Jérôme Amaudrut, Ph.D.

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French nationality
Married, two children

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Computer-Aided Drug Design Expert and Consultant

Competences :

- Molecular modeling
- Cheminformatics
- Drug Design
- Scientific research
- Data mining and analysis
- Programming / Coding
- Oral communication
- Innovation, creativity, pragmatism
- Focus on project advancement
- Team player in multicultural environment
- Organic chemistry
- English language

Experience :

- **Computer-Aided Drug Design** for pharmaceutical research for **25 years**
  - In-Silico Scientific Solutions (Consultant and founder, 2020-present)
  - Inventiva (senior scientist, 2012-2019)
  - Abbott (senior scientist, 2010-2012)
  - Solvay Pharmaceuticals (senior scientist 2006-2010)
  - Laboratoires Fournier (scientist, 2003-2006)
  - Pfizer (post-doc, 2001-2003)
- Computational Chemistry, Institute of Organic Chemistry, University of Basel, Switzerland (post-doc with Prof. Bernd Giese, 2000-2001)

Education :

- Ph.D. in Physical Organic Chemistry at the University of Notre Dame, IN, USA under the supervision of Prof. Olaf Wiest, in 2000
- “Diplôme d'Ingénieur” from ESCIL (Lyon School of Industrial Chemistry) in 1996

Skills / Achievements :

- **Design of new molecular entities**
  Participated to the design of new drugs (14 patents, three preclinical candidates, one currently in clinical trials) in a team with organic chemists ; internally and within collaborations (Abbvie, Boehringer Ingelheim, IRBM).
- **Virtual Screening**
  Performed many successful virtual screens (on various targets including nuclear receptors, enzymes and PPI) for internal projects and also as a service to customers. Hits underwent optimization by medical chemists, one even reached the pre-clinical phase.
- **Molecular Library Design**
  Built the “Mimesis” library (10K small molecules mimicking viral peptides), which delivered trackable hits in 6 phenotypic assays for Enyo Pharma. This project received a 2.5M€ grant from the EU under Horizon 2020.
  Selected molecules (> 100K) for enrichment of corporate libraries using multi-objective optimizations.
- **Pharmaceutical Research**
  Participated to the drug discovery process from target identification to lead optimization. Implemented a “Database of Ideas” at Inventiva, a tool used by all medicinal chemists to store molecular ideas and predict properties using CADD developed models.
- **Predictive Models – Machine Learning**
  Built models to predict activity, solubility and ADME properties of molecules, proposing new and relevant descriptors.
- **Molecular Modeling Softwares**
  Schrödinger, OpenEye, Biovia. Expert Pipeline Pilot user, RDKit
- **Informatics**
  Linux administration, programming in python, shell, SQL

Publications

"Viruses Traverse the Human Proteome through Peptide Interfaces That Can Be Biomimetically Leveraged for Drug Discovery."
Meyniel-Schicklin, Laurène, Jérôme Amaudrut, Pierre Mallinjoud, et al.
Proceedings of the National Academy of Sciences 121, no. 5 ***2024****, e2308776121.*

"Discovery of a Novel Series of Potent SHP2 Allosteric Inhibitors."
Petrocchi, Alessia, Alessandro Grillo, Luca Ferrante, et al.
ACS Medicinal Chemistry Letters 14, no. 5 ***2023****, 645–51.*

"Discovery of a Novel Series of Imidazopyrazine Derivatives as Potent SHP2 Allosteric Inhibitors."
Torrente, Esther, Valentina Fodale, Alina Ciammaichella, et al.
ACS Medicinal Chemistry Letters 14, no. 2 ***2023****, 156–62.*

"SAR Evolution towards Potent C-Terminal Carboxamide Peptide Inhibitors of Zika Virus NS2B-NS3 Protease."
Colarusso, Stefania, Federica Ferrigno, Simona Ponzi, et al.
Bioorganic & Medicinal Chemistry 57, ***2022****, 116631.*

"Discovery of Novel Quinoline Sulphonamide Derivatives as Potent, Selective and Orally Active RORγ Inverse Agonists"
Amaudrut, J.; Argiriadi, M. A.; Barth, M.; Breinlinger, E. C.; Bressac, D.; Broqua, P.; Calderwood, D. J.; Chatar, M.; Cusack, K. P.; Gauld, S. B.; et al.
Bioorganic & Medicinal Chemistry Letters **2019**, 1799-1806.

