



Annual Scientific Report 2025

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113 Researchers
10 PhD theses
8 Research stays
8 New postdocs
16 New PhD Students

18 Invited talks
19 Research visits





117 Publications
2 book chapters
9 Covers

20+ Outreach activities
90+ IQCC news
150+ Social media





21 Awards and recognitions



5 European Projects
7 National Projects
3 Regional Projects
12 Other project

5 Industry internships



2025



1. Preamble

The third 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 2025 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 third one.

As you will see in the next pages, 2025 has been a year plenty of activities in research, education, and science communication. We have successfully defended 10 doctoral theses, which represents ca. 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: 2 Nat. Catal., 1 Nat. Commun., 1 Nat. Methods, 2 ACS Central Sci., 1 PNAS, 6 JACS, 1 JACS Au, 6 Angew. Chem., 7 Chem. Sci., 8 ACS Catal., etc. We have obtained 21 research awards and incorporated 8 new postdocs. We have achieved new research projects, among which the ERC Consolidator Grant from Prof. Marc Garcia-Borràs and two MSCA-Doctoral Network from Prof. Sílvia Osuna stands out. We have continued with the IQCC networking activity, which helps to establish stronger links between IQCC members, especially among the younger ones, the Christmas lunch and IQCC Day. We have continued with an intense activity of communication and dissemination of research through C4D. 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 2025.

I hope you enjoy reading this annual report for 2025.

Xavi Ribas
Director

2. IQCC members

At the end of the 2025, the institute consisted of 113 researchers (7 full professors, 9 associate professors, 3 ICREA Senior researchers, 2 Ramón y Cajal researchers, 3 ex-professors, 19 postdocs, 70 PhD students) and 8 support staff (1 project manager, 3 technicians, 4 administrative staff). The changes during 2025 have been the following:

New members:

- MSc. Giuseppe Campanile, PhD student (A. Call and M. Costas)
- MSc. Maria Cabrero, FPI PhD student (M. Solà)
- MSc. Sergi Llanet, FPU PhD student (F. Feixas, M. Planas and L. Feliu)
- MSc. Rupal Sharma, IF-UdG PhD student (M. Swart and S. Osuna)
- MSc. Visvesvarar P Murugan, IF-UdG PhD student (LI. Blancafort)
- MSc. Fiza Fariha, FPI PhD student (M. Swart and A. Lledó)
- MSc. Maria Martínez, DI PhD student (J. Mestres and Chemotargets, M. Solà)
- David Aguirre, staff
- MSc. Raquel Parrondo, PhD student (J. Mestres and Chemotargets, M. Solà)
- MSc. Nikola Panajotovikj, PhD student (J. Mestres and Chemotargets, M. Solà)
- MSc. Mariona Isern, PhD student (J. Mestres and Chemotargets, M. Solà)
- MSc. Itzel Muro, PhD student (M. Garcia-Borràs and F. Feixas and CSIC)
- MSc. Fiza Fariha, FPI PhD student (M. Swart and A. Lledó)
- MSc. Louis Van Nyvel, PhD student (M. Solà, F. de Proft (VUB), M. Alonso (VUB))
- Dr. Aleria Garcia, MSCA-PF postdoc (M. Costas)
- Dr. Sergio Fernández, JdC postdoc (M. Costas)
- Dr. Hannes Meinert, postdoc (S. Osuna)
- Dr. Francesco Zaccaria, MSCA-PF postdoc (M. Costas)
- MSc. Zanira Mushtaq, FI PhD student (M. Swart and A. Lledó)
- Dr. Anton Stasyuk, postdoc (M. Solà)
- MSc. Evgeniia Konstina, MSCA-DN PhD Student (S. Osuna)
- MSc. Adrià Montal, FPU PhD student (A. Pla-Quintana)

Changes:

- MSc. Enrico Chianese, IF-UdG PhD student (M. Costas)

- Dr. Eduard Masferrer, JdC postdoc (S. Osuna)
- Dr. Najoua Choukairi, postdoc (M. Costas)
- Prof. Xavi Ribas, IQCC Director
- Dr. Albert Artigas, Beatriu de Pinós postdoc (M. Solà)
- MSc. Nil Insa, FI-SDUR PhD student (A. Pla-Quintana and M. Costas)
- MSc. Arslan Ahmad, FI PhD student (A. Poater)
- Dr. Cristina Duran, postdoc (S. Osuna)
- Dr. Daniel Bosch, postdoc (M. Garcia-Borràs, F. Feixas)
- MSc. Esther Pruna, FI-STEP PhD Student (S. Osuna)
- Prof. Jordi Mestres, part time full professor
- MSc. Arslan Ahmad, FPU PhD student (A. Poater)

Members that left the Institute:

