

ML-based structure prediction of human transglutaminases

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Transglutaminases (TGases) are a unique group of enzymes that facilitate the post-translational modification of proteins by forming isopeptide bonds. Understanding that diverse processes such as normal and cancerous cell growth, reproduction, and cell death rely on sufficient levels of transglutaminases and that these enzymes can influence the differentiation and proliferation of various cell types has led many researchers to explore these intriguing molecules. Additionally, transglutaminases play a role in several diseases, including celiac disease and neurological disorders. In mammals, nine distinct isoenzymes of TGases have been identified at the genomic level. However, only a limited number of proteins possess reliable structures for future studies, while most have only partial structures.

We have obtained fully resolved models for proteins from the transglutaminase family for the first time using AlphaFold predictions. We constructed theoretical small angle X-ray scattering (SAXS) curves for each model using CRY SOL and demonstrated the ability to distinguish transglutaminase family proteins using SAXS.

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