Uchigashima Documentation August 2016

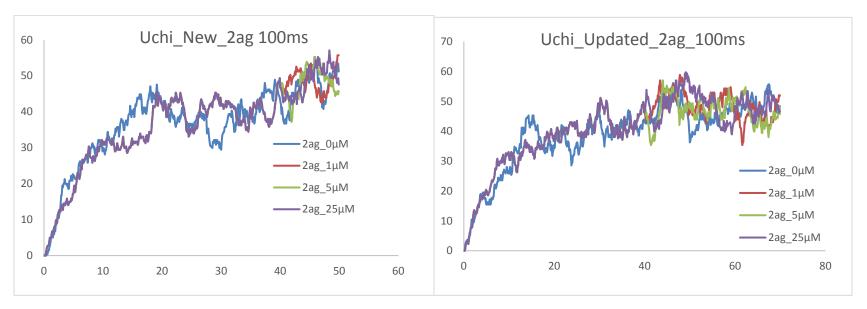
Changes made in the github MSPN table

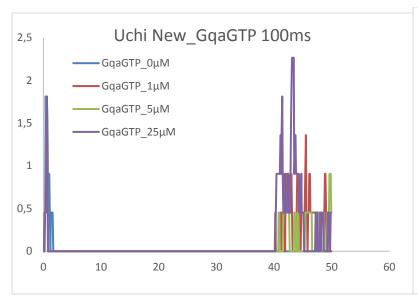
	Github rates (New MSPN table)					Updated			
Reactions	kf (nM ⁻¹ s ⁻¹)	kb (s ⁻¹)	kcat (s ⁻¹)	Kd or Km (nM)		kf (nM ⁻¹ s ⁻¹)	kb (s ⁻¹)	kcat (s ⁻¹)	Kd or Km (nM)
Gqabg + GluMglu ⇔ GqabgGluMglu⇒ GqaGTP + GluMglu	0.0015	0.68	0.5	453.33		0.0075	3.39	2.5	786.66
PlcCa + GqaGTP ⇔ PlcCa-GqaGTP → PlcCa+GaqGDP	0.0035	0.7	12	200		0.0175	51.49	12	3628
Plc + GqaGTP ⇔ PlcGqaGTP → PLC+GaqGDP	0.0007	0.7	12	1000		0.0035	51.49	12	18142.4
PlcGqaGTP Ca ⇔ PlcCaGqaGTP	0.0025	1		400		0.0125	53	12	5200

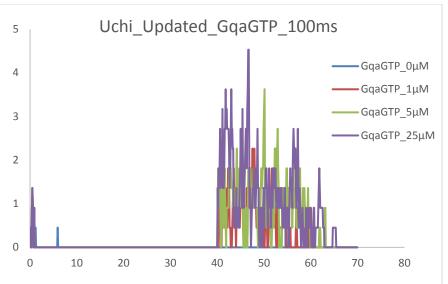
Two set of Uchigashima simulations were carried out:

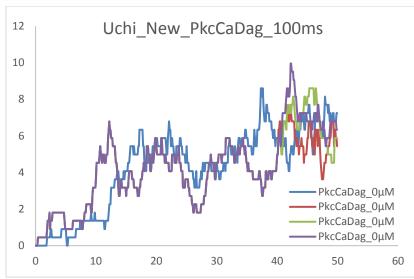
- 1. Uchi_new: Reaction rates from the new MSPN table. Reactions were carried out for 50s.
- 2. Uchi_updated: Modified reaction rates of the MSPN table where the reactions were speeded up 5 times. K_f was speeded up 5 times and K_b was calculated accordingly. Kcat and Km were kept the same with the exception of GqaGTP (Gqabg + GluMglu \Leftrightarrow GqabgGluMglu \Rightarrow GqaGTP + GluMglu) reaction, where the Kcat was increased so we have GqaGTP available. Reactions were carried out for 70s. Updated rates are in red in table.
- 3. Calcium comes at 40s.