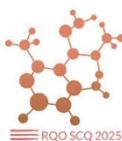
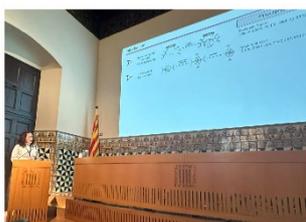
- Dr. Cristina Castanyer, now working at Pharma Hispania (Barcelona)
- Dr. Miquel Estévez-Gay, now postdoc researcher at University of Bern (Switzerland)
- Dr. Alejandro Iglesias
- Dr. Michele Tomasini, now postdoc researcher at University of Salerno (Italy)
- Dr. Gibu George, now postdoc researcher at the ICIQ (Tarragona)
- MSc. Giuseppe Campanile
- David Aguirre
- Dr. Gerard Comas, now postdoc researcher at Università degli Studi di Perugia (Italy)
- Enrico Chianese
- Dr. Ricard López
- Dr. Adrià Juvanteny
- Dr. Laia Vicens, now working at Esteve Química (Celrà)
- Laia Ramoneda
- Dr. Najoua Choukairi, now working at Medichem (Celrà)

3. Awards and Recognitions



2025 Global Women's Breakfast (GWB) - IQCC

Dr. Carles Fuertes wins oral presentation and Christos Cristou wins poster prize at the II RQIO-SCQ - IQCC



Valentina Iannace wins the best oral presentation at the I RQO-SCQ - IQCC

Guillem Pey wins poster prize at the II RQTC-SCQ - IQCC



MSCA Doctoral Network (COMENZE)

Silvia Osuna receives BIOTRANS 2025 Junior Award





Sílvia Escayola receives Josep Castells award of RSEQ-Cat

Marc Garcia-Borràs receives Emerging Scientific Talent 2025 award of Societat Catalana de Química



Premios Tesis Doctorales 2024



Jorge Labella Santodomingo



Patricia Izquierdo Garcia



Carls Bobi Corstant



Sílvia Escayola Gordts



Sílvia Escayola receives an accesit PhD Thesis Award 2024 of GENAM (RSEQ-RSEF)

Carles Alcaide receives the premi Sant Jordi -TFG award of IEC-SCQ



Prof. Miquel Solà receives the 2025 RSEQ Medal

Research teams of Profs. Guo, Que and Swart have been awarded a 2025 Horizon Prize by the Royal Society of Chemistry



Silvia Escayola awarded best PhD thesis 2024 in Chemistry at UdG

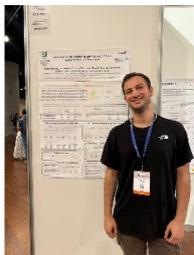
Aqza Elza John wins Best Presentation Award at JODOC 2025



Xavi Ribas wins Research Excellence Award Serra Hünter

Marc Garcia-Borràs appointed ICREA Research Professor





Filippo Scarchilli wins poster prize at the XL Bienal RSEQ



XLIX "A. CORBELLA" INTERNATIONAL SUMMER SCHOOL
ON ORGANIC SYNTHESIS - ISOS 2025
Gargagnano (BS), 13th-19th June 2025

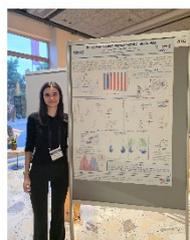


Filippo Scarchilli wins poster prize at the ISOS 2025



Silvia Osuna receives the IX Banc Sabadell Foundation award on Sciences and Engineering

Hande Abes wins poster prize at the WATOC 2025



Jordi Soler wins RSEQ-GEQC Prize for best computational chemistry paper in 2024

Seven IQCC researchers have been included in Stanford University global list of 2% top scientists



IQCC-UdG Leads Green Chemistry Breakthrough in BBVA Foundation's Fundamentos Program

New MSCA postdoctoral project for Francesco Zaccaria



Marc Garcia-Borràs granted an ERC Consolidator grant

Roger Monreal wins Best Presentation Award at TraPCat4 2025





Generalitat de Catalunya
Departament de Recerca
i Universitats

Agència
de Gestió
d'Ajuts
Universitaris
i de Recerca
AGAUR



Albert Poater repeats the Academy of Excellence Program -ICREA award

New Full Professor Prof. Jordi Mestres

iQCC
Institut de Química
Computacional i Catalític



Universitat
de Girona

4. Research visits and invited talks

- Prof. Louis Fensterbank (Sorbonne Université, France) (A. Pla-Quintana), 13/01/25
- MSc. Kathrin Hörnschemeyer (Technische Universität München, Germany) (S. Osuna), 13/01/25-11/04/25
- Dr. Alba Cervera (BSC) (M. Solà), 21/01/25
- Prof. Robert Zalesny (Wroclaw University of Science and Technology, Poland) (JM. Luis), 23/01/25-04/02/25
- MSc. Itzel Mercado (Universidad de Guanajuato, Mexico) (S. Osuna), 27/01/25-01/11/25
- Dr. Fedor Goumans (SCM, The Netherlands) (M. Swart and S. Osuna), 29/01/25
- Dr. Sergio Posada-Pérez (Vrije Universiteit Brussel, Belgium) (A. Poater), 30/01/25
- MSc. Chiara Campi (Giessen University, Italy) Prof. Sigfried Schindler (M. Costas), 01/02/25-01/06/25
- Dr. Massimo Christian D'Alterio (University of Naples Federico II, Italy) (A. Poater), 01/02/25-30/04/25
- BSc. Zehra Evla (Yeditepe Üniversitesi, Turkey) (S. Osuna), 03/02/25-30/03/25
- MSc. Marius Schnutenhaus (University of Bielefeld, Germany) Prof. Stephan Hammer (M. Garcia-Borràs), 03/02/25-30/04/25
- BSc. Natàlia Cabré (Utrecht University, The Netherlands), Prof. Alexandre Bonvin (S. Osuna), 03/02/25-29/07/25

