

**Abstract for MIT Webinar: Wednesday Nov 24<sup>th</sup> 2021**

**Computational Enzymology: Towards using knowledge of structure and function to predict enzyme transformations and mechanisms.**

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Enzymes catalyse most of the chemical reactions which are essential for life. They are powerful catalysts that have evolved over millions of years to perform the functions in an organism that are necessary for survival. Using structural data and computational biology we seek to understand and predict how enzymes work and how they evolve to perform new enzyme functions. In this talk I will present our ongoing work to 'perform catalysis' in the computer. Using methods developed in cheminformatics, combined with information derived from 3D enzyme structures, we are developing tools to predict transformations and mechanisms.

<https://www.ebi.ac.uk/research/thornton/>