

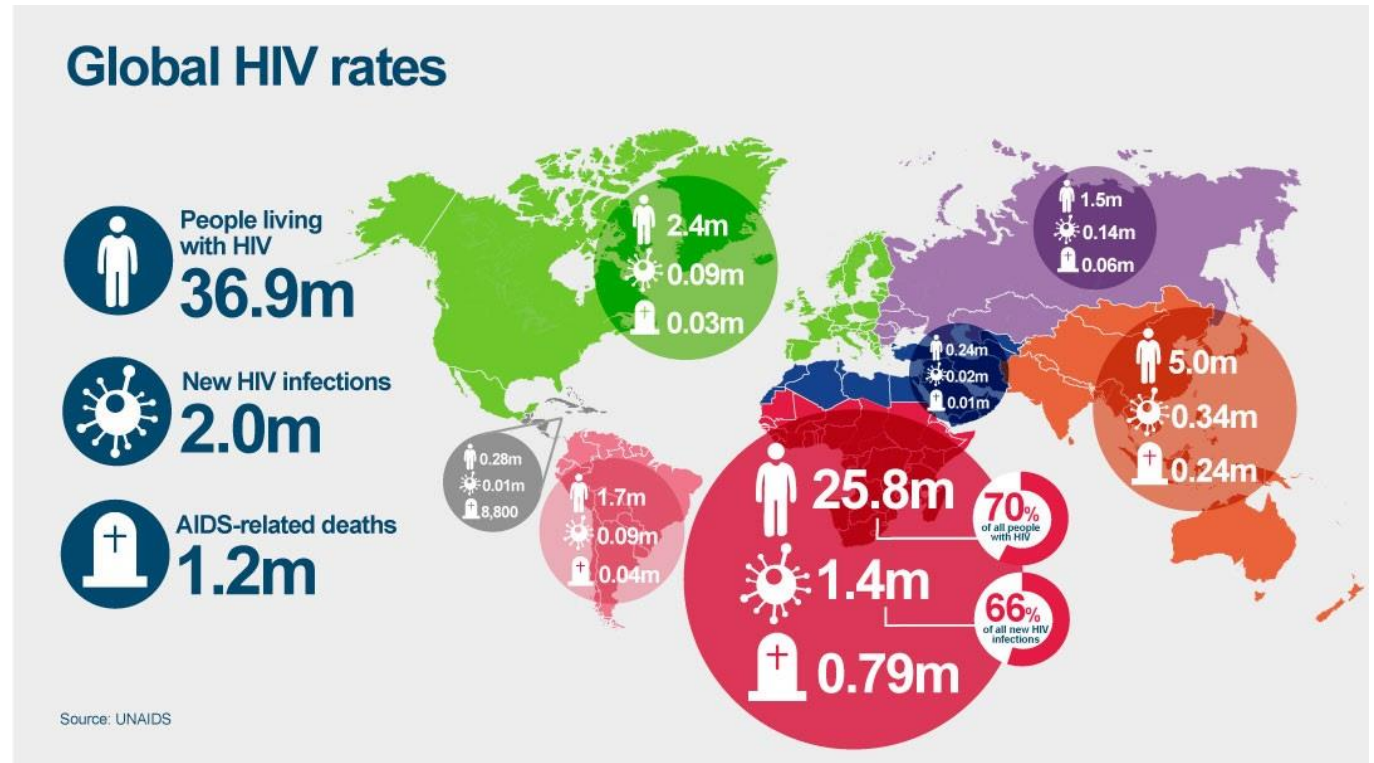
Development and analysis of AIDS epidemic agent-based computer model applying an algorithm for explicit calculation of HIV replicability

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The AIDS epidemic is an extreme problem that is relevant not only for Russia, but also for the whole world. According to statistics, about 1% of the Russian population is HIV-infected. HIV has a large number of genetic variants that differ in both replication and virulence. The duration of the incubation period and the severity of the disease in the active phase also depend on these factors. Currently, a large number of mathematical and computer models of HIV infection have been created that consider infection at different levels of biological organization: from population-epidemiological to molecular-genetic. However, in the modern literature, we have not encountered models that combine the genetic and population-ecological levels



The statistical method [1] of computer prediction of the affinity of the TBP/TATA complex was used to assess the replication and virulence of various genetic variants of HIV. The Python programming language was used to process the HIV strain database and visualize the data. MAFFT and BioPython were used to build a phylogenetic tree. The agent model of the AIDS epidemic is developed in the C++programming language.

