Supplementary Materials

Table S1. Distribution of demographic information and clinical measurements of EMBARC MDD patients included in our study (N=233).

Item	Sub-scales	Mean±Std	Range
Demographics	Age	36.3±18.5	18-65
	Gender	67.4% Female	
HAMD (Hamilton Depression Rating Scale)	17-item total score	18.4±4.2	7-32
ASRM (Altman Self-Rating Mania Scale)	/	1.5±1.9	0-11
AAQ (Anger Attack Questionnaire)	/	0.4±0.5	0-1
CTQ (Childhood Trauma Questionnaire)	emotional abuse	13.1±5.6	5-25
	emotional neglect	13.5±4.9	5-24
	physical abuse	8.3±4.3	5-25
	physical neglect	8.3±3.5	5-20
	sexual abuse	8.3±5.6	5-25
CAST (Concise Associated Symptoms Tracking)	/	30.3±9.2	7-57
CHRTP (Concise Health Risk Tracking-Self Report)	propensity	26.4±8.1	3-49
	risk	5.2±2.4	0-10
MASQ (Mood and Anxiety Symptoms Questionnaire)	anxious arousal	17.4±5.4	10-35
	anhedonic depression	43.7±5.3	16-50
	general distress	32.1±7.9	13-50
MDQ (Mood Disorder Questionnaire)	/	4.1±3.0	0-13
NEO-FFI (NEO-Five Factor Inventory)	agreeableness	32.0±7.0	7-47
	conscientiousness	23.6±8.3	3-44
	extraversion	19.4±7.6	4-43
	neuroticism	35.2±6.3	15-48
	openness	31.8±7.5	14-48
QIDS (Quick Inventory of Depressive Symptomatology)	/	16.8±2.8	10-26
SCQ (Self-Administered Comorbidity Questionnaire)	/	1.9±2.7	0-17
SHAPS (Snaith–Hamilton Pleasure Scale)	continuous score	33.5±5.4	18-51
SAS (Social Adjustment Scale)	overall mean score	2.6±0.6	1.1-4
SAPAS (Standardised Assessment of Personality – Abbreviated Scale)	/	3.9±1.4	1-8

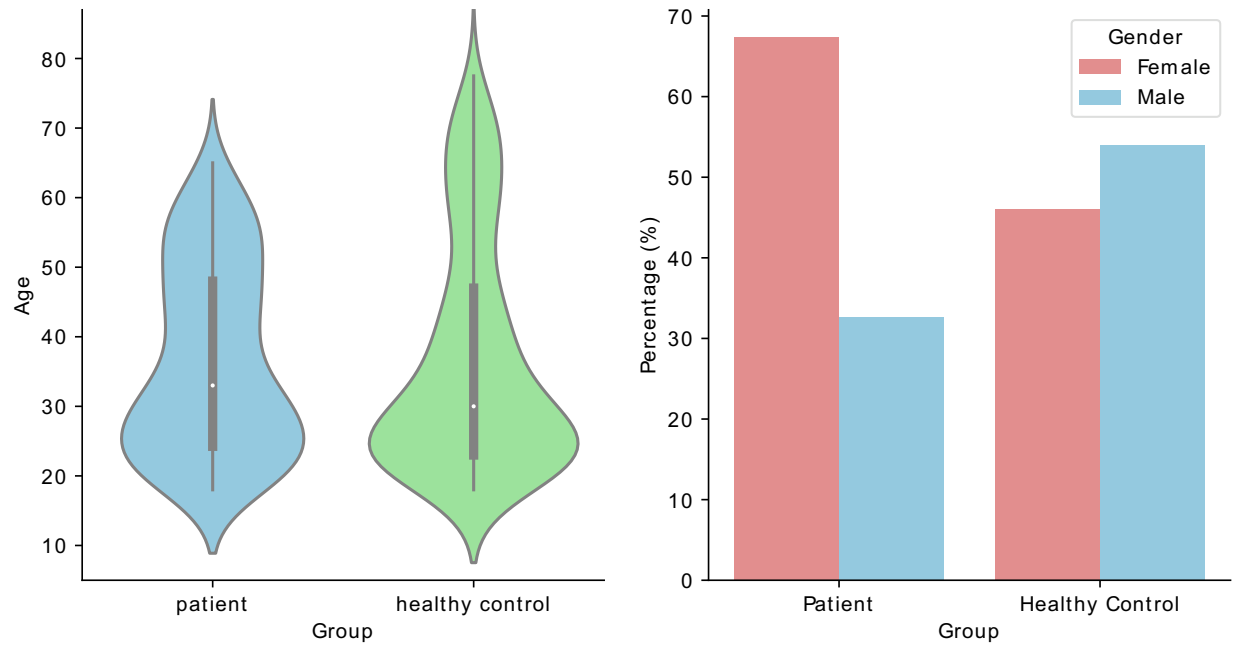**Table S2.** Demographic information of healthy controls included in our study.

