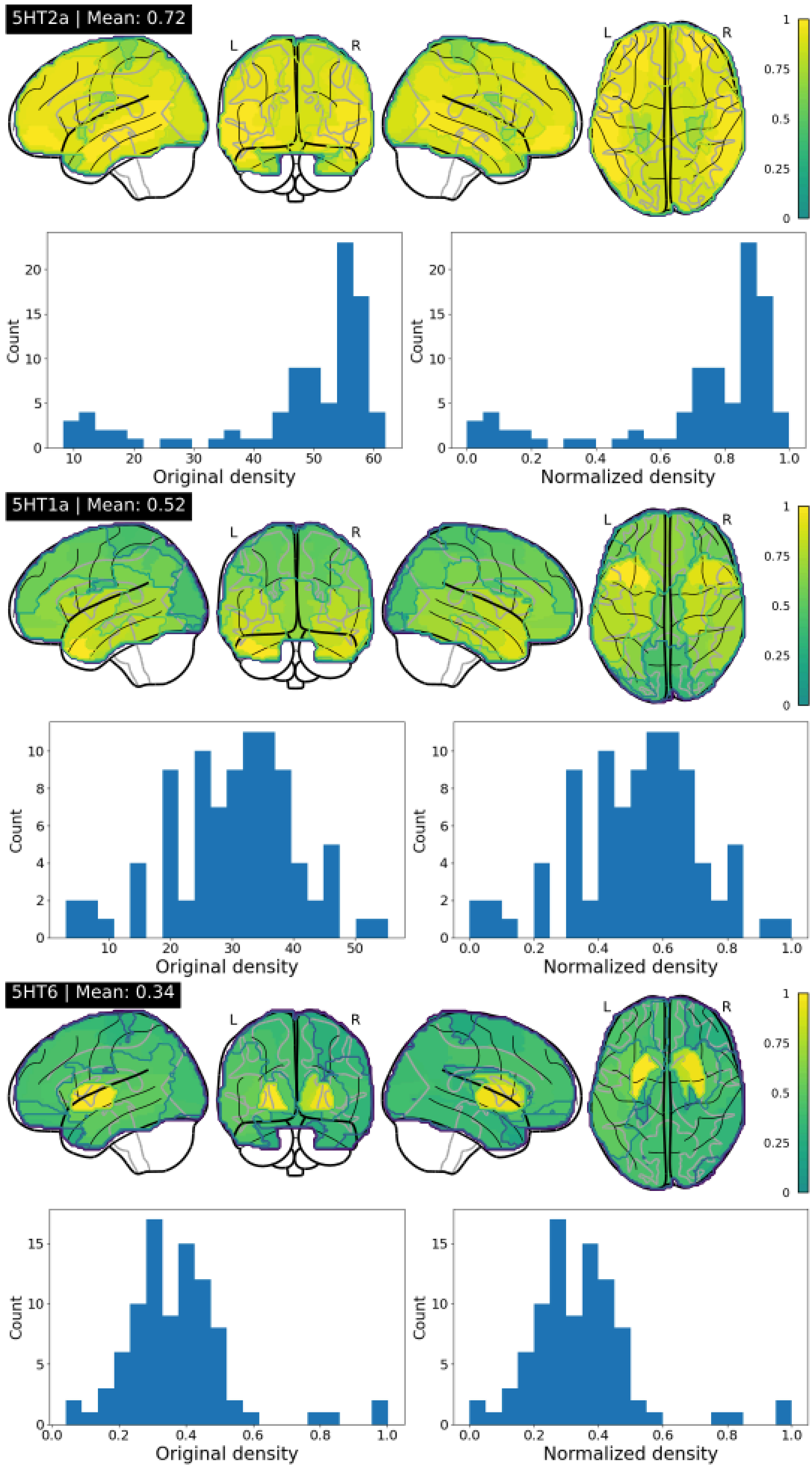
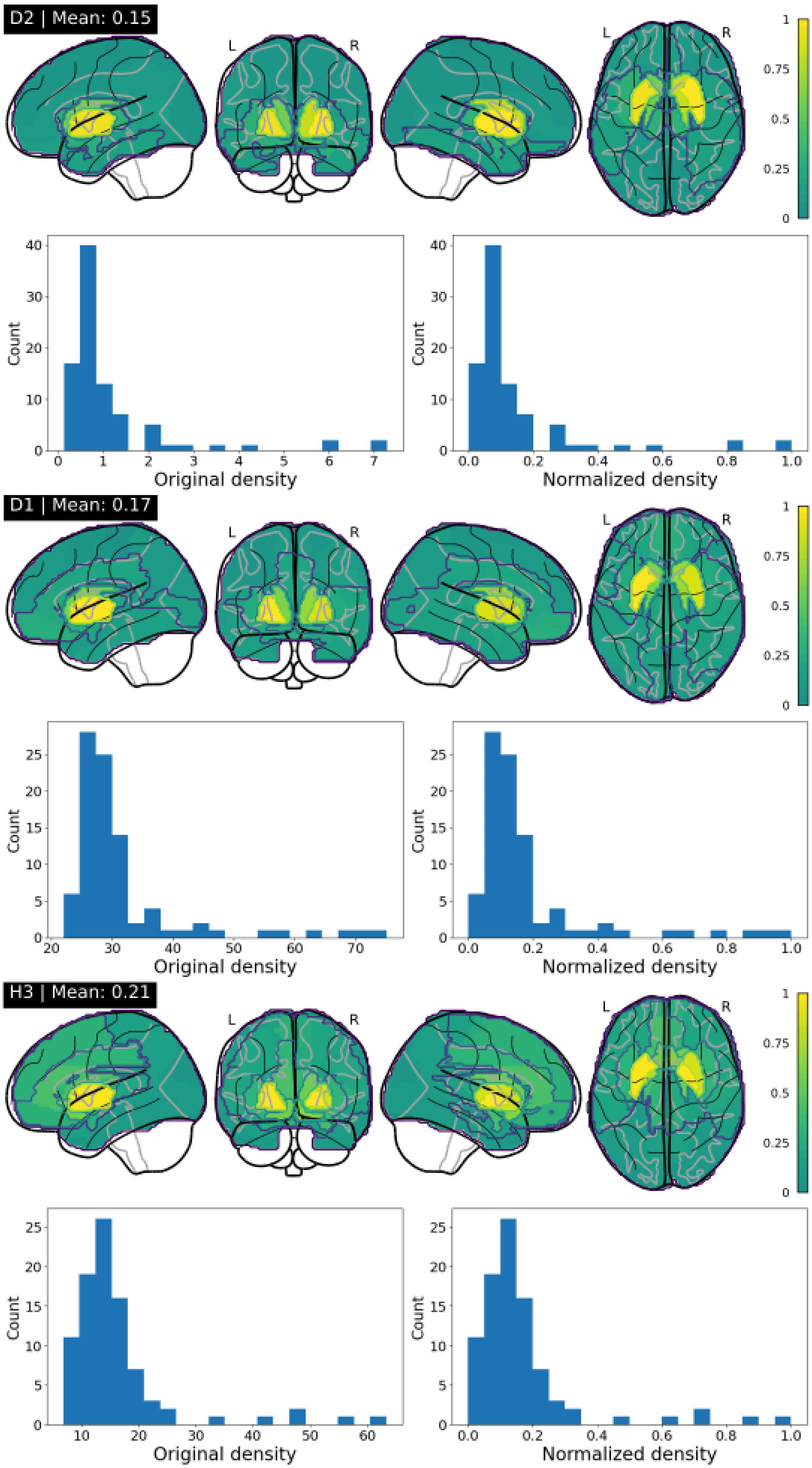
