

Spectroscopy and Structural Properties of Biogene Amines (Serotonine, Histamine, γ -amino oil acid) and Account for Laser and Neutron Capture Effects

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Paper is devoted to the Monte-Carlo computational studying the structural and spectroscopic properties for the biogene amines: serotonine (ST), histamine (HM), γ -amino oil acid (AC) and the laser and neutron capture action on the indicated properties of studied molecules. The ST (or 5-hydroxitriptamine, 5-HT) is produced by means of the hydroxycilation of essential amine acid of the triptophane [1]. ST influences mainly in a place of its appearance and calls for blood vessel narrowing in places of the trombocytes decay. Probably, serotonine ST is the mediator for transition of the nervous pulses in some branch of the brain. HM is produced in cells (mastocides) from the histidine amino acid. The γ -amino oil acid AC is produced in the brain substance and probably plays a role of the mediator or inhibitor of pulses. Many biomolecules (BM) are composed not only by hydrophilic, but also by hydrophobic groups, in the vicinity of which the water-water (or blood plasma) interaction is expected to be present even in the zeroth approximation. We present results of the Monte-Carlo calculating the cluster consisting of the serotonine ST (histamine HM) molecules and 100 molecules of water. All relevant interaction potentials are obtained by means of quantum calculation [1]. The water-water interaction potential was found by Matsouka etal by CI method. The BM-water interaction potential was obtained in the SCF approximation. Calculation is carried out at T=300K; All molecules are treated as rigid. The results for interaction energies are given below in table:

Potential / $kJmol^{-1}$	Neutral molecule	zwitterion
Water-water	-27.7 ± 0.8	-27.2 ± 0.7
ST-water	-59.5 ± 2.0	-348.5 ± 15.0
HM-water	$-37,8 \pm 2.0$	$-178,4 \pm 15.0$

The zwitterion appears as expected to be strongly favoured with respect to neutral molecule. The HM in the “zwitterion” more intensively (on the order) catalyses the gastric juice secretion and secretion from other endocrine glands. The similar situation is with action of the HM in the inflammatory and allergic reactions with further increasing vessel walls permeability and action of the ST with further blood-vessel narrowing in places of the trombocytes decay. We at first consider the possibilities of laser and neutron capture action on different of molecules, including an analysis of Szilard-Chalmers (n, γ), (n,n), Mössbauer and GM [2] effects. Some new bio-nano-technologies are analysed.

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