



Nationality : French

Born in 19/07/1995

Address : 8 rue Callisto,
25300 Doubs

Driving Licence : Category B

Phone : +33 6 48 27 39 56

COMPETENCY

Molecular Modeling software:

Linux, Python
Gaussian16 (DFT),
ChemCraft,
ChemDraw, COPASI
MestreNova, RDkit

Data Scientist / ML software :

PyTorch, Scikit-Learn,
Numpy, Pandas, Spark,
Matplotlib, Seaborn, Git,
GitHub, SQL, Power BI, SAP
ERP

LANGUAGES

English : Fluent
Spanish : Intermediate
French : Native

LORIS GELIN

WITH A PHD IN MOLECULAR MODELING AND
STRONG KNOWLEDGE OF THE FIELD OF DATA
SCIENCE AND MACHINE LEARNING ALGORITHMS.

WORK EXPERIENCES

Doctorat (2020-2023) - Synthesis and theoretical studies of innovative molecules based on 1,2,4,5-tetrazine and 1,3,4-oxadiazole. Burgundy Institute of molecular chemistry (ICMUB - UMR6302)
Pr P. FLEURAT-LESSARD et Dr J. ROGER.

- The Master 2 internship project progressed by adding new molecules based on 1,3,4-oxadiazole. 22h of training courses achieved.

Master 2 internship (2019-2020) - Theoretical and experimental study of the formation of metallacycles based on s-tetrazine. Burgundy Institute of molecular chemistry (ICMUB - UMR6302)
Pr P. FLEURAT-LESSARD et Dr J. ROGER

- Experimental and theoretical studies of functionalization by C-H activation of s-aryltetrazine derivatives in organometallic catalysis using transition metals (Ir, Rh, Ru).
- Total autonomy in my research work (DFT Calculs, organic and inorganicsynthesis, NMR characterisation, exact mass, elementaryanalysis, UV-vis)

Master 1 internship (2018-2019) - Study of organometallic compounds with highly electropositive elements and evaluation of their catalytic activity in several processes.

University of Castilla-La-Mancha (Spain), Dr. FERNANDER GALAN Rafael

- Synthesis, characterisation and reactivities of guanidine and phosphinoguanidine ligand. Synthesis under inert atmosphere in Schlenk.

Bachelor 3 intership (2017-2018) - Chemistry bachelor at Burgundy institute of molecular chemistry (ICMUB - UMR6302)
Dr VERVANDIER-FASSEUR Dominique.

- Synthesis and characterisation of resveratrole derivatives using the Wittig reaction.

Student employee (2013-2020) - Temporary assignments, construction industry, food delivery.

EDUCATION - CHEMISTRY

University of Burgundy

Master of molecular chemistry, T2MC :
Transition Metals in Molecular Chemistry
M2 (2018-2019) : 13,9/20 - (Grading : 2nd/15)
M1 (2017-2018) : 13,6/20 - (Grading : 1st/11)

3rd bachelor degree of Science, Technology and Health degree in Chemistry
L3 (2016-2018) : 11,7/20

1st and 2nd bachelor degree of Life, Earth and Environmental Sciences Parcours Chemistry-Biochemistry
L2 (2015-2016) : 10,4/20
L1 (2014-2015) : 10,3/20

Mail : Loris.gelin.2@gmail.com

Kaggle : GELIN Loris

Linkedin : www.linkedin.com/in/gelin-loris-0824172a5

GitHub : <https://github.com/LGBEUT/Data-Scientist-Portfolio>

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PUBLICATIONS

- Palladium catalyzed C5-arylation of 1,3,4-oxadiazole derivated. L. Gelin, H. Sabadin, H. Cattey, J.-C. Hierso, P. Fleurat-Lessard, J. Roger.
- Oxidative Rhodium(III)-Catalyzed N-Directed C-H Arylation of s-Aryltetrazine with Aryl boronic Acids. O. Abidi, G. Divoux, L. Gelin, H. Cattey, P. Fleurat-Lessard, J.-C. Hierso, and J. Roger. (under preparation)
- Selective Deshydrogenative Cross-coupling Rhodium- or Iridium-Catalyzed (Hetero)Arylation of s-Aryltetrazines. O. Abidi, L. Gelin, G. Divoux, H. Cattey, J.-C. Hierso, P. Fleurat-Lessard and J. Roger. (under preparation)
- Experimental and theoretical study of Palladacycle of s-tetrazine and oxadiazole. L. Gelin, O. Aroule, I. Tolbatov, C. Testa, F. Akhssas, P. Ghesquierre, M. Ponce Vargas, H. Cattey, J.-C. Hierso, J. Roger, P. Fleurat-Lessard, under preparation (under preparation)

COMMUNICATION

- C.O. Meeting of theoretical chemists from the Grand-Est region (RCTGE) - Dijon, 2-3 Juin, 2022
- C.A. GreenCat 2020 -Rennes, March 30-April 2 , 2020

TEACHING AND SUPERVISION

- Supervision of two students on work experience. (15 days), Licence 3rd bachelor degree of chemistry, University of Burgundy.
- 20 hours, student's professional project, 2022, 1st bachelor degree level, University of Burgundy

FORMATION - DATA SCIENTIST / MACHINE LEARNING ENGINEER

- **Python/SQL for Data Analysis :** Analyzing and manipulating extensive databases containing several million records across diverse datasets, including chemical datasets featuring SMILES notation.
- **Machine & Deep Learning :** Implementing machine & deep learning algorithms, such as Graph Neural Networks (GNNs), in various fields, including chemistry
- **Data Visualization :** Proficient in using visualization libraries to graphically represent data (Matplotlib, Seaborn, RDkit).

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GitHub : <https://github.com/LGBEUT/Data-Scientist-Portfolio>