

## PAOLA PELUSO

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## CURRICULUM VITAE

### MAIN RESEARCH INTERESTS

#### Chiral Chromatography and Molecular Recognition

- HPLC enantioseparations, method development, multimodal elution conditions
- Recognition mechanisms on polysaccharide-based chiral stationary phases
- Recognition mechanisms with cyclodextrin-based selectors
- Enantioseparation of atropisomeric compounds
- Design and preparation of new chiral stationary phases
- Applications of polysaccharide-based polymers for molecular recognition
- $\sigma$ - and  $\pi$ -hole bonds

#### Organic Chemistry

- Chirality
- Stereochemistry
- Molecular recognition

### LANGUAGES

- Italian
- English (CAE, Cambridge Assessment 186IT0305026, level C1)
- French

### EDUCATION

- 2003 - PhD Degree in Chemical Sciences, Università Ca' Foscari di Venezia in the group of Prof. O. De Lucchi. Subject: *Desymmetrization reactions of polycyclic alkenes*.
- 1993 - Laurea (MS Degree) in Chemistry, Università degli Studi di Pisa in the group of Prof. Rita Menicagli. Subject: *Synthesis and applications of new chiral stationary phases based on 1,3,5-triazine derivatives*.

### EDITORIAL ACTIVITY

- Member of the Editorial Board of Electrophoresis (Wiley) and Journal of Pharmaceutical and Biomedical Analysis Open.
- Guest Editor for *Molecules* (MDPI) – Special Issue “Chiral Stationary Phases for Enantioseparations: Fundamentals, Preparation, Methods, Applications and Chiral Recognition Mechanisms”.

### COLLABORATIONS

- Prof. Bezhan Chankvetadze, Tbilisi State University, Tbilisi, Georgia.
- Dr. Victor Mamane, Institut de Chimie de Strasbourg, France, UMR CNRS 7177, Equipe LASYROC.
- Prof. Gerhard K.E. Scriba, Friedrich Schiller University, Jena, Germany.
- Dr. Carlo Gatti, SCITEC-CNR, Milan, Italy.
- Prof. Sergio Cossu, Università Ca' Foscari di Venezia, Italy.

### PUBLICATIONS 2018-2023

1. Peluso, P.; Mamane, V.; Dallochio, R.; Dessì, A.; Villano, R.; Sanna, D.; Aubert, E.; Pale, P.; Cossu, S. Polysaccharide-based chiral stationary phases as halogen bond acceptors: A novel strategy for detection of stereoselective  $\sigma$ -hole bonds in solution, *J. Sep. Sci.* **2018**, *41*, 1247-1256 (Special Issue on *Chiral Separations* dedicated to Prof. Benedetto Natalini on the occasion of his 70<sup>th</sup> birthday).
2. Dallochio, R.; Dessì, A.; Solinas, M.; Arras, A.; Cossu, S.; Aubert, E.; Mamane, V.; Peluso, P. Halogen bond in high-performance liquid chromatography enantioseparations: description, features and modelling, *J. Chromatogr. A* **2018**, *1563*, 71–81 (invited article on Special Issue *Enantioseparation 2018*).
3. Peluso, P.; Gatti, C.; Dessì, A.; Dallochio, R.; Weiss, R.; Aubert, E.; Pale, P.; Cossu, S.; Mamane, V. Enantioseparation of fluorinated 3-arylthio-4,4'-bipyridines: insights into chalcogen and  $\pi$ -hole bonds in high-performance liquid chromatography, *J. Chromatogr. A* **2018**, *1567*, 119–129 (invited article on Special Issue *Enantioseparation 2018*).
4. Peluso, P.; Dessì, A.; Dallochio, R.; Mamane, V.; Cossu, S. Recent studies of docking and molecular dynamics simulation for liquid-phase enantioseparations, *Electrophoresis* **2019**, *40*, 1881-1896 (invited article on Special Issue *Enantioseparation 2019*).
5. Weiss, R.; Aubert, E.; Peluso, P.; Cossu, S.; Pale, P.; Mamane, V. Chiral chalcogen bond donors based on the 4,4'-bipyridine scaffold, *Molecules* **2019**, *24*, 4484.