- BSc. Johan Daniel de Smet (Vrije Universiteit Brussel, Belgium) (M. Solà), 10/02/25-31/05/25
- Dr. Joelle N. Pelletier (Université de Montréal, Canada) (S. Osuna), 24/02/25-28/02/25
- Prof. Matthew Sigman (University of Utah, USA), 25/02/25
- BSc. Francesco Dellaversano (Università degli Studi di Napoli Federico II, Italy) (A. Poater), 01/03/25-31/05/25
- Dr. Rosa Axet (CNRS, France) (A. Company), 07/03/25
- Prof. Francesco Zaccaria (University of Naples and Xplore Ltd, Italy) (M. Costas), 21/03/25
- MSc. Hannes Meinert (University of Greifswald, Germany) (S. Osuna), 22/04/25-11/05/25
- Prof. Araceli González Campaña (University of Granada, Spain) (M. Solà), 24/04/25
- MSc. Gerardo Hernández Juárez (Cinvestav, Mexico) (M. Solà), 05/05/25-31/07/25
- Dr. Xingang Xu (Zhejiang Sci-Tech University, China), 26/05/25
- Prof. Francisco Martin-Martinez (King's College London, UK) (F. Feixas), 29/05/25
- Prof. Dominik Munz (Universität des Saarlandes, Germany) (A. Pla-Quintana), 09/06/25
- Dr. Bo Durbeej (Linköping University, Sweden) (Ll. Blancafort), 29/07/25
- Dr. Marco D'Abramo (University Roma La Sapienza, Italy) (F. Feixas), 29/07/25
- MSc. Fabio Ioele (University of Rome Tor Vergata, Italy), Prof. Massimo Bietti (M. Costas) 01/09/25-24/12/25
- Prof. Connie Lu (University of Bonn, Germany) (A. Company), 02/09/25
- Dr. Peter Stockinger (ZHAW, Switzerland), Prof. Rebecca Buller (S. Osuna) 15/09/25-26/09/25
- Dr. Michael Neidig (University of Oxford, UK) (M. Costas), 25/09/25
- BSc. Giuseppe d'Amico (University of Pavia, Italy), Prof. Davide Ravelli (M. Costas) 01/10/25-31/01/26
- BSc. Marie Ronnader (University of Minnesota, USA) (S. Osuna) 20/10/25-17/07/26
- PhD. Beatrice Rassati (Universität Bern, Switzerland), Prof. Francesca Paradisi (S. Osuna) 03/11/25-30/04/26
- Dr. Martí Gimferrer (Georg-August Universität Göttingen, Germany) (A. Poater) 08/12/25-11/12/25

- Prof. Núria Lòpez Alonso (Institut Català d'Investigació Química – ICIQ, Spain) (M. Swart) 18/12/25

5. Research stays

- MSc. Denis Diatlov - Xiamen University (China), Dr. Pavlo O. Dral [5 months]
- MSc. Clara Sabrià - Politecnico di Torino (Italy), Prof. Giovanni Pavan, [3.5 months]
- MSc. Neus Pagés - University of Groningen (The Netherlands), Prof. Wesley R Browne, [3 months]
- Prof. Anna Roglans - Mukogawa Women's University (Japan), Prof. Tetsutaro Kimachi, [1.5 months]
- MSc. Judith Sala– Universität Heidelberg (Germany), Prof. Milan Kivala [3 months]
- Prof. Miquel Solà – Kaust Catalysis Center, King Abdullah University of Science and Technology, Thuwal (Saudi Arabia), Prof. Luigi Cavallo [4 months]
- MSc. Athul Santha Bhaskaran– University of Stuttgart (Germany), Prof. Johannes Kästner [3 months]
- MSc. Thalia Ortiz-Garcia – Università degli Studi di Milano Bicocca (Italy), Prof. Sergio Tosoni [3 months]

6. Funding

EU Funding

Project Title	Reference	Amount (€)	Principal Investigator	Period
BioRelnt	ERC-2025-COG-101232334	1.999.562	M. Garcia-Borràs	2026-2031
ELEGANCE	HORIZON-MSCA-2024-DN-101226960	4.470.727,68 (UdG: 282.188)	S. Osuna	01/01/2026 – 31/12/2029
HaloVerse	HORIZON-MSCA-2024-DN-JD-101226357	3.869.142 (UdG: 376.250)	S. Osuna	01/01/2026-31/12/2030

RePolHyCA	HORIZON- MSCA-2024- PF-101205901	209.914	F. Zaccaria (M. Costas)	01/10/2025 – 30/09/2027
Cyb-org	HORIZON- TMA-MSCA- 2024-PF-GF- 101206634	322.164	A. Roca (M. Costas)	01/07/2025 – 31/12/2027

