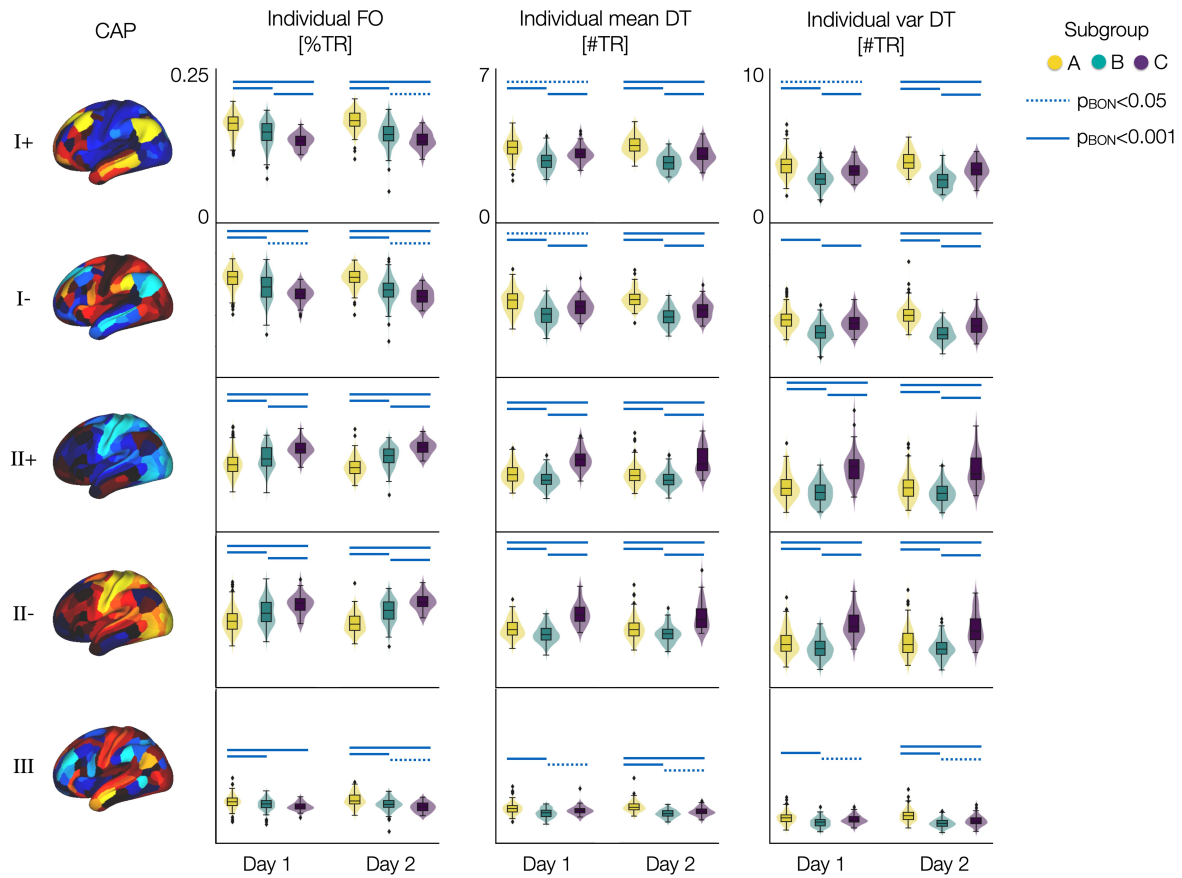


Fig. S12. Within-subject variance of FO across 5 CAPs across permutations.

