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XXI MENDELEEV CONGRESS
on general and applied chemistry

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Book of abstracts in 6 volumes

Saint Petersburg
9 –13 September

XXI Mendeleev Congress on General and Applied Chemistry.
Book 5: Abstracts. – Saint Petersburg, 2019 – p. 352
ISBN - 978-5-6043248-4-4
Book 5. The periodic table and new elements.
Medical chemistry: fundamental and applied aspects.

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ISBN 978-5-6043248-4-4
9 785604 324844

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CAGE STRUCTURES – INHIBITORS OF FLAVIVIRUS P7 ION CHANNEL

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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.

The research is funded by RFBR, project 18-33-00994 mol_a.