MICINN Funding

Project Title	Reference	Amount (€)	Principal Investigator	Period
Catalyst design to exert chemoselectivity control in biologically inspired oxidation catalysis	PID2024- 162777NB-I00	387.500 + FPI	M. Costas A. Company	01/09/2025 – 31/12/2028
Rational design of efficient therapeutic enzymes	PID2024- 155349NB-I00	237.500+FPI	S. Osuna	01/09/2025 – 31/12/2028
Going to selectivity in mild conditions in C-C bond formation by chemical tools	PID2024- 155989NB-I00	177.500+FPI	A. Poater	01/09/2025 – 31/12/2028
Juan de la Cierva	JDC2024- 054354-I	76.600	A. Fadeev (M. Costas)	01/03/2026- 28/02/2028
Juan de la Cierva	JDC2024- 055132-I	76.600	S. Kapse (A. Poater)	01/06/2026- 31/05/2028
Red de investigación en fotovoltaica orgánica-inorgánica de nueva generación	RED2024- 154178-T	28.000	A. Lledó M. Solà	2025-2027
Consolidación Investigadora	CNS2025- 165326	192.390	F. Feixas	2026-2028

ICREA Acadèmia Awards

Project Title	Reference	Amount (€)	Principal Investigator	Period
ICREA Academia 2025	2025 ICREA 00110	200.000	A. Poater	01/01/2027-31/12/2031

AGAUR Funding

Project Title	Reference	Amount (€)	Principal Investigator	Period
Doctorat Industrial	2025 DI 079	37.800	J. Mestres Chemotargets	2026-2028
Beatriu de Pinós	2024 BP 00034	161.400	S. Fernández (M. Costas)	01/01/2026 – 31/12/2028
Indústria del Coneixement	2025 PROD 00025	150.000	S. Osuna	16/09/2025-15/03/2027

Other Funding

Project Title	Type	Amount (€)	Principal Investigator
6a edició de IQCC open doors 2025	University of Girona – Consell social	810	X. Ribas
I, per a què serveix la teva Recerca? Activitat associada a La Nit Europea de la Recerca UdG	University of Girona – Consell social	1.200	S. Simon
Any Internacional de la Ciència i la Tecnologia Quàntica (IYQ)	University of Girona – Consell social	400	S. Simon
X Campus d'Estiu de Màgia i Ciència	University of Girona – Consell social	1.680	M. Duran
La Ciència de la Casa Màgica	University of Girona – Consell social	400	M. Duran
(Pre)-escolars & Ciència	University of Girona – Consell social	3.600	S. Osuna

IQCC en fires de divulgació científica 2025	University of Girona – Consell social	975	X. Ribas
PROMOTORS_UdG2025/13	University of Girona	49.675	X. Ribas
TalentUdG2025	University of Girona	85.525	A. Call
RETICAT	BBVA Fundamentos	247.687	M. Costas, D. Maspoch, X. Ribas, A. Call
Breakfast IUPAC-UdG	Breakfast IUPAC	340	Ll. Blancafort
Diseño computacional de nuevos catalizadores para reacciones de acoplamiento cruzado, metástasis de olefinas y funcionalización de enlaces C–H	ONCE INVESTIGA	30.000	O. El Bakouri

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 and others have just started on a new joint industry-IQCC PhD thesis.

Interdisciplinary collaboration to address health challenges through computational chemistry

The Dr. Josep Trueta Biomedical Research Institute of Girona (IDIBGI) and the Institute of Computational Chemistry and Catalysis (IQCC) of the University of Girona (UdG) have organized a joint event with the goal of fostering collaboration between researchers from different disciplines. The meeting, held at the IDIBGI in Salt, allowed the sharing of research lines, identification of synergies, and exploration of new collaboration opportunities.

During the session, researchers from the IQCC presented their research on the chemical synthesis of pharmacologically interesting products and the computational analysis of reaction mechanisms in enzymes. Meanwhile, the IDIBGI teams presented their projects developed in the five major health areas: cardiovascular and respiratory, metabolism and inflammation, neurosciences, oncohematology, and mental health.

This first exchange of synergies highlighted the potential of joining efforts between two institutions that share a commitment to society, scientific excellence, and innovation. “This meeting is a great opportunity to create synergies with the patron institutions of IDIBGI and combine efforts in the Girona region to advance in the mission of improving the health and quality of life of people,” emphasized the director of IDIBGI, Marga Nadal.

On the other hand, the director of IQCC highlighted that “this first meeting, which we hope will be the first of many, has established an initial contact between researchers from two powerful research institutes in Girona, IDIBGI and IQCC. In this way, researchers from both institutions realized that, despite working on topics that may seem distant at first glance, there are overlapping areas in which they can collaborate and help each other.” This alliance could be key to the development of new therapeutic tools, predictive models, and applications that address current health challenges.