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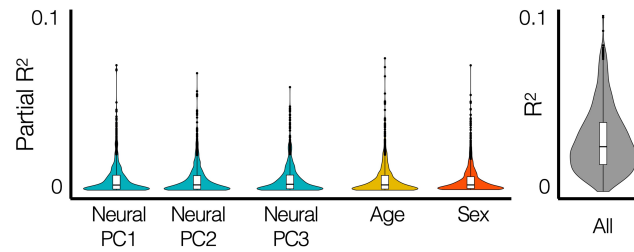


**Fig. S13. Distribution of individual neural measures of spatio-temporal CAP dynamics differ between subgroups.** The distributions of individual FO, mean DT, and var DT of each CAP state are color-coded by the three subgroups. Results from days 1 and 2 data are shown separately and compared between groups. Each data-point indicates a subject. Blue lines:  $p$ -values with Bonferroni-correction across five CAPs are estimated using two-sided two-sample *t*-tests between groups,  $p_{BON} < .001$  (bold) and  $p_{BON} < .05$  (dotted).

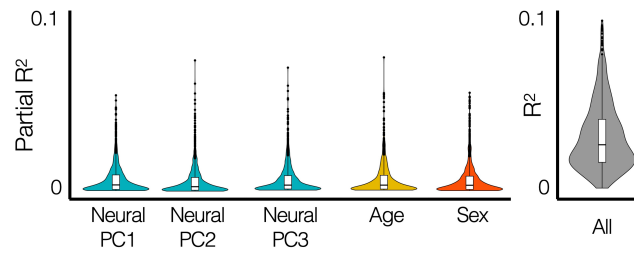
1 - MMSE_Score	91 - Language_Task_Story_Avg_Difficulty_Level	181 - DSM_Somp_T
2 - PSQI_Score	92 - Language_Task_Math_Acc	182 - DSM_Avoid_T
3 - PicSeq_AgeAdj	93 - Language_Task_Math_Median_RT	183 - DSM_Adh_T
4 - CardSort_AgeAdj	94 - Language_Task_Math_Avg_Difficulty_Level	184 - DSM_Antis_T
5 - Flanker_AgeAdj	95 - Relational_Task_Acc	185 - SSAGA_ChildhoodConduct
6 - PMAT24_A_CR	96 - Relational_Task_Median_RT	186 - SSAGA_PanicDisorder
7 - PMAT24_A_SI	97 - Relational_Task_Match_Acc	187 - SSAGA_Agoraphobia
8 - PMAT24_A_RTCT	98 - Relational_Task_Match_Median_RT	188 - SSAGA_Depressive_Ep
9 - ReadEng_AgeAdj	99 - Relational_Task_Rel_Acc	189 - SSAGA_Depressive_Sx
10 - PicVocab_AgeAdj	100 - Relational_Task_Rel_Median_RT	190 - Total_Drinks_7days
11 - ProcSpeed_AgeAdj	101 - Social_Task_Perc_Random	191 - Num_Days_Drank_7days
12 - DDisc_SV_1mo_200	102 - Social_Task_Perc_TOM	192 - Avg_Weekday_Drinks_7days
13 - DDisc_SV_6mo_200	103 - Social_Task_Perc_Unsure	193 - Avg_Weekend_Drinks_7days
14 - DDisc_SV_1yr_200	104 - Social_Task_Median_RT_Random	194 - Total_Beer_Wine_Cooler_7days
15 - DDisc_SV_3yr_200	105 - Social_Task_Median_RT_TOM	195 - Avg_Weekday_Beer_Wine_Cooler_7days
16 - DDisc_SV_5yr_200	106 - Social_Task_Median_RT_Unsure	196 - Avg_Weekend_Beer_Wine_Cooler_7days
17 - DDisc_SV_10yr_200	107 - Social_Task_Random_Perc_Random	197 - Total_Malt_Liquor_7days
18 - DDisc_SV_1mo_40K	108 - Social_Task_Random_Median_RT_Random	198 - Avg_Weekday_Malt_Liquor_7days
19 - DDisc_SV_6mo_40K	109 - Social_Task_Random_Perc_TOM	199 - Avg_Weekend_Malt_Liquor_7days
20 - DDisc_SV_1yr_40K	110 - Social_Task_Random_Perc_Unsure	200 - Total_Wine_7days
21 - DDisc_SV_3yr_40K	111 - Social_Task_TOM_Perc_TOM	201 - Avg_Weekday_Wine_7days
22 - DDisc_SV_5yr_40K	112 - Social_Task_TOM_Median_RT_TOM	202 - Avg_Weekend_Wine_7days
23 - DDisc_SV_10yr_40K	113 - Social_Task_TOM_Perc_Unsure	203 - Total_Hard_Liquor_7days