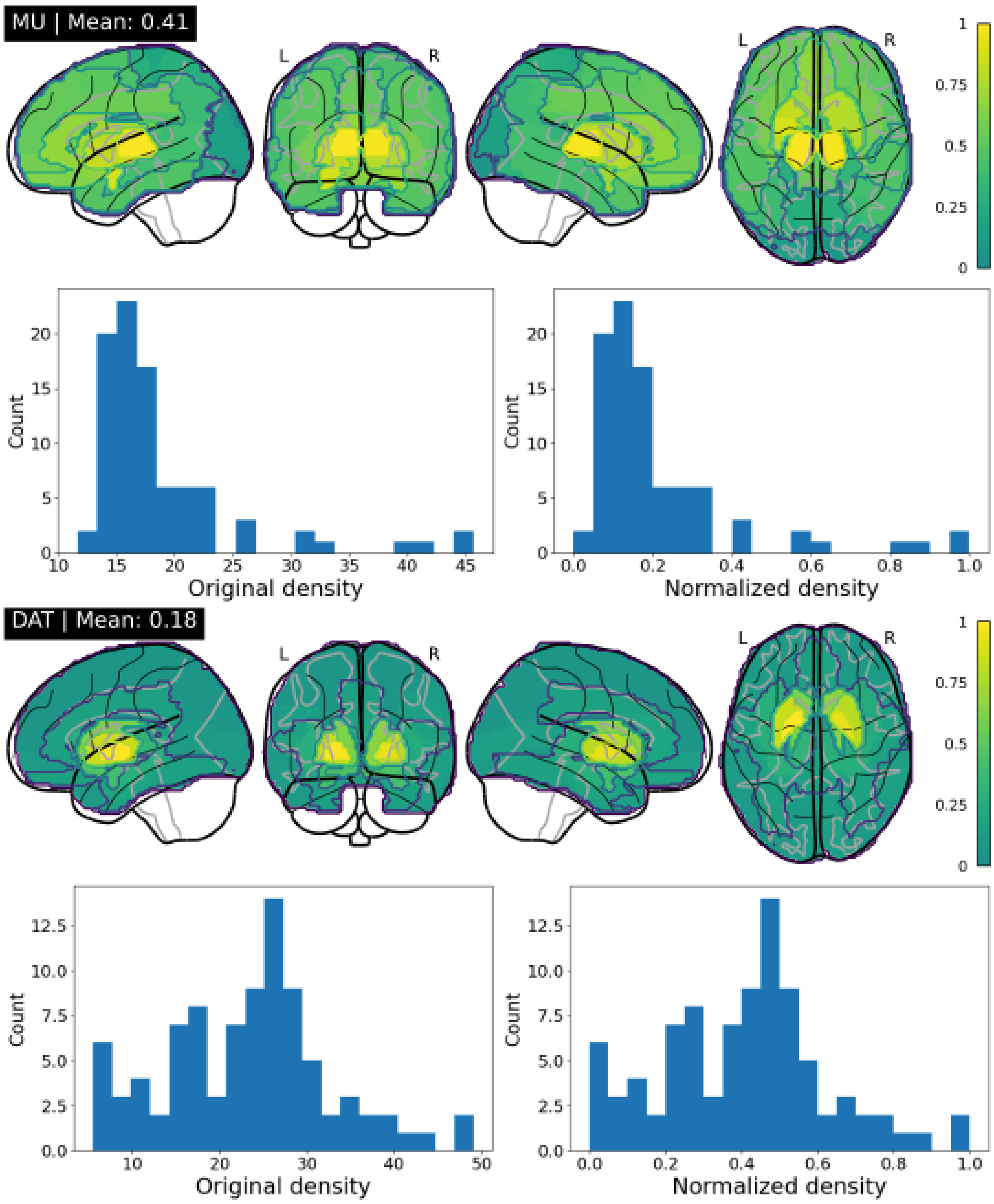
Supplementary Material for : "Whole brain modelling for simulating pharmacological interventions on patients with Disorders of Consciousness"

