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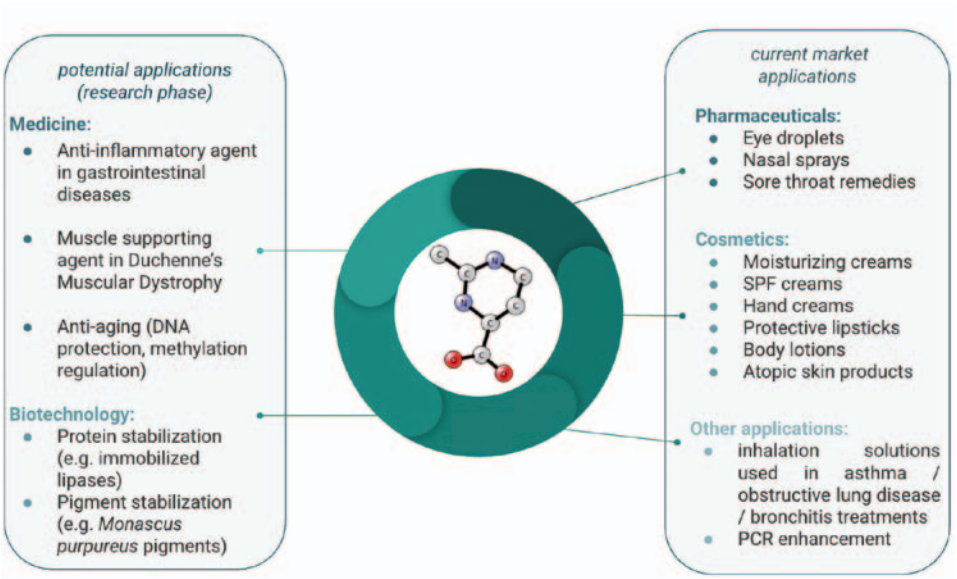
The interview with the author of the PhD thesis:
„Computational studies on ectoine synthase"

What inspired you to dedicate yourself to research on ectoine synthase?

What really inspired me to get into research were the amazing scientists I had the chance to work with. During my master's studies, Dr. Anna Wójcik-Augustyn was the one who first sparked my passion for computational chemistry. It was later fuelled by Professor Tomasz Borowski and the amazing Theoretical and Experimental Biocatalysis group at the Institute of Catalysis and Surface Chemistry (IKIFP PAN). They played a big role in supporting my growth as I dove deeper into enzyme research. Professor Borowski's mentorship played a key role throughout my research journey. It helped me push through the more challenging parts of my PhD and made the small and big wins even more rewarding. The project itself was incredibly motivating, as it presented a real challenge: first, I needed to figure out the unusual coordination of the iron ion in the enzyme's active site and determine its spin state; then, model the actual movements of the protein using molecular dynamics simulations; and finally, run quantum mechanical calculations to uncover the fine details of the chemical reaction taking place in the enzyme. There was also a practical side to all of this that I found exciting. The reaction's product, ectoine, is used in many skincare products, which I personally use as well. Knowing that my research could help deepen our understanding of natural production of ectoine and its role in bacterial systems was an extra source of inspiration for me.



Ectoine applications

Could you briefly introduce this topic to our readers?

Ectoine synthase is a protein primarily found in bacteria adapted to survive in extreme conditions, such as high salinity or temperature, where it catalyses the production of ectoine, a natural compound known for its protective role in cells. Although ectoine was discovered back in the 1980s, it has been gaining increasing interest, primarily due to its moisturizing and anti-inflammatory properties. As

a result, it is now used as an ingredient in pharmaceuticals and skincare products, while the new potential applications are still being explored. The bacterial biosynthesis of ectoine is well understood, but the final step of the pathway, being the conversion of the N-γ-ADABA substrate into ectoine, which takes place in the active site of ectoine synthase, remains unclear. In my research, I used molecular simulations and quantum mechanical calculations to uncover the three-step reaction mechanism, along with the associated energy barriers. It includes ring closure with deprotonation of the substrate's amino group, proton transfer from a tyrosine residue (one of the iron-coordinating amino acids) to the product's oxygen, and finally, the elimination of a hydroxyl group leading to the formation of ectoine. A better understanding of the reaction catalysed by ectoine synthase could support the development of more efficient biocatalysts for industrial scale ectoine production.

How did the Cyfronet resources help in your research?

The resources provided by Cyfronet were essential for my research on ectoine synthase. Series of simulations and quantum mechanical calculations consumed hundreds of computing hours from grants, for which I expressed my gratitude in publications and conference presentations. Among the most critical tools in my research were three computational chemistry tools: the AMBER suite, Gaussian, and ORCA.

What are the biggest myths or misconceptions about your field?

I've heard many times, especially from scientists working in laboratory, that computational biochemistry seems too difficult or inaccessible. In reality, once you grasp the basics and carry out your first calculations on real protein models, you begin to see the logic and find your way in the world of modeling. Patience and persistence are key, as quantum mechanical calculations can take weeks and often require corrections or revisiting earlier assumptions, sometimes it results in bringing the researcher back to square one. Still, I believe that every mistake is a valuable lesson and experience that enriches the research toolbox.

What advice would you give to someone planning to start a scientific career?

Before starting a scientific career, especially a PhD, it's essential to carefully choose the research environment. Getting to know your supervisor and the project is crucial, as it can determine whether your experience is fulfilling or frustrating. Inspiring mentors are one of the most important factors in a research career. Perseverance is also key: a PhD is a constant balance between successes and failures, so it's important to seek support from peers who share similar experiences and build mental resilience together. Recognizing that failure is part of the process helps you better appreciate progress and achievements. Networking is another vital aspect, offering practical insights not always found in textbooks. And while it's important to set realistic goals and work toward them, maintaining a healthy work-life balance is just as crucial. My advice to aspiring scientists is simple: don't forget there's life beyond the lab. Sometimes, taking a break and spend some time in the nature can be more rewarding than expected, and even spark new ideas.

What are your future goals in the context of scientific research?

Currently, I'm expanding my knowledge in data analysis, both in medical and biochemical contexts, as a postdoctoral researcher in data science. Given the rapid technological advancements, I believe it's crucial to add programming, machine learning, and other AI tools to my skill set. I think these skills are increasingly valuable in biochemistry and biotechnology, as IT industry and biomedical sciences are becoming more integrated.