



Wisconsin Virtual Learning SMART Team

Amber Wicklund, Catherine Minter, Chenoah Gad, Elizabeth Merkel, Rachel Mangiulli

Teacher: Karen O'Donnell

Mentors: Andrew Karls, Ph.D.¹ and Audra Kramer, M.S.¹

¹Marquette University

Modeling P2X4

PDB: 4DW1

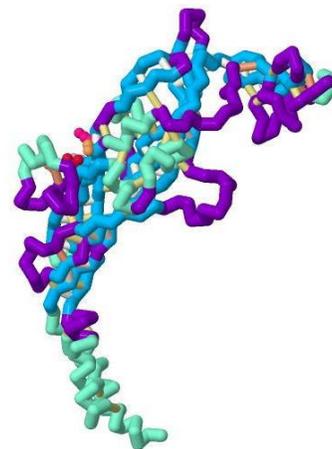
Primary Citation: Hattori, M. and Gouaux, E. (2012). Molecular Mechanism of ATP Binding and Ion Channel Activation in P2X Receptors. *Article* 485: 207-212.

Format: Alpha carbon backbone

RP:----- Zcorp with plaster

Abstract:

To someone who has excessive P2X4 receptors, simple gestures like hugs could cause unbearable pain. P2X4, a protein receptor located on the membrane of neurons, plays a large role in neuronal communication and pain perception. Ion channels on dendrites, located on one end of a neuron, allow ions to enter, causing an electrical current that continues through the cell. Once a current reaches the axon terminals, neurotransmitters are released to the next neuron, opening more ion channels and allowing transmission of the signal. This relay between neurons causes the perception of pain. In its resting position, P2X4 is closed inhibiting ions to enter the neuron, signaling no pain. In order for the receptor to open, ATP acts as the neurotransmitter attaching to the binding site of P2X4. In some, repeated sensory injury can lead to a need for extra receptors to be produced leading to chronic pain. Current studies are finding ways to block ATP from binding to receptors, keeping the receptor closed. P2X4 consists of 3 units forming the quaternary structure of the protein and 3 binding sites allowing for ATP to attach, opening the structure. Wisconsin Virtual Learning's SMART (Students Modeling A Research Topic) Team, using 3D printing technology, has modeled an open structure of P2X4, highlighting amino acids Leu 217, Leu 191,



Lys 193, Lys 70, Thr 189, and Ile 232 from PDB file 4DW1. With more knowledge of P2X4, scientists can unravel the mystery of chronic pain. This program is supported by a grant from NIH-CTSA.

Specific Model Information:

The amino acid Leu217 is colored coral.

The amino acid Lys193 is colored goldenrod.

The amino acid Lys70 is colored deeppink.

The amino acid Thr189 is colored sandybrown.

The amino acid Leu191 is colored plum.

The amino acid Ile232 is colored crimson.

We highlighted these amino acids because they are the ATP binding site on P2X4.

The hydrogen bonds are colored ivory.

The disulfide bonds are colored lightsalmon.

The support struts are colored khaki.

The backbone is colored darkmagenta.

The alpha helices are colored aquamarine.

The beta sheets are colored deepskyblue.

<http://cbm.msoc.edu/smartTeams/>

The SMART Team Program is supported by the National Center for Advancing Translational Sciences, National Institutes of Health, through Grant Number 8UL1TR000055. Its contents are solely the responsibility of the authors and do not necessarily represent the official views of the NIH.