24 - DDisc_AUC_200	114 - WM_Task_Acc	204 - Avg_Weekday_Hard_Liquor_7days
25 - DDisc_AUC_40K	115 - WM_Task_Median_RT	205 - Avg_Weekend_Hard_Liquor_7days
26 - VSPLOT_TC	116 - WM_Task_2bk_Acc	206 - Total_Other_Alc_7days
27 - VSPLOT_CRTE	117 - WM_Task_2bk_Median_RT	207 - Avg_Weekend_Other_Alc_7days
28 - VSPLOT_OFF	118 - WM_Task_Obk_Acc	208 - SSAGA_Alc_D4_Dp_Sx
29 - SCPT_TP	119 - WM_Task_Obk_Median_RT	209 - SSAGA_Alc_D4_Ab_Dx
30 - SCPT_TN	120 - WM_Task_Obk_Body_Acc	210 - SSAGA_Alc_D4_Ab_Sx
31 - SCPT_FP	121 - WM_Task_Obk_Body_Acc_Target	211 - SSAGA_Alc_D4_Dp_Dx
32 - SCPT_FN	122 - WM_Task_Obk_Body_Acc_Nontarget	212 - SSAGA_Alc_12_Drinks_Per_Day
33 - SCPT_TPRT	123 - WM_Task_Obk_Face_Acc	213 - SSAGA_Alc_12_Frq
34 - SCPT_SEN	124 - WM_Task_Obk_Face_Acc_Target	214 - SSAGA_Alc_12_Frq_5plus
35 - SCPT_SPEC	125 - WM_Task_Obk_Face_ACC_Nontarget	215 - SSAGA_Alc_12_Frq_Drk
36 - SCPT_LRNR	126 - WM_Task_Obk_Place_Acc	216 - SSAGA_Alc_12_Max_Drinks
37 - IWRD_TOT	127 - WM_Task_Obk_Place_Acc_Target	217 - SSAGA_Alc_Age_1st_Use
38 - IWRD_RTC	128 - WM_Task_Obk_Place_Acc_Nontarget	218 - SSAGA_Alc_Hvy_Drinks_Per_Day
39 - ListSort_AgeAdj	129 - WM_Task_Obk_Tool_Acc	219 - SSAGA_Alc_Hvy_Frq
40 - ER40_CR	130 - WM_Task_Obk_Tool_Acc_Target	220 - SSAGA_Alc_Hvy_Frq_5plus
41 - ER40_CRT	131 - WM_Task_Obk_Tool_Acc_Nontarget	221 - SSAGA_Alc_Hvy_Frq_Drk
42 - ER40ANG	132 - WM_Task_2bk_Body_Acc	222 - SSAGA_Alc_Hvy_Max_Drinks
43 - ER40FEAR	133 - WM_Task_2bk_Body_Acc_Target	223 - Total_Any_Tobacco_7days
44 - ER40HAP	134 - WM_Task_2bk_Body_Acc_Nontarget	224 - Times_Used_Any_Tobacco_Today
45 - ER40NOE	135 - WM_Task_2bk_Face_Acc	225 - Num_Days_Used_Any_Tobacco_7days
46 - ER40SAD	136 - WM_Task_2bk_Face_Acc_Target	226 - Avg_Weekday_Any_Tobacco_7days
47 - AngAffect_Unadj	137 - WM_Task_2bk_Face_Acc_Nontarget	227 - Avg_Weekend_Any_Tobacco_7days
48 - AngHostil_Unadj	138 - WM_Task_2bk_Place_Acc	228 - Total_Cigarettes_7days
49 - AngAggr_Unadj	139 - WM_Task_2bk_Place_Acc_Target	229 - Avg_Weekday_Cigarettes_7days
50 - FearAffect_Unadj	140 - WM_Task_2bk_Place_Acc_Nontarget	230 - Avg_Weekend_Cigarettes_7days
51 - FearSomat_Unadj	141 - WM_Task_2bk_Tool_Acc	231 - Total_Cigars_7days
52 - Sadness_Unadj	142 - WM_Task_2bk_Tool_Acc_Target	232 - Avg_Weekday_Cigars_7days
53 - LifeSatisf_Unadj	143 - WM_Task_2bk_Tool_Acc_Nontarget	233 - Avg_Weekend_Cigars_7days
54 - MeanPurp_Unadj	144 - WM_Task_Obk_Body_Median_RT	234 - Total_Chew_7days
55 - PsaAffect_Unadj	145 - WM_Task_Obk_Body_Median_RT_Target	235 - Avg_Weekday_Chew_7days
56 - Friendship_Unadj	146 - WM_Task_Obk_Body_Median_RT_Nontarget	236 - Avg_Weekend_Chew_7days
