

A computational approach to evaluate how molecular mechanisms impact large-scale brain activity

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Supplementary Information

1 Fitting parameters

Cell Type	P_0	$P_{\mu V}$	$P_{\sigma V}$	$P_{\tau N}^V$	$P_{\mu V}^2$	$P_{\sigma V}^2$	$P_{(\tau N)}^V)^2$	$P_{\mu V}\sigma V$	$P_{\mu V}\tau N^V$	$P_{\sigma V}\tau N$
RS-cell	-50.17	4.52	-7.94	-2.08	-0.55	3.42	-11.56	1.95	2.74	-10.67
FS-cell	-51.85	6.16	-14.04	1.67	-2.06	3.18	-31.13	6.57	1.72	-45.16

Supplementary Table 1: Fitting parameters expressed in mV

2 Model parameters

Supplementary Table 2: Model Parameters

Parameter name	Symbol	Awake	NMDA- block	GABA _A agonism	NREM sleep	Unit
Cellular Properties						
Leak conductance	g_L		10			nS
Membrane capacitance	C_m		200			pF
Resting voltage	v_{rest}		-65			mV
Action Potential threshold	v_{thr}		-50			mV
Refractory period	T_{refr}		5			ms
Adaptation time constant	τ_w		500			ms
<i>Excitatory Neuron</i>						
Leak reversal potential	E_L		-64			mV
Spike sharpness	Δ_e		2			mV
Adaptation current increment	b_e	5	30	30	120	pA
Adaptation conductance	a_e		0			nS
<i>Inhibitory Neuron</i>						
Leak reversal potential	E_L		-65			mV
Spike sharpness	Δ_i		0.5			mV
Adaptation current increment	b_i		0			pA
Adaptation conductance	a_i		0			ns
Synaptic Properties						
<i>Excitatory Neuron</i>						
Reversal potential	E_e		0			mV
Quantal conductance	Q_e		1.5			nS
Decay time of synaptic conductance	τ_e	5	3.75	5	5	ms
<i>Inhibitory Neuron</i>						
Reversal potential	E_i		-80			mV
Quantal conductance	Q_i		5			nS
Decay time of synaptic conductance	τ_i	5	5	7	5	ms
Network Properties						
Total network size	N		10000			
Global Coupling Factor	G		0.3			
Signal Propagation Speed	V_c		4.0			mm/ms
Connectivity probability	p		0.05			
Fraction of inhibitory cells	g_{ei}		0.2			

3 Statistical Analysis

3.1 Statistical analysis reported in Figure 5

The correlations between structural and functional connectivity correspond to the Pearson correlation between the vectorized structural and functional matrices.

Supplementary Table 3: Statistical Summary and Mann-Whitney U Test Results for the experimental data

Statistic	Awake	Anesthesia
Mean	0.2974	0.3304
Variance	0.0003	0.0007
Standard Deviation	0.0184	0.0272
Minimum	0.2582	0.2692
Maximum	0.3445	0.3835
Median	0.2956	0.3314
Q1 (25th percentile)	0.2882	0.3082
Q3 (75th percentile)	0.3049	0.3470
Mann-Whitney U Test	U statistic = 108.0, p-value = 2.6677e-05	

Supplementary Table 4: Statistical Summary and Mann-Whitney U Test Result for the simulated data

Statistic	Awake	Anesthesia
Mean	0.2998	0.3938
Variance	0.0002	0.0001
Standard Deviation	0.0141	0.0101
Minimum	0.2747	0.3771
Maximum	0.3184	0.4114
Median	0.2990	0.3923
Q1 (25th percentile)	0.2883	0.3874
Q3 (75th percentile)	0.3146	0.4013
Mann-Whitney U Test	U statistic = 256.0, p-value = 1.5449e-06	

3.2 Statistical analysis reported in Figure 6

Following the rejection of the Kruskal-Wallis ($H = 114.9, p = 9.5e - 25$), we used the Conover post-hoc test to perform pairwise comparisons between the simulated different conditions (median and Interquartile range (IQR) for GABA_A: 0.109(0.149 – 0.076), NMDA-block: 0.099(0.135 – 0.078), NREM sleep: 0.152(0.198 – 0.086), Wakefulness: 0.360(0.378 – 0.345)).

In Table 5, we report the p-values for each of the pairwise comparisons, adjusted for multiple comparisons using the Holm-Bonferroni method:

In Table 6, we also report the T-statistic of the Mann-Whitney U test between each pair of groups calculated as:

$$T = \frac{U - \frac{n_1 \cdot n_2}{2}}{\sqrt{\frac{n_1 \cdot n_2 \cdot (n_1 + n_2 + 1)}{12}}}$$

Supplementary Table 5: Pairwise p-values for comparisons of PCI values among conditions

	GABA _A -agonism	NMDA-block	NREM sleep	Wakefulness
GABA _A -agonism	1.0	5.83e-01	4.81e-03	1.06e-28
NMDA-block	5.83e-01	1.0	1.75e-02	5.73e-27
NREM sleep	4.81e-03	1.75e-02	1.0	1.2e-18
Wakefulness	1.06e-28	5.73e-27	1.2e-18	1.0

where U is the Mann-Whitney U statistic, and n_1 and n_2 are the sample sizes of the two groups compared.

Supplementary Table 6: Pairwise T-statistics for comparisons of PCI values among conditions

	GABA _A -agonism	NMDA-block	NREM sleep	Wakefulness
GABA _A -agonism	1.00	-0.05	-2.89	9.27
NMDA-block	-0.05	1.00	-2.36	8.10
NREM sleep	-2.89	-2.36	1.00	8.12
Wakefulness	9.27	8.10	8.12	1.00

Effect sizes were calculated using the T-statistics from the previous section as:

$$r = \frac{T}{\sqrt{2 \cdot n}}$$

where n is the sample size for each group. For each pairwise comparison, the effect size was computed and is summarized in Table 7:

Supplementary Table 7: Pairwise Effect Sizes (r) for comparisons of PCI values among conditions

	GABA _A -agonism	NMDA-block	NREM sleep	Wakefulness
GABA _A -agonism	1.00	-0.00	-0.26	0.85
NMDA-block	-0.00	1.00	-0.22	0.74
NREM sleep	-0.26	-0.22	1.00	0.74
Wakefulness	0.85	0.74	0.74	1.00