



Annual Scientific Report 2023

Summary

1. Preamble.....	2
2. IQCC members	3
3. Awards	5
4. Research visits.....	8
5. Research stays	9
6. Funding	10
7. Industrial Collaborations.....	14
8. PhD Thesis	17
9. Publications.....	20
10. Books	33
11. Book Chapters	33
12. Journal Covers.....	34
13. Outreach activities.....	35

1. Preamble

The first annual report of the Institute of Computational Chemistry and Catalysis (IQCC) of the University of Girona (UdG) containing the most important activities developed by the IQCC during 2023 is presented below. Writing an annual report is a valuable practice that goes beyond fulfilling regulatory requirements. It serves as a tool for communication, reflection, and strategic planning, contributing to the overall success and positive reputation of the institute. The present report is the first one, but we expect it will not be the last. The idea is that, from now on, we will publish an annual report collecting the activities of each year.

As you will see in the next pages, 2023 has been a year plenty of activities in research, education, and science communication. We have celebrated the 30 years of existence of the Institute and the celebration has allowed us to meet again with old colleagues. We have successfully defended 12 doctoral theses, which represents more than 10% of UdG theses. We have once again overcome the barrier of 100 articles, some of which have been published in journals of high scientific reputation: 1 Nat. Chem., 3 Nat. Cat., 1 Nat. Commun., 7 J. Am. Chem. Soc., 6 Angew. Chem., 4 Chem. Sci., 5 ACS Catal., etc. We have obtained 10 research awards and incorporated 5 new postdocs. We have achieved new research projects, among which the ERC Consolidator Grant from Prof. Sílvia Osuna stands out. We have approved the 2024–2026 strategic plan. We have started the IQCC networking activity, which will make it possible to establish stronger links among IQCC members, especially among the younger ones. We have set up the Alumni Association, which will allow us to keep in touch with ex-members of the IQCC. We have continued with an intense activity of communication and dissemination of research through C4D. And it has also been a year of elections and changes in the government team of the IQCC. In short, an intense year with plenty of great activities and excellent results.

Finally, I want to congratulate and acknowledge all members of the Institute for their effort and enthusiastic work during 2023.

I hope you enjoy reading this annual report for 2023.

Miquel Solà
Director

2. IQCC members

At the end of the 2023, the institute consisted of 104 researchers (6 full professors, 9 associate professors, 2 ICREA Senior researchers, 2 Ramón y Cajal researchers, 3 ex-professors, 24 postdocs, 58 PhD students) and 6 support staff (1 research manager, 3 technicians, 2 administrative staff). The changes during 2023 have been the following:

New members:

- Dr. Nikita Chaudhary, postdoc - MSCA-PF (A. Lledó group)
- MSc. Athul Santha Bhaskaran, PhD student - IFUdG2022 (M. Swart group)
- Dr. Albert Artigas, postdoc - REQ – Margarita Salas (M. Solà group)
- MSc. Marc Rubio, PhD student – AGAUR Doctorat Industrial (A. Pla-Quintana group)
- MSc. Nicolás Ramírez, PhD student – IF-UdG PhD student (M. Costas and A. Call group)
- Dr. Carles Fuertes, postdoc - Margarita Salas (X. Ribas group)
- MSc. Filippo Scarchilli, PhD student (M. Costas group)
- Dr. Eduard Masferrer, postdoc (S. Osuna group)
- MSc. Elias Romero, PhD student – FI (A. Roglans and A. Pla-Quintana group)
- MSc. Guillem Vila, PhD student – FI (J.M. Luis group)
- MSc. Judith Sala, PhD student – FI (X. Ribas group)
- MSc. Janet Sánchez, PhD student – FPI (S. Osuna group)
- MSc. Christos Christou, PhD student (M. Costas group)
- MSc. Jonnelly Rissell Luizaga, PhD student (S. Osuna group)
- MSc. Diana Maria Tenica, PhD student (M. Costas group)
- Dr. Jordi Mestres, visitant professor (M. Solà group)
- MSc. Thalia Ortiz, PhD student – IF-UdG (A. Poater group)
- MSc. Cristina Berga, PhD student – IF-UdG (M. Garcia-Borràs, F. Feixas, S. Simon group)

Changes:

- Dr. Muthuramalingam Sethuraman, postdoc - Juan de la Cierva (X. Ribas group)
- Dr. Christian Curado, postdoc (S. Osuna group)
- Dr. Marco Galeotti, postdoc - MSCA-PF (M. Costas group)
- Dr. Laia Vicens, postdoc (M. Costas group)
- Dr. Miquel Estévez-Gay, postdoc (S. Osuna group)
- Dr. Carla Calvó-Tusell, postdoc (M. Garcia-Borràs and F. Feixas group)
- Dr. Jordi Soler, postdoc (M. Garcia-Borràs group)

