Abstract (EN)

Nucleic acids are among the largest and most complex compounds in nature and without a doubt the most important molecules for the existence of life. Understanding the chemical behaviour and thermodynamic parameters of their building components enables us to make ever so increasingly accurate predictions of nucleic acid structures, reactions and functions. These predictions in turn provide great help in research fields such as DNA nanotechnology, nucleic acid targeted drug development and DNA material sciences. My research work targeting nucleobases and their analogues is focused on exploring effects of their conformational isomers and tautomers on the thermodynamics of intermolecular complexes that these compounds can theoretically form with each other through hydrogen bonds.

Doc. RNDr. Martin Dračínský, Ph.D. and I have conducted two separate studies concerning this topic at the NMR department of the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences. The first research project concentrated on developing a method for the determination of nucleobase-pairing free energies from rotamer equilibria of various 2-(methylamino)pyrimidines [1], while the second project aimed to shed light on the tautomerism of guanine analogues [2].

Keywords

Nuclear Magnetic Resonance (NMR) Spectroscopy, Rotational Isomers, Tautomerism, Complex Formation