Alessio Ragno, Ph.D.

alessio.ragno.ai@gmail.com @spideralessio spideralessio
http://alessio.ragno.info/ Last Update: April 2026

Employment History

Apr 2026 – · · · · **Associate Professor.** EPITA Lyon.
Explainable AI and Graph Neural Networks

Jan 2026 – Mar 2026 **Postdoctoral Researcher.** EPITA Lyon.
Explainable AI and Graph Neural Networks
Supervisor: Prof. Marc Plantevit.
Research Project on Explainable AI and Graph Neural Networks.

Mar 2025 – Dec 2025 **Postdoctoral Researcher.** INSA Lyon.
Explainable AI and Graph Neural Networks
Supervisor: Prof. Céline Robardet.
Research Project on Explainable AI and Graph Neural Networks. The contract will be extended to a Postdoc after defending the PhD. Founded within the ANR 22-PEAE-0008 (WAIT4) Project.

Sep 2025 – Dec 2025 **Lecturer.** EPITA Lyon.
Deep Learning Course at the M.Sc. in Computer Engineering.
Supervisor: Prof. Marc Plantevit.
Deep Learning Contract Professor at the Engineering in Computer Science Master's Degree on: Fully-Connected Neural Networks, Convolutional Neural Networks, Transformers, Generative Models, Explainable AI.

Oct 2019 – · · · · **Artificial Intelligence Consultant.** Online.
Self-employed consultant.
Consultant, tutor, and teacher for several private clients and companies, working on Machine Learning and Artificial Intelligence projects, including Neural Networks, RAG Systems, Multi-Agent AI, and Generative AI.

Sept 2016 – · · · · **Machine Learning Engineer.** Rome Center for Molecular Design, Rome, Italy.
Long-lasting collaboration.
Participation with the research group developing web apps and developing Machine Learning models for Pharmaceutical Chemistry.

Nov 2024 – Mar 2025 **Research Engineer.** INSA Lyon.
Topic: *Explainable AI and Graph Neural Networks*
Supervisor: Prof. Céline Robardet.
Research Project on Explainable AI and Graph Neural Networks. The contract will be extended to a Postdoc after defending the PhD. Founded within the ANR 22-PEAE-0008 (WAIT4) Project.

Oct 2024 – Dec 2024 **Lecturer.** EPITA Lyon.
Deep Learning Course at the M.Sc. in Computer Engineering.
Supervisor: Prof. Marc Plantevit.
Deep Learning Contract Professor at the Engineering in Computer Science Master's Degree on: Fully-Connected Neural Networks, Convolutional Neural Networks, Transformers, Generative Models, Explainable AI.

Jul 2024 – Sep 2024 **Lecturer.** BoostCamp Fullstack Course, Online.
Python and AI Teacher at the BoostCamp FullStack Course.
Hired as Professor for a course on Introduction to Programming and AI with Python.

Employment History (continued)

Jan 2022 – Dec 2023 — **Teaching Assistant.** Sapienza University of Rome, Rome, Italy.
Programming Teaching Assistant at the Advanced Course on Bioinformatics.

Jan 2022 – Dec 2022 — **Teaching Assistant.** Sapienza University of Rome, Rome, Italy.
Programming Teaching Assistant at the course "Introduction to Programming with Python" at the Bachelor's Degree in Computer and Control Engineering.

Jan 2018 – May 2021 — **Secretary Assistant.** Sapienza University of Rome, Rome, Italy.
Secretary Assistant during study-work scholarships at the Department of Computer, Control and Management Engineering "Antonio Ruberti" of Sapienza University of Rome.

Education

Nov 2021 – Jan 2025 — **Ph.D. in Artificial Intelligence,** Sapienza University of Rome.
Thesis title: *Topology-based Explanations for Neural Networks.*
Supervisor: Prof Roberto Capobianco
Grade: with honors (Top 5%).
Doctor Europaeus Title: Abroad internship at EPITA Lyon and INSA Lyon.

Sept 2019 – May 2021 — **M.Sc. Artificial Intelligence and Robotics,** Sapienza University of Rome.
Thesis title: *Explainable AI in Drug Design: Perturbation based molecular attributions using Graph Convolutional Networks.*
Supervisor: Prof Roberto Capobianco
Grade: 110/110 with honors (Excellence Program).
Among the best graduated students of 2021 from Sapienza University of Rome.
Best Student according to Sapienza "Exam Bonus" Award.

