Andrea Darù

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Working experience

20 Oct 2020 - present **Postdoctoral Associate** - The Scripps Research Institute (CA, USA)
Field Computational chemistry applied to metal catalysis and origin of life
PI Prof. Donna Blackmond

Jan - Feb 2018 **Visiting PhD Student** - Syngenta (Stein, CH)
Project Reactivity study with Fukui functions as molecular descriptors

Education

21 Feb 2020 **PhD Marie Skłodowska-Curie Fellow** - KU Leuven (Belgium)
Thesis title Non-noble metal catalysis for cross-coupling reactions: computational insights
Project NoNoMeCat: Non-Noble Metal Catalysis Horizon2020
Supervisors Prof. Jeremy N. Harvey, Prof. Xile Hu [EPFL]

17 Dec 2015 **Postgraduate Degree** - University of Zaragoza (Spain)
Subjects Organic Synthesis, Computational Chemistry
Supervisors Prof. Pedro Merino, Prof. Tomas Tejero

12 Dec 2013 **MSc Degree in Chemical Science** - University of Ferrara (Italy)
Thesis title Synthesis of self-concentrating biocides as polymeric additives
Supervisors Prof. Marco Fogagnolo, Dr. Giancarlo Fantin

16 Dec 2011 **BSc Degree in Chemistry** - University of Ferrara (Italy)
Thesis title Strategies for conjugation of oligonucleotides
Supervisor Prof. Alessandro Massi

Academic experience

1-3 Nov 2021 **Virtual Simons Collaboration on the Origin of Life Annual Symposium**
Poster: Computational insights into the origin of stereoselectivity of the Strecker reaction

14 Jun 2019 **NoNoMeCat Symposium** - Syngenta (Stein - CH)
Poster: Computational Study of Nickel-catalysed Negishi Arylation of Propargylic bromides

04 Jun 2019 **VSC User Day** - Brussels (BE)
Poster: Computational Study of Nickel-catalysed Negishi Arylation of Propargylic Bromides

19 May 2019 **Open Day KU Leuven - Discovering chemistry & life sciences**
Task: Organizer for the Quantum Chemistry division

8–11 Jul 2018 **ECIRM: European Colloquium on Inorganic Reaction Mechanisms** - Barcelona (ES)
Talk: Computational Study of Olefin Reductive Coupling Reaction Catalyzed by Iron Bromide

13–15 Jun 2018 **Computational Catalysis for Sustainable Chemistry** - Tarragona (ES)
Poster: Computational Study of Nickel-catalysed Negishi Arylation of Propargylic Bromides

22 May 2018 **VSC User Day** - Brussels (BE)
Poster & Talk: Computational Expenses of Inorganic Computational Chemistry Calculations

17–20 Jul 2018 **EJD-TCCM Conference** - Leuven (BE)
Task: Web designing and management of participants

28 May 2018 **Symposium: Chemical Bonding in the 21st Century** - Brussels (BE)

30 Jan 2018 **QCB13: Quantum Chemistry in Belgium** - Brussels (BE)
Poster: Computational Study of Olefin Reductive Coupling Reaction Catalyzed by Iron Bromide

02 Jun 2017 **VSC User Day** - Brussels (BE)
Poster: Computational Study of Olefin Reductive Coupling Reaction Catalyzed by Iron Bromide

20 May 2017 **Open Day of KU Leuven - 200 years advanced curiosity**
Task: Organizer for the Quantum Chemistry division

19–22 March 2017 **CMS Conference** - University of Warwick (UK)
Poster: Computational Study of Olefin Reductive Coupling Reaction Catalyzed by Iron Bromide

Computer skills

Coding	Linux-Bash, Python
OS	Linux, Windows, Android
DRMS - HPC	Torque, Slurm
Chemistry	Gaussian, Molpro, ORCA, Turbomole, NAMD/VMD, Multiwfn, CREST, xtb
Tools	Office Suite, LaTeX, Adobe Photoshop, Gimp, Inkscape, AutoCad

Languages skills

Mother tongue	Italian
Foreign languages	English, Spanish

Teaching activity

2^{nd} semester 2019 **Stuctural Bioinformatics Exercise** - KU Leuven (BE)
Task: Assistant of Prof. Harvey for practical exercise part

a.y. 2017/2018 **Master Thesis Supervision** - KU Leuven (BE)
Title: Computational study of the mechanism of the triazolization reaction

9–13/01/2017 **Workshop: Introduction to Computational Chemistry** - KU Leuven (BE)
Task: Teaching and exercise for NoNoMeCat memebers

Publications

[Submitted] 2022 **Darù, A.***; Martín-Fernandez, C.; Harvey, J. N. Iron-catalyzed Kumada cross-coupling Reaction Involving $Fe_8Me_{12}^-$ and Related Clusters: A Computational Study.

