Abstract

Quantum mechanics and biology used to be two distinct disciplines with no direct connection, since quantum mechanics describes physical systems on length scales much too small to be considered in biology. This changed with the concept of quantum biology, i.e. the idea that the special properties of quantum systems might be utilized by biological systems, which to date is still controversial. A specific area where quantum effects are proposed to play a key role in a biological system is the study of avian magnetoreception, the magnetic compass sense that migratory song birds rely on twice a year for travelling vast distances across the continents. The avian magnetic compass was proposed to rely on the spin dynamics of transient spin-correlated radical pairs through what is known as the radical pair mechanism. This mechanism exploits the quantum phenomenon known as entanglement to enable magnetic field-dependent chemical reactions. As the radical pair mechanism mediates a chemical response to changes in an external magnetic field, the mechanism may also be affected by the magnetic component of electromagnetic radiation, especially radiofrequency radiation. Such radiation was shown to disrupt the avian magnetic compass sense in accordance with the radical pair mechanism, but weak radiofrequency radiation has also been shown to affect the production of reactive oxygen species in biological cells. This effect on cells is possibly due to the radical pair mechanism and is, therefore, another possible case of quantum biology. Thus even weak radiofrequency radiation might potentially affect our health and this possibility calls for more research into spin dynamics in biological systems.

Various molecular systems, such as the putative magnetosensor protein cryptochrome, has been studied using a variety of computational methods. These methods include all-atom molecular dynamics and quantum chemical methods such as density functional theory. Additionally, many investigations have relied on simulation of spin dynamics, and unlike molecular dynamics or quantum chemical methods no general computational tool exists for spin dynamics. Much effort was therefore put into the development of such a general-purpose spin dynamics simulation tool, MolSpin. In addition to the development of MolSpin, several studies were carried out on cryptochrome proteins. Cryptochrome may contain a *flavin adenine dinucleotide* (FAD) co-factor as well as a set of tryptophan amino acids, which form a radical pair upon photoexcitation of FAD. In particular, the absorption spectrum of the FAD co-factor was computed for a variety of cryptochromes. It was also demonstrated using computational means that ascorbic acid, a previously suggested interaction partner, is unable to sufficiently affect the radical pairs hosted by cryptochrome to be relevant for magnetoreception. Research into the possible adverse health effects of radiofrequency radiation was initiated by construction of a general workflow for evaluating radiation effects in specific biological systems. The preliminary steps towards an investigation of the electron transfer flavoprotein using the workflow were taken.