Understanding water-repellent enzymes

June 16 2020, by David Bradley

The ability of some molecules, such as fatty or oily molecules, to repel water is known as hydrophobicity. The opposite, water attracting, is hydrophilicity. The hydrophobic force that keeps water molecules at bay is one of the most fundamental of chemical interactions, but it is not only about why oil and water do not mix, it lies at the heart of how the proteins, the molecular machinery of our cells fold into their active form and indeed how they work to keep us and every other living thing alive.

Research published in the *International Journal of Computational Biology and Drug Design*, has investigated the properties of two types of hydrophobic groups in six specific kinds of proteins, the biological catalysts known as enzymes. Anindita Roy Chowdhury (Chakravarty) of the GD Goenka University, in Haryana and her colleagues H.G. Nagendra of the Sir M Visvesvaraya Institute of Technology, in Bengaluru, and Alpana Seal of the University of Kalyani, in West Bengal, India, explain how the hydrophobic properties of aliphatic and aromatic groups on the amino acids that build up a protein chain then allow the chain to twist and turn and fold in on itself to form its active structure. Aliphatic groups, or residues, are essentially chains of carbon and hydrogen atoms while aromatic groups are commonly rings of carbon and hydrogen atoms joined to the amino acid structure.

The researchers had previously identified those aromatic and aliphatic residues that contribute the most and the least to hydrophobic character in six enzyme classes. In the current work, they have examined the relative contributions towards hydrophobicity of the different hydrophobic amino acids in both aromatic and aliphatic categories.

They have found that there is an inverse relationship between residues of similar hydrophobic strength both in aromatic and aliphatic categories. So, for instance, the presence of an amino acid such as tryptophan which contains an aromatic group has the inverse effect to one like phenylalanine . A similar relationship is found in pairs of amino acids with aliphatic side chains, such as isoleucine and leucine. Leucine, isoleucine, and phenylalanine are essential for creating a hydrophobic, non-polar, environment at the core of an enzyme that has to bind non-polar molecules.

"This analysis is likely to provide insight for finer analysis of the enzyme molecule," the team writes.

More information: Anindita Roy Chowdhury (et al. Correlation among hydrophobic aromatic and aliphatic residues in the six enzyme classes, *International Journal of Computational Biology and Drug Design* (2020). DOI: 10.1504/IJCBDD.2020.107318

Provided by Inderscience