Contribution ID: 1709

Type: Oral

Novel structure-based transglutaminase 2 inhibitors

Wednesday 30 October 2024 15:50 (15 minutes)

Among all of the human transglutaminases (TGases), transglutaminase 2 (TG2) is the most present one, existing in all of the tissues and organs of the human body. The protein has several conformations and functions, including protein crosslinking, apoptosis, immune response and calcium signaling. Moreover, TG2 also has the least variability in its coding sequence among the family of proteins, being the most conservative TGase. All of these facts combined highlight the necessity of the protein in the normal development of human organism and show the importance of studying it.

We obtained the first completely resolved TG2 structure using AlphaFold2 and validated it with developed molecular docking and molecular dynamics protocols. We also assembled a library of compounds similar to the existing TG2 inhibitors and verified the efficiency of novel compounds using in silico techniques.

We acknowledge the support from the Ministry of Science and Higher Education of the RF, project FSMF-2023-0010; "Integrated structural biology and genetics for the production of protein preparations and biologically active substances as new food and non-food products."

Primary author: IVASHCHENKO, Sergey (Moscow Institute of Physics and Technology)

Co-authors: Dr VLASOV, Alexey (Moscow Institute of Physics and Technology); ALEXANDROVA, Anastasia (Moscow Institute of Physics and Technology); Dr SHULGA, Dmitry (Department of Chemistry, Moscow State University); ZINOVEV, Egor (Moscow Institute of Physics and Technology); AKULININ, Mikhail (Moscow Institute of Physics and Technology); IVASHCHENKO, Vladimir (Moscow Institute of Physics and Technology)

Presenter: IVASHCHENKO, Sergey (Moscow Institute of Physics and Technology)

Session Classification: Life Science

Track Classification: Life Science