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A quantum-chemical model of the inhibition of HIV-1 integrase action by molecular iodine

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A distinctive feature of the drugs having anti-HIV and anti-viral action (AHD) [1-2] is that they contain not only an iodine-polymer complex, but also lithium and potassium halogenides.

Using X-ray data for iodine-α-dextrin complexes and the results of quantum-chemical ab initio RHF/3-21G** level calculations a model of the active complex (AC) of AHD was proposed. It is suggested that the drug active complex contains molecular iodine located inside the α-dextrin helix and coordinated by lithium halogenides and polypeptides. Electronic structure of I2 in this complex differs from its characteristics in complexes with organic ligands or the free I2. In the AC under study the molecular iodine displays the acceptor (donor) properties towards polypeptides (lithium halogenides) [1]. In paper [3] UV- and IR-spectroscopy has been used to study the water-glycine - KI3 - LiCl –ethanol system that forms AC of AHD. It has been shown that in this system conditions are created for the formation of an iodine complex compound, in which the molecular iodine reveals the acceptor properties towards glycine, and the donor properties towards the LiCl-ethanol complex.

A mechanism of AHD anti-HIV action has been proposed. Under the influence of molecular iodine contained in the AC of AHD the structure of HIV DNA is modified: the nucleotides of the viral DNA that are more π-donor-active than peptides form a stable complex with molecular iodine and lithium halogenides [1].

Using UV- and IR-spectroscopy and quantum-chemical DFT/B3PW9 we have confirmed the existence of the molecular iodine complex coordinated by lithium halogenides with nucleotide (nucleotideI2 LiCl) in the system containing the AGA nucleotides triplet and the AC complex of AHD.

The interaction of molecular iodine coordinated by lithium halogenides with the viral DNA and the HIV-1 integrase co-factor has been studied by DFT/B3PW9 method.

Calculations have shown that complex nucleotideI2 LiCl may prevent the active catalytic fragment of HIV-1 integrase from interacting with the virus DNA. Complex nucleotideI2 LiCl may become the center of another nucleoprotein complex in which molecular iodine interacts both with the virus DNS and the active catalytic domain of HIV-1 integrase

Experimental data on the anti-HIV effect of AHD [2] and the results of calculations suggest that the molecular iodine coordinated by lithium halogenides can be regarded as a compound inhibiting the catalytic center of integrase.

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