

5.10: Other Applications of NMR

Magnetic resonance imaging

In the introduction to this chapter, we heard two stories about people whose lives were potentially saved when brain tumors were discovered during a magnetic resonance imaging (MRI) scan. MRI is a powerful diagnostic technique because it allows doctors to visualize internal body tissues while sparing the patient from surgery and potentially harmful, high energy x-rays. The basis for MRI is essentially the same as for NMR: an MRI scanner has a very strong superconducting magnet large enough to completely surround a whole person, much the same way in which a small glass sample tube in an NMR experiment is surrounded by the instrument's magnet. Once exposed to the strong magnetic field, water protons in the body resonate at different radio frequencies - the variation in resonance frequencies is due to water binding in different ways to different tissue types, creating slightly different electronic environments for the protons. The software in the MRI scanner then translates variations in resonance frequencies to a color scheme, which creates a visual image of the body tissues in the scanned area.



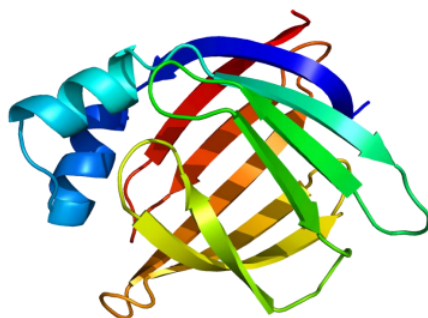
NMR of proteins and peptides

In this chapter you have learned enough about NMR to be able to understand how it is used to solve the structures of relatively small organic molecules. But what about really big organic molecules, like proteins?

X-ray crystallography, not NMR, is the most common way to determine the precise three-dimensional structure of a protein, and in a biochemistry class you will look at many images of protein structures derived from x-ray crystallography. While it is an immensely powerful tool for analyzing protein structure, crystallography has two major drawbacks. First, it relies on a researcher being able to get a protein to form regular, ordered crystals, which can be very challenging. Most proteins are globular, meaning they are (very roughly) spherical in shape. For a molecule to form crystals, it must pack together tightly in an ordered, repeating way: think of a neat stack of cube-shaped objects. Spheres, however, are inherently difficult to pack this way. Imagine trying to make a pile of tennis balls - they just roll apart, because so little of each ball's surface area comes into contact with its neighbor, thus there is very little friction (ie. noncovalent interactions!) holding them together. A large percentage of known proteins simply will not crystallize under any conditions that have been tried - therefore, we cannot determine their structure using x-ray crystallography.

Secondly, a lot of what is most interesting about proteins is how they move: flaps open and close when a substrate binds, or one part of the protein moves over to connect with another part. Protein action is dynamic. A crystal, on the other hand, is static, or frozen. A protein structure determined by x-ray crystallography is like a still photograph of a leaping dancer: we can infer from the picture what kind of movement might be taking place, but we can't get a full appreciation of the motion.

This leads to NMR, which of course is done in solution. It is easy to get most proteins into aqueous solution, so there are no worries about trying to make crystals. Also, a protein in solution is free to move, so NMR can potentially capture elements of protein dynamics. So why don't scientists always use NMR to look at proteins?



After working through a few NMR structure determination problems in this chapter, you have an appreciation for the brainwork required to figure out the structure of a small organic molecule based on its NMR structure: now imagine doing this with a protein, with its thousands of carbon and hydrogen atoms! Nevertheless, spectroscopists are gradually getting better and better at using NMR and computer-power to do just this. The advanced NMR techniques and methods of analysis are far beyond the scope of our discussion here, but you can see how useful it could be to protein scientists to be able to 'see' what a protein looks like using NMR, and if you are interested in this area of research you can learn about it in more advanced courses.

Note: The [Spectral Database of Organic Compounds](#) is a great resource for looking at NMR spectra (both proton and carbon) for a large number of compounds - the more examples you see, the better!

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