

Fecha del CVA	28/01/2025
---------------	------------

## Parte A. DATOS PERSONALES

Nombre	Abel		
Apellidos	de Cózar Ruano		
Sexo	Hombre	Fecha de Nacimiento	17/10/1981
DNI/NIE/Pasaporte	05689199B		
URL Web	http://adecozar.com		
Dirección Email	abel.decozar@ehu.es		
Open Researcher and Contributor ID (ORCID)	0000-0001-8430-4076		

### A.1. Situación profesional actual

Puesto	Ikerbasque Research Associate Professor		
Fecha inicio	2017		
Organismo / Institución	Universidad del País Vasco		
Departamento / Centro	Química Orgánica I / Facultad de Ciencias Químicas		
País	España	Teléfono	943015753
Palabras clave	Mecanismos de reacción		

### A.2. Situación profesional anterior (incluye interrupciones en la carrera investigadora - indicar meses totales, según texto convocatoria-)

Periodo	Puesto / Institución / País
2012 - 2017	Ikerbasque Research Fellow / Universidad del País Vasco
2011 - 2012	Postdoctoral fellow / Vrije Universiteit. Amsterdam
2009 - 2011	Personal Investigador Contratado / Universidad del País Vasco
2009 - 2011	Personal Investigador Contratado / Universidad del País Vasco
2009 - 2009	Personal Investigador / Universidad de Castilla-La Mancha
2004 - 2008	becario predoctoral / Universidad de Castilla-La Mancha

### A.3. Formación académica

Grado/Master/Tesis	Universidad / País	Año
Programa Oficial de Doctorado en Química Sostenible	Universidad de Castilla-La Mancha	2008
Diploma de estudios avanzados de Doctorado	Universidad de Castilla-La Mancha	2007
Certificado de aptitud pedagógica	Universidad de Extremadura	2005
Licenciado en ciencias químicas	Universidad de Castilla-La Mancha	2004

## Parte B. RESUMEN DEL CV

During my undergraduate studies, I developed my skills as a synthetic chemist in the Dept. of Organic Chemistry at the University of Castilla - La Mancha (UCLM). In 2008 I obtained the degree of European Doctor in Chemical Sciences (summa cum laude, UCLM, Prof. A. Díaz-Ortiz and Dr. P. Prieto) combining the synthesis of heterocyclic systems with the use of microwave radiation (JCCM grant). I reinforced the multidisciplinary character of the thesis with a 4-month stay (José Castillejo programme, (JCCM)) at the U. of Cambridge (Prof. J. Goodman, UK), introducing me on the use of computational tools. That was the beginning of my interest in the combined theoretical-experimental study to understand chemical processes. I did a postdoctoral stay at the University of the Basque Country (UPV/EHU) in the Bioorganic Chemistry and Molecular Modelling group (Prof. F. P. Cossío) where I developed models for pericyclic reactions and silylated compounds, in close collaboration with experimentalists. I published 13 articles in international journals (Angew. Chem. Int. Ed. 2011,50,1092-1096;2011,50, 6060-6064 (cover); 2011 50, 10414-10416; Chem. Sci. 2012,3,1486-1491). In 2011 I decided to deepen my knowledge of the quantum-physical

basis of chemistry by doing a postdoctoral stay at the Dept. of Theoretical Chemistry of the Vrije U. of Amsterdam (VU, Prof. F. M. Bickelhaupt, The Netherlands). There I developed a more realistic method for analysing reaction profiles including solvent effects explicitly (Chem. Eur. J. 2016,22, 4431-4439, corresponding author, cover page) that has been used in numerous subsequent works. I participated in the practical classes of the Computational Chemistry course of the Master's programme in Chemistry (VU). At the end of 2012 I rejoined the Dept. of Organic Chemistry I (UPV/EHU) after obtaining the Ikerbasque Fellow position. With the experience gained on the mechanisms of synthesis of heterocyclic compounds, my interest in the usefulness of these species began: how to predict their properties, modify and improve them. Thus, I started my independent research career based on three main research lines: (a) Predictive computational analysis in the selectivity of chemical reactions; (b) Improvement of the synthetic processes and the optoelectronic and pharmacological properties of heterocyclic compounds and (c) study of the reactivity of organic and organometallic radicals and their photoexcited derivatives. As a result, I have published 17 articles as a corresponding author. I have elucidated the reaction mechanism of synthesis of organophosphorus derivatives, allowing access to a new family of compounds with interesting optoelectronic and pharmacological properties (Chem. Eur. J. 2017 23,13919- 13928 (cover, highlighted as hot paper); 2017 23, 17487-17496 (cover); 2019 25, 9035-9044). In addition, I have demonstrated the predictive character of computational methods in pericyclic reactions (J. Org. Lett. 2017,82,6298-6312, ChemPhysChem 2021,1805-1813) and substitution (J. Org. Lett. 2018,83,15101-15109; Chem. Asian. J. 2018,13,1138-1147 (cover)) by designing more selective synthetic methodologies. As a result, I obtained my consolidation as an independent Ikerbasque Research Associate in 2017. Since 2021 I have participated as a lecturer in master classes of the Chemistry and Industrial programme (UPV/EHU) and master's degree in chemistry (UCLM). In 2023 I obtained the I3 certification. Since July 2023 I am member of the editorial board of Int. J. Quantum Chem. journal.

