

P.26

Development and application of virtual screening protocol, as a tool to support the process of finding new drugs

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The presentation shows research on the development of new chemoinformatic tools and methods used in the search of new drugs. At first, the virtual screening protocol for fast searching of chemical libraries in order to identify new potential serotonergic 5-HT₇ receptor ligands was built. Out of the Enamine screening database, consisting of approximately 730,000 commercially available drug-like compounds, 26 virtual hits were finally selected and biologically evaluated. Two benzodioxane derivatives with significant affinity for 5-HT₇ receptors were found. Next, the improved protocol was used to search for new serotonin transporter (SERT) inhibitors. In the screening of five commercial database (containing approximately 3.24 M molecules) the 202 compounds were selected, out of which 23 showed high affinity for SERT. In the next stage, the virtual screening protocol was used for the analysis of virtual combinatorial library, developed on the reaction scheme for the synthesis of analogs of long-chain arylpiperazines - one of the largest classes of 5-HT₇R ligands. Finally, the new algorithm of pharmacophore model generation using the information about the structure of the ligand-receptor complexes was presented. A fast algorithm to search for linear combination of pharmacophore models showing much better efficacy in the identification of active compounds in chemical libraries than the single hypothesis, was also developed.

Presented research might be especially helpful for those who is aimed on developing a new material with desired properties (agricultural, material engineering, etc.).

P.27

Miniaturowe narzędzia do diagnostyki rzadkich schorzeń genetycznych

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Prowadzone przeze mnie badania dotyczą opracowania zarówno narzędzia jak i metody do wczesnej diagnostyki rzadkich schorzeń genetycznych na przykładzie chorób spichrzeniowych. Diagnostyka rzadkich chorób jest obecnie ogromnym wyzwaniem dla lekarzy, diagnostów i naukowców. Pacjent powinien być zdiagnozowany w pierwszych tygodniach życia, by rozpocząć odpowiednią terapię zanim wystąpią poważne, nieodwracalne uszkodzenia organów.