Miquel Estévez-Gay,PhD

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Professional Summary

I'm a dedicated researcher with extensive experience in bioinformatics, catalysis, and enzyme design. I hold a PhD in Bioinformatics from Universitat de Girona. My research has been published in prestigious journals and has significantly advanced our understanding of enzyme mechanisms and their applications in catalysis. I am skilled in computational and experimental techniques, working as a postdoc managing a lab.

Experience

- Postdoctoral Researcher | 13/07/2023 - Actuality
OsunaLab, IQCC - Universitat de Girona | Girona

- Lab management and research.
- Set up a Biochemistry and protein engineering lab.
- Design of new PLP-dependent enzymes for the synthesis of non-canonical amino acids
- Protocol design and streamlining for enzyme design and screening
- Co-supervision of PhD students and visitors.

- Predoctoral Researcher | 20/06/2017 - 13/07/2023
CompBioLab, IQCC - Universitat de Girona | Girona

- Computational design of new halohydrin dehalogenases (HHDH). Creating computational protocols based on molecular mechanics to design new halohydrin dehalogenases to synthesize useful building blocks. The results culminated in my PhD thesis and multiple published papers.
- Computational study of HHDHs for increasing activity and selectivity.
- Computational study of HHDHs for increasing substrate scope and functionality.
- Creating new computational tools and protocols for analyzing the molecular dynamics simulation of complex and flexible systems.
- Experimental production and study of HHDH properties.

Skills

Biochemistry | Lab Management | Molecular Dynamics simulations | Python | Statistics | Quantum Mechanics | Bioinformatics | Enzyme Design

Education

- PhD in Bioinformatics, Universitat de Girona
  Girona, 2023
- Master in Molecular Biology and Biomedicine, Universitat de Girona
  Girona, 2017
- Specialized Training - Python for Scientists, Universitat de Barcelona,
  Barcelona, 2017
- Degree in Biology, Universitat de Girona
  Girona, 2016

Publications

1. **Miquel Estévez-Gay.** PhD Thesis: Computational exploration and design of HHDH variants with novel synthetically useful functionalities. Universitat de Girona (*Cum Laude*). http://hdl.handle.net/10256/23828

2. **Miquel Estévez-Gay**; Javier Iglesias-Fernández; Sílvia Osuna. Conformational Landscapes of Halohydrin Dehalogenases and Their Accessible Active Site Tunnels. Catalysts. 10-12, pp. 1403. 2020.

3. Guillem Casadevall; Cristina Durán; **Miquel Estévez-Gay**; Sílvia Osuna. Estimating conformational heterogeneity of tryptophan synthase with a template-based Alphafold2 approach. Protein Science. 31-10, 2022.

4. Sophie Staar; **Miquel Estévez-Gay**; Felix Kaspar; Sílvia Osuna;Anett Schallmey. Engineering of Conserved Sequence Motif 1 Residues in Halohydrin Dehalogenase HheC Simultaneously Enhances Activity, Stability, and Enantioselectivity. ACS Catalysis. 2025 *15* (7), 5257-5272.

5. Marcel Staar; Lina Ahlborn; **Miquel Estévez-Gay**; Katharina Pallasch; Sílvia Osuna; Anett Schallmey. A Dynamic Loop in Halohydrin Dehalogenase HheG Regulates Activity and Enantioselectivity in Epoxide Ring Opening. ACS Catalysis 2024 *14* (21), 15976-15987.

6. Lei Wang; Marzia Marciello; **Miquel Estévez-Gay**; Paul E.D.S. Rodriguez; Yurena Luengo Morato; Javier Iglesias-Fernández; Xin Huang; Sílvia Osuna; Marco Filice; Samuel Sanchez.Enzyme Conformation Influences the Performance of Lipase-Powered Nanomotors. Angewandte Chemie. 59-47, pp. 21080-21087, 2020.

7. Julia Wessel; Giovanna Petrillo; **Miquel Estevez-Gay**; Sandra Bosch; Margarita Seeger; Willem P. Dijkman; Javier Iglesias-Fernández; Aurelio Hidalgo; Isabel Uson; Sílvia Osuna; Anett Schallmey. Insights into the molecular determinants of thermal stability in halohydrin dehalogenase HheD2. Febs Journal, 2021.

8. Martin Floor; Kengjie Li; **Miquel Estévez-Gay**; Luis Agulló; Pau Marc Muñoz-Torres; Jenn-Kang Hwang; Sílvia Osuna; Jordi Villà-Freixa. SBMOpenMM: A Builder of Structure-Based Models for OpenMM. Journal of Chemical Information and Modeling. 61-7, pp. 3166-3171. American Chemical Society, 2021.