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Computational And Experimental Studies Of New Cage Compounds – Potential Antiviral Drugs

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The influenza A virus, with 27 known subtypes that range from low to high pathogenicity in the bird population, also infects humans and other mammals. Adamantane derivatives have been used successfully for the prevention and treatment of influenza A virus infection for more than 30 years. It is proposed that these drugs inhibit influenza A virus replication by blocking the M2-protein ion channel.

Our work [1] and previous [2] has shown that the high biological and antiviral activity show the cage substances that posses amino-, amido- and carboxy- groups. Based on these data we have synthesized the relevant derivatives of Cs- and D3- trishomocubanes.

Binding of blockers to the Influenza A M2 ion-channel is studied using automated docking calculations. Our study present various binding sites for the studied cage compounds within the TM-M2 region.

[1] A.V. Gayday, I.A. Levandovskiy, K.G. Byler, T.E. Shubina, "Mechanism of Influenza A M2 Ion-Channel Inhibition: a Docking and QSAR Study" in *Lecture notes in Computer Science* **5102**, Springer, (2008), pp. 360-368.

[2] (a) F.N. Stepanov et al, *Zh. Org. Khim.* **6**, (1970), 1823; (b) S.D. Isaev et al., *Virus inhibitors and mechanism of their inhibition* Riga, 1977; (c) M.K. Indulen et al. *Interaction of viruses and cells* Riga, 1977; (d) A.G. Yurchenko et al. *Patents USSR*, 1979, 1981, 1984, 1989.