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Mathematical Design of Ion Channel Selectivity

Technology

Reference

R231

Keyword

Drug Discovery

Contact

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Interested in studying ion channels as physical objects, trying to use the tools of physics, chemistry, engineering, and applied mathematics to understand how they work. Ion channels are proteins with a hole down their middle that are the gatekeepers for cells. Ion channels control an enormous range of biological function in health and disease. But ion channels have simple enough structure that they can be analyzed with the usual tools of physical science

Field

Molecular Biophysics and
Physiology

Patent Status

US and PCT Patents Pending

This invention relates to a method for designing ion channels with selectivity for different ions. The method was developed through collaboration between an ion channel researcher and mathematicians specializing in alternative modeling techniques.

AREAS OF APPLICATION

Development of selective ion channels for:

- Research into disorders caused by ion channel deficiencies.
- Identification and clinical development of compounds that preferentially mediate ion channels.
- Creation and testing of channel libraries

ADVANTAGES

- Improves speed and functionality of rational drug design process.
- Creates opportunities for monitoring impact of new compounds on non-targeted channels.
- Allows a new perspective into research on the causes of disease related to ion channel function.

THE TECHNOLOGY

This method is a major advance in the design of ion channels for synthesis and R&D. The manufacture of ion channels is sufficiently understood such that if channels can be designed to specification they can be built using the well-developed techniques of molecular engineering, such as site directed mutagenesis. However, there are present shortcomings in the ability to understand how the structure of an ion channel dictates its function. Thus the technical ability to make an ion channel is not sufficient to allow for their broad use to study structure-function relationships and to identify effectors and drug candidates. Researchers have yet to predetermine a particular selectivity for an ion channel, and then successfully attempt to determine the physical characteristics of a channel with that selectivity. This patent application describes how to perform ion channel design and identification. It represents a merger of physiological research with mathematical modeling. In the method, a class of models is first used to describe the function of ion channels where all of the parameters and boundary conditions are predetermined. Then novel algorithms are used to efficiently and stably solve the structural character and specificity of the channel. The combination of techniques provides a method for rapid, specific identification of the physical parameters necessary to create a selective channel. Existing molecular techniques are then employed to create the desired channel for further investigation.

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