Newcastle University

PDBe
Protein Data Bank in Europe

Name:
Date:

WP1 – PDBe Worksheet

The sodium-potassium pump is found in cellular membranes – its main job is to generate an ion gradient by pumping sodium ions out of the cell, and potassium ions in. To do this it gets energy from ATP. As more and more sodium leaves the cell, an electrical gradient and a concentration gradient are created. These gradients are vital for tasks such as transmitting nerve signals and controlling the osmotic pressure in cells.

Visit the PDBe homepage (www.ebi.ac.uk/pdbe) and load up the summary page for the sodium-potassium pump 2zxe. Explore the information and answer the questions below.

1. Which species is this protein from? State its scientific name, and find out its common name online.
   ***Squalus acanthias* – Spiny Dogfish**

2. View the protein in 3D using the 'Visualisation' tab or loading up the structure into PyMol. What do you notice about this protein? Describe the key structural features you can see.
   This protein has **three different polypeptide chains**. **Most of the ligands are attached to one of the chains** at one end of the protein. The protein is mainly composed of **α-helices**, most of these are stacked in the centre of the structure. At either end of the protein there are **β-sheets** too.

3. What is the most common secondary structure present in this protein? What do you know about this secondary structure?
   The most common secondary structure is the **α-helix**. This is a **regular, repeating rod-like structure**. The coil is held together by **hydrogen bonds** between a carbonyl oxygen, and the amine hydrogen **four residues ahead.**

4. How many different polypeptide (macromolecular) chains are present in this molecule? Why do you think it's beneficial to have more than one?
   3. Multiple chains give **more options to the protein structure and therefore function**.

5. Using the structure analysis tab, you'll find details of each of the macromolecules in the protein. By combining the number of amino acids in each polypeptide chain, work out the total number of amino acids in the protein pump.
   Chain B=305 amino acid residues
   Chain A=1028 amino acid residues
   Chain G=74 amino acid residues
   Total=**1407** amino acids

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6. <u>The Structure Analysis section lists the different polypeptide chains under Macromolecules. Each chain has a subsection called InterPro. This breaks the chain down into common domains and shows the different important sites in the polypeptide chain. Which of these chains do you think is most important to the overall function of the protein, and why?</u>
   Chain A appears to be the most important as it has the greatest number of InterPro domains. This means that it has **more key sites** which could be useful in the protein's function. Also, **this chain is much larger** than the other two, having many more amino acids. It is a good rule of thumb that a larger polypeptide chain has the potential for more possible functions, because it has more domains than other chains. A very small polypeptide chain is less likely to be able to form as many useful active sites and domains.

7. <u>List the different types and numbers of ligands bound to this protein. Which is the most common ligand?</u>
   There are 6 different types of ligands, and a total of 9 ligands.
   1x tetrafluromagnesate, MgF_4^{2-}
   1x magnesium ion, Mg^{2+}
   3x potassium ions, K^+
   1x cholesterol
   2x n-acetyl-d-glucosamine
   1x 2-acetylamino-2-deoxy-A-D-glucopyranose

8. <u>Using the Function and Biology Section, list all the different biochemical functions of this protein. How does the size of the protein and number of amino acids in the protein relate to its total number of functions?</u>
   Sodium-potassium exchanging ATPase activity
   Ion channel activity
   Nucleotide binding
   Hydrolase activity
   Metal ion binding
   ATP binding
   There are many different biochemical functions seen in this protein. In general, these are possible because there are so **many amino acids in this protein**, and because the **protein is large**, it can **perform many functions**. However, this is just a general rule, and there are exceptions.

9. <u>By considering the biological process of this protein, explain the general difference between a biological process and the biochemical functions of a protein?</u>
   In this case, the biological process is **ion transportation**. The **biological process is the overall aim of the protein**. For a protein to work effectively, it has to perform many different biochemical functions. For example, this protein must allow ATP to bind, because this provides the protein with the energy necessary to generate the ion gradients necessary for ion transport.