Members that left the Institute:

- Dr. Martí Gimferrer, now postdoc at University of Göttingen, Germany
- Dr. Jordi Vila, now process chemist at AGC Pharma Chemicals Europe, Spain
- Dr. Carla Calvó-Tusell, now postdoc (Schmidt AI in Science program) at University of California, USA
- Dr. Nikita Chaudhary
- Dr. Ruben Álvarez, now process chemist at AGC Pharma Chemicals Europe, Spain
- Dr. Daniel Trujillo, now associate professor in the Facultad de Ingeniería Ambiental de la Universidad Santo Tomás, sede Villavicencio (Colombia)
- Dr. Frederico Martins, now postdoc at Technical University Darmstadt, Germany
- Dr. Pau Font
- Dr. Nicolas Joly, now postdoc at CEA Paris-Saclay at University of Paris-Saclay, France

3. Awards



[Valentina Iannace wins poster prize at First Inorg/OrgMet Conference of Societat Catalana de Química - IQCC \(udg.edu\)](#)

[Janet Sánchez wins poster prize at First CompChem Conference of Societat Catalana de Química - IQCC \(udg.edu\)](#)



[Najoua Choukairi wins best flash talk award at European-Winter School on Physical Organic Chemistry - IQCC \(udg.edu\)](#)

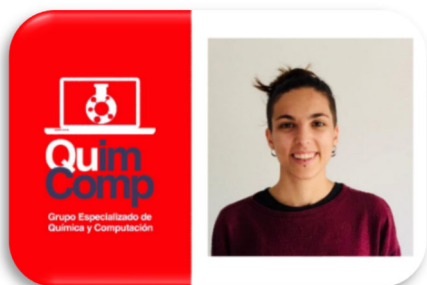
[Sergio Fernández wins Josep Castells award of RSEQ-Cat - IQCC \(udg.edu\)](#)





Lorena Capdevila awarded best PhD thesis 2022

[Artur Brotons-Rufes wins poster prize at the XXXIX Biental of RSEQ - IQCC \(udg.edu\)](#)



[Carla Calvó-Tusell wins RSEQ-GEQC Prize for best computational chemistry paper in 2022 - IQCC \(udg.edu\)](#)

[Miquel Costas receives medalla Rafael Uson award GEQO-RSEQ 2023 - IQCC \(udg.edu\)](#)





[Silvia Osuna receives Emerging Scientific Talent 2023 award of Societat Catalana de Química - IQCC \(udg.edu\)](#)

[Silvia Osuna receives the National Research Award 'María Teresa Toral' 2023 - IQCC \(udg.edu\)](#)



[Anton Stasyuk wins the best oral presentation at the EuChemS CompChem - IQCC \(udg.edu\)](#)

[Miguel Solà new Fellow of the Royal Society of Chemistry - IQCC \(udg.edu\)](#)



4. Research visits

- MSc. Alessandro Nardi, Università La Sapienza (Ll. Blancafort), 10/01/23-30/06/23
- Prof. Roberto Chica, University of Ottawa (S. Osuna), 10/01/23-10/03/23
- MSc. Niayesh Zarifi, University of Ottawa (S. Osuna), 11/01/23-15/04/23
- BSc. Andrea Grillo, Università degli Studi di Napoli Federico II (A. Poater), 01/03/23-31/10/23
- BSc. Unai Merino (M. Garcia-Borràs), 02/03/23-10/10/23
- Dr. Vladimir Motornov, Institute of Organic Chemistry and Biochemistry of the CAS (X. Ribas), 17/04/23-16/06/23
- MSc. Celine Nieuwland, Univ. Amsterdam (M. Swart), 02/05/23-20/06/23
- MSc. Emely Jockmann, University of Freiburg (M. Garcia-Borràs), 14/05/23-17/06/23
- BSc. Petru Milev, Wrocław University of Science and Technology (JM Luis), 14/07/23-15/08/23
- MSc. Keren Iudanov, Ben-Gurion University of the Negev (A. Poater), 01/09/23-30/09/23
- MSc. Amir Lebcir, Badji Mokhtar University (M. Solà), 01/09/23-31/12/23
- Prof. Robert Zalesny, Wrocław University of Science and Technology (J. M. Luis), 06/11/23-21/11/23