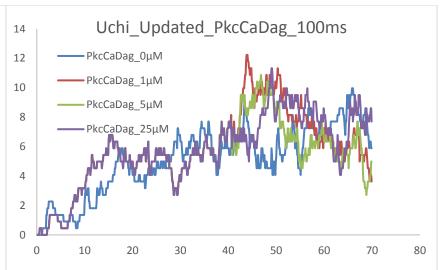
Plots
100ms depolarization

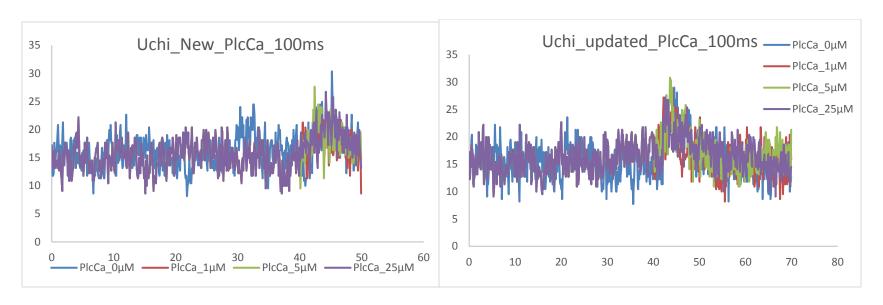




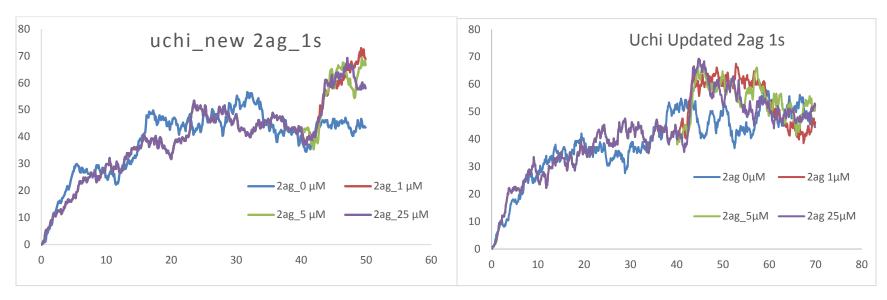


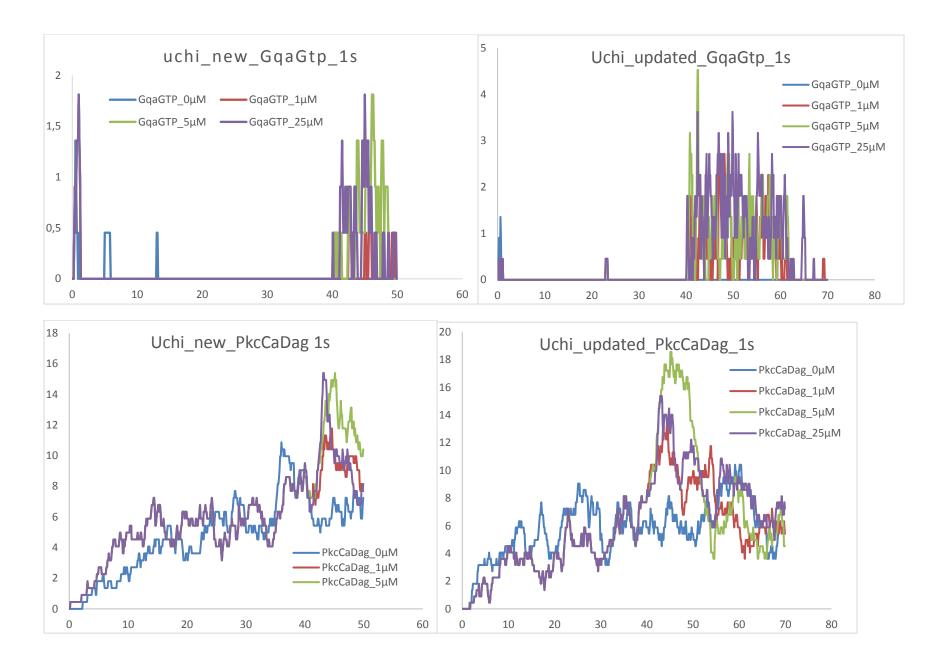


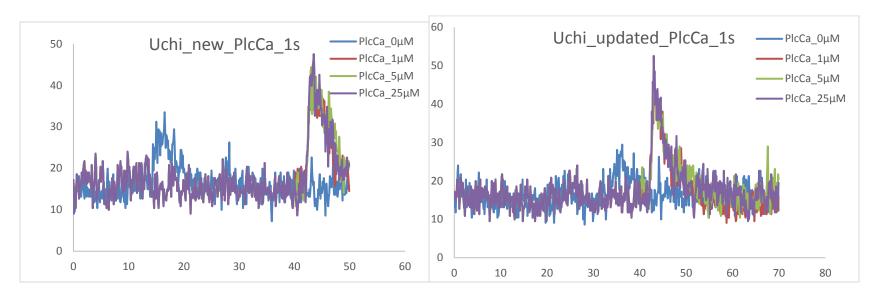




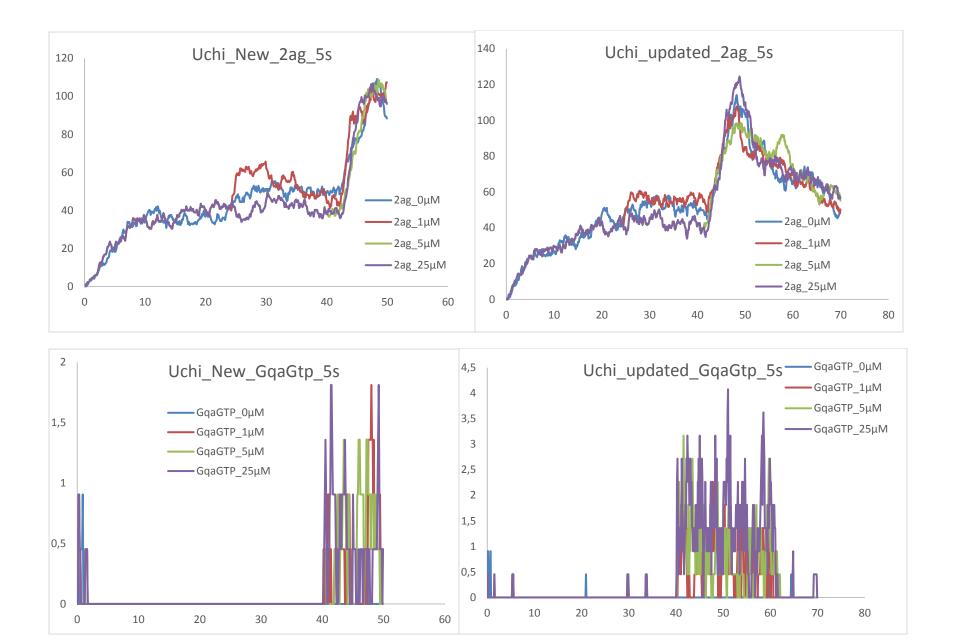
1 Second Depolarization

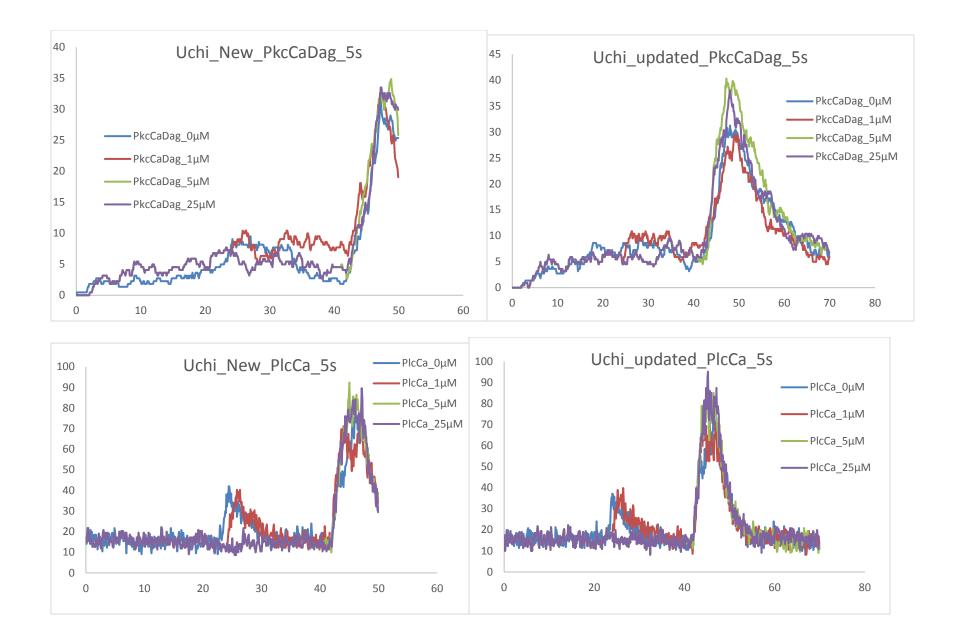






5s depolarization





Notes:

- 1. GqGTP produced is too little in both the github and updated version. The speeding up of 5 times didn't show any significant increase in the production of GqGTP.
- 2. Active PKC in both Github and Updated is too little and there is almost no difference with changing Dhpg concentration.
- 3. The amounts of G protein is lower in the github MSPN table compared to the published model, but a large difference is in amount of the G protein present.

Published Model	Github
Gq are 3500 nM	Gs, Gi and Gq are around 2000 nM
mGluR1 is 5000nM	mGluR1 is 150nM