Sept 2016 – Mar 2019 — **B.Sc. Computer and Control Engineering,** Sapienza University of Rome.
Thesis title: *Deep Deterministic Policy Gradient for Regularity Rally in TORCS Simulator.*
Supervisor: Prof Roberto Capobianco
Grade: 110/110 with honors.
Best Student of the third year according to Sapienza "Exam Bonus" Award.

Research Publications

Journal Articles

1. R. Astolfi, A. Oliva, A. Raffo, *et al.*, "Essential oils as antimicrobials against acinetobacter baumannii: Experimental and literature data to definite predictive quantitative composition–activity relationship models using machine learning algorithms," *Journal of Chemical Information and Modeling*, 2025.
2. A. Kamal, A. Ragno, M. Plantevit, and C. Robardet, "Leveraging internal representations of gnns by shapley values," *Data Mining and Knowledge Representation*, 2025.
3. M. Proietti, A. Ragno, and R. Capobianco, "Xai-guided continual learning: Rationale, methods, and future directions," *WIREs Data Mining and Knowledge Discovery. Accepted, will be published soon*, 2025.
4. M. Proietti, A. Ragno, B. L. Rosa, R. Ragno, and R. Capobianco, "Explainable ai in drug discovery: Self-interpretable graph neural network for molecular property prediction using concept whitening," *Machine Learning*, vol. 113, no. 4, pp. 2013–2044, 2024.
5. E. Proia, A. Ragno, L. Antonini, *et al.*, "Ligand-based and structure-based studies to develop predictive models for sars-cov-2 main protease inhibitors through the 3d-qsar. com portal," *Journal of Computer-Aided Molecular Design*, vol. 36, no. 7, pp. 483–505, 2022.

6. A. Ragno, B. La Rosa, and R. Capobianco, "Prototype-based interpretable graph neural networks," *IEEE Transactions on Artificial Intelligence*, vol. 5, no. 4, pp. 1486–1495, 2022.

7. A. Ragno, A. Baldisserotto, L. Antonini, *et al.*, "Machine learning data augmentation as a tool to enhance quantitative composition–activity relationships of complex mixtures. a new application to dissect the role of main chemical components in bioactive essential oils," *Molecules*, vol. 26, no. 20, p. 6279, 2021.

Conference Proceedings

1. F. Di Valerio, M. Proietti, A. Ragno, and R. Capobianco, "Cip-net: Continual interpretable prototype-based network," in *AAAI 2026*, Accepted, will be published soon, 2026.

2. A. Ragno and R. Capobianco, "Impo: Interpretable memory-based prototypical pooling," in *WSDM 2025*, ACM, 2025.

3. A. Ragno, M. Plantevit, and C. Robardet, "Faithful explanations for graph classification using logic," in *ECML-PKDD 2025*, Springer Lecture Notes in Computer Science Series, 2025.

4. A. Ragno, M. Plantevit, and C. Robardet, "On logic-based self-explainable graph neural networks," in *NeurIPS 2025*, Accepted, will be published soon, 2025.

5. A. Borghini, F. Di Valerio, A. Ragno, and R. Capobianco, "Identifying candidates for protein-protein interaction: A focus on nkp46's ligands," in *CEUR Workshop Proceedings*, CEUR-WS, 2024.

6. A. Ragno, M. Plantevit, C. Robardet, and R. Capobianco, "Transparent explainable logic layers," in *ECAI 2024*, IOS Press, 2024.

7. C. Borzillo, A. Ragno, and R. Capobianco, "Understanding deep rl agent decisions: A novel interpretable approach with trainable prototypes," in *CEUR Workshop Proceedings Vol-3518*, 2023.

8. M. Proietti, A. Ragno, and R. Capobianco, "Memory replay for continual learning with spiking neural networks," in *2023 IEEE 33rd International Workshop on Machine Learning for Signal Processing (MLSP)*, IEEE, 2023, pp. 1–6.

Books and Chapters

1. M. Proietti, R. Astolfi, and A. Ragno, "Applied artificial intelligence for drug discovery," in A. Lavecchia, Ed. Springer Nature, 2025, ch. Explainable Artificial Intelligence in Drug Discovery.