5. Research stays

- MSc. Roger Monreal-Corona, Laboratoire de Chimie de Coordination (France), Dr. Rosa Axet, 09/01/23-08/03/23
- MSc. Gibu George, Medical University of Graz (Austria), Prof. Pedro A. Sánchez Murcia, 13/02/23-14/05/23
- MSc. Àlex Díaz, Universidad de Huelva (Spain), Dr. Anna Caballero and Prof. Pedro Pérez, 01/03/23-31/03/23
- Prof. Miquel Solà, Vrije Universiteit Amsterdam (The Netherlands), 04/03/23-04/04/23
- Prof Lluís Blancafort, Ohio State University (United States), 13/03/23–05/05/23
- MSc. Cristina Duran, University of Regensburg (Germany), Prof. Reinhard Sterner, 01/05/23-31/07/23
- MSc. Guillem Casadevall, University of Regensburg (Germany), Prof. Reinhard Sterner, 01/05/23-31/07/23
- Dr. Ouissam El Bakouri, Uppsala University (Sweden), Prof. Henrik Ottosson, 01/05/23-31/05/23
- MSc. Roger Monreal-Corona, Vrije Universiteit Brussel (Belgium), Dr. Mercedes Alonso 01/09/23-30/11/23
- MSc. Adrià Juventeny, University of Illinois Urbana-Champaign (United States), Prof. Liviu M. Mirica, 14/09/23-12/12/23
- Prof. Miquel Solà, King Abdulhah University of Science and Technology (Saudi Arabia), Prof. Luigi Cavallo, 01/11/23-31/1/24

6. Funding

EU Funding

Project Title	Reference	Amount (€)	Principal Investigator	Period
ConfiMet	H2020-MSCA-IF-2020-101027049	160.932	N. Chaudhary (A. Lledó)	01/01/2023 – 31/09/2023
Computational design of industrial enzymes for green chemistry (GREENZYME)	ERC-2022-PoC2-101112805	150.000	S. Osuna	01/05/2023 – 31/10/2024
ICAT-PACHO	H2020-MSCA-2022-PF-101106196	165.312	M. Galeotti (M. Costas)	01/05/2023 – 30/04/2025
Fast yet accurate routine rational design of novel enzymes (FASTEN)	ERC-2022-CoG-101088032	1.996.250	S. Osuna	01/10/2023 – 30/09/2028
Full-Fission	H2020-MSCA-2022-PF-101106492	181.152	A. Artigas (M. Solà)	03/04/2024 – 02/04/2026

MICINN Funding

Project Title	Reference	Amount (€)	Principal Investigator	Period
Organometallic Chemistry for Sustainable Solutions	RED2022-134074-T	20.390	A. Pla-Quintana M. Costas	2023 – 2024
Fotovoltaica Avanzada	RED2022-134939-T	20.390	M. Solà A. Roglans	2023 – 2024

Catálisis Asimétrica	RED2022-134331-T	20.390	M. Solà	2023 – 2024
Estructura electrónica, propiedades y reactividad de moléculas bajo campos eléctricos	PID2022-140666NB-C22	131.250	J. M. Luis P. Salvador	01/09/2023 – 31/08/2026
Modelado Computacional Integrativo de Procesos Bioquímicos y Biocatalíticos: Desde la Comprensión hasta el Diseño	PID2022-141676NB-I00	168.750	M. Garcia-Borràs F. Feixas	01/09/2023 – 31/08/2026
Funcionalización regioselectiva de moléculas esféricas con máscaras supramoleculares y síntesis bottom-up de nanografenos	PID2022-136970NB-I00	281.250	X. Ribas	01/09/2023 – 31/08/2026
Simulating Phase Effects on Excited States	PID2022-138062NB-I00	131.250	Ll. Blancafort	01/09/2023 – 31/08/2026
Estancias de personal docente y/o investigador senior en centros extranjeros 2022	PRX22/00057	10.247	M. Solà	01/11/2023 – 31/01/2024
Estancias de personal docente y/o investigador senior en centros extranjeros 2022	PRX22/00196	10.265	Ll. Blancafort	01/03/2024 – 31/05/2024
Juan de la Cierva	JDC2022-049287-I	67.400	M. Ansari M. Swart	01/03/2024 – 28/02/2026
Programa Ramón y Cajal	RYC2022-038031-I	244.350	A. Call	01/03/2024 – 28/02/2029

AGAUR Funding

Project Title	Reference	Amount (€)	Principal Investigator	Period
Disseny i Modelatge de Reaccions Catalitzades per Metalls de Transició (DIMOCAT)	2021 SGR 00623	60.000	A. Roglans	01/01/2022 – 31/12/2024
Química Bioinspirada, Supramolecular i Catàlisi (QBIS-CAT)	2021 SGR 00475	60.000	A. Company	01/01/202 – 31/12/2024
Theoretical Chemistry of Biosystems (TCBioSys)	2021 SGR 00487	60.000	S. Osuna	01/01/2022 – 31/12/2024
Formulació de resines pel sector químic, utilitzades en la reparació de vehicles comercials i/o industrials i/o pel sector de l'anclatge químic.	2022 DI 095	33.960	A. Pla-Quintana J. Tarres	20/02/2023 – 19/02/2026
Beatriu de Pinós	2022 BP 00078	152.348	C. Fuertes (X. Ribas)	01/01/2024 – 31/12/2026

