

TARGET-ORIENTED APPROACH TO NEW INHIBITORS ION CHANNELS RNA-GENOMIC VIRUSES BASED ON FRAMEWORK STRUCTURE COMPOUNDS



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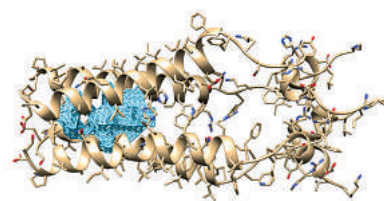
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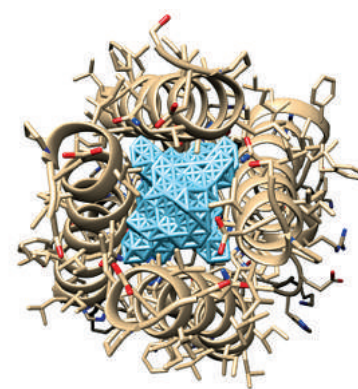
OBJECTIVES

Computer design of new inhibitors of viral reproduction by virtual screening of frame structure compounds, development of optimal synthesis schemes and detection of anti-virus activity in vitro



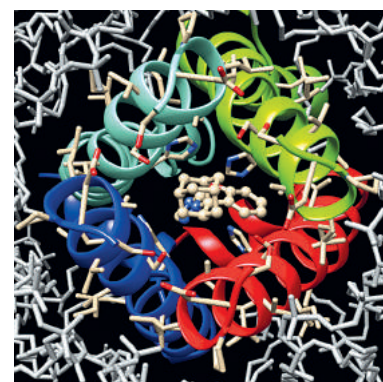
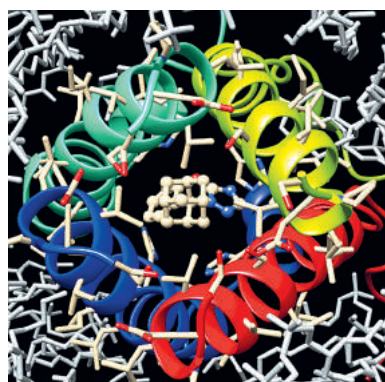
AREAS OF USE

Chemical Industry, Pharmaceutical Industry, Medical Industry

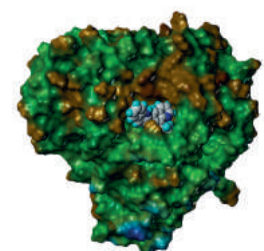
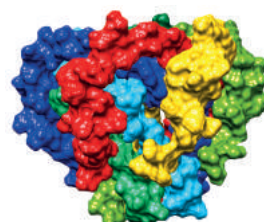
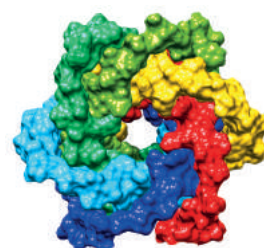


PECULIARITIES

Computer design of fundamentally new inhibitors reproduction RNA-genomic virus, development of methods for their production and determination of antiviral activity spectrum.



The project is devoted to creation of new orally available potential inhibitors of viral reproduction for further development and clinical studies of compounds. During research models of proteins influenza virus A, Hepatitis C and variola virus were developed and the data about binding of a large array of caged compounds with protein targets was obtained. Moreover, the Project allowed to select the most promising candidates for synthesis and testing of biological activity. Also, new methods of obtaining the most promising candidates of frame structure, a system of modification of polarity of functional groups and variation of steric load responsible for binding molecule centers were developed. Physicochemical characteristics of new synthesized samples (IR and NMR spectroscopy, mass spectrometry, gas-liquid chromatograph, x - ray structural analysis, elementary analysis) are determined. The study also resulted in obtaining data on virus-inhibition action of the synthesized samples in vitro concerning RNA and DNA genome viruses (influenza viruses A and virus of bovine diarrhea as a surrogate model of hepatitis C virus, variola virus). The obtained results are expected to lead to creation of new national pharmaceuticals for various viral diseases therapy. This will allow to reduce the number of ill people among the population of Russia, as well as to solve the problem of import substitution in health care. The Project will also contribute to the development of the pharmaceutical industry through the creation of innovative antiviral agents.



CORE COMPETENCIES

#ANTIVIRAL ACTIVITY, # FRAMEWORK STRUCTURE, #DOCKING,
MOLECULAR MODELING, # OPTIMAL SYNTHESIS SCHEMES, #VIRAL
INFECTION, #RESISTIBILITY

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