"Existence of a Preferred Orientation for the Methoxy Group on an Extended Aromatic System."
Amaudrut, J.; Braccini, I.; Duhamel, E.; Montalbetti, C.
ChemistrySelect **2018**, 6750–6755.

"Design, Synthesis, and Evaluation of a Novel Series of Indole Sulfonamide Peroxisome Proliferator Activated Receptor (PPAR) α/γ/δ Triple Activators: Discovery of Lanifibranor, a New Antifibrotic Clinical Candidate."
Boubia, B.; Poupardin, O.; Barth, M.; Binet, J.; Peralba, P.; Mounier, L.; Jacquier, E.; Gauthier, E.; Lepais, V.; Chatar, M.; et al.
J. Med. Chem. **2018**, 2246–2265.

"Electron Delocalization in the Radical Cation of 1,3,6,8-Tetraazatricyclo[4.4.1.1]dodecane, a 4-Nitrogen-7-Electron System"
Zwier, J. M.; Brouwer, A. M.; Keszthelyi, T.; Balakrishnan, G.; Offersgaard, J. F.; Wilbrandt, R.; Barbosa, F.; Buser, U.; Amaudrut, J.; Gescheidt, G.
J. Am. Chem. Soc. **2002**, *124,* 159-167.

"Ion Pairing in Radical Cations: the Example of 9,9'-Bianthryl"
Khan, M. N.; Palivan, C.; Barbosa, F.; Amaudrut, J.; Gescheidt, G.
J. Chem. Soc, Perkin Trans. 1 **2001**, 1522-1526.

"Direct observation of hole transfer through DNA by hopping between adenine bases and by tunnelling"
Giese, B.; Amaudrut, J.; Kohler, A. K.; Spormann, M.; Wessely, S.
Nature **2001**, *412,* 318-320.

"Epoxide Formation by Ring Closure of the Cinnamyloxy Radical."
Amaudrut, J.; Wiest, O.
Org. Lett. **2000**, 2, 1251-1254.

"The Thermal Sulfenate-Sulfoxide Rearrangement: A Radical Pair Mechanism."
Amaudrut, J.; Wiest, O.
J. Am. Chem. Soc. **2000**, *122*, 3367-3374.

"Theoretical Studies of the Sulfenate-Sulfoxide Rearrangement"
Amaudrut, J.; Pasto, D. J.; Wiest, O
J. Org. Chem. **1998**, *63*, 6061-6064.

Presentations

"Screening Library Enrichment : Criteria that matter, timely manner."
Eurocup VII, May 2014, Mery-sur-Oise. (Poster)

"Compound and sample selection for an optimal screening library at Inventiva."
8th International Conference on Chemical Libraries, October 2012, Berlin (Invited talk)

"A Brief guide of fluorine-protein interaction for the medicinal chemist"
Advances and Progress in Drug Design, February 2012, London. (Invited talk)

"A Brief guide of fluorine-protein interaction for the medicinal chemist"
Rencontres Internationales de Chimie Thépateutiques, July 2011, Lyon. (Invited talk)

"Selection of plates for screening using Pareto"
Accelrys European User Group Meeting, October 2009, Barcelone.