	UCLA CNP (N=83)	LEMON (N=103)	AOMIC (N=72)	EMBARC (N=27)	Total (N=285)
Age	35.31±8.26	45.22±20.72	21.96±1.86	42.75±12.84	36.73±16.48
Female %	43.3	33.0	56.9	60.8	46

**Table S3.** Cognitive and emotional tasks included in our study and their measurements.

Task	Item	Measurements
A not B task	Overall accuracy	Working memory
Choice reaction time task	Overall reaction time	Interference and post-error adjustments
Flanker task	Accuracy difference between incongruent and congruent trials	Cognitive control, conflict monitoring
	Reaction time difference between incongruent and congruent trials	Cognitive flexibility, conflict processing speed
Word fluency task	Total valid number of words	Psychomotor slowing
Probabilistic reward task	Overall response bias	Reward learning
Emotion conflict task	Reaction time difference between incongruent-following and congruent-following incongruent trials	Resolution and adjustment behavior in response to emotional conflict

Table S4. Chi-square test between the population distribution in high/low FC dimension score groups and remission rates within different treatment groups (sertraline and placebo). Remission is defined as HAM-D score $\leqslant$ 7 at week 8. For each dimension, high/low groups are divided by the median FC dimension score from all population. All p-values > 0.05, indicating that there is no significant relation between high/low dimension scores and remission.

| Internalizing-externalizing symptoms dimension						
Sertraline	Observed		Expected		Statistics	
	Remission	Non-remission	Remission	Non-remission	χ2	1.20
High group	14	42	17.19	38.81	p	0.27
Low group	21	37	17.81	40.19	samples	114
Placebo	Observed		Expected		Statistics	
	Remission	Non-remission	Remission	Non-remission	χ2	0.00
High group	16	45	15.89	45.11	p	1.00
Low group	15	43	15.11	42.89	samples	119
Depression-protective personality dimension						
Sertraline	Observed		Expected		Statistics	
	Remission	Non-remission	Remission	Non-remission	χ2	0.71
High group	21	39	18.42	41.58	p	0.40
Low group	14	40	16.58	37.42	samples	114
Placebo	Observed		Expected		Statistics	
	Remission	Non-remission	Remission	Non-remission	χ2	0.48
High group	17	40	14.85	42.15	p	0.49
Low group	14	48	16.15	45.85	samples	119

