

## PhD Seminar

# **Selenium organic compounds: *in silico* chemical insight on their antioxidant and antiviral action**

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## **Abstract**

For more than fifty years, organoselenium compounds have been attracting interest for their potential antioxidant glutathione peroxidase (GPx) mimetic activity.<sup>1</sup> This family of enzymes mitigate oxidative stress in the cell by reducing hydroperoxides thanks to selenium, which is present in the catalytic pocket in the form of selenocysteine.<sup>2</sup> But so far, no successful application of Se-based GPx mimics has been reported.<sup>1</sup> Conversely, one of the best known organoselenium compound, i.e. ebselen (1,2-phenyl-1,2-benzisoselenazol-3(2H)-one) has proved to be a promising drug in various contexts including as antiviral.<sup>3</sup> The theoretical analysis of the elementary reactions in which organoselenium compounds are involved may provide a (chemical) unified picture of the biological as well as pharmacological role of this element. Mechanistic results on the redox (bio)chemistry of selenocompounds will be presented and discussed.

1. L. Orian, S. Toppo *Organochalcogen peroxidase mimetics as potential drugs: a long story of a promise still unfulfilled* *Free Rad. Biol. Med.* **66**, 65-74 (2014).

2. L. Flohé, S. Toppo, L. Orian *The glutathione peroxidase family: discoveries and mechanism* *Free Rad. Biol. Med.* **187**, 113-122 (2022)

3. P. A. Nogara, J. B. T. Rocha, C. S. Oliveira, L. Orian *The long history of Ebselen* in *Chalcogen Chemistry: fundamentals, advances and applications*, (2023) Ed. RSC, in press (Feb 2023).