In total, the scientific relevance of my work is reflected in the authorship of 89 publications (9 covers, 6 as first author and 20 as corresponding author) in highly prestigious international scientific journals (Angew. Chem. Int. Ed., J. Am. Chem. Soc., Nature Commun., Chem. Eur. J., Chem. Sci.), co-authorship of a book chapter; presentation in 20 national and international scientific congresses (11 oral communications) and 7 invited conferences in universities in Spain, The Netherlands, Sweden, France and UK. In addition, I have been member of the local organizing committee of 4th Brazil- Spain Workshop in Organic Chemistry (2014) and IX International School on Organometallic Chemistry Marcial Moreno Mañas (2016) as well as organizer of 1st Spanish Workshop on Phosphorus Chemistry (1SWPC, 2021), 2SWPC (2022) and 19th European Workshop on Phosphorus Chemistry & 3SWPC (2023). I have participated in 11 research projects and I am a reviewer for 25 international journals. I have been the supervisor of 1 PhD thesis (plus 2 in progress), 1 Master's thesis and supervisor of 2 Bachelor's theses (plus 2 in progress). In addition, I have been a member of 11 doctoral theses (U. Oxford, U. Stockholm, VU Amsterdam, UPV/EHU, U. Extremadura (UEx), UCLM, U. de Málaga and U. Alicante (UA), 4 master's theses (Univ. de Navarra-UPV/EHU) and 20 final degree theses (UPV/EHU).

## Parte C. LISTADO DE APORTACIONES MÁS RELEVANTES

### C.1. Publicaciones más importantes en libros y revistas con “peer review” y conferencias

AC: Autor de correspondencia; (nº x / nº y): posición firma solicitante / total autores. Si aplica, indique el número de citaciones

- 1 Artículo científico.** J Sanchez-Quesada; C López-Cruz; A de Cózar; A Arrieta; I Arrastia; F. P. Cossío. 2024. Dehydration of alcohols catalyzed by copper(ii) sulfate: type II dyotropic reactions and stepwise mechanisms. Organic and Biomolecular Chemistry. RSC. 22-9, pp.1800-1811.

- 2 **Artículo científico.** A Ugartemendia; J. M. Mercero; E Jimenez-Izal; A de Cózar. 2024. Doping Effects on Ethane/Ethylene Dehydrogenation Catalyzed by Pt<sub>2</sub>X Nanoclusters. *ChemPhysChem*. Wiley. 25-12, pp.e202400095.
- 3 **Artículo científico.** A López-Francés; Z Serna-Burgos; X del Corte; J. M. de los Santos; A de Cózar; J Vicario. 2024. Exploring the Reactivity of Rigid 1-Azadienes Derived from Methylene  $\gamma$ -Lactams. Applications to the Stereoselective Synthesis of Spiro- $\gamma$ -Lactams. *Journal of Organic Chemistry*. ACS. 89-13, pp.9502-9515.
- 4 **Artículo científico.** A de Cózar; A Arrieta; F. P. Cossío. 2024. On the Role of the Solvent in the Synthesis of Spirocycles from Alkyne Cations Catalyzed by Triflic Acid: A DFT Study. *European Journal of Organic Chemistry*. Wiley. 2733-33, pp.e202400347.
- 5 **Artículo científico.** (1/3) Abel de Cózar (AC); Ana Arrieta; Fernando P. Cossío. 2023. Selectivity in Cationic Cyclizations Involving Alkynes: A Computational Study on the Biomimetic Synthesis of Ste. *Chemistry a European Journal*. WILEY-V C H VERLAG GMBH. 29-19, pp.e202300666-e202300666-13. ISSN 0947-6539. <https://doi.org/10.1002/chem.202204028>
- 6 **Artículo científico.** (1/2) Abel de Cózar (AC); Carlos Romero-Nieto. 2023. Boundaries of the Hyperconjugation from it-Extended Six- Membered Phosphorus Heterocycles. *Inorganic Chemistry*. AMER CHEMICAL SOC. 61-10, pp.4097-4105. ISSN 1520-510X. <https://doi.org/10.1021/acs.inorgchem.2c03884>
- 7 **Artículo científico.** A López-Francés; X del Corte; Z Serna-Burgos; J. M. de los Santos; A de Cózar; J Vicario. 2023. Chiral self-recognition in a bispericyclic cyclodimerisation reaction of 1-azadienes. *Organic Chemistry Frontiers*. RSC. 10-24, pp.6103-6111.
- 8 **Artículo científico.** A de Cózar; A Arrieta; I Arrastia; F. P. Cossío. 2023. Higher-Order Electrocyclizations in Biological and Synthetic Processes. *ChemPlusChem*. Wiley. 88-11, pp.e202300482.
- 9 **Artículo científico.** (1/1) Abel de Cózar (AC). 2022. Diastereoselectivity on Intramolecular Alder-ene Reaction of 1,6-Di. *ChemPhysChem*. WILEY-V C H VERLAG GMBH. 23-23, pp.e202200377-e202200377-9. ISSN 1439-7641. <https://doi.org/10.1002/cphc.202200377>
- 10 **Artículo científico.** Ana Gonzalez Moreno; (2/5) Abel de Cózar (AC); Pilar Prieto; Eva Dominguez; Antonio Heredia. 2022. Radiationless mechanism of UV deactivation by cuticle phenolics in plants. *Nature Communications*. Nature. 13, pp.1786-1786-11. <https://doi.org/10.1038/s41467-022-29460-9>

