

# One step closer to green chemistry and improved pharmaceuticals

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Proteins are the workhorses of our cells. They help to digest our food, are at the core of our immune system, and literally shape our body from top to toe. Proteins also play an important role in biotechnology in the form of enzymes, which are important in the creation of anything from pharmaceuticals to bread, washing powder and much more. Their possibilities are virtually without limit.

To take advantage of their great potential, a detailed understanding of the three-dimensional shape of proteins is necessary. This is normally achieved through a complicated and expensive process in the laboratory. For years, researchers have tried to replace these experiments by computer simulations.

Now, two researchers at the Department of Biology at the University of Copenhagen, Assoc. professor Thomas Hamelryck and PhD-student Wouter Boomsma, have solved an important part of the problem of modeling the three dimensional shape of proteins. After 5 years of research, they have succeeded in developing a mathematical model that incorporates knowledge from physics, probability theory and geometry to describe the structure of proteins. This has given protein researchers a valuable new tool for the improved understanding of the shape and function of proteins.

"Each individual protein has its own unique chemical composition, consisting of 20 different amino acids in various different combinations. There are an endless number of such combinations, each giving rise to

its own shape. We have developed a simple mathematical model that captures these different shapes. This means that it will become easier for industry and researchers to use proteins to achieve their goals. For example in the development of green chemistry, where dangerous chemicals are replaced with protein-based products, which are more environment friendly", says Thomas Hamelryck.

Thomas also points to the fact that their computer model can have a great impact on the pharmaceutical industry.

"Proteins and illness are highly related, and most pharmaceuticals are targeted at proteins in our body. As we increase our knowledge of these proteins, the chance of finding more efficient pharmaceuticals for illnesses such as cancer, diabetes and AIDS are greatly enhanced", Thomas continues.

The two researchers at the University of Copenhagen are currently collaborating closely with partners in the biotech industry to explore these possibilities.

Source: University of Copenhagen

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