About [IDIBGI](#): The Dr. Josep Trueta Biomedical Research Institute of Girona (IDIBGI) focuses on translational research with the aim of improving health and healthcare. Organized into 24 research groups, it employs over 400 professionals and conducts research in the five major scientific areas. IDIBGI is a private foundation within the public sector of the Generalitat of Catalonia and is part of the Research Centers of Catalonia (CERCA).

About [IQCC](#): The Institute of Computational Chemistry and Catalysis (IQCC) focuses its research on theoretical chemistry, homogeneous and enzymatic catalysis. As such, research and education are its two missions, naturally intertwined. With an international vision, it promotes cooperation between theoretical and experimental teams to tackle the major challenges in chemical sciences, contributing to the transition towards a circular economy. The IQCC consists of 112 researchers organized into three research units and [fifteen research teams](#).



Collaboration with Givaudan, Concentrol, AGC Pharma Chemicals, Esteve and Nanobots Therapeutics industries for five MACMoM students

During February, five of the Master in Advanced Catalysis and Molecular Modelling (MACMoM) students started an internship in [Givaudan](#), [Concentrol](#), [AGC Pharma Chemicals](#), [Esteve](#), [Nanobots Therapeutics](#) to perform their Master research project (TFM).

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.



Hands-on Amsterdam Modeling Suite workshop 2025

During last week (Jan 29th) there was the Hands-on Amsterdam Modeling Suite workshop at the Parc-UdG organized by SCM and Prof. Marcel Swart and Prof. Sílvia Osuna, ICREA researchers at the Institute of Computational Chemistry and Catalysis (IQCC), to learn hands-on how easy it is to use the powerful Amsterdam Modeling Suite for understanding and predicting chemical and materials properties.



8. PhD tesis



Title: Exploring the use of Rh-catalyzed cyclization reactions for the functionalization of fullerenes

Author: Castanyer Caballé, Cristina

Director: Pla-Quintanta, Anna; Solà, Miquel; Roglans, Anna

Defense date: 2025-02-14



Title: Asymmetric oxidative dearomatization of arenes with biologically inspired oxidation catalysts

Author: Choukairi Afailal, Najoua

Director: Costas, Miquel

Defense date: 2025-03-18



Title: Intermolecular interactions between fluorophores carrying BF/BF₂ group and halogenated fluorobenzenes

Author: Iglesias Reguant, Alejandro

Director: Luis, Josep Maria; Osmialowski, Borys

Defense date: 2025-04-07

Title: DFT calculations towards predictive organo/organometallic chemistry
Author: Tomasini, Michele
Director: Poater, Albert; Caporaso, Lucia; Falivene, Laura
Defense date: 2025-04-24



Title: Computational study and design of materials for photovoltaic applications
Author: George, Gibu
Director: Solà, Miquel; Stasyuk, Anton
Defense date: 2025-04-25



Title: Extracting Chemical Concepts with Effective Fragment Orbitals
Author: Comas i Vilà, Gerard
Director: Salvador, Pedro
Defense date: 2025-06-10



Title: Rational design of tryptophan synthases through conformation and correlation-based allosteric networks
Author: Duran i Rebenaque, Cristina
Director: Osuna, Sílvia
Defense date: 2025-06-12



Title: Generation of theoretical DHICA melanin models for the simulation of optical spectra
Author: Bosch Coch, Daniel
Director: Blancafort, Lluís
Defense date: 2025-07-28



Title: Functional Cavitands as Artificial Enzymes: Bridging Computational and Synthetic Strategies for Supramolecular Catalysis and Beyond
Author: López Coll, Ricard
Director: Lledó, Agustí
Defense date: 2025-07-31



Title: Getting insight into C-H functionalization and cross-coupling reactions mediated by nickel and other first-row transition metals

