Alessio Ragno, Ph.D.

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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. A. Ragno, P.-A. Peyrie, M. Plantevit, R. Pensa, and C. Robardet, "Differentiable parameter-less co-clustering using graph neural networks," *ECML-PKDD Journal Track @ Data Mining and Knowledge Discovery*, 2026.
2. 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*, vol. 65, no. 3, pp. 1378–1391, Jan. 2025, ISSN: 1549-960X. DOI: 10.1021/acs.jcim.4c02389.
3. A. Kamal, A. Ragno, M. Plantevit, and C. Robardet, "Leveraging internal representations of gnns with shapley values," *Data Mining and Knowledge Discovery*, vol. 39, no. 6, Oct. 2025, ISSN: 1573-756X. DOI: 10.1007/s10618-025-01159-7.
4. M. Proietti, A. Ragno, and R. Capobianco, "Xai-guided continual learning: Rationale, methods, and future directions," *WIREs Data Mining and Knowledge Discovery*, vol. 15, no. 4, Oct. 2025, ISSN: 1942-4795. DOI: 10.1002/widm.70046.

5. A. Ragno, B. L. Rosa, and R. Capobianco, "Prototype-based interpretable graph neural networks," *IEEE Transactions on Artificial Intelligence*, vol. 5, no. 4, pp. 1486–1495, Apr. 2024, ISSN: 2691-4581. DOI: 10.1109/tai.2022.3222618.

6. 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, Oct. 2023, ISSN: 1573-0565. DOI: 10.1007/s10994-023-06369-y.

7. 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, ISSN: 1573-4951. DOI: 10.1007/s10822-022-00460-7.

8. 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, Oct. 2021, ISSN: 1420-3049. DOI: 10.3390/molecules26206279.

Conference Proceedings

1. F. Di Valerio, M. Proietti, A. Ragno, and R. Capobianco, "Cip-net: Continual interpretable prototype-based network," 25, vol. 40, Association for the Advancement of Artificial Intelligence (AAAI), Mar. 2026, pp. 20 772–20 780. DOI: 10.1609/aaai.v40i25.39216.

2. A. Marzo, A. Ragno, and R. Capobianco, "This state looks like that: Self-interpretable reinforcement learning agents using prototype soft actor-critic," in *ICML 2026*, Accepted, will be published soon, 2026.

3. S. Plumbo, A. Ragno, R. Capobianco, M. Plantevit, and C. Robardet, "Plex: Edge-aware logic-based self-explainable graph neural networks with polyadic predicates," in *ECML-PKDD 2026*, Accepted, will be published soon, 2026.

4. M. E. Russo, A. Borghini, F. Di Valerio, A. Ragno, and R. Capobianco, "Ppi candidate ranking: Large-scale evaluation of a domain knowledge–guided pipeline," in *ICML 2026*, Accepted, will be published soon, 2026.

5. A. Ragno, M. Plantevit, and C. Robardet, "Faithful explanations for graph classification using logic," in *Machine Learning and Knowledge Discovery in Databases. Research Track*, Springer Nature Switzerland, 2025, pp. 113–129, ISBN: 9783032060785. DOI: 10.1007/978-3-032-06078-5_7.

6. A. Ragno, M. Plantevit, and C. Robardet, "On logic-based self-explainable graph neural networks," in *Advances in Neural Information Processing Systems*, D. Belgrave, C. Zhang, H. Lin, *et al.*, Eds., vol. 38, Curran Associates, Inc., 2025, pp. 116 138–116 166. URL: https://proceedings.neurips.cc/paper_files/paper/2025/file/a8c893712cb7858e49631fb03c941f8d-Paper-Conference.pdf.

7. 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.

8. 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.

Books and Chapters

1. M. Proietti, R. Astolfi, and A. Ragno, "Explainable artificial intelligence in drug discovery," in *Applied Artificial Intelligence for Drug Discovery*. Springer Nature Switzerland, 2026, pp. 525–555, ISBN: 9783031980220. DOI: 10.1007/978-3-031-98022-0_17.

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.

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.

Miscellaneous Experience (continued)

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.

2010 **DELF**: A1 Level.

References

Prof Roberto Capobianco
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