Figure S1. Demographic information comparison between patient (N=233) and healthy control groups (N=285). The age distribution of the patient population and the healthy population was matched, with a Kolmogorov-Smirnov test yielding a p-value of 0.052.
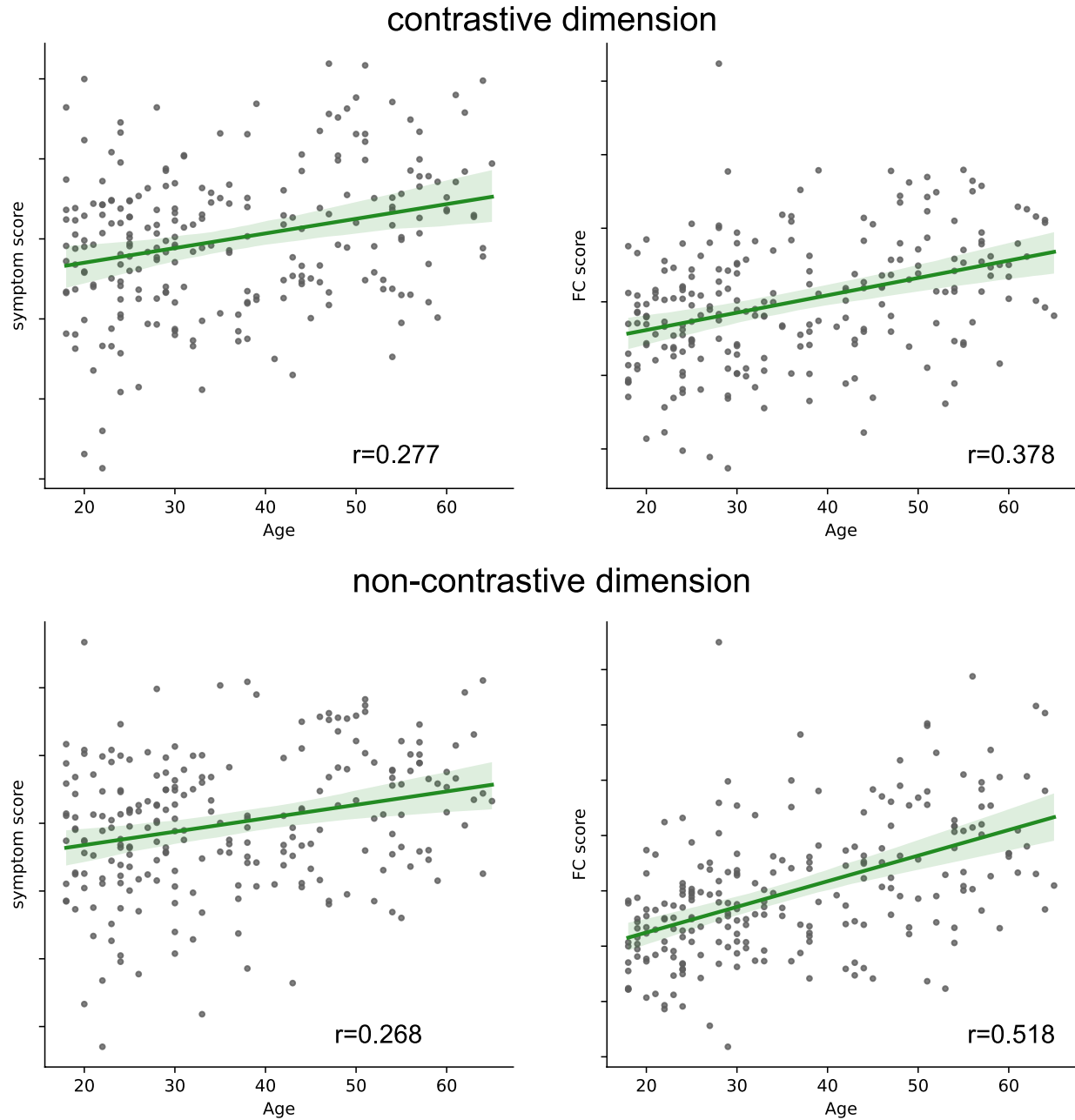
Figure S2. Comparison of the age-correlation of the best symptom/FC dimensions derived from cPCA and regular PCA components. Contrastive learning marginally reduced the age-related component in