Author: Juvanteny Palomerias, Adrià

Director: Company, Anna

Defense date: 2025-09-03

9. Publications

1. R. Barzaga, B. Kerkeni, D.A. García-Hernández, X. Ribas, T. Pelachs, M. Manteiga, A. Manchado, M.A. Gómez-Muñoz, T. Huertas-Roldán, G. Ouerfelli
Peculiarities in the infrared emission of polycyclic aromatic hydrocarbon-C₆₀ adducts
A&A, **2025**, *704*, A300 [DOI: 10.1051/0004-6361/202554031](https://doi.org/10.1051/0004-6361/202554031)
2. Mostafa Ahmadi, Yasothaa Thavayogarajah, Josep Duran, Albert Poater, Sebastian Seiffert
Reconfigurable Transient Polymer Networks Based on Heteroleptic Metal-Ligand Complexes
ACS Appl. Polym. Mater., **2025**, *7*, 16427-16433 [DOI: 10.1021/acspm.5c03436](https://doi.org/10.1021/acspm.5c03436)
3. Judith Münch, Jordi Soler, Ofir Gildor-Cristal, Sarel J. Fleishman, Marc Garcia-Borràs, Martin J. Weissenborn
Computationally Designed Peroxygenases That Exhibit Diverse and Selective Terpene Oxyfunctionalization
ACS Catal., **2025**, 12741-12755 [DOI: 10.1021/acscatal.5c02412](https://doi.org/10.1021/acscatal.5c02412)
4. Stuart C.D. Kennington, Mou Mandal, Roger Monreal-Corona, Arijit Saha, Albert Poater, Anna Roglans, Anna Pla-Quintana
Head-to-Tail Selective [2 + 2 + 2] Cycloadditions of Bisallenes Enabled by Ligand-Free Nickel(0)
ACS Catal., **2025**, *15*, 15043-15049 [DOI: 10.1021/acscatal.5c04046](https://doi.org/10.1021/acscatal.5c04046)
5. Bittu Chandra, Chupeng Li, Mursaleem Ansari, Jin Xiong, Alex Lovstedt, Yisong Guo, Marcel Swart, Lawrence Que
Million-Fold Activation of C-H Bonds by Fluorinated Nonheme Fe^{IV}=O Complexes via Second Sphere Equatorial Substitution and Catalytic Epoxidation to Boot
ACS Catal., **2025**, 17361-17372 [DOI: 10.1021/acscatal.5c04331](https://doi.org/10.1021/acscatal.5c04331)
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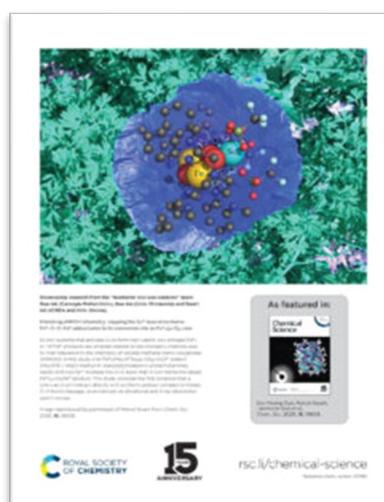
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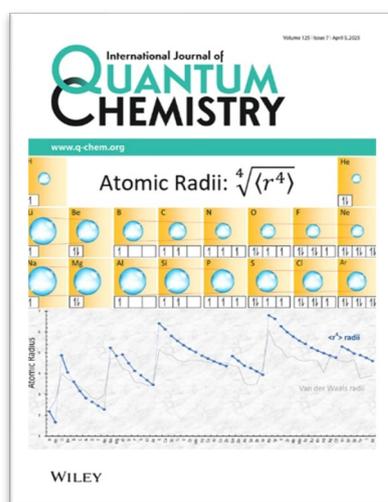
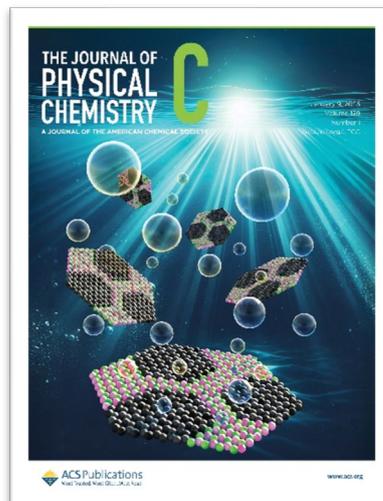
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10. Book Chapters

1. A. Artigas and M. Solà
“Aromaticity and Antiaromaticity in Nanographenes: An Overview”
Book: *Molecular Nanographenes: Synthesis, Properties and Applications*
DOI: [10.1002/9783527845019.ch1](https://doi.org/10.1002/9783527845019.ch1)
2. E. Marguí, E. de Almeida, E. Besalú, I. Queralt, Y. Bolaños & F. L. Melquiades
“X-Ray Fluorescence Spectroscopy and Chemometrics”
Book: *Data Analysis and Chemometrics in X-Ray Fluorescence and Applications*
DOI: [10.1007/978-3-031-98375-7](https://doi.org/10.1007/978-3-031-98375-7)

11. Journal Covers





12. 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 2025

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 30th January, it was the turn for the visit of 22 high-school students from INS Pla de l'estany, 27 from INS Llagostera, 22 from INS La Bisbal, 20 from school Immaculada Concepció, 37 from school Les Alzines, 9 from Montjuic Girona International School, 35 from INS Salvador Espriu and 38 from INS Celrà. In the first part, the director of Science Culture and Digital Communication (C4D) and IQCC researcher (Sílvia Simon) gave a brief summary of the IQCC institute and two researchers of IQCC (Arnau Call and Josep Maria Luis) explained their research at the IQCC. Afterwards, the pupils attended two workshops (Analysis of Fullerenes by Thin Layer Chromatography (TLC) and Computational simulations to experience in real life the research in chemistry with the help of some PhD students and postdocs from IQCC (Dr. Hugo Marchi, Enrico Chianese, David Capellán, Andrea Álvarez, Anju Manickoth, Rosa Mollfulleda and Denis Diatlov).



Chemistry Department open doors 2025

Last 30th January the Chemistry Department of the University of Girona opened its doors and gives the opportunity to high-school students to know our work through 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.

Some IQCC members have participated (Aythami Soto, Esther Pruna, Raúl Lago, Núria Alsina, Ricard López, Dr. Ferran Feixas, Dr. Albert Poater, Dr. Sílvia Simon, Dani Masó) with two workshops (virtual reality and experimental workshop).



