

Table 1. Model Parameters

<u>Reaction</u>	<u>Param</u>	<u>Value</u>	<u>Units</u>
<u>Receptor Activation</u>			
add_Ligand	t_Ladd	2160	s
add_Ligand	L_pipette	0	uM
add_Ligand	tauL	1	s
bind_L_b1AR	Kf	1000	uM-1.s-1
bind_L_b1AR	Kr	285	s-1
bind_Lb1AR_Gs	Kf	1000	uM-1.s-1
bind_Lb1AR_Gs	Kr	62	s-1
bind_b1AR_Gs	Kf	1000	uM-1.s-1
bind_b1AR_Gs	Kr	33000	s-1
bind_L_b1ARGs	Kf	1000	uM-1.s-1
bind_L_b1ARGs	Kd	0.535714	s-1
<u>Receptor inhibition/desensitization</u>			
add_propranolol	t_propadd	2420	s
add_propranolol	Propranolol_pipette	0	uM
add_propranolol	tauPropranolol	1	s
bind_b1AR_propranolol	Kf	1000	uM-1.s-1
bind_b1AR_propranolol	Kr	8	s-1
desens_bark	k_barkp	0.0011	s-1
resens_bark	k_barkm	0.0022	s-1
desens_pka	kpkap	0.0036	uM-1.s-1
desens_pka	kpkam	0.0022	s-1
<u>Gs activation</u>			
LRG_activation	k_gact	16	s-1
RG_activation	k_gact	16	s-1
Gs_gtp_hydrolysis	khyd	0.8	s-1
Gs_reassociation	k_reassoc	1210	uM-1.s-1
<u>cAMP synthesis</u>			
bind_Gs_AC	Kf	1000	uM-1.s-1
bind_Gs_AC	Kr	400	s-1
cAMP_synthesis_GsAC	Km	315	uM
cAMP_synthesis_GsAC	Vmax	(k_ac_gsa * GsAC_cell)	uM.s-1
cAMP_synthesis_GsAC	k_ac_gsa	2.5	s-1
bind_FskAC	Kf	1000	uM-1.s-1
bind_FskAC	Kr	860000	s-1
cAMP_synthesis_FskAC	Km	860	uM
cAMP_synthesis_FskAC	Vmax	(kfsk * FskAC_cell)	uM.s-1
cAMP_synthesis_FskAC	kfsk	7.3	s-1
cAMP_photolysis	kphot	0.1	uM-1.s-1
cAMP_photolysis	ton_global_light	0	s
cAMP_photolysis	toff_global_light	0	s
cAMP_photolysis	ton_local_light	0	s
cAMP_photolysis	toff_local_light	0	s
<u>cAMP degradation</u>			

bind_PDEcAMP	Kf	1000	uM-1.s-1
bind_PDEcAMP	Kr	1300	s-1
cAMP_degradation	kpde	5	s-1
inhibit_PDE	Kf	1000	uM-1.s-1
inhibit_PDE	Kr	30000	s-1

### PKA activation

bind_RC_cAMP	Kf	1000	uM-1.s-1
bind_RC_cAMP	Kr	9140	s-1
bind_cAMP_ARC	Kf	1000	uM-1.s-1
bind_cAMP_ARC	Kr	1640	s-1
bind_A2R_PKAC	Kf	4375	s-1
bind_A2R_PKAC	Kr	1000	uM-1.s-1
inhib_PKAC	Kf	1000	uM-1.s-1
inhib_PKAC	Kr	0.2	s-1

### AKAR phosphorylation

bind_PKAC_AKAR	Kf	1000	uM-1.s-1
bind_PKAC_AKAR	Kr	21000	s-1
AKAR_phosph	kpka_akar	54	s-1
bind_AKARp_PP	Kf	1000	uM-1.s-1
bind_AKARp_PP	Kr	7000	s-1
AKARp_dephosph	kcat_PP_AKARp	8.5	s-1