

## Phylogenetical, structural and conformational characterization of ureases

Ligabue-Braun, R.<sup>1</sup>, Andreis, F. C.<sup>2</sup>, Carlini, C.R.<sup>1,2</sup>, Verli, H.<sup>1,3</sup>

<sup>1</sup>PPGBCM-CBiot, UFRGS; <sup>2</sup>IB-UFRGS; <sup>3</sup>FF-UFRGS, Porto Alegre, Brazil

Ureases are nickel-dependent enzymes catalyzing the hydrolysis of urea. Also, activities as insecticidal, fungitoxic and induction of exocytosis were described as unrelated to catalysis, pointing to potential biotechnological implications. The current work aims to enlighten these functions by combining sequence, structure and dynamics. Phylogenetic analyses were conducted in the search for an evolutionary basis for the difference between single-chain (Eukaryotes) and multi-chain ureases (Prokaryotes). MD simulations were employed searching for insights into protein dynamics and oligomerization, and docking calculations for obtaining the complex formed by urease and its accessory proteins, required for enzyme activation. While plant and fungi ureases present a phylogenetical separation, their relations to bacterial ureases are still elusive. Such separation does not seem to correlate to differences at the conformational level. The monomeric, trimeric and hexameric forms of ureases became more globular in aqueous solution when compared to crystalline medium. Finally, the trimeric form of *Klebsiella aerogenes* (UreABC)<sub>3</sub> was complexed to its accessory proteins following previous mechanistic and SAXS data. The data obtained so far contribute in the structural biology of ureases, relating sequence to structure and, ultimately, to dynamics, offering atomic-level insights that may contribute in the elucidation of its moonlighting properties.

Keywords: urease, conformation, dynamics.

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