

Projekt: Discovery of CCR7 small molecule inhibitors by virtual screening and hit-to-lead optimization

Trajanje projekta: 2017 - 2020

Koordinator: Leuven Catholic University (KU), Virology and Chemotherapy, (prof. dr. Dominique Schols)

Vodja projekta na UL FFA: prof. dr. Stanislav Gobec

Povzetek projekta:

S proteinom G sklopljeni receptorji so dobro validirane tarče, saj nanje deluje ena tretjina vseh zdravil na tržišču. CCR7 je primer takšnega receptorja, ki pa je slabo raziskan kljub udeležnosti v številnih človeških boleznih (npr. rak, vnetne in imunske bolezni). V projektu bomo s pomočjo vrednotenja kemijske knjižnice, virtualnega rešetanja in optimizacije že znanih neselektivnih ligandov skušali odkriti selektivni ligand za receptor CCR7. Modulacijo delovanja receptorja bomo potrdili z različnimi *in vitro* biološkimi testi.

Project summary:

Protein G coupled receptors are well-validated targets targeted by one third of all medicinal products on the market. CCR7 is an example of such a receptor, although it is poorly studied despite being involved in many human diseases (e.g. cancer, inflammatory and immunodeficiency diseases). In the project, the discovery of selective ligand for the CCR7 receptor will be attempted through the use of the chemical library, virtual screening and optimization of the already known non-selective ligands. Modulation of the receptor action will be confirmed by various *in vitro* biological tests.

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