

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

CURRICULUM VITAE

Laura Orian



1 Short CV

Laura Orian (ORCID: 0000-0002-1673-5111) got her degree in Chemistry at Università degli Studi di Padova in 1997 (Mark: 110/110 *summa cum laude* and Supervisor: Prof. P.L. Nordio), and, in the same group (Theoretical Chemistry), got the PhD in Chemistry in 2000. Since 2016, she is employed as Associate Professor of Physical Chemistry at the Department of Chemical Sciences in Padova. Her research interest aims at elucidating central physical phenomena in chemistry rooted in the properties of atoms, molecules, and materials. A deep rationalization and interpretation of experimental evidence is pursued through improvement of the fundamental description of chemical systems (chemical theory), and the applications of new and existing techniques to chemical, physical and biological problems (chemical computation) The ultimate goal of her research is to predict the chemical properties of a chemical system in advance of the experiment, for a rational design of functional molecules and materials assisted by computer. She has been regular visiting scientist (almost yearly) at VU Amsterdam since 2006 and at UFSM in Brasil in 2019. She has been appointed in international research evaluation panels in Portugal and Sweden. She is currently member of the editorial board of three journals and serves as referee of theoretical-computational papers for several editorial groups, including RSC, ACS and Wiley. L.O. is also active in scientific divulgation in the schools for pupils and in STEM activities for the Secondary school students and shares numerous chemistry projects with their teachers. Since 2015, she is referent for Piano Lauree Scientifiche Chimica in her university.

2 Bibliometric data

L.O. has co-authored more than 110 papers published in international peer-reviewed journals (h.index 25 and more than 2400 citations), 15 non-ISI publications and 8 book chapters; she has edited/co-edited three books.

3 Selection of the 10 most relevant recent publications

1. Madabeni, S. Zucchelli, P.A. Nogara, J. B. T. Rocha and L. Orian *In the chalcogenoxide elimination panorama: systematic insight into a key reaction* *J. Org. Chem.* **87**, 11766–11775 (2022).
2. **BCSJ Awarded article** R. Masuda, S. Kuwano, S. Sase, M. Bortoli, A. Madabeni, L. Orian and K. Goto *Model study on the catalytic cycle of glutathione peroxidase utilizing selenocysteine containing tripeptides: elucidation of the protective bypass mechanism involving selenocysteine selenenic acid* *Bull. Chem. Soc. Jap.* **95**, 1360–1379 (2022) (with **COVER**)
3. G. Ribaudó, M. Bortoli, C. E. Witt, B. Parke, S. Mena, E. Oselladore, G. Zagotto, P. Hashemi, L. Orian *ROS-scavenging fluoxetine derivatives inhibit in vivo serotonin reuptake* *ACS Omega*, **7**, 8314-8322 (2022).
4. L. Orian, L. Flohé *Selenium catalyzed reduction of hydroperoxides in chemistry and biology* *Antioxidants*, **10**, 1560 (2021).
5. A. Madabeni, M. Bortoli, P. A. Nogara, J. B. T. Rocha, L. Orian *Effect of methylmercury binding on the peroxide reduction potential of cysteine and selenocysteine* *Inorg. Chem.* **60**, 4646-4656 (2021). (with **COVER**)
6. M. Dalla Tiezza, F. M. Bickelhaupt, L. Flohé, M. Maiorino, F. Ursini, L. Orian, *A dual attack on the peroxide bond. The common principle of peroxidatic cysteine or selenocysteine residues.* *Redox Biol.* **34**, 101540 (2020).
7. M. Bortoli, M. Dalla Tiezza, C. Muraro, C. Pavan. G. Ribaudó, A. Rodighiero, C. Tubaro, G. Zagotto, L. Orian *Psychiatric Disorders and Oxidative Injury: Antioxidant Effects of Zolpidem Therapy disclosed in silico* *Comp. Struct. Biotech. J.*, **17**, 311-318 (2019).
8. G. Ribaudó, M. Bellanda, I. Menegazzo, L. P. Wolters, M. Bortoli, G. Ferrer-Sueta, G. Zagotto, L. Orian *Mechanistic insight into the oxidation of organic phenylselenides by H₂O₂* *Chem. Eur. J.*, **23**, 2405-2422 (2017).
9. **VIP PAPER** M. Bortoli, M. Torsello, F. M. Bickelhaupt, L. Orian *Role of the chalcogen (S, Se, Te) in the oxidation mechanism of the glutathione peroxidase active site* *ChemPhysChem*, **18**, 2990-2998 (2017). (with **COVER**)
10. M. Bortoli, L. P. Wolters, L. Orian, F. M. Bickelhaupt *Addition-Elimination or Nucleophilic Substitution? Understanding the Energy Profiles for the Reaction of Chalcogenolates with Dichalcogenides* *J. Chem. Theory. Comput.* **12**, 2752-2761 (2016).