6. Peluso, P.; Mamane, V.; Dessì, A.; Dallochio, R.; Aubert, E.; Gatti, C.; Mangelings, D.; Cossu, S. Halogen bond in separation science: overview, concepts and perspectives, *J. Chromatogr. A* **2020**, *1616*, 460788 (Special Issue *HPLC2019 Milan*).
7. Dessì, A.; Peluso, P.; Dallochio, R.; Weiss, R.; Andreotti, G.; Allocca, M.; Aubert, E.; Pale, P.; Mamane, V.; Cossu, S. Rational design, synthesis, characterization and evaluation of iodinated 4,4'-bipyridines as new transthyretin fibrillogenesis inhibitors, *Molecules* **2020**, *25*, 2213 (Special Issue *Exclusive Papers of the Editorial Board Members of the Organic Chemistry Section of Molecules*).
8. Peluso, P.; Mamane, V.; Dallochio, R.; Dessì, A.; Cossu, S. Noncovalent interactions in high-performance liquid chromatography enantioseparations on polysaccharide-based chiral selectors, *J. Chromatogr. A* **2020**, *1623*, 461202 (invited article on Special Issue *Enantioseparations 2020*).
9. Peluso, P.; Sechi, B.; Lai, G.; Dessì, A.; Dallochio, R.; Cossu, S.; Aubert, E.; Weiss, R.; Pale, P.; Mamane, V.; Chankvetadze, B. Comparative enantioseparation of chiral 4,4'-bipyridine derivatives on coated and immobilized amylose-based chiral stationary phases, *J. Chromatogr. A* **2020**, *1625*, 461303 (invited article on Special Issue *Enantioseparations 2020*).
10. Gatti, C.; Dessì, A.; Dallochio, R.; Mamane, V.; Cossu, S.; Weiss, R.; Pale, P.; Aubert, E.; Peluso, P. Factors impacting  $\sigma$ - and  $\pi$ -hole regions as revealed by the electrostatic potential and its source function reconstruction: the case of 4,4'-bipyridine derivatives, *Molecules* **2020**, *25*, 4409 (invited article on Special Issue *Electron Density Analysis Tools*).
11. Mamane, V.; Peluso, P.; Aubert, E.; Wenger, E.; Cossu, S.; Pale, P. Disubstituted ferrocenyl iodo- and chalcogeno-alkynes as chiral halogen and chalcogen bond donors, *Organometallics* **2020**, *39*, 3936-3950.
12. Peluso, P.; Chankvetadze, B. The molecular bases of chiral recognition in 2-(benzylsulfinyl) benzamide enantioseparation, *Anal. Chim. Acta* **2021**, *1141*, 194-205.
13. Peluso, P.; Dessì, A.; Dallochio, R.; Sechi, B.; Gatti, C.; Chankvetadze, B.; Mamane, V.; Weiss, R.; Pale, P.; Aubert, E.; Cossu, S. Enantioseparation of 5,5'-dibromo-2,2'-dichloro-3-selanyl-4,4'-bipyridines on polysaccharide-based chiral stationary phases: exploring chalcogen bonds in liquid-phase chromatography, *Molecules* **2021**, *26*, 221 (Special Issue *Chiral Stationary Phases for Enantioseparations: Fundamentals, Preparation, Methods, Applications and Chiral Recognition Mechanisms*).
14. Giunta, D.; Arras, A.; Peluso, P.; Solinas, M. Synthesis of "Click BOX" ligands and preliminary results on their application in the asymmetric copper catalysed Henry reaction of *o*-methoxybenzaldehyde, *Results in Chemistry* **2021**, *3*, 100122.
15. Dallochio, R.; Sechi, B.; Dessì, A.; Chankvetadze, B.; Cossu, S.; Mamane, V.; Weiss, R.; Pale, P.; Peluso, P. Enantioseparations of polyhalogenated 4,4'-bipyridines on polysaccharide-based chiral stationary phases and molecular dynamics simulations of selector-selectand interactions, *Electrophoresis* **2021**, *42*, 1853-1863 (invited article on Special Issue *Enantioseparations 2021*).
16. Gogolashvili, A.; Lomsadze, K.; Chankvetadze, L.; Takaishvili, N.; Peluso, P.; Dallochio, R.; Salgado, A.; Chankvetadze, B. Separation of tetrahydrozoline enantiomers in capillary electrophoresis with cyclodextrin-type chiral selectors and investigation of chiral recognition mechanisms, *J. Chromatogr. A* **2021**, *1643*, 462084 (invited article *Electromigration and Related Liquid-Phase Separation Techniques dedicated to Dr. Salvatore Fanali on the occasion of his 70th birthday*).
17. Peluso, P.; Chankvetadze, B. Native and substituted cyclodextrins as chiral selectors for capillary electrophoresis enantioseparations: structures, features, application, and molecular modeling, *Electrophoresis* **2021**, *42*, 1676-1708 (invited article on Special Issue *Enantioseparations 2021*).
18. Aubert, E.; Wenger, E.; Peluso, P.; Mamane, V. Convenient access to functionalized non-symmetrical atropisomeric 4,4'-bipyridines, *Compounds* **2021**, *1*, 58-74 (Special Issue *Feature Papers in Compounds*).
19. Krait, S.; Salgado, A.; Peluso, P.; Malanga, M.; Sohajda, T.; Benkovics, G.; Naumann, L.; Neusüß, C.; Chankvetadze, B.; Scriba, G. K. E. Complexation of daclatasvir by single isomer methylated  $\beta$ -cyclodextrins studied by capillary electrophoresis, NMR spectroscopy and mass spectrometry, *Carbohydrate Polymers* **2021**, *273*, 118486.
20. Cossu, S.; Peluso, P. Bridged polycyclic benzocyclotrimers: concepts, synthesis, and applications, *Curr. Org. Chem.* **2021**, *25*, 2912-2937.
21. Aubert, E.; Doudouh, A.; Wenger, E.; Sechi, B.; Peluso, P.; Pale, P.; Mamane, V. Chiral Ferrocenyl-Iodotriazoles and -Iodotriazoliums as Halogen Bond Donors. Synthesis, Solid State Analysis and Catalytic Properties, *Eur. J. Inorg. Chem.* **2022**, *2022*(5), e202100927 (Special Collection *Ferrocene Chemistry*).
22. Dallochio, R.; Dessì, A.; Sechi, B.; Chankvetadze, B.; Cossu, S.; Mamane, V.; Aubert, E.; Rozzo, C.; Palmieri, G.; Y. Spissu, Peluso, P. Exploring interaction modes between polysaccharide-based selectors and biologically active 4,4'-bipyridines by experimental and computational analysis, *J. Chromatogr. Open* **2022**, *2*, 100030 (invited article on Special Issue *Advances in liquid phase separation techniques applied to pharmaceutical and biomedical analysis*).
23. Dessì, A.; Sechi, B.; Dallochio, R.; Chankvetadze, B.; Pérez-Baeza, M.; Cossu, S.; Mamane, V.; Pale, P.; Peluso, P. Comparative enantioseparation of planar chiral ferrocenes on polysaccharide-based chiral stationary phases, *Chirality* **2022**, *34*, 609-619 (Special Issue to Celebrate the 80th Birthday of Professor Yoshio Okamoto).
24. Sechi, B.; Dessì, A.; Gatti, C.; Dallochio, R.; Chankvetadze, B.; Cossu, S.; Mamane, V.; Pale, P.; Peluso, P. Unravelling functions of halogen substituents in the enantioseparation of halogenated planar chiral ferrocenes on polysaccharide-based