Other Funding

Project Title	Type	Amount (€)	Principal Investigator
Activitats d'Igualtat de Gènere	University of Girona	1.000	S. Simon
Passejant entre molècules	University of Girona – Consell social	892	M. Solà
Campus d'Estiu de Màgia i Ciència 2023 (VI)	University of Girona – Consell social	714	M. Duran

7. Industrial Collaborations

One of the priorities of the IQCC is to **strengthen the connections with industry**, both nationally and internationally. Apart from projects, collaborations, and research stays of undergrad, Master and PhD students, many of the IQCC Alumni find positions within industry in the participating companies. Furthermore, the IQCC also participates actively in the Industrial Doctorates research *programme* of the *Generalitat de Catalunya*, with several students having already finished their thesis in collaboration with Concentrol (chemical company in the Girona area), and others have just started on a new joint industry-IQCC PhD thesis.

Fourth IndustryQCC Forum

Last 16th November, the IQCC organized the fourth edition of the IndustryQCC Forum with four national and international companies (**Concentrol, UQUIFA, AGC Pharma Chemicals Europe and Chemotargets**) during the Science Week.

The IndustryQCC Forums provide young (and more advanced) researchers of IQCC the opportunity to get to know the research carried out in (bio)chemical industry in different parts of the world; vice versa, for the companies the meetings provide an opportunity to learn about the research of the IQCC, and meet highly qualified researchers with the potential of becoming future employees. This networking activity encourages creating new connections between IQCC/IQCC-researchers and industry in a relaxed and informal manner. This meeting is organized every year since 2020 during the Science Week.

Some companies have shown interest in hosting Master's students for their Master research project and joint research projects have been considered. The event was attended by researchers, postdocs, doctoral students and Master's students from the UdG who were able to speak directly with companies. This facilitated the attraction to the outside world of industry and, at the same time, increases the links between the IQCC and companies to bring research closer to society.



Collaboration with the MACMoM master

During February and March, six of the Master in Advanced Catalysis and Molecular Modelling (MACMoM) students did a internship in Concentrol, Roberlo, Novartis and P&G company (Belgium) to perform their Master research project (TFM) 2022-2023.

Internship in a company is an optional module of the MACMoM Master, in which the students can perform a full-time internship in a company for up to 4-5 months and a maximum of 750h. In these cases, the Master Thesis is associated with the work carried out in the company, and is co-supervised by a supervisor at the company and a supervisor of the IQCC. The internship corresponds to training undertaken by a student in a national or foreign company, with the aim of applying and complementing the training acquired in the master's degree, bringing the student closer to the reality of the environment in which he/she will exercise his/her professional activity. Every year, some companies have shown interest in hosting Master's students.



Collaboration agreement

Industry	Principal Investigator	Period
<p>REPSOL</p> 	<p>Marc Garcia-Borràs</p>	<p>2023-2024</p>
<p>SEQENS</p> 	<p>Sílvia Osuna</p>	<p>2023-2024</p>
<p>BRIOLF</p> 	<p>Anna Pla-Quintana</p>	<p>2023-2026</p>
<p>Fundació Instiut Jaume Vicens Vives de Girona</p>	<p>Ferran Feixas</p>	<p>2023-2027</p>

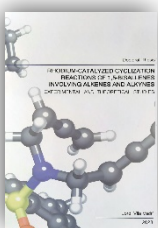
8. PhD tesis



Title: Elucidating the role of conformational dynamics of *Aspergillus niger* monoamine oxidase towards enzymatic chiral amines synthesis
Author: Curado Carballada, Christian
Director: Osuna Oliveras, Sílvia; Feixas Geronès, Ferran
Defense date: 2023-03-13



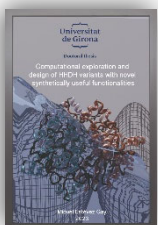
Title: Development and application of new methodologies for chemical bonding analysis
Author: Gimferrer Andrés, Martí
Director: Salvador Sedano, Pedro
Defense date: 2023-03-27



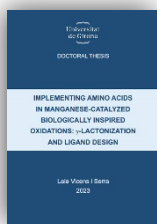
Title: Rhodium-Catalyzed Cyclization Reactions of 1,5-bisallenenes Involving Alkenes and Alkynes: Experimental and Theoretical Studies
Author: Vila Vadrí, Jordi
Director: Roglans Ribas, Anna; Pla Quintana, Anna
Defense date: 2023-04-21



