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# Volume 5

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in 6 volumes**

**Saint Petersburg  
9 –13 September**

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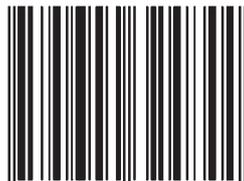
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## CAGE STRUCTURES – INHIBITORS OF FLAVIVIRUS P7 ION CHANNEL

Klimochkin Yu.N.<sup>a</sup>, Shiryaev V.A.<sup>a</sup>, Leonova M.V.<sup>a</sup>, Palyulin V.A.<sup>b</sup>, Radchenko E.V.<sup>b</sup>,  
Bormotov N.I.<sup>c</sup>, Serova O.A.<sup>c</sup>, Shishkina L.N.<sup>c</sup>

<sup>a</sup>Samara state technical university, Molodogvadeyskaya 244, Samara, 443100, Russia,  
e-mail: orgchem@samgtu.ru

<sup>b</sup>M.V. Lomonosov Moscow state university, Leninskie gory 1/3, Moscow, 119991

<sup>c</sup>State research center of virology and biotechnology VECTOR, Koltsovo, Novosibirsk region, 630559

Cage fragments are relatively often found in the structure of medicines, including the well-known antiviral drugs. Hepatitis C virus is one of the most dangerous viruses. Currently, there are direct-acting antivirals (DAA) for hepatitis C, their targets are NS3 / 4A protease, NS5A replication activator and NS5B polymerase, however their successful application is complicated due to the high variability of the virus and drug resistance. There is another potential target - the viral protein p7, which functions as an ion channel. The development of potential inhibitors of hepatitis C virus reproduction was performed for the p7 proteins produced by viruses of the most common genotypes Gt1a, Gt1b, Gt2a and Gt2b (protein primary structures UniProt: P26664, P26663, P26660, P26661, respectively). The three-dimensional structures of ion channels were obtained using molecular dynamics. Molecular docking of more than 800 structures revealed compounds potentially active against hepatitis C virus and bovine diarrhea virus (BVDV). Based on the results obtained, a series of adamantane and homoadamantane derivatives were synthesized. Testing of antiviral activity was carried out in the SRC VB "Vector". Most of the synthesized compounds showed pronounced antiviral activity *in vitro* against bovine diarrhea virus as a surrogate model of the hepatitis C virus, one of the compounds showed high activity and can be used as a leader for further research.

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