The study of the correlation of the binding energy of peptide ligand complexes with hybrid antibiotics vancomycin-azithromycin and eremomycin-azithromycin with antibacterial activity

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One of modern strategies that can solve the problem of antibacterial resistance is the development of dual-acting hybrid antibiotics – structures that contain two covalently linked antimicrobial drugs that interact with different targets in a bacterial cell [1]. Antibacterial activity of hybrid antibiotics vancomycin-azithromycin (C11, C12-carbonate) and eremomycin-azithromycin (C11, C12-carbonate) was evaluated. Quantum chemical calculations of energy these hybrid antibiotics with a model tripeptide ligand α,ε-di-Ac-L-Lys-D-Ala-D-Ala by the semiempirical PM6 method using a software package Spartan-10[2] provided data on geometrical parameters of these complexes along with the energy of their formation and the influence of protonation of the NHCH₃ group. A correlation between the energy of formation of antibiotics-ligand complexes and antibacterial activity of hybrid antibiotics against Gram-positive bacterial strains was found.

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References
