

## Application of fragment-based drug design to the discovery of novel anti-HIV microbicides

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The development of potent microbicides is a great challenge in the field of battle with the HIV/AIDS. The complex mechanism of virus-human cell interaction provides the difficulties in the search for novel pharmaceuticals that prevent the virus intrusion into the human organism. We propose to apply PASS approach (<http://pharmaexpert.ru/PASSonline/>) for fragment-based design of novel multitargeted potential microbicides. Suggested method has been validated in the virtual experiments (Filz et al., SAR & QSAR Environ. Res., 2012) and in the design of novel COX-1/2 and LOX inhibitors (Eleftheriou et al., Eur. J. Med. Chem., 2012). Fragment library is constructed focused on inhibitors of known anti-HIV targets (HIV-1 integrase, reverse transcriptase, etc.) as well as on inhibitors of proteins playing a role in the formation of virus-host contacts. An application of fragment library to the design of novel microbicides will be discussed.

Acknowledgement. The work was partially supported by RFBR/NIH grant No. 12-04-91445-NIH\_A/RUB1-31081-MO-12.