Mindlin I [1] , Herzog R , Belloli L, Manasova D , Monge-Asensio M ,
Vohryzek J ., Escrichs, A. , Alnagger N , Núñez P , Gosseries O , Kringelbach ML,
Deco G, Tagliazucchi E, Naccache L , Rohaut B , Sitt JD , Sanz Perl Y

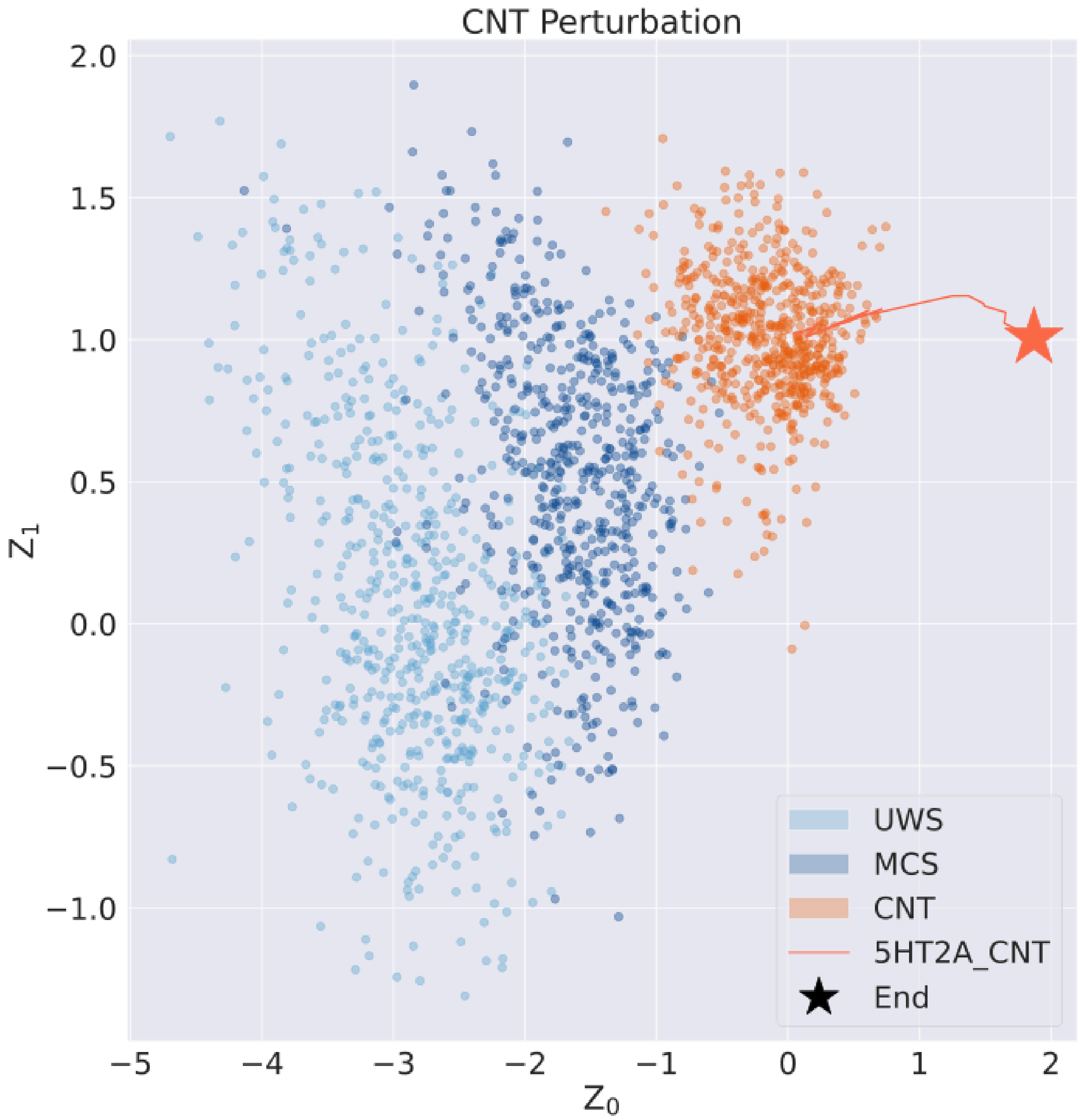


5HT2a | Mean: 0.72
L
R
Count
Original density
Normalized density
5HT1a | Mean: 0.52
L
R
Count
Original density
Normalized density
5HT6 | Mean: 0.34
L
R
Count
Original density
Normalized density

