

SELENIUM ORGANIC COMPOUNDS: CHEMICAL INSIGHT ON THEIR ANTIOXIDANT AND ANTIVIRAL ACTION THROUGH COMPUTATIONAL MODELLING

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SEPTEMBER 29th, 11:00 am, room 1A (1st floor), building D

For more than fifty years, organoselenium compounds have been prepared and studied for their potential antioxidant glutathione peroxidase (GPx) mimetic activity.^{1,2} This family of enzymes is involved in keeping at bay oxidative stress in the cell by reducing hydroperoxides. This occurs thanks to the presence of selenium, which is found in the catalytic pocket in the form of selenocysteine.³ Unfortunately, so far, no successful application of Se-based GPx mimics has been reported.¹ In contrast, the most popular 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.⁴ 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 selenoproteins and selenocompounds will be illustrated and rationalized.

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. P. A. Nogara, M. Pereira, C. S. Oliveira, L. Orian, J. B. T. Rocha *Organic selenocompounds: are they the panacea to human illnesses?* *New J. Chem.* **47**, 9959-9988 (2023)

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

4. 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.

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