Table S4: Dissociation constants and rate constants in Kai reaction network. (The values in the round brackets are specific for simulations that consistent with experiments by Rust et al., and details can be found in section 2.6 in the Text S1.)

Dissociation constants for KaiA-KaiC binding-unbinding: Ka_s^t (μM)							
T432 / S431	0	1	2	3	4	5	6
0	0.3009	0.3009	0.3009	0.3009	0.3009	0.3009	0.3009
1	0.3825	0.3825	0.3825	0.3825	0.3825	0.3825	0.3825
2	0.5616	0.5616	0.5616	0.5616	0.5616	0.5616	0.5616
3	1.0382	1.0382	1.0382	1.0382	1.0382	1.0382	1.0382
4	2.7747	2.7747	2.7747	2.7747	2.7747	2.7747	2.7747
5	13.3752	13.3752	13.3752	13.3752	13.3752	13.3752	13.3752
6	165.6677	165.6677	165.6677	165.6677	165.6677	165.6677	165.6677
Dissociation constants for KaiA-KaiBC binding-unbinding: Kba_s^t (μM)							
T432 / S431	0	1	2	3	4	5	6
0	0.0003 (0.0001)	0.0008 (0.0005)	0.0028 (0.0017)	0.0091 (0.0058)	0.0298 (0.0198)	0.0890 (0.0585)	0.1656 (0.0755)
1	0.0011 (0.0007)	0.0031 (0.0020)	0.0086 (0.0056)	0.0234 (0.0160)	0.0616 (0.0431)	0.1419 (0.0941)	0.2316 (0.1183)
2	0.0050 (0.0034)	0.0116 (0.0080)	0.0263 (0.0188)	0.0585 (0.0428)	0.1218 (0.0887)	0.2217 (0.1515)	0.3220 (0.1856)
3	0.0225 (0.0167)	0.0425 (0.0323)	0.0787 (0.0608)	0.1388 (0.1076)	0.2276 (0.1730)	0.3384 (0.2438)	0.4450 (0.2911)
4	0.0980 (0.0802)	0.1487 (0.1231)	0.2157 (0.1787)	0.2992 (0.2454)	0.3969 (0.3190)	0.5034 (0.3923)	0.6105 (0.4565)

5	0.3720 (0.3366)	0.4254 (0.3817)	0.4864 (0.4329)	0.5561 (0.4909)	0.6359 (0.5567)	0.7271 (0.6313)	0.8314 (0.7159)
6	0.6162	0.6810	0.7526	0.8318	0.9193	1.0160	1.1228

Rate constants for KaiB-KaiC association: kb_s^t ($\mu M^{-2}h^{-1}$)

T432 / S431	0	1	2	3	4	5	6
0	0.000E+00	0.000E+00 (2.990E-01)	2.261E+00 (2.990E-01)	2.261E+00 (2.990E-01)	2.261E+00 (2.990E-01)	2.261E+00 (2.990E-01)	2.261E+00 (2.990E-01)
1	1.225E+01 (2.186E+00)	1.225E+01 (2.186E+00)	1.225E+01 (2.186E+00)	1.225E+01 (2.186E+00)	1.225E+01 (2.186E+00)	1.225E+01 (2.186E+00)	1.225E+01 (2.186E+00)
2	5.926E+01 (1.428E+01)	5.926E+01 (1.428E+01)	5.926E+01 (1.428E+01)	5.926E+01 (1.428E+01)	5.926E+01 (1.428E+01)	5.926E+01 (1.428E+01)	5.926E+01 (1.428E+01)
3	2.483E+02 (8.075E+01)	2.483E+02 (8.075E+01)	2.483E+02 (8.075E+01)	2.483E+02 (8.075E+01)	2.483E+02 (8.075E+01)	2.483E+02 (8.075E+01)	2.483E+02 (8.075E+01)
4	8.657E+02 (3.801E+02)	8.657E+02 (3.801E+02)	8.657E+02 (3.801E+02)	8.657E+02 (3.801E+02)	8.657E+02 (3.801E+02)	8.657E+02 (3.801E+02)	8.657E+02 (3.801E+02)
5	2.389E+03 (1.416E+03)	2.389E+03 (1.416E+03)	2.389E+03 (1.416E+03)	2.389E+03 (1.416E+03)	2.389E+03 (1.416E+03)	2.389E+03 (1.416E+03)	2.389E+03 (1.416E+03)
6	4.891E+03 (3.913E+03)	4.891E+03 (3.913E+03)	4.891E+03 (3.913E+03)	4.891E+03 (3.913E+03)	4.891E+03 (3.913E+03)	4.891E+03 (3.913E+03)	4.891E+03 (3.913E+03)

