CIS COLLABORATIVE DRUG DISCOVERY HUB: ADDRESSING THE CHALLENGES IN DRUG DISCOVERY

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Drug discovery and development nowadays are facing considerable challenges due to the progressive escalation of intellectual, material and financial cost of research and development (R&D). In order to solve the problem, new directions appear at the junction of new scientific areas using novel technological and organizational approaches. One way to an effective solution is the creation of cooperative global networks of professionals in drug R&D as "virtual clusters", in which scientists join their experience and abilities to provide a "brain-storming" effect in finding a solution for particular drug discovery problems.

A significant part of the CIS and Russian scientific resources in organic and medicinal chemistry, pharmacology and toxicology, bio- and chemoinformatics is still not involved in such International cooperative networks, and remains underexploited. To overcome this gap, we propose creating a CIS Collaborative Drug Discovery Hub (CDD Hub), which will provide the general framework for: collection of information about the experience and potential in pharmaceutical R&D of CIS, Russian and worldwide research teams; collecting and sharing of information about the diseases, pharmacological targets and small organic molecules as potential pharmaceutical agents, identification of medical needs, which can be considered as objectives for CDD Hub activities; recognition of "hot spots" where unmet medical needs can be matched with the available CDD Hub resources; etc.

As initial "seeds" for creating CDD Hub we may offer the web-service for prediction of biological activity spectra for organic drug-like compounds (http://pharmaexpert.ru/passonline), which is provided for scientific community during the past ten years. Currently, the number of registered users includes ~7,000 researchers from ~60 countries; over 200,000 molecules have been submitted for prediction of bioactivity; over 40 papers, where the prediction results are confirmed by the subsequent synthesis and biological testing of compounds, have been published.

Recently, in the framework of European FP6 collaborative project *No*. 037590 (Net2Drug) on the basis of PASS prediction for ChemNavigator library (contained at that time ~24 mln unique structures) we have identified two promising antitumor agents. These compounds have been shown to be active against breast cancer and melanoma cell lines. One of these compounds is shown to exhibit the synergistic action with known p53 reactivator RITA (Galina Selivanova, Karolinska Institute, Sweden, unpublished data), which was the aim of the project.

Some prototype of CDD Hub is available at: https://cis-cdd.ibmc.msk.ru/.