57 - Loneliness_Unadj	147 - WM_Task_Obk_Face_Median_RT	237 - Total_Other_Tobacco_7days
58 - PercHostil_Unadj	148 - WM_Task_Obk_Face_Median_RT_Target	238 - Avg_Weekday_Other_Tobacco_7days
59 - PercReject_Unadj	149 - WM_Task_Obk_Face_Median_RT_Nontarget	239 - Avg_Weekend_Other_Tobacco_7days
60 - EmotSupp_Unadj	150 - WM_Task_Obk_Place_Median_RT	240 - SSAGA_FTND_Score
61 - InstruSupp_Unadj	151 - WM_Task_Obk_Place_Median_RT_Target	241 - SSAGA_HSI_Score
62 - PercStress_Unadj	152 - WM_Task_Obk_Place_Median_RT_Nontarget	242 - SSAGA_TB_Age_1st_Cig
63 - SelIEff_Unadj	153 - WM_Task_Obk_Tool_Median_RT	243 - SSAGA_TB_DSM_Diffculty_Quitting
64 - NEOFAC_A	154 - WM_Task_Obk_Tool_Median_RT_Target	244 - SSAGA_TB_DSM_Tolerance
65 - NEOFAC_O	155 - WM_Task_Obk_Tool_Median_RT_Nontarget	245 - SSAGA_TB_DSM_Withdrawal
66 - NEOFAC_C	156 - WM_Task_2bk_Body_Median_RT	246 - SSAGA_TB_Hvy_CPD
67 - NEOFAC_N	157 - WM_Task_2bk_Body_Median_RT_Target	247 - SSAGA_TB_Max_Cigs
68 - NEOFAC_E	158 - WM_Task_2bk_Body_Median_RT_Nontarget	248 - SSAGA_TB_Reg_CPD
69 - Emotion_Task_Acc	159 - WM_Task_2bk_Face_Median_RT	249 - SSAGA_TB_Smoking_History
70 - Emotion_Task_Median_RT	160 - WM_Task_2bk_Face_Median_RT_Target	250 - SSAGA_TB_Still_Smoking
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72 - Emotion_Task_Face_Median_RT	162 - WM_Task_2bk_Place_Median_RT	252 - SSAGA_TB_Yrs_Smoked
73 - Emotion_Task_Shape_Acc	163 - WM_Task_2bk_Place_Median_RT_Target	253 - SSAGA_Times_Used_Illicits
74 - Emotion_Task_Shape_Median_RT	164 - WM_Task_2bk_Place_Median_RT_Nontarget	254 - SSAGA_Times_Used_Cocaine
75 - Gambling_Task_Perc_Larger	165 - WM_Task_2bk_Tool_Median_RT	255 - SSAGA_Times_Used_Hallucinogens
76 - Gambling_Task_Perc_Smaller	166 - WM_Task_2bk_Tool_Median_RT_Target	256 - SSAGA_Times_Used_Opiates
77 - Gambling_Task_Median_RT_Larger	167 - WM_Task_2bk_Tool_Median_RT_Nontarget	257 - SSAGA_Times_Used_Sedatives
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79 - Gambling_Task_Reward_Perc_Larger	169 - ASR_Witd_T	259 - SSAGA_Mj_Use
80 - Gambling_Task_Reward_Median_RT_Larger	170 - ASR_Soma_T	260 - SSAGA_Mj_Ab_Dep
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84 - Gambling_Task_Punish_Median_RT_Larger	174 - ASR_Rule_T	
85 - Gambling_Task_Punish_Perc_Smaller	175 - ASR_Intr_T	
86 - Gambling_Task_Punish_Median_RT_Smaller	176 - ASR_Intr_T	
87 - Language_Task_Acc	177 - ASR_Extn_T	
88 - Language_Task_Median_RT	178 - ASR_Totp_T	
89 - Language_Task_Story_Acc	179 - DSM_Depr_T	
90 - Language_Task_Story_Median_RT	180 - DSM_Anxi_T	

