

Table S5: Parameters in the estimation of free energies of all reaction and interaction processes in Kai network.

Parameters in the estimation of free energies of activation in KaiC (and its complexes) phosphorylation and dephosphorylation				
	free KaiC	KaiAC	KaiBC	KaiABC
$\Delta G_p^{\ddagger*} (k_B T)$	25	25	25	25
$\Delta G_d^{\ddagger*} (k_B T)$	20	20	20	20
$\Delta \Delta E_p^{\ddagger} (k_B T)$	----	-13.5	----	-11.4
$\Delta \Delta E_d^{\ddagger} (k_B T)$	-10.6	----	-10	-10.6
$\sigma_{00Tp}^{\ddagger}$	----	0.3704	----	0.5412 (0.5439)
$\sigma_{01Tp}^{\ddagger}$	----	0.3704	----	0.5088 (0.5263)
$\sigma_{00Sp}^{\ddagger}$	----	0.2778 (0.2222)	----	0.3684 (0.2807)
$\sigma_{10Sp}^{\ddagger}$	----	0.4593 (0.4741)	----	0.6316 (0.6491)
$\sigma_{10Tdp}^{\ddagger}$	0.3962 (0.3774)	----	0.38 (0.42)	0.2075
$\sigma_{11Tdp}^{\ddagger}$	0.3774	----	0.4	0.4528
$\sigma_{01Sdp}^{\ddagger}$	0.4906	----	0.46	0.4151
$\sigma_{11Sdp}^{\ddagger}$	0.4906	----	0.3 (0.24)	0.2642

λ_{00}	1	1	1	1
λ_{01}	0.8696	1	0.8696	0.9
λ_{10}	1	1	1	1.1
λ_{11}	0.9259	1	0.9259	1.05
ω	0.23	0.41	0.41	0.41
Apt_0 (h ⁻¹)	----	657.3658 (648.9298)	----	146.0928 (144.2179)
Aps_0 (h ⁻¹)	----	18.8379 (18.5961)	----	44.8530 (44.2774)
$Adpt_0$ (h ⁻¹)	79.8605 (118.2535)	----	88.0171 (86.8875)	27.0190 (4.4454)
$Adps_0$ (h ⁻¹)	4.4438 (4.3868)	----	11.6599 (11.5103)	0.5629 (0.6668)
Parameters in estimation of free energies for association-dissociation of Kai proteins				
	KaiA-KaiC	KaiB-KaiC	KaiA-KaiBC	
ΔG_{00} ($k_B T$)	-1	-2.2 (-2.5)	4 (4.1)	
ΔG_{01} ($k_B T$)	-1	-0.1	2.5	
ΔG_{10} ($k_B T$)	-1	-2.2 (-2.5)	2.8 (2.85)	
ΔG_{11} ($k_B T$)	-1	-0.1	2.4	
h_{00}	1.0	1.2	0.2	
h_{01}	1.6	1.53	1.2	

h_{10}	1.0	1.2	1.1 (1.2)
h_{11}	1.6	1.53	1.2
$\Psi (k_B T)$	-0.4	-0.5	0.4
$K_0 (\mu\text{M})$	5e-4	kb_0 ($\mu\text{M}^{-2}\text{h}^{-1}$)	5.4e6 (4.4e6)
		$kdb_0 (\text{h}^{-1})$	90
			6.65e6

Apt_0 , Aps_0 , $Adpt_0$ and $Adps_0$ are the pre-exponential factors in Arrhenius equation for calculation of the rate constants for KaiC phosphorylation and dephosphorylation. K_0 is the pre-exponential factor for calculation of the dissociation constants. The values in the round brackets are specific for simulations that consistent with experiments by Rust et al. (details see section 2.6 in the Text S1).