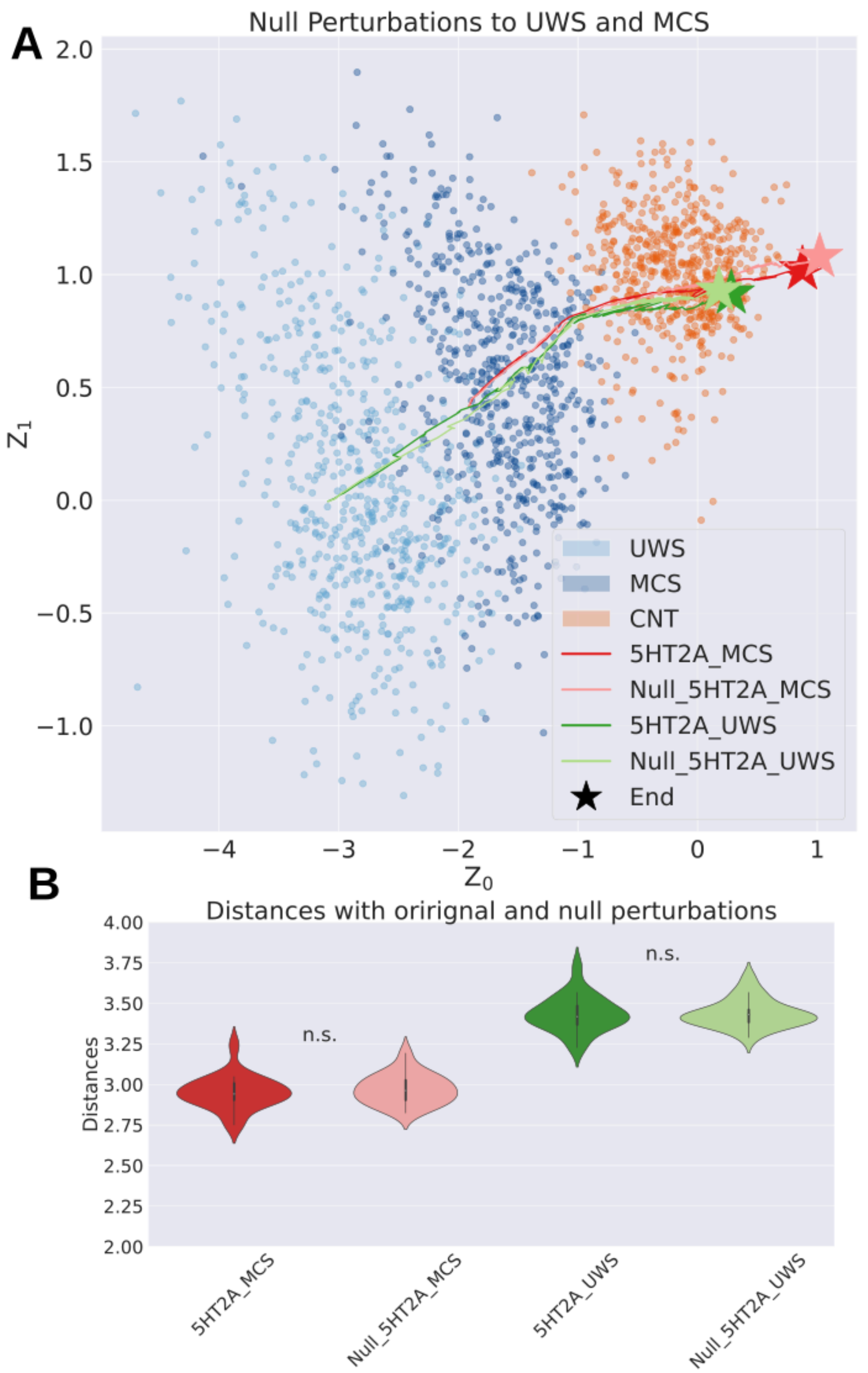

D2 | Mean: 0.15
L
R
1
0.75
0.5
0.25
0
Count
Original density
Normalized density
D1 | Mean: 0.17
L
R
1
0.75
0.5
0.25
0
Count
Original density
Normalized density
H3 | Mean: 0.21
L
R
1
0.75
0.5
0.25
0
Count
Original density
Normalized density



