

Nationality : French
Born in 19/07/1995
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GitHub (PortFolio) : <https://github.com/LGBEUT/Data-Scientist-Portfolio>

Loris GELIN

With a PhD in molecular modeling, I have transitioned to the field of data science and machine learning algorithms.

Work Experiences

2020 – 2023

Lenght : 3 years

Doctorat 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.

2019 – 2020

Lenght : 5 months

Master 2 internship 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 inorganic synthesis, NMR characterisation, exact mass, elementary analysis, UV-vis)

2018 – 2019

Lenght : 3 months

Master 1 internship 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.

2017 – 2018

Lenght : 2 months

Bachelor 3 intership Chemistry bachelor at Burgundy institute of molecular chemistry (ICMUB - UMR6302)

Dr VERVANDIER-FASSEUR Dominique.

Synthesis and characterisation of resveratrole derivatives using the Wittig reaction.

2013 – 2018

Student employee Temporary assignments, construction industry, food delivery.

Formation

2018 – 2020

University of Burgundy

Master of molecular chemistry, T2MC : Transition Metals in Molecular Chemistry

M2 : 13,9/20 – (Grading : 2nd/15).

M1 : 13,6/20 – (Grading : 1st/11).

2016 – 2018

University of Burgundy

3rd bachelor degree of Science, Technology and Health degree in Chemistry

L3 : 11,7/20

2014 – 2016

University of Burgundy

1st and 2nd bachelor degree of Life, Earth and Environmental Sciences Parcours

Chemistry-Biochemistry

L2 : 10,4/20

L1 : 10,3/20

Competency

- Software: Python, PyTorch, Scikit-Learn, Numpy, Pandas, Spark
RDkit, SQL, Git, GitHub, Power BI
- Molecular modelling: Gaussian16 (DFT), ChemCraft, ChemDraw, MestreNova, COPASI
- Organic/Organometallic Chemistry/Catalysis Synthesis

Languages

- English : Fluent
- Spanish : intermediate
- French : Native

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Publications

1. Experimental and theoretical study of s-tetrazine mono-ortho-metallation catalyzed by iridium and rhodium. O. Adibi, L. Gelin, G. Divoux, H. Cattey, J.-C. Hierso, P. Fleurat-Lessard, J. Roger, under preparation.
2. Theoretical and experimental comparison of s-tetrazine mono and di-ortho-metallation catalyzed by iridium and rhodium. L. Gelin, O. Adibi, H. Cattey, J.-C. Hierso, J. Roger, P. Fleurat-Lessard, under preparation.
3. Palladium catalyzed C5-arylation of 1,3,4-oxadiazole derivated. L. Gelin, H. Sabadin, H. Cattey, J.-C. Hierso, P. Fleurat-Lessard, J. Roger.
4. 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.

Communication

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

Teaching and Supervision

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