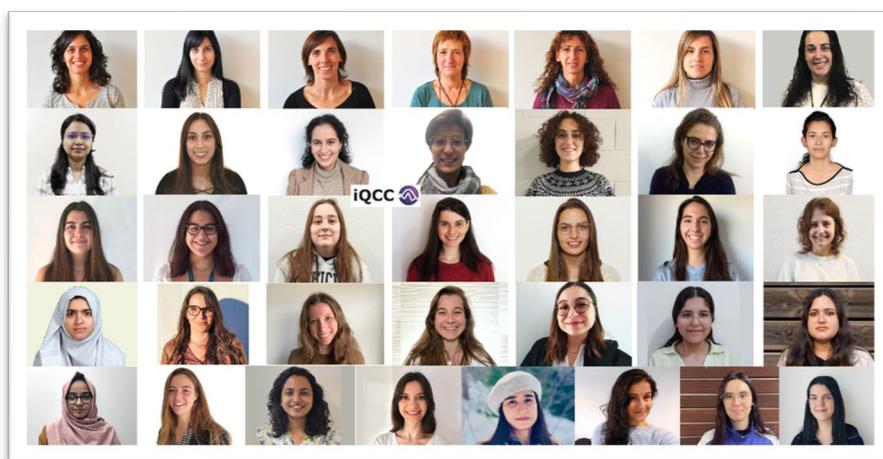
International Day of Women and Girls in Science at IQCC 2025

This coming Tuesday (11th of February) is 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 (54%), PhD level (47%), postdocs (21%) 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, next week Dr. Sílvia Simon will moderate the round table with Dr. Laia Vicens about "[Impulsem les vocacions científiques](#)" (Centre Cultural La Mercè – Girona, 10am). On 14th of February, Dr. Sílvia Simon will participate in a round table at [Ràdio Girona FM](#). Also, Dr. Sílvia Simon will do a talk a #100tifiques (Institut Castell d'Estela, Amer) and Dr. Laia Vicens will participate at exposition "[Ciència amb Denominació d'Origen Girona; Les nostres veïnes, les nostres científiques](#)" (10-16/02,

Girona). On 15th of February, MSc. Cristina Berga, Núria Alsina and Dr. Sílvia Simon will be at [“ciència en joc”](#) (La Marfà – Girona, 10-12h).

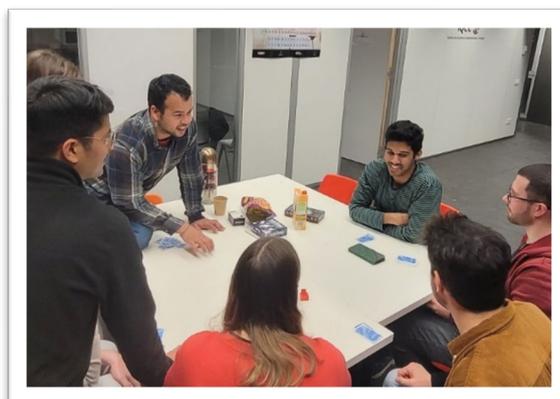
Furthermore, 11 of our IQCC women (Dr. Anna Pla-Quintana, Dr. Sílvia Simon, Prof. Sílvia Osuna, Prof. Anna Roglans, MSc. Cristina Duran, MSc. Najoua Choukairi, Dr. Laia Vicens, MSc. Helena Giramé, MSc. Anju Manickoth, MSc. Judit Gálvez, MSc. Núria Alsina) are participating in the [International Day of Women and Girls in Science initiative of UdG](#), where more than 50 researchers are being recognized as #ExpertaUdG.



IQCC networking: February 2025

Since 2023 every two months, the IQCC is organizing some sessions of IQCC networking. This activity is trying to promote networking between the people of the all Institute (PIs, postdocs, PhD students, master students and staff) and it is a chemistry-free event,

On Friday 14th February took place a new session of IQCC networking, we did a board/cards games session.



2025, International Women's Day – Women's IQCC Forum

8th of March is International Women's Day. The IQCC has currently a rather favourable balance in gender ratio of staff members, both at the Master level (54%), PhD level (47%), postdocs (21%) 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, on the 7th of March there was the fifth IQCC Forum: Women's edition, open to the general public. The IQCC Forum: Women's edition provides the opportunity for an invited speaker and IQCC researchers to present their work to society.



Forum

IQCC Institut de Química Computacional i Catalísi

Universitat de Girona

IQCC Forum: Women's edition

7th March 2025

11:30 - 13:00 h

Join us!

		
Dr. M. Rosa Axet CNRS, France	Dr. Mou Mandal IQCC-University of Girona, Spain	MSc. Valentina Iannace IQCC-University of Girona, Spain
<i>Supporting Metal Nanoparticles and Single-atom Catalysts for Hydroconversion and Hydroformylation</i>	<i>Ligand-Free Ni(0)-Catalyzed [2+2+2] Cycloadditions of 1,5-Bisallenenes with Acetylenes: A Chemo- and Regioselective Approach</i>	<i>Regioswitchable Bingel bis-Functionalization of Fullerene C70 via Supramolecular Masks</i>

IQCC Day 2025

Since 2023 every two months, the IQCC is organizing some sessions of IQCC networking. This activity is trying to promote networking between the people of the all Institute (PIs, postdocs, PhD students, master students and staff) and it is a chemistry-free event.