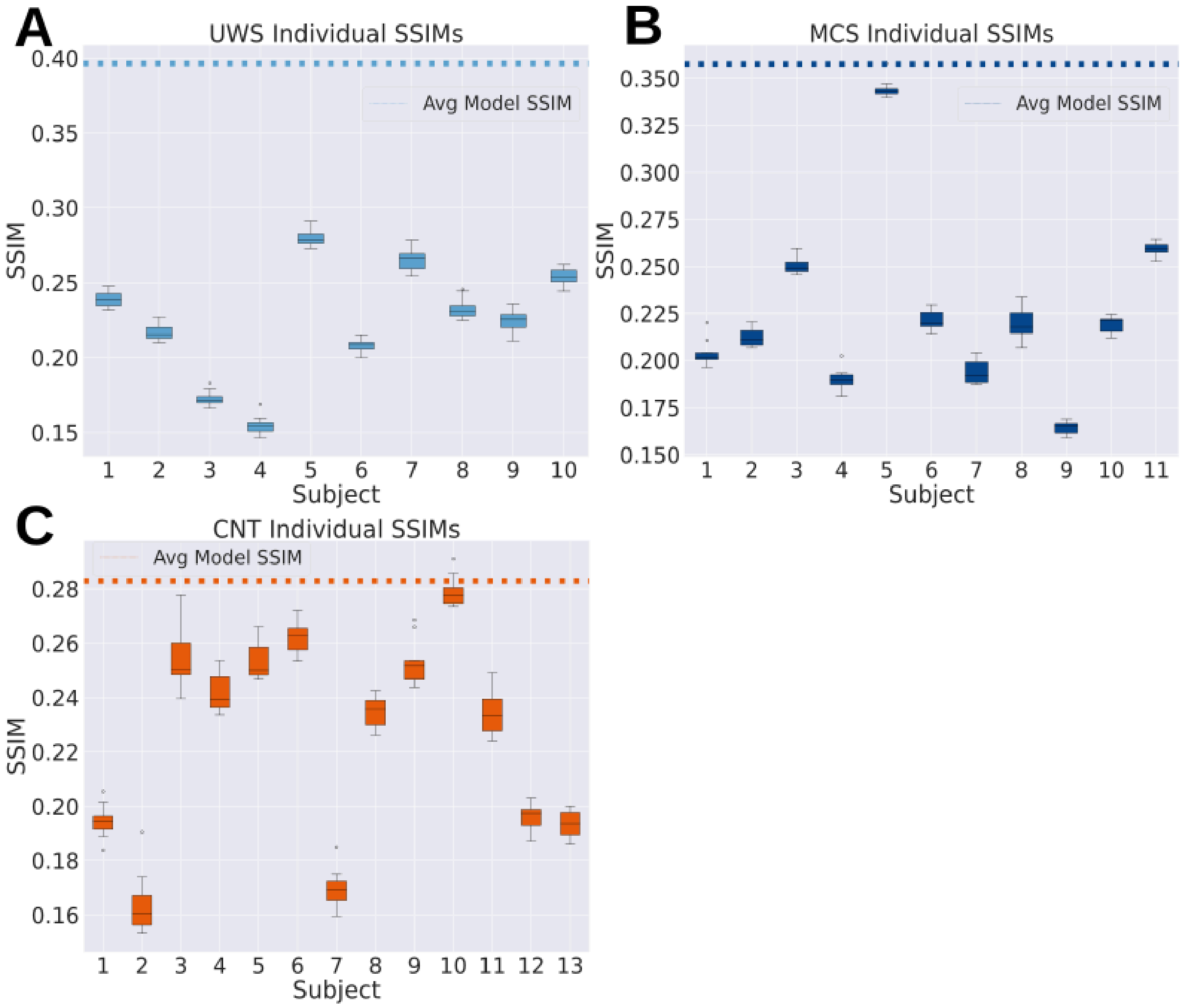
Supp Fig 1. Brain renders of the normalized receptor density maps along with histogram before and after normalization. Count is the amount of regions with each density value



Supp Fig 2. Modeling the effects in brain dynamics during the psychedelic state by modulating the serotonergic receptors parametrized by the scaling parameter. Interestingly, this intervention is represented in the 2D latent space as a trajectory that moves towards the direction opposite to that of reduced states of consciousness.



Supp Fig 3. Null comparison of 5HT2A perturbation. We generated a randomized null version of the 5HT2A receptor where the spatial autocorrelation and mean density is preserved. **(A)** Projection of the null and original receptor map perturbation to the patient models. **(B)** Violinplots showing the distance traveled distribution for the group of perturbations. After performing a Wilcoxon test on the distributions we saw no significant difference between the distributions.



Supp Fig 4. Individual vs. group level model fitting performance A) Comparison between the SSIM of each subject-level model vs. the group level model performance for UWS patients. B,C) Same as panel A but for MCS and CNT groups, respectively.

	Precision	Recall	F1-Score
UWS	0.9921	0.9921	0.9921
MCS	0.9523	0.9375	0.9448
CNT	0.9158	0.9333	0.9245

Supplementary Table 1. Because we observe the neuromodulatory effect in the latent space we used Support Vector Machines (SVM) in the projected baseline FC matrices to show that the resulting clusters were distinguishable. The data from three latent clusters (UWS, MCS, CNT) was concatenated to form the feature matrix and corresponding labels. The dataset was split into training and testing sets using an 80-20 split. The SVM model from the scikit-learn library was used with a default radial basis function (RBF) kernel and was trained on the training set. The model's performance was evaluated on the test set using precision, recall, and F1 score, as provided by scikit-learn. The SVM's parameters were chosen based on default settings without additional hyperparameter tuning