DENSITY FUNCTIONAL THEORY APPLICATION TO THE STEROID HORMONES SPECTROSCOPIC BIOCLASSIFICATION

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Abstract

The steroid hormones carry out the most important regulatory functions and influence many physiologic processes. The steroid hormone molecules are built of a standard four-ring system (three six-member rings and one five-member ring). How these similar-type compounds can provide various complicated biological functions based on recognition of numerous receptors and their modification actions on DNA? Vibrational spectroscopy together with quantum density functional theory (DFT) calculations provide a good bioinformatics background for classification and biospecification of their structure-activity relationship.

The presence of the four rings provides a specific structure with conformational flexibility and a large number of low-frequency vibrations. Minor alterations in position of side functional groups result in essential change of binding processes with steroid receptors. In this work we present our studies of teraherz time-domain (THz) and infrared (IR) spectra of a number of hormones and compare their absorption THz-IR spectra with Raman scattering. The Raman and THz spectra were measured in the temperature range from 83 K to 297 K. Based on quantum chemical calculations of frequencies by the DFT B3LYP/6-31 G (d,p) approximation we can assign the vibrational bands in both, the THz-IR absorption and Raman spectra.

The chosen steroid hormones (progesterone, 17α-hydroxyprogesterone, cortisol, cortisone and acetate cortisone) differ in the sequential addition of OH groups to the progesterone core. Low frequency vibrational spectra of steroid hormones contain vibrational modes which include deformation of the whole molecule (30-35 cm^{-1}, twisting of steroid rings), and modes of side chain (75-77 cm^{-1}). Position and intensity of lines depends on the structure of molecules, the presence and quantity of hydrogen atoms and intermolecular bonds. The knowledge of vibrational modes presented here is important for understanding of hormone-receptor binding.