**Fig. S14. 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](https://wiki.humanconnectome.org/display/PublicData/HCP-YA+Data+Dictionary--Updated+for+the+1200+Subject+Release). Check <https://wiki.humanconnectome.org/display/PublicData/HCP-YA+Data+Dictionary--Updated+for+the+1200+Subject+Release> for details.

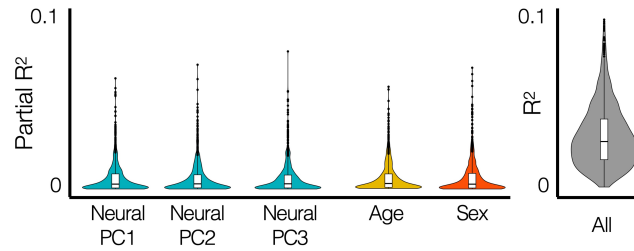
**A** Null Behavioral PC 1 Prediction (1,000 Split-half Permutations)



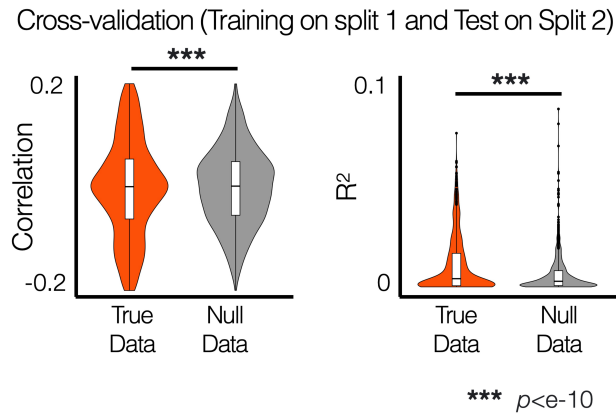
**B** Null Behavioral PC 2 Prediction (1,000 Split-half Permutations)



