

Novel structure-based transglutaminase 2 inhibitors

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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.

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