The first step was a genetic analysis of the HIV strains obtained from the NCBI database. Based on the analysis of 1336 HIV strains using statistical methods for predicting the affinity of the TBP/TATA complex, clustering into 3 visible groups was obtained (Fig. 1).

On the phylogenetic tree, the obtained clustering was confirmed for two groups (Fig. 2)

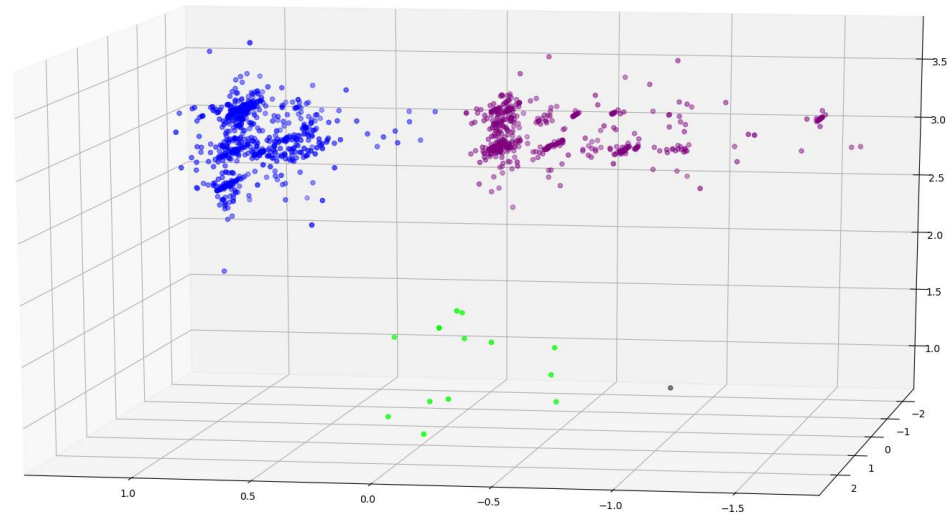


Fig. 1. Groups obtained based on the analysis of 1336 HIV strains

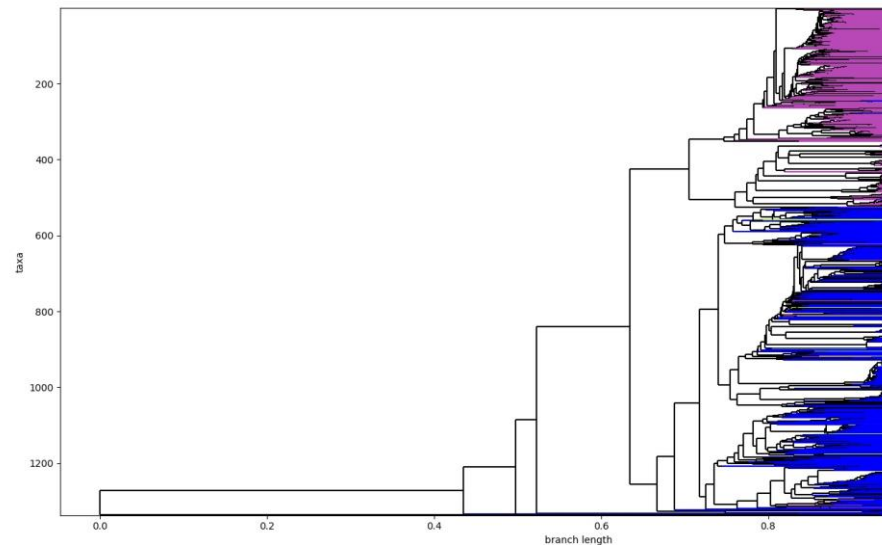


Fig. 2. The phylogenetic tree of 1336 HIV strains.