**C** Null Behavioral PC 3 Prediction (1,000 Split-half Permutations)



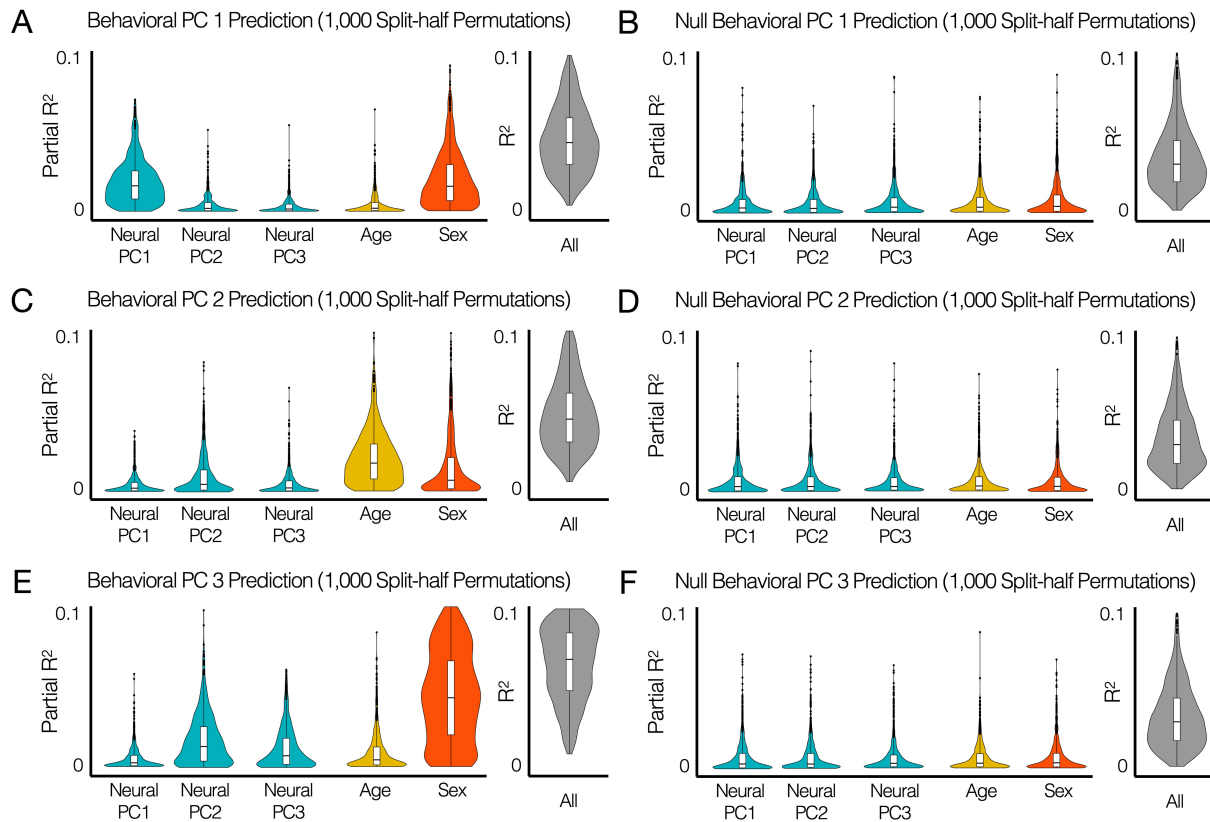
**Fig. S15.** Null data were generated by shuffling individual subjects in behavioral data. Null distributions of partial  $R^2$  were estimated for each predictor in the neuro-behavioral association model trained from a split data across 1,000 split-half permutations.



**Fig. S16. Split-half permutation based cross-validation of the prediction model of predicting behavioral PC 1 from neural PCs. The multiple linear regression models were trained using split 1 data and tested on split 2 data in each permutation. Null data were generated by shuffling individual subjects in behavioral data.**

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n=309 subjects excluding 28 subjects with high motion



**Fig. S17. Repeating the analysis of neuro-behavioral association excluding subjects with high motion did not change the results.** Among 337 subjects, 28 subjects with excessive motion ( $FD > 0.5mm$ ) were excluded. Across 1,000 permutations, a split of subjects ( $n = 154$ ) was randomly selected, and PCA was performed on neural measures from these subjects. Multiple linear regression models for predicting behavioral PCs from these subjects were estimated. Null data were generated by shuffling individual subjects in behavioral data.