Using Enzymes to Selectively Form C-C Bonds

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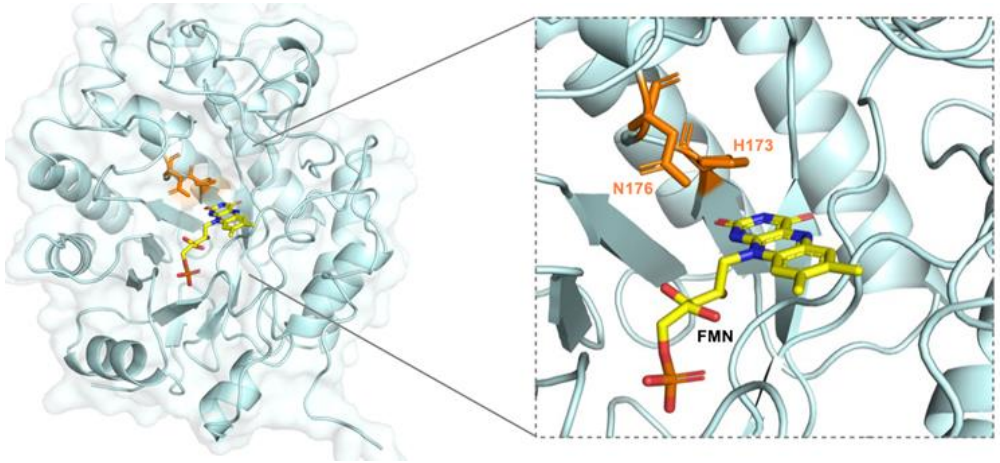
AMX



Overall crystal structure and active site of wild-type CsER (PDB code: 7TNB). Residues H173 and N176 responsible for substrate binding and the flavin mononucleotide (FMN) cofactor are labeled.

Scientific Achievement

Scientists use an enzyme to form unique C-C bonds with unprecedented selectivity that is not possible with traditional metal-catalyzed small-molecule chemistry.

Significance and Impact

The ability to precisely control the construction of new molecules enables the synthesis of new drugs for the pharmaceutical industry.

Research Details

- The ‘ene’-reductase from Caulobacter segnis (CsER) with a flavin cofactor was used to template a light-induced reaction to form the C-C bond.
- X-ray crystallography was performed on the flavin-bound enzyme at the NSLS-II AMX beamline.
- The crystal structure and docking model helped clarify the substrate binding site and reaction mechanism.

H. Fu, J. Cao, T. Qiao, Y. Qi, S.J. Charnock, S. Garfinkle, T.K. Hyster. An asymmetric sp3–sp3 cross-electrophile coupling using ‘ene’-reductases. Nature (2022). https://doi.org/10.1038/s41586-022-05167-1

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