- chiral stationary phases: experimental and electrostatic potential analyses, *J. Chromatogr. A* **2022**, *1673*, 463097 (invited article on Special Issue Enantioseparations 2022).
25. Peluso, P.; Mamane, V. Stereoselective processes based on  $\sigma$ -hole interactions, *Molecules* **2022**, *27*, 4625 (invited article on Special Issue A Wonderful Journey in the Asymmetric Catalysis World: A Themed Issue in Honor of Prof. Henri B. Kagan)
  26. Peluso, P.; Chankvetadze, B. Recognition in the domain of molecular chirality: from noncovalent interactions to separation of enantiomers, *Chem. Rev.* **2022**, *122*, 13235-13400.
  27. Peluso, P.; Mamane, V. Ferrocene derivatives with planar chirality and their enantioseparation by liquid-phase techniques, *Electrophoresis* **2023**, *44*, 158-189 (invited article on Special Issue Young and Inspiring Scientists).
  28. Dallochio, R.; Dessì, A.; Sechi, B.; Chankvetadze, B.; Jibuti, G.; Cossu, S.; Mamane, V.; Peluso, P. Enantioseparation of planar chiral ferrocenes on cellulose-based chiral stationary phases: benzoate versus carbamate pendant groups, *Electrophoresis* **2023**, *44*, 203-216 (invited article on Special Issue Young and Inspiring Scientists).
  29. Peluso, P.; Landy, D.; Nakhle, L.; Dallochio, R.; Dessì, A.; Krait, S.; Salgado, A.; Chankvetadze, B.; Scriba, G. K. E. Isothermal titration calorimetry and molecular modeling study of the complex formation of daclatasvir by  $\gamma$ -cyclodextrin and trimethyl- $\beta$ -cyclodextrin, *Carbohydrate Polymers* **2023**, *313*, 120870.
  30. Sechi, B.; Mamane, V.; Dallochio, R.; Dessì, A.; Cossu, S.; Jibuti, G.; Peluso, P. Enantioseparation of new axially chiral carboxylic acids on polysaccharide-based chiral stationary phases under normal phase elution conditions, *J. Pharm. Biomed. Anal. Open* **2023**, *1*, 100011.

