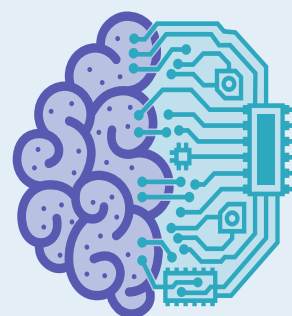


TIME FOR THE ENZYME TO HOP ONLINE!

By Camdyn Peace

Digitizing and Predicting Enzyme Mechanisms

Preconceived knowledge of enzyme mechanisms has been discovered by scientists studying enzyme-substrate complex structure, then conveying their findings into mechanistic function². Using all known enzyme mechanisms stored in the Mechanism and Catalytic Site Atlas (M-CSA), there is a push in the industry to predict mechanisms for uncharacterized enzymes based on similarity in structure and which catalytic transformation they are performing¹. The first mechanism generating automated software system, EzMechanism, has been developed as a result to propose solutions for the enzymes with currently undefined mechanisms¹. It is crucial that these generated mechanisms are confirmed by scientists in the field before publishing, therefore the evolution of this work will result in computational chemists evaluating their validity using quantum mechanic calculations¹. These future developments will be advantageous in biotechnology progressions with DNA sequencing, protein engineering, and biocatalysis-- all of which utilize enzyme mechanisms!²



Nature of Science Connection

This area of research combines contributions from a variety of sources in order to expand enzyme mechanism knowledge beyond its modern capacity, while illustrating the Nature of Science. The newly developed technological software has collaborated with prior work from researchers who used tools such as X-ray crystallography, NMR, and cryo-EM to obtain enzyme structures for further discoveries². Furthermore, EzMechanism's generated proposals must be interpreted using human discretion and advanced technological tools like high performance computer clusters to source out any errors the software may overlook¹. Overall, all pieces of this principle are required to work in tandem to support a common enzymatic goal!

Why is This Important?

This Nature of Science principle is relevant as it displays to learners and educators how scientific conclusions should never depend on a single source, but should encompass layers of knowledge from both foundational and futuristic approaches. This outlook supports quality education because it conceptualizes the process of breaking down an overarching question into smaller pieces, using different methods of discovery that best suit each piece to approach a collective answer. In addition, this principle reveals how scientific ambiguities are not typically solved with standalone work, as they require knowledge from specialized instruments and pre-existing material for best results.

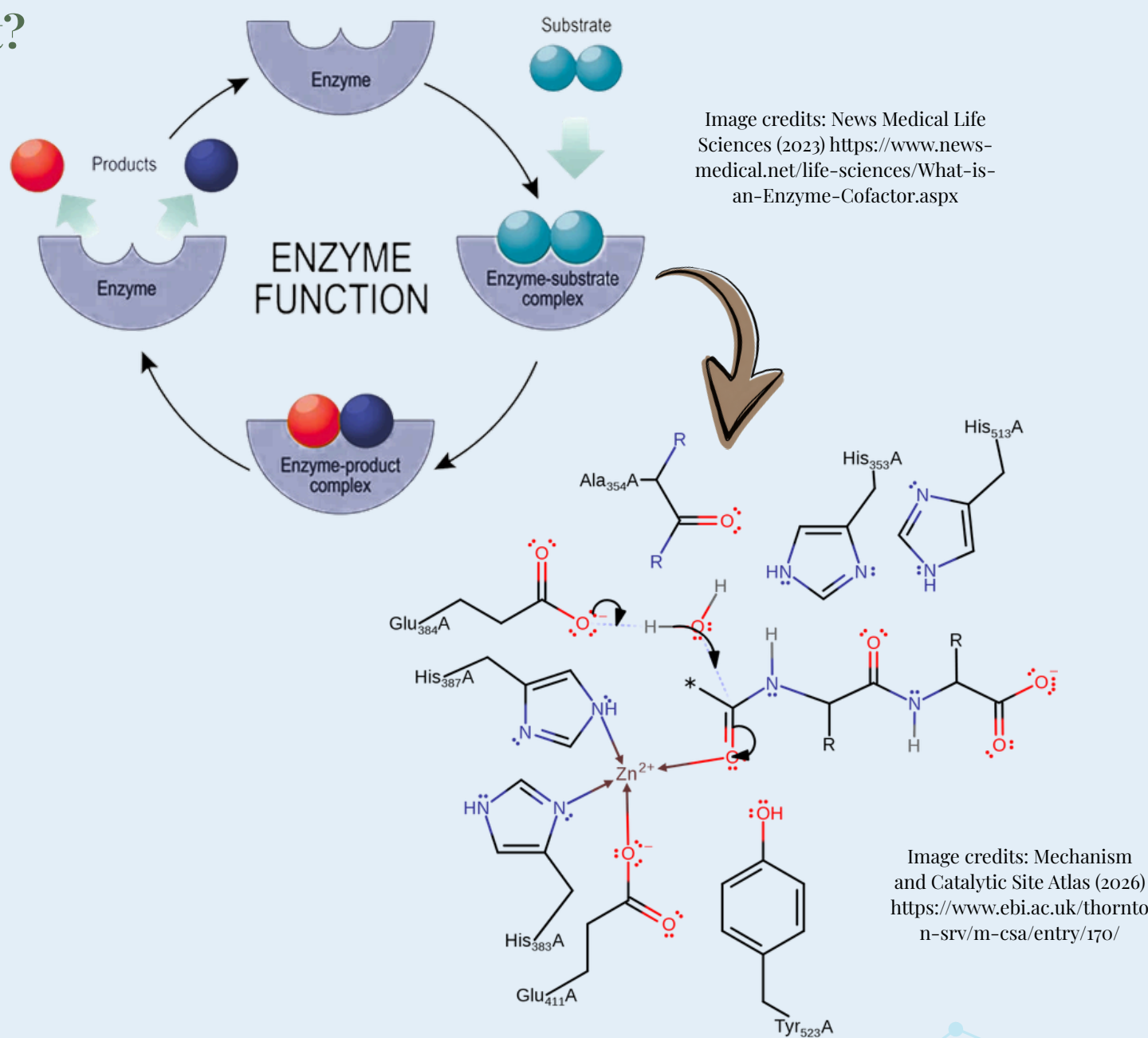


Figure 1. Step one of **peptidyl-dipeptidase A** mechanism, displaying electron flow after enzyme-substrate complex forms.

Resource Use in Classrooms

This case card could be used by an instructor as a discussion prompt in a classroom to spark conversation about ways human involvement with science will continue to evolve as technology advances, and ways it will likely never change. Perhaps the mention of artificial intelligence in science could also align seamlessly into this idea, as it begins to inevitably impact all industries.



References

1. Borkakoti, N., Ribeiro, A. J. M., & Thornton, J. M. (2025). A structural perspective on enzymes and their catalytic mechanisms. *Current Opinion in Structural Biology*, 92. <https://doi.org/10.1016/j.sbi.2025.103040>
2. Gao., T., Damborsky., J., Janin, Y. L., & Marek., M. (2023). Deciphering enzyme mechanisms with engineered ancestors and substrate analogues. *ChemCatChem*, 15(19), 1–15. <https://doi.org/10.1002/cctc.202300745>

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