THE INHIBITION OF MYCOBACTERIUM TUBERCULOSIS CULTURE BY ISONIAZID, VITAMIN B_6 AND PYRIDOXALPHOSPHATE IN VITRO. "STRUCTURE — ACTIVITY" CORRELATION WITH APPLICATION OF QUANTUM-CHEMICAL CALCULATIONS

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Summary

The attempt of prediction of antituberculous activity of vitamin B_6 and pyridoxalphosphate in comparison with isoniazid was performed. The ability of vitamin B_6 and pyridoxalphosphate to inhibit the grows of Mycobacterium tuberculosis culture was studied. It was established, that MIC of pyridoxalphosphate was 62,5 mcg/ml. Vitamin B_6 inhibited the growth of MBT on 25 % at concentrations of 50 mcg/ml (isoniazid MIC — 0,03 mcg/ml). The biological study indicated a synergetic action of drugs combinations. The inhibitory concentration of vitamin B6 in combination with isoniazid exceeded the MIC of separately administered vitamin B_6 in 8 times and isoniazid — in 10 times. For combination of pyridoxalphosphate with isoniazid the inhibiting concentrations increased a by 8,6 and 10 times, accordingly, in comparison with their separate administration. The antituberculous activity of these medications correlated with the following molecular properties, such as electronegativity, energy of the highest held molecular orbital, energy of the lower free molecular orbital, value of a charge on 4C core of pyridine, value of a charge on Carbon atom of oxo- or hydroxymethylen- groups and molecular volume.