Last Thursday 20th March the 2nd **IQCC Day** took place. This activity is part of the Networking IQCC activities. We did a **BBQ**.



Ciència en Equip 2025 at IQCC

Every year in April since 2014 is organizing the *Ciència en equip*. It is a science fair mainly led by secondary school students from various institutes in the Girona region, aimed at the general public. This year, 5th of April 2025, the *Ciència en Equip* took place in Girona. The event started at 10 am until 2 pm at Pati de les Magnòlies (Seu de la Generalitat). The IQCC participated in an stand on “Catàlisi: a on la trobem?” by some IQCC members (Dr. Sílvia Simon, Dr. Mou Manda, Dr. Arijit Saha, Dr. Hugo Marchi, MSc. Maria Cabrer and Dr. Teresa Corona) to show our chemistry to the society.



Petits grans científics i científiques 2025 at IQCC

Every year in May since 2008 is organizing the *Ciència en equip – Petits grans científics i científiques*. Its goal is to promote scientific education among young people. By applying the scientific method, students observe phenomena, formulate hypotheses, conduct experiments, draw conclusions, and develop theories related to the scientific concepts they are working on. This year, 7th of May 2025, the *Ciència en Equip-Petits grans científics i científiques* took place in Girona. The event started at 10 am to 12pm at Parc del Migdia. The IQCC participated in an stand on “*Sigues el millor catalitzador!*” by some IQCC members ([Prof. Lluís Blancafort](#), Dr. Silvia Simon and BSc. Carles Alcaide) to show our chemistry to the childrens from 4-7 years old from 18 schools (Àgora, Cassià Costal, Joan Bruguera, Josep Dalmau Carles, FEDAC Pont Major, EE Font de l’Abella, Font de la Pólvara, Marta Mata, Dr. Masmitjà, Migdia, Montfalgars, Pericot, EE Palau, Pla de Girona, Santa Eugènia, Sagrada Família, Taialà and Vedruna).



European Researchers' Night 2025 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. Sivia Simon** (researcher of IQCC) and others entities (<https://lanitdelarecerca.cat>).

On September 26, 2025, the European Researchers' Night took place in Girona. The main event was organized from 10 am to 9 pm, where there were different workshops. The IQCC participated in different ways, **Dr. Sílvia Simon** as organizer, researcher **Prof. Miquel Duran**, **MSc. Carles Alcaide** “Any Internacional de la Ciència i la Tecnologia Quàntiques” workshops; **Dr. Ferran Feixas**, **Dr. Marc Garcia-Borràs**, **MSc. Aqza John**, **MSc. Hande Abes**, **MSc. Helena Giramé** with the “Les cadenes d’aminoàcids”; **MSc. Raúl Lago**, **MSc. Judit Gálvez** with “Passejant entre molècules”; **Dr. Albert Artigas**, **MSc. Maria Cabrero**, **MSc. Iqra Sarfraz**, **MSc. Rabab Maqsood**, **MSc. Faiza Ahsan** “Construeix el teu propi nanografè” workshop; **MSc. Omkar Charapale**, **MSc. Guillem Pey**, **MSc. Guillem Vila** with “Kaprekar Constant: Un descobriment màgic” workshop; **Prof. Sílvia Osuna**, **Dr. Hannes Meinert**, **MSc. Jonnelly Luizaga**, **MSc. Janet Sánchez** and **MSc. Akram Doustmohammadi** with the “Contes de ciència per a nens i pintem enzims” workshop and **Dr. Daniel Bosch** with “Música i AI” workshop and **MSc. Cristina Berga** and **MSc. Núria Alsina**. Furthermore, the researcher **Dr. Agustí Lledó** did a microtalk about “Processos químics sostenibles inspirats en la natura” at CaixaForum (25th Sept).



IQCC Science Slam 2025, October 8th 12:30h

Since 2015 the IQCC is organizing a Science Slam. On Wednesday October 8th the IQCC organizes the X 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 will be briefly summarized by the PIs (2 minutes).



IQCC networking: October 2025

Since 2023 every two months, the IQCC is organizing some sessions of IQCC networking. This activity is trying to promote networking between the people of the all Institute (PIs, postdocs, PhD students, master students and staff) and it is a chemistry-free event,

On Thursday October 2nd took place a new session of IQCC networking, we did a soccer match, trival and a dinner.



Science Week – Diada de Sant Albert at IQCC and Science Faculty UdG 2025

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 14, 2025, the Diada de Sant Albert took place at Science Faculty of UdG. The event was organized from 09.00h to 13.00h, where there were different workshops and stands. The IQCC participated in an stand on “Catàlisi: a on la trobem?” by two bachelor students (Iman Aguerram and Kabil Karunanithi) and a PhD student (Guillem Pey) to show our chemistry to more than 600 high-school students.