Skills

Languages	Italian: Mother Tongue. English: Advanced communicative and comprehensive skills. French: Intermediate communicative and comprehensive skills.
Coding	Python, MATLAB, Octave, Java, C, C++, Objective-C, Assembly IA32, PHP, JavaScript, VisualBasic, SQL, HTML, CSS, Django, RDKit, Open Babel, ROS, scikit-learn, Tensorflow, PyTorch, MXNet, OpenCV, PCL, Android Java, Docker.
Research Fields	Explainable AI, Graph Neural Networks, Reinforcement Learning, Computational Chemistry, Continual Learning
Misc.	Academic research, teaching, training, consulting.

Miscellaneous Experience

Awards and Achievements

2026 **Seal of Excellence - European Commission Horizon Europe** for the project proposal submitted under the Horizon Europe Marie Skłodowska-Curie Actions call.

Miscellaneous Experience (continued)

2025 **NeurIPS Travel Grant** for attending NeurIPS 2025.

2024 **EurAI Travel Grant** for the 27th European Conference on Artificial Intelligence.

2024 **Sapienza PhD Mobility Grant** for the research project "Obtaining topology-based explanations through relevant subgraphs".

2022 **EurAI Travel Grant** for the Joint EurAI Advanced Course on AI, TAILOR Summer School 2022.

2022 **EuroQSAR Travel Grant** for the 23rd European Symposium on Quantitative Structure-Activity Relationship.

2022 **Sapienza Starting Grant** for the research project on "Topology-based Explanations for Neural Networks".

2021 **Ernesto & Iole De Maggi Scholarship**, awarded for academic excellence in Engineering.

Posters and Presentations

2025 **Distilling Rules from GIN: Logic-based Explanations for Graph Neural Networks**. Workshop: L'explicabilité via le prisme de la décision algorithmique et des jeux. Sorbonne Université. Paris, France.

2022 **Self-explainable Graph Neural Network for Molecular Property Prediction using Concept Whitening**. 3rd MMCS: Shaping Medicinal Chemistry for the New Decade. Sapienza University of Rome. Rome, Italy.

2021 **Semi-Supervised GCN for Learning Molecular Structure-Activity Relationships**. ELLIS Machine Learning for Molecules Workshop (ML4Molecules). NeurIPS 2021. Online.

2021 **Molecule Generation from Input-Attributions over Graph Convolutional Networks**. ELLIS Machine Learning for Molecules Workshop (ML4Molecules). NeurIPS 2021. Online.

Invited Seminars

2025 **On Logic-based Explanations for Graph Neural Networks: From post-hoc approaches to self-explainable neural networks**. EPITA Lyon. Lyon, France.

2025 **Logic-based Explanations for Graph Neural Networks**. Sapienza University of Rome. Rome, Italy.

2025 **Transparent Explainable Logic Layers**. Sony AI. Online.

Review Activity

2026 ICML 2026, ECML-PKDD 2026, NeurIPS 2026.

2025 AAAI 2026, ICLR 2026, Nature Scientific Reports.

2024 Computational and Structural Biotechnology Journal, Information Processing & Management.

Conference Organization

2024 **Workshop in eXplainable AI approaches for deep reinforcement learning**. Organizing Committee. AAAI 2024. Vancouver Canada.

2021 **6th International Conference on Polyamines: Biochemical, Physiological and Clinical Perspectives**. Organizing Secretariat. Tivoli, Italy.

Certifications

2019 **ACTFL Oral Proficiency Interview by Computer (OPIc)**: Advanced Mid Level.

2012 **Cambridge English: Preliminary (PET)**: B1 Level.

Miscellaneous Experience (continued)

2010 **DELF**: A1 Level.

References

Prof Roberto Capobianco
PhD Supervisor
Senior Researcher & Contract Professor
Sony AI & Sapienza University of Rome
roberto.capobianco@sony.com

Prof Marc Plantevit
PostDoc Supervisor
Full Professor
EPITA Lyon
marc.plantevit@epita.fr

Prof Celine Robardet
PostDoc Supervisor
Full Professor
INSA Lyon
celine.robardet@insa-lyon.fr

Dr Biagio La Rosa
Collaborator
PostDoc Researcher
University of California Santa Cruz
bilarosa@ucsc.edu