its FC dimension, with a Fisher's z test showing near-significant results (p = 0.059).
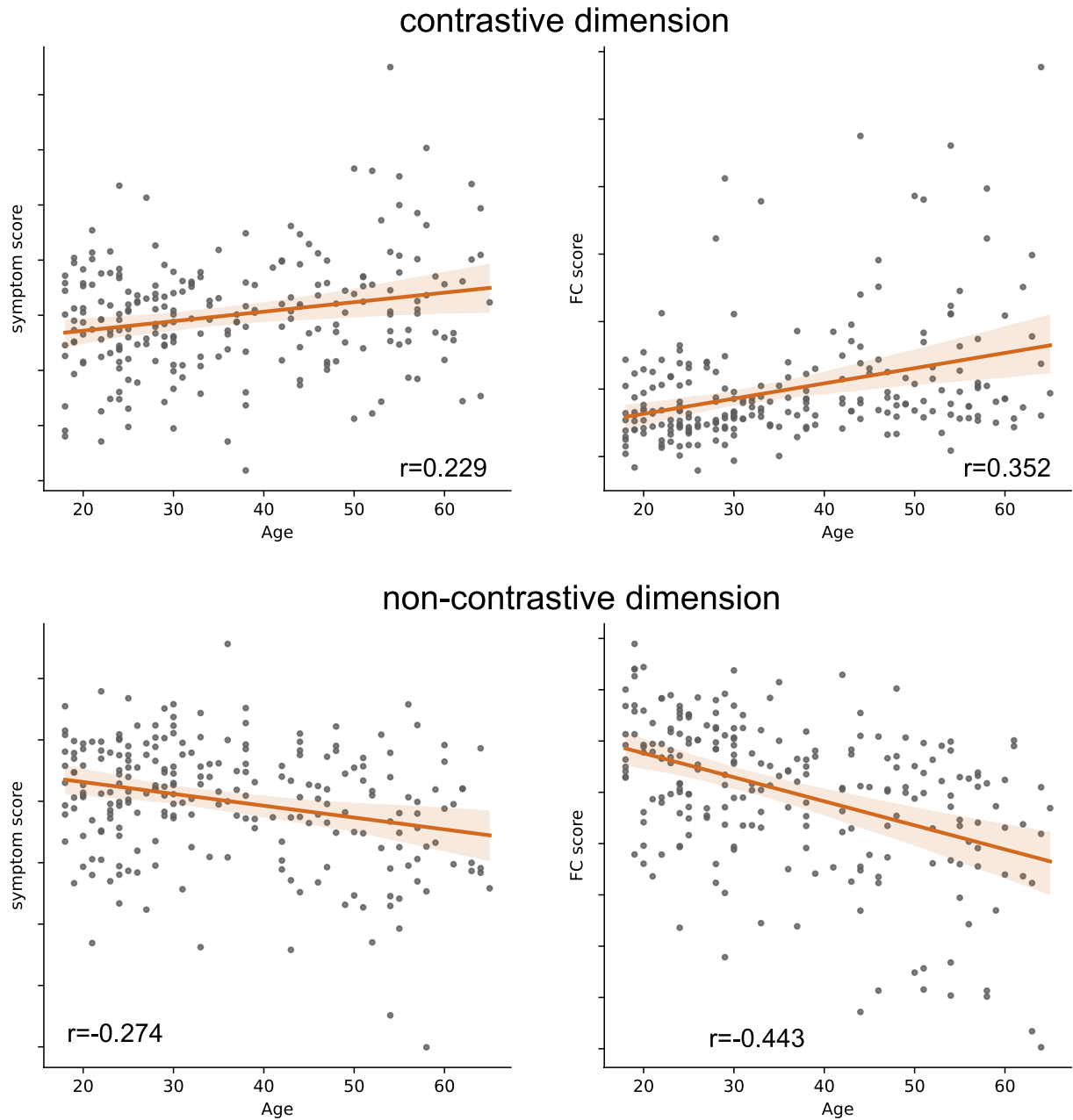
Figure S3. Comparison of the age correlation in the second-best symptom/FC dimensions derived from cPCA and regular PCA components. Contrastive learning reduced the age-related component in both symptom and FC dimensions, but the reduction was not statistically significant (p > 0.1).
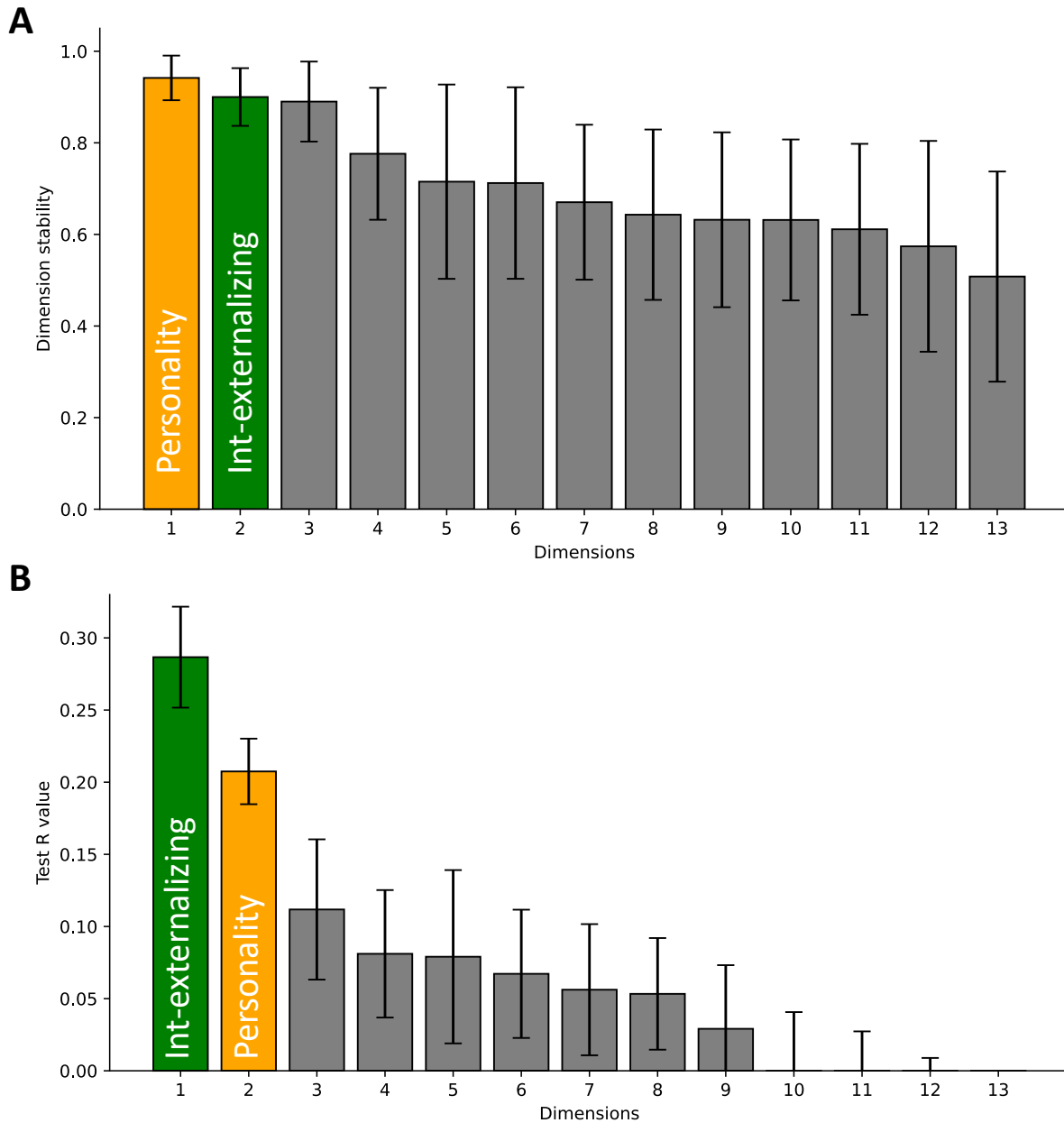
Figure S4. (A) Overall dimension stability for all 13 dimensions given by sCCA, measured by the average of the cosine similarity between each pair of FC dimensions and each pair of symptom dimensions from 10×10 folds. All dimensions have an overall stability over 0.5. (B) For the 13 dimensions, only two dimensions survived FDR correction in permutation test, shown in colors. The raw p-values are: p<0.001 for internalizing-externalizing symptoms dimension, and p=0.001 for depression-protective personality dimension.