2022 Hao, W.; Joe, C. L.; **Darù, A.**; Ayers, S.; Ramirez, A.; Sandhu, B.; Daley, R.A.; Chen, J. S.; Schmidt, M. A.*; Blackmond, D. G.* Kinetic and Thermodynamic Considerations in the Rh-Catalyzed Enantioselective Hydrogenation of 2-Pyridyl-Substituted Alkenes. *ACS Cat.* **2022**, 12, 5961–5969.

2022 Hao, W.; Joe, C. L.; Ayers, S.; **Darù, A.**; Daley, R. A.; Domanski, M.; Chen, J. S.; Schmidt, M. A.*; Blackmond, D. G.* Ru-Catalyzed Enantioselective Hydrogenation of 2-Pyridyl Substituted Alkenes and Substrate-Mediated H/D Exchange. *ACS Cat.* **2022**, 12, 1150-1160.

2021 Legnani, L.; **Darù, A.**; Jones, A. X.; Blackmond, D. G.* Mechanistic Insight Into the Origin of Stereoselectivity in the Ribose-Mediated Strecker Synthesis of Alanine. *J. Am. Chem. Soc.* **2021**, 143, 7852-7858.

2020 Harvey, J. N.; **Darù, A.**. Computational Chemistry and Non-noble Metal-catalyzed Cross-coupling Reaction Mechanisms. *Chimia* **2020**, 74, 467-469.

2020 Pérez–García, P. M.; **Darù, A.**; Scheerder, A. R.; Lutz, M.; Harvey, J. N.*; Moret, M-E.* Oxidative Addition of Aryl Halides to a Triphosphine Ni(0) Center to Form Pentacoordinate Ni(II) Aryl Species. *Organometallics* **2020**, 39, 1139-1144. [shared first authorship]

2020 Ploeger, M. L.; **Darù, A.**; Harvey, J. N.*; Hu, X.* Reductive Cleavage of Azoarene as a Key Step in Nickel-Catalyzed Amidation of Esters with Nitroarenes. *ACS Cat.* **2020**, 10, 2845-2854. [shared first authorship]

2020 **Darù, A.**; Hu, X.*; Harvey, J. N.* Iron-Catalyzed Reductive Coupling of Alkyl Iodides with Alkynes to Yield Cis-Olefins: Mechanistics Insights from Computation. *ACS Omega* **2019**, 5, 1586-1594.

2017 Ríos-Gutiérrez, M.; **Darù, A.**; Tejero, T.; Domingo, L. R.; Merino, P.* A Molecular Electron Density Theory Study of the [3 + 2] Cycloaddition Reaction of Nitrones With Ketenes. *Org. Biomol. Chem.* **2017**, 15, 1618-1627.

2016 Roca-López, D.; **Darù, A.**; Tejero, T.; Merino, P.* Revisiting Oxime-Nitrone Tautomerism. Evidences of Nitrone Tautomer Participation in Oxime Nucleophilic Addition Reactions. *RSC Adv.* **2016**, 6, 22161-22173.

2016 **Darù, A.**; Roca-López, D.; Tejero, T.; Merino, P.* Revealing Stepwise Mechanisms in Dipolar Cycloaddition Reactions: Computational and Topological Study of the Reaction between Nitrones and Isocyanates *J. Org. Chem.* **2016**, 81, 673-680.

2016 Matute, R.; García-Viñuales, S.; Hayes, H.; Ghirardello, M.; **Darù, A.**; Tejero, T.; Delso, I.; Merino, P.* Recent Advances in the Preparation of Enantiomerically Pure Hydroxylamines from Nitrones. *Curr. Org. Synth.* **2016**, 13, 669-686.

References

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`https://www.scripps.edu/blackmond/index.html`

PhD supervisor Prof. Jeremy Harvey, Professor of Theoretical Chemistry at KU Leuven (Belgium)
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Postgrad supervisor Prof. Pedro Merino, Professor of Organic Chemistry at the University of Zaragoza (Spain)
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