Abstract

Magnetic field sensing in animals has been a long standing scientific question, historically surrounded with scepticism and interest from many different fields. In recent years the general understanding of this phenomena has expanded significantly, however, there are still many unanswered questions, as to the exact mechanism. In general there are two main hypothesis, the first being that animals use magnetite, or other magnetic materials, to sense the magnetic field. The other theory is the radical pair mechanism, where animals would sense the magnetic field by using the quantum mechanical properties of radical pairs.

Both of these theories are likely true, some animals using magnetite, and some using the more exotic radical pair mechanism.

This thesis is a computational study of the believed host molecule for the radical pair mechanism, the cryptochrome protein, in relation to magnetoreception. It has two main objectives. The investigation of the creation of the radical pair in cryptochrome, and the study of different structural models of avian cryptochrome proteins.

The created models are investigated using molecular dynamics, to study their dynamic properties, which arise from the motions of the atoms in the protein. By subjecting known crystal structures of the cryptochrome proteins from non-migratory species, and the models of avian cryptochrome to molecular dynamics simulations we probe the different dynamics and functions these proteins might have.

To investigate the creation of the radical pair formation we utilize quantum mechanical methods that accounts for the electronic structure in the protein, and allows for investigation of the movement of the electrons that form the radical pairs in question.

When possible the investigations are linked to experimental results, to heighten the understand of the *in vivo* activity.