Rate constants for KaiB-KaiC dissociation: kdb_s^t (h^{-1})

T432 / S431	0	1	2	3	4	5	6
0	90	90	90	90	90	90	90
1	90	90	90	90	90	90	90
2	90	90	90	90	90	90	90
3	90	90	90	90	90	90	90
4	90	90	90	90	90	90	90

5	90	90	90	90	90	90	90
6	90	90	90	90	90	90	90
Rate constants for KaiAC phosphorylation at T432: $kapt_s^t$ (h^{-1})							
T432 / S431	0	1	2	3	4	5	6
0	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	---
1	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	---
2	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	---
3	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	---
4	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	---
5	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	---
6	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	7.6771 (7.5786)	---
Rate constants for KaiAC phosphorylation at S431: $kaps_s^t$ (h^{-1})							
T432 / S431	0	1	2	3	4	5	6
0	0.0378 (0.0129)	0.0671 (0.0288)	0.1194 (0.0640)	0.2124 (0.1423)	0.3777 (0.3163)	0.6717 (0.7032)	1.1947 (1.5635)
1	0.0378 (0.0129)	0.0671 (0.0288)	0.1194 (0.0640)	0.2124 (0.1423)	0.3777 (0.3163)	0.6717 (0.7032)	1.1947 (1.5635)
2	0.0378 (0.0129)	0.0671 (0.0288)	0.1194 (0.0640)	0.2124 (0.1423)	0.3777 (0.3163)	0.6717 (0.7032)	1.1947 (1.5635)
3	0.0378 (0.0129)	0.0671 (0.0288)	0.1194 (0.0640)	0.2124 (0.1423)	0.3777 (0.3163)	0.6717 (0.7032)	1.1947 (1.5635)
4	0.0378 (0.0129)	0.0671 (0.0288)	0.1194 (0.0640)	0.2124 (0.1423)	0.3777 (0.3163)	0.6717 (0.7032)	1.1947 (1.5635)

5	0.0378 (0.0129)	0.0671 (0.0288)	0.1194 (0.0640)	0.2124 (0.1423)	0.3777 (0.3163)	0.6717 (0.7032)	1.1947 (1.5635)
6	---	---	---	---	---	---	---

Rate constants for KaiABC phosphorylation at T432: $kabpt_s^t$ (h^{-1})

T432 / S431	0	1	2	3	4	5	6
0	1.0876 (1.1200)	1.7927 (1.8506)	3.0494 (3.1561)	5.3665 (5.5696)	9.7982 (10.1988)	18.6165 (19.4382)	---
1	0.6574 (0.7032)	1.1007 (1.1830)	1.9089 (2.0623)	3.4394 (3.7362)	6.4600 (7.0586)	12.6958 (13.9595)	---
2	0.4099 (0.4533)	0.6945 (0.7739)	1.2235 (1.3742)	2.2487 (2.5472)	4.3294 (4.9493)	8.7719 (10.1271)	---
3	0.2630 (0.2995)	0.4496 (0.5173)	0.8018 (0.9328)	1.4982 (1.7637)	2.9473 (3.5140)	6.1374 (7.4191)	---
4	0.1733 (0.2025)	0.2981 (0.3529)	0.5366 (0.6444)	1.0164 (1.2393)	2.0368 (2.5251)	4.3464 (5.4868)	---
5	0.1171 (0.1399)	0.2021 (0.2454)	0.3664 (0.4527)	0.7014 (0.8832)	1.4279 (1.8355)	3.1141 (4.0950)	---
6	0.0810 (0.0987)	0.1400 (0.1738)	0.2549 (0.3230)	0.4920 (0.6380)	1.0149 (1.3491)	2.2563 (3.0832)	---

Rate constants for KaiABC phosphorylation at S431: $kabps_s^t$ (h^{-1})

T432 / S431	0	1	2	3	4	5	6
0	0.0208 (0.0050)	0.0558 (0.0167)	0.1649 (0.0628)	0.5408 (0.2714)	1.9857 (1.3591)	8.2507 (8.0048)	39.2369 (56.3038)
1	0.0148 (0.0039)	0.0387 (0.0123)	0.1120 (0.0446)	0.3627 (0.1868)	1.3271 (0.9184)	5.5560 (5.3834)	26.9805 (38.3157)
2	0.0107 (0.0030)	0.0274 (0.0092)	0.0776 (0.0322)	0.2478 (0.1309)	0.9018 (0.6308)	3.7951 (3.6728)	18.7696 (26.3878)
3	0.0080 (0.0024)	0.0198 (0.0070)	0.0548 (0.0236)	0.1724 (0.0932)	0.6227 (0.4401)	2.6278 (2.5403)	13.2042 (18.3830)
4	0.0060 (0.0019)	0.0145 (0.0054)	0.0394 (0.0176)	0.1219 (0.0675)	0.4365 (0.3116)	1.8434 (1.7802)	9.3894 (12.9488)