"Fast Scaffold Hopping using ROCS and Pipeline Pilot"
Eurocup II, April 2008, Strasbourg. (Poster)

"Sulfenate-Sulfoxide Thermal Rearrangement: Diradical Mechanism."
219th ACS National Meeting, March 26-30, 2000, San Francisco, CA (ORGN 458)

"The Photo-Induced Decomposition of Arenesulfenates and Its Application to the Studies of Substituted Oxiranylmethyl Radicals."
214th ACS National Meeting, September 7-11, 1997, Las Vegas, NV (Poster, ORGN 94)

Patents

"Flavivirus Inhibitors."
Ontoria, Ontoria Jesus Maria, Christian Montalbetti, Antonio Quotadamo, et al.
Patent WO2025114399A1, filed November 27, 2024, and issued June 5, 2025.

"Flavivirus Inhibitors"
Ontoria, Ontoria Jesus Maria, Christian Montalbetti, Jerome Amaudrut, et al.
Patent EP4563146A1, filed November 28, 2023, and issued June 4, 2025.

"Flavivirus Inhibitors."
Alli, Cristina, Alberto Bresciani, Fabio Romano Di, et al.
Patent EP4532476A1, filed May 25, 2023, and issued April 9, 2025.

"Flavivirus Inhibitors"
Alli, Cristina, Alberto Bresciani, Fabio Romano Di, et al.
Patent EP4282862A1, filed May 25, 2022, and issued November 29, 2023.

"Quinazolinone Derivatives and Uses Thereof for Treating a Cancer."
Meyniel-Schicklin, Laurène, Peter Machin, Eric Meldrum, et al.
Patent EP4126847A1, , filed March 29, 2021, and issued February 8, 2023.

"Quinazolinone Derivatives and Uses Thereof for Treating a Cancer."
Meyniel-Schicklin, Laurène, Peter Machin, Eric Meldrum, et al.
Patent WO2021198191A1, filed March 29, 2021, and issued October 7, 2021.

"Nuclear Receptor Modulators (ror) for the Treatment of Inflammatory and Autoimmune Diseases."
Argiriadi, Maria a, Eric C. Breinlinger, Kevin P. Cusack, et al.
Patent EP3636643A, filed June 8, 2016, and issued April 15, 2020.

"Thiophene derivatives as antiviral agents"
Meldrum, Eric, Chassey Benoît De, Laëtitia Lines, et al.l.
Patent EP3562818A1, filed December 28, 2017, and issued November 6, 2019.

"Azetidine Carboxylic Compounds for Treating Diseases Involving the Nurr1 Nuclear Receptors."
Boubia, Benaîssa, Christine Massardier, Fabrice Guillier, Jerôme Amaudrut, Mireille Tallandier, and Christian Montalbetti.
Patent WO2017025695A1, filed August 12, 2016, and issued February 16, 2017.

"Nuclear Receptor Modulators (ror) for the Treatment of Inflammatory and Autoimmune Diseases."
Argiriadi, Maria a, Eric C. Breinlinger, Kevin P. Cusack, et al.
Patent EP3307734A1, filed June 8, 2016, and issued April 18, 2018.

"Ror Nuclear Receptor Modulators."
Argiriadi, Maria a, Eric Breinlinger, Kevin P. Cusack, et al.
Patent WO2016198908A1, filed June 9, 2015, and issued December 15, 2016.

"New Phenylazetidine, Carboxylate or Carboxamide Compounds."
Boubia, Benaïssa, Christine Massardier, Fabrice Guillier, et al.
Patent EP3107910A1, filed February 19, 2015, and issued December 28, 2016.

"New Benzoic Pyrrolopyridine Derivatives and Their Use for the Treatment of Parkinson's Disease."
Amaudrut, Jerome, Benaissa Boubia, Fabrice Guillier, and Olivia Poupardin-Olivier.
Patent EP2521727A1, filed January 7, 2011, and issued November 14, 2012.

"Use of indole derivatives as NURR-1 activators for their application as a medicament for the treatment of Parkinson's disease."
Amaudrut, Jerome, Benaissa Boubia, Dongen Maria Johanna Petronella Van, Fabrice Guillier, and Olivia Poupardin-Olivier.
Patent EP2475642A1, filed September 10, 2010, and issued July 18, 2012.