Title: Computational Strategies for Understanding the Molecular Bases of Biochemical and Biocatalytic Processes
Author: Calvó Tusell, Carla
Director: Osuna Oliveras, Sílvia; Garcia Borràs, Marc
Defense date: 2023-06-02



Title: Computational Exploration and Design of Halohydrin Dehalogenase variants with novel synthetically useful functionalities
Author: Estévez Gay, Miquel
Director: Osuna Oliveras, Sílvia
Defense date: 2023-07-07



Title: Implementing amino acids in manganese-catalyzed biologically inspired oxidations: γ -lactonization and ligand design

Author: Vicens Serra, Laia

Director: Costas Salgueiro, Miquel

Defense date: 2023-07-18

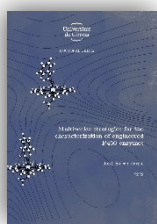


Title: Alkylations by Hydrogen Autotransfer: From Experiments to Reaction Mechanisms and Vice-Versa

Author: Joly, Nicolas

Director: Renaud, Jean-Luc; Poater, Albert

Defense date: 2023-09-13

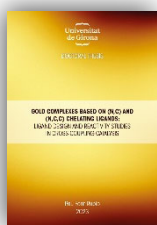


Title: Multiscalar strategies for the characterization of engineered P450 enzymes

Author: Soler i Parpal, Jordi

Director: Osuna Oliveras, Sílvia; Garcia Borràs, Marc

Defense date: 2023-09-19

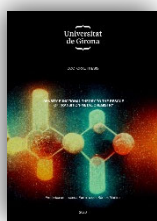


Title: Gold complexes based on (N,C) and (N,C,C) chelating ligands: ligand design and reactivity studies in cross-coupling catalysis

Author: Font Rubio, Pau

Director: Ribas Salamaña, Xavi

Defense date: 2023-10-06

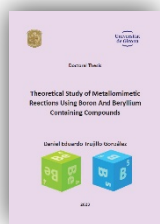


Title: Density functional theory to the rescue of transition-metal chemistry

Author: Martins, Frederico

Director: Swart, Marcel

Defense date: 2023-10-09



Title Theoretical Study of Metallomimetic Reactions Using Boron And Beryllium Containing Compounds

Author: Trujillo González, Daniel Eduardo

Director: Solà, Miquel; Jiménez Halla, J. Óscar; González García, Gerardo

Defense date: 2023-10-23



Title: Development of flexible cavitand receptors based on calixarene.

Rational design, synthesis and study of their properties

Author: Álvarez Yebra, Rubén

Director: Lledó, Agustí

Defense date: 2023-11-07

9. Publications

1. L. Á. Turcio-García, H. Valdés, A. Arenaza-Corona, S. Hernández-Ortega and D. Morales-Morales
"Electronic properties and supramolecular study of selenoureas with fluorinated-NHC ligands derived from imidazo[1,5-a]pyridines"
New J. Chem. **2023**, 47, 2090-2095 DOI: [10.1039/D2NJ04699G](https://doi.org/10.1039/D2NJ04699G)
2. G. George, O.A. Stasyuk, A. A. Voityuk, A. J. Stasyuk and M. Solà
"Aromaticity controls the excited-state properties of host-guest complexes of nanohoops"
Nanoscale **2023**, 15, 1221-1229 DOI: [10.1039/D2NR04037A](https://doi.org/10.1039/D2NR04037A)
3. H. Ottosson, B. Durbeej and M. Solà
"Excited state aromaticity and antiaromaticity special issue"
J. Phys. Org. Chem. **2023**, 36, e4468 DOI: [10.1002/poc.4468](https://doi.org/10.1002/poc.4468)
4. M. Shehata, A. Ünlü, J. Iglesias-Fernández, S. Osuna, O. U. Sezerman and E. Timucin
"Brave new surfactant world revisited by thermoalkalophilic lipases: computational insights into the role of SDS as a substrate analog"
Phys. Chem. Chem. Phys. **2023**, 25, 2234-2247 DOI: [10.1039/d2cp05093e](https://doi.org/10.1039/d2cp05093e)
5. O. Stasyuk, A. Stasyuk, M. Solà and A. Voityuk
"γ-graphyne: A promising electron acceptor for organic photovoltaics"
Mater. Des. **2023**, 225, 111526- DOI: [10.1016/j.matdes.2022.111526](https://doi.org/10.1016/j.matdes.2022.111526)
6. D. E. Trujillo-González, G. González-García, T. A. Hamlin, F. M. Bickelhaupt, H. Braunschweig, J. O. C. Jiménez-Halla and M. Solà
"The Search for Enhanced σ-Donor Ligands to Stabilize Boron-Boron Multiple Bonds"
Eur. J. Inorg. Chem. **2023**, 26, e202200767 DOI: [10.1002/ejic.202200767](https://doi.org/10.1002/ejic.202200767)
7. A. Vicens, L. Vicens, G. Olivo, O. Lanzalunga, S. Di Stefano and M. Costas
"Site-selective methylene C-H oxidation of an alkyl diamine enabled by supramolecular recognition using a bioinspired manganese catalyst"
Faraday Discuss. **2023**, 244, 51-61 DOI: [10.1039/D2FD00177B](https://doi.org/10.1039/D2FD00177B)
8. M. Mitra, A. Brinkmeier, Y. Li, M. Borrell, A. Call, J. Lloret Fillol, M. G. Richmond, M. Costas and E. Nordlander
"An investigation of steric influence on the reactivity of Fe^V(O)(OH) tautomers in stereospecific C-H hydroxylation"
Dalton Trans. **2023**, 52, 3596-3609 DOI: [10.1039/D2DT00725H](https://doi.org/10.1039/D2DT00725H)
9. A. Rahbar, B. Falcone, G. Pareras, M. Nekoomanesh-Haghighi, N. Bahri-Laleh and A. Poater
"Chain Walking in the AlCl₃ Catalyzed Cationic Polymerization of α-Olefins"
ChemPlusChem **2023**, 88, e202200432 DOI: [10.1002/cplu.202200432](https://doi.org/10.1002/cplu.202200432)

