**Simulation in Biology Abstract**

**Group:** Molecular

**Project name:** Neurotransmission Simulation

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**Project description:**

Within the cell there are proteins used that are coupled with G protein effector systems. Upon the existence of a transmitter protein in a receptor, G protein is activated, where adenylyl is stimulated. This causes ATP to be converted into cAMP, which intern activates protein kinase A and allows phosphorylation of potassium channels. Changing the amount of transmitter and length of degradation could change the effectiveness of the G protein.

**Agents and rules:**

*Transmitter rules:*

1. Generated at the leisure of the simulation runner
2. When collided to Receptor it attaches for a set time specified by a slider then removes itself
3. Moves randomly
4. Decays after set time
5. Moves outside of cell
6. Shape: circle

*Cell Membrane*: Patches

*Receptor rules:*

1. When Transmitter is attached, G-protein is released and charged along the neuronal membrane indicated by patches
2. Shape: triangle

*G-Protein rules:*

1. Follows along the neuronal membrane until collision with PLC where ATP -> cAMP
2. Can have inhibitory or supplestory states
3. Has field of has GTP/GDP
4. Shape: circle (different color than transmitter)

*ATP/cAMP rules:*

1. ATP is free floating within the neuronal membrane
2. When ATP attached to PLC it changes state to cAMP
3. cAMP can attach to PKA
4. cAMP is able to degrade
5. Shape: Diamond

Adeniline Cyclaze

1. turns ATP to cAMP
2. Shape: Triangle

*PKA rules:*

1. PKA when cAMP is attached to it can phosphorylate potassium channels
2. Shape: square

*Potassium Channels rules:*

1. Have a closed and opened state
2. Start on closed
3. Upon interaction with PKA+cAMP change state
4. Extra ions move through the channel when open
5. Shape: ovals

*Other ions:*

1. Shape: Small circle (different color)

**Model validation:**

1) As transmitter amount increases, more channels will open as they are phosphorylated.

2) As decay time decreases the less likely anything will occur

3) Phosphorylation occurs for some time after release

**Hypotheses / Predictions:**

1) Influence on the decay time effects the amount of cAMP produced

2) Inhibitory status mixed with suppletory states will dynamically change the state of the channel in such a way that its state will alter to that of a wave function.

**Evaluation (graphs, statistics):**

1. Graphs of the populations of agents over time
2. Number of open channels

**User Interaction (sliders, buttons):**

1) Sliders allow changes in environmental conditions (temperature)

2) Sliders allow changes in decay time of receptors per agent interaction (time)

3) Sliders allow to change amount of inhibitory / supplementary G-protein

**References:**

<https://bmcresnotes.biomedcentral.com/track/pdf/10.1186/1756-0500-5-608?site=bmcresnotes.biomedcentral.com>

<https://onlinelibrary.wiley.com/doi/abs/10.1111/jipb.12648>

<https://www.youtube.com/watch?v=FD3oksR-bhk>