

## **Bulgarian Innovative Company Micar Innovation (Micar 21) with a breakthrough in a fight with COVID-19**

### ***Detection of the first class of CCR5 / 7 dual antagonists for COVID-19***

Despite that CCR5/7 are a key targets for HIV, Coronavirus, various Cancer metastasis and many other diseases only few antagonists have been developed up to date for CCR5 and non for CCR7. However, one of CCR5 antibody antagonists is under clinical trial in US now (phase 1b/2).

**Micar21** aimed to identify the first in class dual CCR5/CCR7 small molecule antagonists. The company used intensive MD simulations (many 1  $\mu$ s runs) to obtain the CCR7 structure and also those of the ligand-CCR5 and 7 complexes.

A combination of structural based pharmacophore, docking, IFD and MD approaches have been employed in a virtual screen of database of 4 million compounds. The most promising compounds were sent to ThermoFisher companies for bioassays to study both their binding capability and biological response; i.e. whether they are agonists or antagonists. The compounds have been also studied for their cascade biological response paths: Ca<sup>+</sup> mobilization and cAMP assays. Based on these results a lead compound was chosen.

The biological response of the lead compound to the ERK path and GTPyS binding is currently under evaluation in a lab located in Belgium.

The company has received very encouraging results from ThermoFisher and Eurofins companies in the Creation of Medicinal Molecules \* phase, which provides a field for the development of derived drug molecule and the further lead optimization.

*The Drug discovery of small Molecules \* includes:*

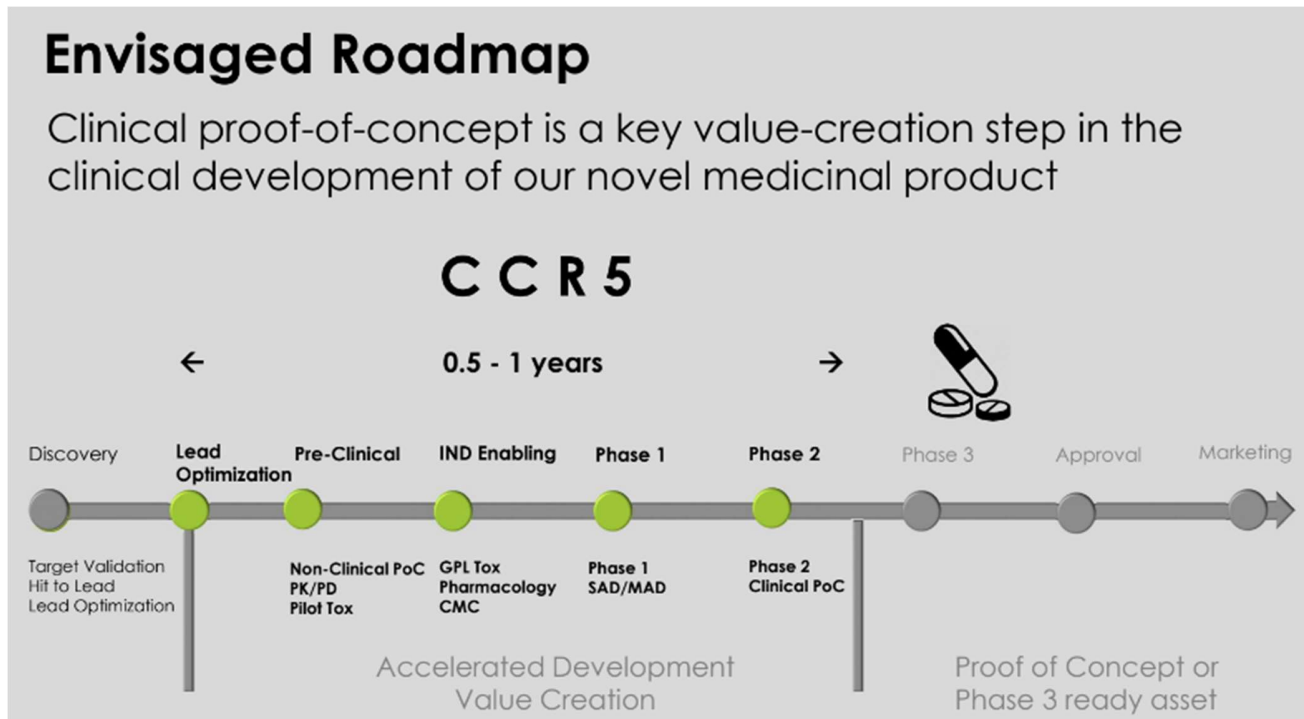
- *Creating a 3D structure*
- *Perform virtual screening, identification of hits and discovery of initial lead compound*
- *Lead optimization of the lead compound by FEP + approach*
- *Advanced ADMET forecasts*

### **Needed action for Micar 21 COVID-19 drug development:**

Partnership and funding for the entire drug molecule discovery process and specifically for the implementation of the pre-clinical phase financing: **between EUR 2.5 and 3 million**

(Recurring costs at this stage include all tests that evaluate product safety and dose determination for use in initial human studies. These tests include animal model studies aimed at demonstrating concept proof, dose determination studies, toxicological studies, genotoxicity and carcinogenicity studies. The results of each of these tests are verified by independent laboratory analysis. One-off costs include the synthesis of drug molecules and the production of test doses.)

Scheme:



### About the company

Micar Innovation (<http://micar21.com/>) is a drug discovery company. The company has found a niche where it is able to create a large societal impact by improving the quality of life through new blockbuster drug molecules for a large class of diseases. Micar Innovation focuses on non-clinical Proof-of-Concepts (POCs) in preclinical R&D and Hit-to-Lead (H2L) achievements in areas such as neuroscience, oncology, cardio-vascularity, dermatology, rare diseases. Micar21 is our drug discovery platform for small molecule drug candidates.

All improvements to the *in silico* process made by the team are validated with over 30 scientific publications in high-impact scientific magazines. Some other achievements are:

- Micar21, is one of the world's 130 companies in Deep Knowledge Analytics report: AI for Drug Discovery Landscape 2018 Q1,2,3,4 & 2019 Q1 Source: <https://www.dka.global/>
- Micar21, is one of the world's 198 companies in Roots Analysis Study report: "In Silico/Computer-Aided Drug Discovery Services Market 2020-2030" Source: [https://www.rootsanalysis.com/reports/view\\_document/in-silico-drug-discovery/298.html](https://www.rootsanalysis.com/reports/view_document/in-silico-drug-discovery/298.html)
- Micar21, is one of the world's 250 companies in Roots Analysis Study report: "Computer-Aided Drug Discovery Services Market 2018-2030" Source: [https://www.rootsanalysis.com/reports/view\\_document/computer-aided-drug-discovery-services-market-2018-2030/207.html](https://www.rootsanalysis.com/reports/view_document/computer-aided-drug-discovery-services-market-2018-2030/207.html)

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