10. M. Bhadra, T. Albert, A. Franke, V. Josef, I. Ivanović-Burmazović, M. Swart, P. Moënne-Loccoz and K. D. Karlin
"Reductive Coupling of Nitric Oxide by Cu(I): Stepwise Formation of Mono- and Dinitrosyl Species *En Route* to a Cupric Hyponitrite Intermediate"
J. Am. Chem. Soc. **2023**, *145*, 2230-2242 DOI: [10.1021/jacs.2c09874](https://doi.org/10.1021/jacs.2c09874)
11. S. Posada-Pérez, M. Solà and A. Poater
"Carbon Dioxide Conversion on Supported Metal Nanoparticles: A Brief Review"
Catalysts **2023**, *13*, 305 DOI: [10.3390/catal13020305](https://doi.org/10.3390/catal13020305)
12. A. Brotons-Rufes, N. Bahri-Laleh and A. Poater
"H-bonding Leading to Latent Initiators for Olefin Metathesis Polymerization"
Faraday Discuss. **2023**, *244*, 252-268 DOI: [10.1039/D2FD00163B](https://doi.org/10.1039/D2FD00163B)
13. R. Carbó-Dorca
"Collatz Conjecture Redefinition on Prime Numbers"
JAMP **2023**, *11*, 147-157 DOI: [10.4236/jamp.2023.111011](https://doi.org/10.4236/jamp.2023.111011)
14. B. J. Bloomer, S. N. Natoli, M. Garcia-Borràs, J. H. Pereira, D. B. Hu, P. D. Adams, K. N. Houk, D. S. Clark and J. F. Hartwig
"Mechanistic and structural characterization of an iridium-containing cytochrome reveals kinetically relevant cofactor dynamics"
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10. Books

M. Solà, A. I. Boldyrev, M. K. Cyranski, T. M. Krygowski, and G. Merino

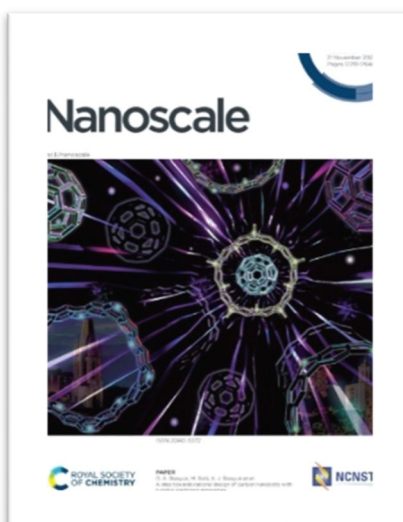
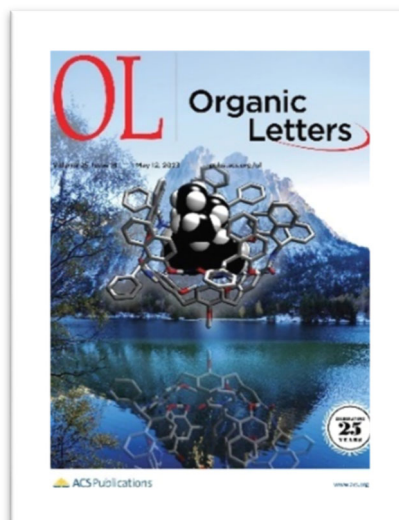
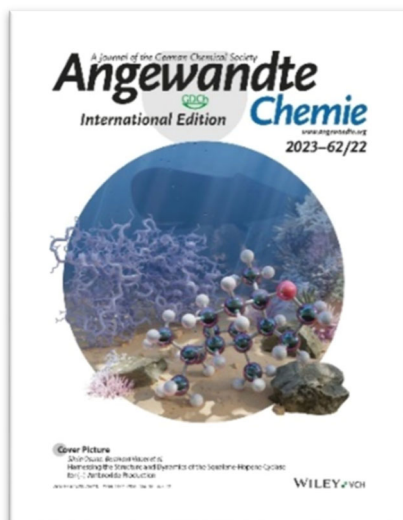
Book: Aromaticity and Antiaromaticity: Basics and Applications, Wiley