5	0.0046 (0.0016)	0.0109 (0.0043)	0.0288 (0.0134)	0.0876 (0.0496)	0.3104 (0.2238)	1.3094 (1.2633)	6.7462 (9.2185)
6	---	---	---	---	---	---	---
Rate constants for free KaiC dephosphorylation at T432: $kdpt_s^t$ (h^{-1})							
T432 / S431	0	1	2	3	4	5	6
0	---	1.1575 (1.3402)	1.1575 (1.3402)	1.1575 (1.3402)	1.1575 (1.3402)	1.1575 (1.3402)	1.1575 (1.3402)
1	---	1.5466 (1.8364)	1.4995 (1.7832)	1.4540 (1.7316)	1.4098 (1.6814)	1.3669 (1.6327)	1.3254 (1.5854)
2	---	2.0965 (2.5667)	1.9645 (2.4112)	1.8416 (2.2661)	1.7273 (2.1307)	1.6207 (2.0042)	1.5214 (1.8860)
3	---	2.8861 (3.6648)	2.6041 (3.3170)	2.3531 (3.0064)	2.1293 (2.7286)	1.9296 (2.4799)	1.7510 (2.2568)
4	---	4.0383 (5.3548)	3.4949 (4.6479)	3.0339 (4.0465)	2.6417 (3.5334)	2.3070 (3.0941)	2.0205 (2.7171)
5	---	5.7494 (8.0216)	4.7516 (6.6429)	3.9486 (5.5310)	3.2988 (4.6294)	2.7701 (3.8945)	2.3377 (3.2922)
6	---	8.3372 (12.3453)	6.5489 (9.6973)	5.1897 (7.6846)	4.1473 (6.1411)	3.3409 (4.9470)	2.7119 (4.0157)
Rate constants for free KaiC dephosphorylation at S431: $kdps_s^t$ (h^{-1})							
T432 / S431	0	1	2	3	4	5	6
0	---	---	---	---	---	---	---
1	0.2204 (0.2175)	0.2204 (0.2175)	0.2204 (0.2175)	0.2204 (0.2175)	0.2204 (0.2175)	0.2204 (0.2175)	0.2204 (0.2175)
2	0.3602 (0.3556)	0.3467 (0.3422)	0.3337 (0.3294)	0.3212 (0.3171)	0.3091 (0.3052)	0.2975 (0.2937)	0.2864 (0.2827)
3	0.6120 (0.6041)	0.5635 (0.5563)	0.5192 (0.5126)	0.4787 (0.4725)	0.4415 (0.4359)	0.4075 (0.4023)	0.3763 (0.3715)
4	1.0850 (1.0711)	0.9493 (0.9371)	0.8321 (0.8214)	0.7307 (0.7213)	0.6429 (0.6346)	0.5666 (0.5593)	0.5002 (0.4938)

5	2.0168 (1.9909)	1.6630 (1.6417)	1.3770 (1.3593)	1.1447 (1.1300)	0.9554 (0.9431)	0.8005 (0.7902)	0.6732 (0.6645)
6	3.9515 (3.9008)	3.0421 (3.0030)	2.3599 (2.3296)	1.8443 (1.8206)	1.4516 (1.4329)	1.1503 (1.1356)	0.9177 (0.9059)

Rate constants for KaiBC dephosphorylation at T432: $kbdpt_s^t$ (h^{-1})

T432 / S431	0	1	2	3	4	5	6
0	---	0.8483 (1.4720)	0.8483 (1.4720)	0.8483 (1.4720)	0.8483 (1.4720)	0.8483 (1.4720)	0.8483 (1.4720)
1	---	1.3064 (2.1487)	1.2603 (2.0651)	1.2159 (1.9847)	1.1730 (1.9075)	1.1316 (1.8333)	1.0917 (1.7619)
2	---	2.0880 (3.2128)	1.9313 (2.9521)	1.7875 (2.7145)	1.6555 (2.4977)	1.5342 (2.2999)	1.4226 (2.1192)
3	---	3.4766 (4.9294)	3.0613 (4.3052)	2.7012 (3.7685)	2.3885 (3.3062)	2.1162 (2.9069)	1.8788 (2.5615)
4	---	6.0563 (7.7752)	5.0350 (6.4126)	4.2054 (5.3148)	3.5283 (4.4259)	2.9733 (3.7027)	2.5164 (3.1117)
5	---	11.0899 (12.6324)	8.6226 (9.7681)	6.7617 (7.6199)	5.3461 (5.9944)	4.2604 (4.7540)	3.4210 (3.7997)
6	---	21.4593 (21.1839)	15.4340 (15.2359)	11.2590 (11.1145)	8.3245 (8.2176)	6.2337 (6.1537)	4.7248 (4.6642)