In the second step, an agent computer model of the HIV epidemic was developed and implemented taking into account socio-epidemic, geographical and genetic factors.

35 strains characteristic of the territory of Russia were selected from a total of 1336 strains. Using the statistical method of computer prediction of the affinity of the TBP/TATA complex, we obtained the virulence values of these strains and integrated them into the agent model. Using the model, forecasts were made for a 10-year period of development of the HIV epidemic in Russia for 5 scenarios of initial parameters.

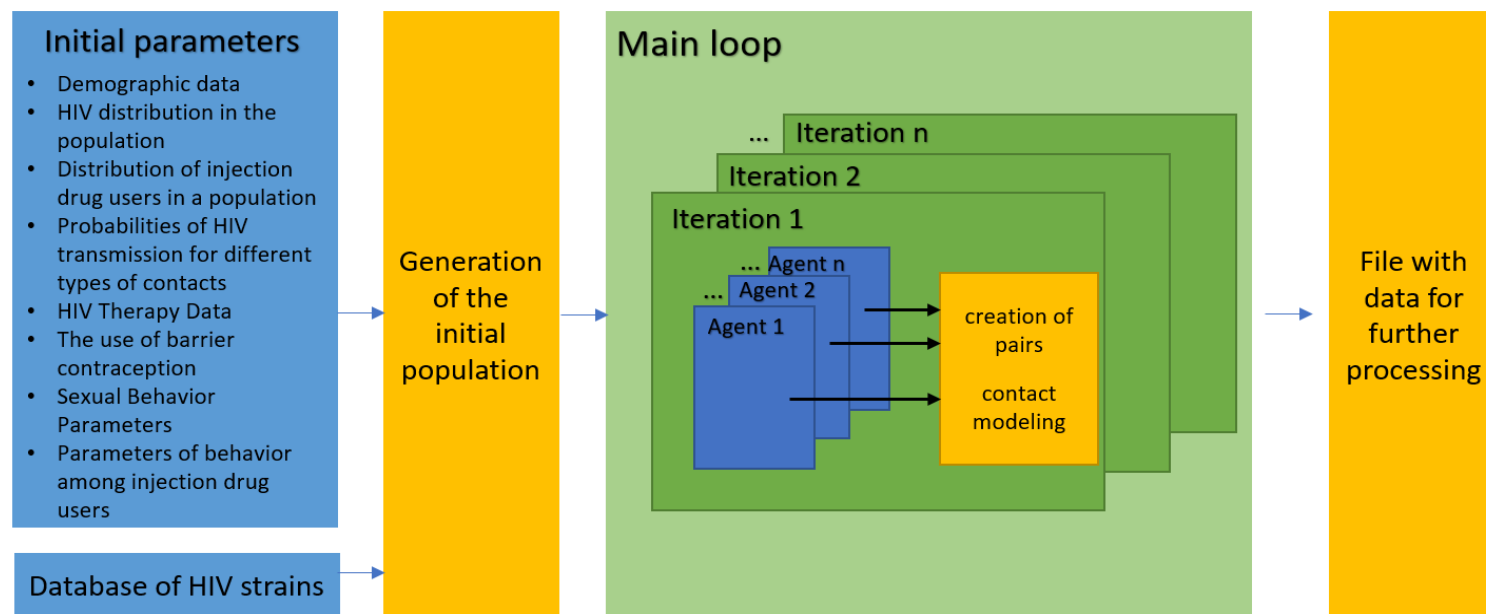


Fig. 3. HIV agent model diagram.

For scenario №1 that simulates the current situation, the model predicts an increase in the number of HIV-infected in the population by more than two times to 2.45%. The percentage of new HIV infections per year remains stable. The most effective strategy was №5, which suggests - 1) an increase in the proportion of men and women using barrier contraception to 0.8 (instead of 0.337 for men and 0.238) 2) a decrease in the share of joint injections to 0.01 (instead of 0.4) and 3) increasing the proportion of patients using treatment to 0.9 and increasing the proportion of patients with reduced viral load among those on treatment to 0.9 (instead of 0.45 and 0.62, respectively). This scenario showed a 3-fold decrease in the percentage of HIV patients in the population from 0.97% to 0.3% over 10 years and an almost complete halt in the growth of new HIV cases.