ISBN:9781119085898 DOI: 10.1002/9781119085928

11. Book Chapters

1. M. Solà
“Aromaticity: Types, rules and quantification”
Book: Comprehensive Computational Chemistry, *volume 2*, 189-209
DOI: [10.1016/B978-0-12-821978-2.00061-1](https://doi.org/10.1016/B978-0-12-821978-2.00061-1)
2. S.F. Vyboishchikov and A.A. Voityuk
“Noniterative solvation energy method based on atomic charges”
Book: Chemical Reactivity - Approaches and applications, *volume 2, chapter 15*,
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DOI: [10.1016/B978-0-32-390259-5.00021-4](https://doi.org/10.1016/B978-0-32-390259-5.00021-4)
3. R. Carbó-Dorca and T. Chakraborty
“Quantum similarity description of a unique classical and quantum QSPR algorithm in
molecular spaces: the connection with Boolean hypercubes, algorithmic intelligence,
and Gödel's incompleteness theorems. “
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4. L. Vicens, A. Palone, M. Costas
“Asymmetric C—H Oxidation with Biologically Inspired Manganese and Iron
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Book: Science of Synthesis - Base Metal Catalysis 2, *chapter 12*, 465-
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5. S. Osuna
“Computational design of industrially relevant enzymes”
Book: New Horizons in Modern Catalysis: Five Different Perspectives, *volumen 72*,
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12. Journal Covers



13. Outreach activities

The IQCC is an active source of dissemination and communication activities and has a proven track record in this area. The unit follows two strategies for communication. The first one is direct communication activities of [IQCC](#), by means of corporate platforms (website, social media) and individual promotion by the researchers or research teams. This includes meetings with the general public (e.g. research presentations at high schools). The second one is the alliance with the [Unit for Science Culture and Digital Communication \(C4D\)](#) of the UdG, which is directed by IQCC researcher Dr. Sílvia Simon and can be considered an offspring of the IQCC.

Open IQCC doors to secondary school students 2023

A few times a year, the IQCC opens its doors and gives the opportunity to high-school students to know our work through exciting lectures and computational and experimental workshops. This provides the secondary school pupils the possibility to get a feel for the research and have real-time chemistry in their hands. Last month, it was the turn for the visit of 50 high-school students from INS Sagulla Blanes, 15 of INS de Clerà, 26 from school Les Alzines, 48 high-school students from INS Vicens Vives, 29 of INS de Llagostera and 34 from INS La Bisbal.



International Day of Women and Girls in Science at IQCC 2023

11th of February of 2023 was the International day of Women and Girls in Science. The IQCC has currently a rather favourable balance in gender ratio of staff members, both at the Master level (50%), PhD level (38%), postdocs (24%) and permanent researchers' staff (29%). Notably, out of the 4 most recent permanent members, 2 are men and 2 are women, reinforcing one of the goals of the IQCC of striving to have a gender-balanced permanent staff in the near future.

In order to celebrate this day of the 11th of February, last week Prof. Sílvia Osuna participated a round-table: "Trencant barreres: claus per ser una dona STEM!" moderated by Dr. Sílvia Simon (Biblioteca Carles Rahola – Girona, 7th Feb). Also, Dr. Sílvia Simon did a talk at [DonesNano 2023](#) (Barcelona – Institut d'Estudis Catalans, 8th Feb) and another talk about "WikiSciW: Wikimedia, Ciencia y Mujeres" at the conference [Género y Comunicación de la ciencia](#) (Bilbao, 9th Feb). Furthermore, 13 of our IQCC women (Dr. Anna Pla-Quintana, Dr. Sílvia Simon, Prof. Sílvia Osuna, Prof. Anna Roglans, Dr. Olga Stasyuk, MSc. Sílvia Escayola, MSc. Cristina Duran, MSc. Míriam Pujals, MSc. Najoua Choukairi, MSc. Laia Vicens, MSc. Helena Giramé, MSc. Anju Manickoth and MSc. Judit Gálvez) were participating in the [International Day of Women and Girls in Science initiative of UdG](#), where more than 50 researchers are being recognized as #ExpertaUdG.