Rate constants for KaiBC dephosphorylation at S431: $kbdps_s^t$ (h^{-1})

T432 / S431	0	1	2	3	4	5	6
0	---	---	---	---	---	---	---
1	0.3472 (0.3427)	0.2384 (0.2044)	0.1637 (0.1219)	0.1124 (0.0727)	0.0772 (0.0433)	0.0530 (0.0258)	0.0364 (0.0154)
2	0.6072 (0.5994)	0.3864 (0.3273)	0.2474 (0.1802)	0.1594 (0.1001)	0.1033 (0.0560)	0.0674 (0.0316)	0.0442 (0.0180)
3	1.1193 (1.1050)	0.6529 (0.5457)	0.3862 (0.2747)	0.2317 (0.1409)	0.1408 (0.0736)	0.0868 (0.0391)	0.0542 (0.0212)
4	2.1893 (2.1612)	1.1552 (0.9516)	0.6246 (0.4328)	0.3458 (0.2032)	0.1959 (0.0983)	0.1135 (0.0490)	0.0672 (0.0252)

5	4.5763 (4.5175)	2.1512 (1.7437)	1.0500 (0.7073)	0.5314 (0.3009)	0.2783 (0.1339)	0.1507 (0.0622)	0.0842 (0.0301)
6	10.3096 (10.1773)	4.2403 (3.3771)	1.8423 (1.2034)	0.8428 (0.4585)	0.4047 (0.1861)	0.2034 (0.0801)	0.1067 (0.0365)
Rate constants for KaiABC dephosphorylation at T432: $kabdpt_s^t$ (h^{-1})							
T432 / S431	0	1	2	3	4	5	6
0	---	0.0497 (0.0082)	0.0423 (0.0070)	0.0363 (0.0060)	0.0314 (0.0052)	0.0274 (0.0045)	0.0241 (0.0040)
1	---	0.1080 (0.0178)	0.0865 (0.0142)	0.0703 (0.0116)	0.0578 (0.0095)	0.0482 (0.0079)	0.0405 (0.0067)
2	---	0.2561 (0.0421)	0.1903 (0.0313)	0.1443 (0.0237)	0.1115 (0.0183)	0.0876 (0.0144)	0.0699 (0.0115)
3	---	0.6683 (0.1100)	0.4522 (0.0744)	0.3150 (0.0518)	0.2254 (0.0371)	0.1652 (0.0272)	0.1237 (0.0204)
4	---	1.9390 (0.3190)	1.1693 (0.1924)	0.7350 (0.1209)	0.4796 (0.0789)	0.3236 (0.0532)	0.2251 (0.0370)
5	---	6.3228 (1.0403)	3.3147 (0.5454)	1.8417 (0.3030)	1.0774 (0.1773)	0.6600 (0.1086)	0.4213 (0.0693)
6	---	23.4598 (3.8598)	10.3869 (1.7089)	4.9824 (0.8197)	2.5643 (0.4219)	1.4043 (0.2310)	0.8124 (0.1337)
Rate constants for KaiABC dephosphorylation at S431: $kabdps_s^t$ (h^{-1})							
T432 / S431	0	1	2	3	4	5	6
0	---	---	---	---	---	---	---
1	0.0230 (0.0273)	0.0121 (0.0143)	0.0067 (0.0079)	0.0039 (0.0046)	0.0023 (0.0028)	0.0015 (0.0017)	0.0010 (0.0011)
2	0.0342 (0.0405)	0.0166 (0.0196)	0.0086 (0.0101)	0.0047 (0.0055)	0.0027 (0.0032)	0.0016 (0.0019)	0.0010 (0.0012)
3	0.0523 (0.0619)	0.0232 (0.0275)	0.0111 (0.0132)	0.0057 (0.0068)	0.0031 (0.0037)	0.0018 (0.0022)	0.0011 (0.0013)
4	0.0823 (0.0975)	0.0331 (0.0392)	0.0147 (0.0174)	0.0071 (0.0084)	0.0037 (0.0044)	0.0021 (0.0024)	0.0012 (0.0014)

5	0.1340 (0.1587)	0.0484 (0.0574)	0.0197 (0.0233)	0.0088 (0.0105)	0.0043 (0.0052)	0.0023 (0.0027)	0.0013 (0.0016)
6	0.2259 (0.2677)	0.0725 (0.0859)	0.0267 (0.0317)	0.0111 (0.0132)	0.0052 (0.0061)	0.0026 (0.0031)	0.0015 (0.0017)