### Book Chapters

1. Peluso, P.; Chankvetadze, B. Fundamentals of enantioselective liquid chromatography, in *Liquid Chromatography: Fundamentals and Instrumentation*, Vol 1, Third Edition, Edited by Fanali, S.; Chankvetadze, B.; Haddad, P. R.; Poole, C. F.; Riekkola, M. -J., Elsevier 2023.
2. Peluso, P.; Chankvetadze, B. Application of enantioselective liquid chromatography, in *Liquid Chromatography: Applications*, Vol 2, Third Edition, Edited by Fanali, S.; Chankvetadze, B.; Haddad, P. R.; Poole, C. F.; Riekkola, M. -J., Elsevier 2023.

### INVITED LECTURES

1. 29<sup>th</sup> International Symposium on Electro- and Liquid Phase-Separation techniques (ITP 2023), Rome – San Felice Circeo, September 13-17, **2023**. *Searching for noncovalent interactions in liquid-phase enantioseparations*.
2. 33<sup>rd</sup> International Symposium of Pharmaceutical and Biomedical Analysis (PBA2023), Ankara (Turkey), July 2-6, **2023**. *Integrating experimental and computational approaches to study enantioselective recognition in liquid-phase enantioseparations*.
3. 11<sup>th</sup> Annual Symposium on Physical and Analytical Chemistry (ASPAC 2022), Tbilisi (Georgia), December 8-10, **2022**.  *$\sigma$ - and  $\pi$ -hole bonds in enantioseparation science*.
4. 1<sup>st</sup> International Conferences on Noncovalent Interactions (ICNI-2019), Lisbon (Portugal), September 2-6, **2019**.  *$\sigma$ - and  $\pi$ -hole bonds: emergent noncovalent interactions in liquid-chromatography enantiodiscrimination*.
5. Université de Strasbourg (Faculté de Chimie) Strasbourg (France), September 17, **2015**. *High-performance liquid chromatography (HPLC) on polysaccharide-based chiral stationary phases. Exploiting the size and shape of molecules to understand chiral recognition mechanisms*.