

Table 2. Performance of classification of OCD clinical outcomes in (A) adult, (B) adult applied NeuroComBat harmonization, (C) pediatric, (D) pediatric applied NeuroCombat harmonization samples. — mean with 95% confidence interval

(A) Adult sample

	OCD (N = 690) vs. HC (N = 646)		unmedicated OCD (N = 429) vs. HC (N = 646)		unmedicated OCD (N = 429) vs. medicated OCD (N = 261)	
	Discovery set	Replication set	Discovery set	Replication set	Discovery set	Replication set
ROC-AUC	67.29 ± 0.26	57.19 ± 3.47	63.96 ± 0.43	62.67 ± 3.84	60.22 ± 0.40	76.72 ± 3.97
Accuracy (%)	66.37 ± 0.27	57.08 ± 3.22	64.64 ± 0.49	61.68 ± 3.58	66.88 ± 0.32	67.15 ± 12.83
Sensitivity (%)	61.96 ± 0.79	75.36 ± 8.49	65.84 ± 1.66	58.82 ± 19.79	58.7 ± 1.53	92.31 ± 2.95
Specificity (%)	71.87 ± 0.73	37.69 ± 29.44	68.44 ± 1.00	63.57 ± 7.92	73.77 ± 1.44	51.76 ± 16.19

For the classification of medication status among OCD patients, some sites (i.e., Amsterdam, Shanghai) containing only unmedicated OCD were excluded from the discovery set.

(B) Adult sample, NeuroComBat

	OCD (N = 690) vs. HC (N = 646)		unmedicated OCD (N = 429) vs. HC (N = 646)		unmedicated OCD (N = 429) vs. medicated OCD (N = 261)	
	Discovery set	Replication set	Discovery set	Replication set	Discovery set	Replication set
ROC-AUC	64 ± 0.05	51.07 ± 3.54	67.35 ± 0.52	52.8 ± 4.18	66.12 ± 3.63	62.24 ± 5.08
Accuracy (%)	63.87 ± 0.07	53.36 ± 3.64	66.44 ± 0.52	60.75 ± 3.09	74.42 ± 0.65	68.6 ± 3.72
Sensitivity (%)	67.14 ± 1.20	37.68 ± 25.16	63.95 ± 1.80	37.65 ± 17.42	76.14 ± 0.71	48.08 ± 13.79
Specificity (%)	60.96 ± 1.24	70 ± 13.74	71.55 ± 0.87	75.97 ± 9.51	70.31 ± 1.35	81.18 ± 4.19

For the classification of medication status among OCD patients, some sites (i.e., Amsterdam, Shanghai) containing only unmedicated OCD were excluded from the discovery set.

(C) Pediatric sample

	OCD (N = 175) vs. HC (N = 142)		unmedicated OCD (N = 105) vs. HC (N = 142)		unmedicated OCD (N = 105) vs. medicated OCD (N = 70)	
	Discovery set	Replication set	Discovery set	Replication set	Discovery set	Replication set
ROC-AUC	69.54 ± 8.59	59.8 ± 7.39	65.96 ± 12.33	48.51 ± 10.14	61.82 ± 15.50	72.45 ± 8.87
Accuracy (%)	73.56 ± 6.82	62.5 ± 6.38	69.15 ± 8.35	57.9 ± 8.06	69.15 ± 11.18	74.3 ± 5.83
Sensitivity (%)	73.25 ± 17.25	65.71 ± 16.03	73.43 ± 14.12	50 ± 25.51	73.43 ± 12.74	95.24 ± 2.43
Specificity (%)	73.03 ± 13.18	58.62 ± 20.58	68.75 ± 9.90	62.5 ± 19.13	68.75 ± 15.95	42.86 ± 29.15

For the classification of medication status among OCD patients, some sites (i.e., Calgary) containing only unmedicated OCD were excluded from the discovery set.

(D) Pediatric sample, NeuroComBat

	OCD (N = 175) vs. HC (N = 142)		unmedicated OCD (N = 105) vs. HC (N = 142)		unmedicated OCD (N = 105) vs. medicated OCD (N = 70)	
	Discovery set	Replication set	Discovery set	Replication set	Discovery set	Replication set
ROC-AUC	66.05 ± 0.41	60.49 ± 7.20	60.71 ± 0.92	55.36 ± 10.15	66.78 ± 0.35	58.2 ± 8.85
Accuracy (%)	67.56 ± 0.38	62.5 ± 6.38	61.46 ± 0.28	71.05 ± 8.06	72.1 ± 0.28	60 ± 5.82
Sensitivity (%)	62.28 ± 1.55	71.43 ± 13.10	84.06 ± 0.91	35.71 ± 25.51	77.5 ± 0.91	47.61 ± 2.43
Specificity (%)	77.16 ± 1.46	51.72 ± 24.63	54.69 ± 2.05	91.67 ± 19.13	68.75 ± 2.05	78.57 ± 29.15

For the classification of medication status among OCD patients, some sites (i.e., Calgary) containing only unmedicated OCD were excluded from the discovery set.