IQCC Science Slam 2023

Since 2015 the IQCC is organizing a Science Slam. Last Tuesday April 25th the IQCC was organized the seven edition to show the most representative research projects of the Institute to a wide audience. The research carried out within each of the research teams of the IQCC was explained briefly summarized by the PIs (2 minutes).



30 years IQC(C) celebration

Last 20th April took place the 30 years IQC(C) celebration. This wonderful moment was celebrated by a symposium and get-together in Girona.



Pint of Science Girona 2023 at IQCC

Every year in May since 2013 is organizing the international Print of Science festival. This year is organizing by ICREA, IDIBGI, BTM, ERAM, and the Scientific Culture and Digital Communication (C4D) unit of the UdG. Print of Science is an international event with the aim to bring science closer to the general public in a bar. This year, 22-24th of May, the Print of Science was taken place in Girona. The event was started at 7:30 pm at three different bars (Cucut, Kerunta and Sbarjo). The IQCC was participated with three different talks: on 22nd of May at Cucut with Dr. Sílvia Simon with her talk about “Tot és química, química quàntica”, on 24th of May at Kerunta with Prof. Marcel Swart and his talk about “El ball del combustible humà” and then Prof. Sílvia Osuna with her talk about “Dissenya el teu propi enzim”.



CampusPreBAT and Young Research Campus 2023

Every year in June and July since 2008, the UdG is organizing the 13th CampusPreBAT with the aim to offer a set of activities that show an overview of the areas of knowledge in which the UdG works, the studies that can be taken there as well as the services available to 4th ESO students and Young Research Campus with the aim to awaken the scientific curiosity of young people who are on the verge of becoming university students.

Last 26-30 June 2023 (Campus PreBAT) and 3-7 July 2023 (the Young Research Campus) took place in the UdG. The campus was organized from 9:30 am to 6pm, where there were

different workshops. The IQCC participated in different ways: the researcher **Dr. Sílvia Simon** as director, the researcher **Prof. Miquel Duran** with the *7 camins cap a un bon Treball de Recerca* workshop at Campus PreBAT, the researcher **Dr. Ferran Feixas** and the PhD students **MSc. Daniel Bosch** and **MSc. Cristina Berga** with the Realitat virtual workshop at the Young Research Campus.



European Researchers' Night 2023 at IQCC

Every year in September since 2008, the IQCC is organizing together with the Scientific Culture and Digital Communication (C4D) unit of the UdG, the Diputació de Girona and the Girona City Council the European Researchers' Night with the aim to bring science closer to the Girona general public. The European Researchers' Night is a coordinated project with Dr. Sílvia Simon (researcher of IQCC) and others entities (<https://lanitdelarecerca.cat>).

On September 29, 2023, the European Researchers' Night took place in Girona. The main event was organized from 5 pm to 8pm, where there were different workshops. The IQCC participated in different ways, **Dr. Sílvia Simon** as organizer, the postdoctoral researcher **Dr. Hugo Valdés** and **Dr. Marco Galeotti** with the "Catalysis" workshop; and the PhD students **MSc. Abhishek Nair**, **MSc. Judit Gálvez**, **MSc. Daniel Bosch** with the "Porphyrins: Aromatic donuts for transporting metals" workshop; **Prof. Sílvia Osuna**, **MSc. Cristina Duran**, **Dr. Miquel Estévez-Gay** and **MSc. Guillem Casadevall** with the "Coloring and drawing" and "What is an enzyme? stories to save the planet" workshop. Furthermore, **Dr. Marc Garcia-Borràs** did a talk about "The chemistry of biology: the directed evolution of

enzymes in the laboratory seen through a computer” at CaixaForum (28th Sept) and at Saint George School (29th Sept); the postdoctoral researcher **Dr. Miquel Estévez-Gay** did a workshop about “Walking between molecules” at CaixaForum (30th Sept) and **Dr. Sílvia Simon** did a talk on “All it is chemistry. Quantum chemistry, of course! at correbar of Olot (30th Sept).



Science Week – Diada de Sant Albert at IQCC and Science Faculty UdG

Every year in November, the IQCC is organizing together with the Scientific Culture and Digital Communication (C4D) unit of the UdG some activities for Science Week with the aim to bring our science closer to the Girona general public.

Last Friday, November 17, 2023, the Diada de Sant Albert took place at Science Faculty of UdG. The event was organized from 9 am to 1 pm, where there were different workshops and stands. The IQCC participated in a stand on “Catàlisi: a on la trobem?” by two bachelor students (Nora Villar and Arnau Cornellà) to show our chemistry to more than 600 high-school students.