## C.2. Congresos

- 1 Abel de Cózar; Ana Arrieta; Fernando P Cossio. Selectivity and solvent effects in alkyne cationic cyclizations. CBOND 2024. VU amsterdam. 2024. Holanda.
- 2 Adrian Lopez-Frances; Javier Vicario; Abel de Cózar. DFT EVALUATION OF STEREOSELECTIVE SYNTHESIS OF TETRASUBSTITUTED  $\alpha$ -AMINOPHOSPHONIC ACID DERIVATIVES. Spanish workshop on Phosphorus chemistry. Universidad del País Vasco- Universidad de Castilla la mancha. 2024.
- 3 Adrian Lopez-Frances; Javier Vicario; Abel de Cózar. Stereoselective Synthesis of Tetrasubstituted  $\alpha$ - Aminophosphonic Acid Derivatives: A Computational Approach. European workshop on Phosphorus chemistry. Julius-Maximilians-Universität Würzburg. 2024. Alemania.
- 4 A. de Cózar. Unraveling reaction mechanisms with theoretical tools. Université de Bordeaux- Institut des Sciences Moleculaires Seminar. Université de Bordeaux. 2023. Francia. Participativo - Plenaria. Jornada.
- 5 Andoni Ugartemendia; Jose M. Mercero; Elisa Jimenez-Izal; Abel de Cózar. Effect of Pt<sub>2</sub>X Doping on Ethane Dehydrogenation. 19th European Workshop on Phosphorus Chemistry & 3rd Spanish Workshop on Phosphorus Chemistry. DIPC-ULCM. 2023. España. Participativo - Ponencia oral (comunicación oral). Congreso.
- 6 Theoretical Studies on Phosphaphenylene Synthesis and their Supramolecular Assemblies. Universidad de Málaga- Organic Chemistry Lecture. Universidad de Málaga. 2023. España. Participativo - Ponencia invitada/ Keynote.

- 7 Theoretical Studies on Phosphaphenalene Synthesis and their Supramolecular Assemblies. Stockholm University- Organic Chemistry Lecture. Stockholm University. 2022. Suecia. Participativo - Ponencia invitada/ Keynote.

### C.3. Proyectos o líneas de investigación

- 1 **Proyecto.** Development and Proof of Concept of Theoretical and Predictive Models of Chemical Reactions with Direct Application in the Organic Synthesis of Fragrance Ingredients. IFF BENICARLO, S.A.. Abel de Cózar Ruano. (Universidad del País Vasco). 01/06/2024-31/05/2026. 87.474,14 €.
- 2 **Proyecto.** QUÍMICA BIOORGANICA, QUÍMICA SUPRAMOLECULAR Y MODELIZACION MOLECULAR. (Universidad del País Vasco). 01/01/2022-31/12/2025. 346.500 €.
- 3 **Proyecto.** Inmunoterapia génica y celular monitorizada mediante nanopartículas para la modulación clínica de la tolerancia inmunológica. Junta de Andalucía. Francisco García-Cozar. (H. Puerto Real). 2018-2020. 499.142,58 €.
- 4 **Proyecto.** Caracterización y desarrollo de nuevas fibras basadas en seda de Nephile Clavides, Nephile Inaurata y otros arácnidos de interes commercial MNS20013. (Universidad Regional Amazónica (IKIAM)). 01/03/2014-01/06/2017. 35.057 €.
- 5 **Proyecto.** Estudios teóricos y experimentales sobre el mecanismo y las aplicaciones en catálisis de las reacciones de cicloadición. (Universidad del País Vasco). 01/01/2014-31/12/2016. 175.450 €.