Abstract

A thorough knowledge of non-covalent amino acid interactions within a protein structure is essential for a complete understanding of its conformation, stability and function. Among all the amino acids that usually make up a protein, tryptophan is distinguished both by its rarity and size of its side chain formed by an indole group. It is able to provide various types of indispensable interactions within the protein and between different polypeptide chains, but also between the protein and a biological membrane. In addition, it is the most commonly used natural fluorophore.

Databases of solved protein structures are commonly used to study amino acid interactions and allow more or less complex analyzes of the issue. Thus many non-covalent interactions that may occur between tryptophan and other amino acids have been found. However, most of these analyzes focus on specific interactions and do not follow up the tryptophan's environment as a whole, where all amino acids interact.

Some newly developed methods have been used in this Thesis, specifically the occurrence profiles of the individual amino acids around the indole group of tryptophan and the results were compared with an available literature. The amino acid that has the greatest preference for tryptophan turned out to be tryptophan again, and these tryptophan pairs were subjected to more detailed analysis.

One of the conclusions of my work is the finding that arginine and lysine show a cation-π interaction described in the literature, but that they do not show an increased occurrence in its surroundings. On the other hand, I did not observe any anion-π interaction in combination with tryptophan and I believe that these are erroneous results in the literature.

Analysis of tryptophan pairs showed how structured the interaction space around tryptophan is. There are different layers, where the orientation of the indole groups of tryptophanes always prevail. Such a non-random distribution is located up to 10 Å distance between the indoles. Therefore, for all analyzes of the properties of the space around tryptophan (and probably other amino acids as well), it is necessary to proceed only in certain specific directions, even at greater distances and not to limit the research to the average properties of the surrounding at once.