Figure 4 shows the dynamics over 10 years of the representation of 35 strains selected for Russia in the population. The most common strain MH330341 is presented 2 times more often than the least represented MK984160.

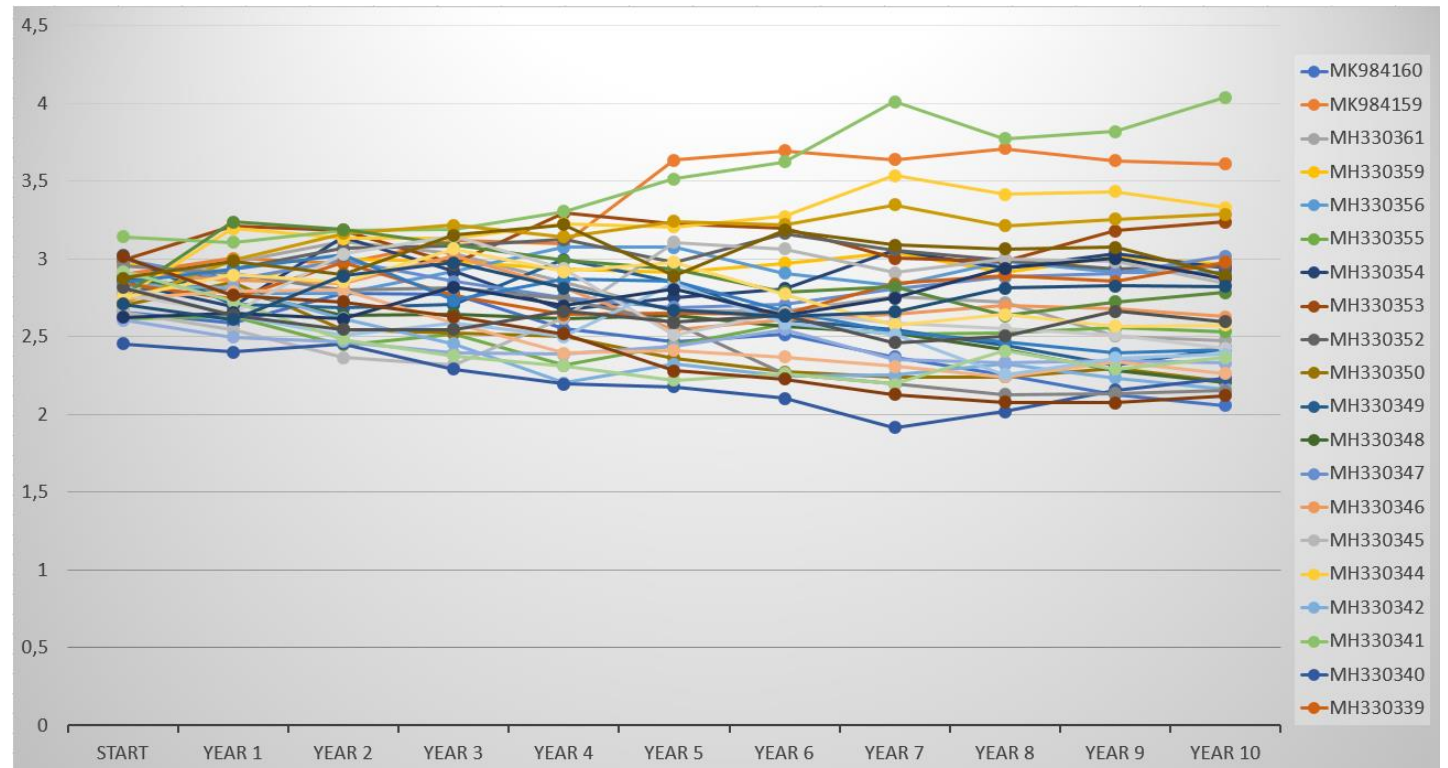


Fig. 4. The dynamics of the representation of strains in the general population over time.