

Part A. PERSONAL INFORMATION		CV date	29/01/2021
First and Family name	ANA CASTRO MORERA		
Social Security, Passport, ID number		Age	
Researcher numbers	Researcher ID	K-8831-2014	
	Orcid code	0000-0001-7526-6717	

A.1. Current position

Name of University/Institution	INSTITUTO DE QUÍMICA MÉDICA (IQM-CSIC)		
Department	Fármacos innovadores y quimioinformática		
Address and Country	Juan de la Cierva, 3, 28006, Madrid (SPAIN)		
Phone number	E-mail	acastro@iqm.csic.es	
Current position	Tenured Scientific/Director IQM	From	2002/2015
Espec. cód. UNESCO	239001, 230206		
Palabras clave	Medicinal Chemistry, organic chemistry, drug design		

A.2. Education

PhD	University	Year
Chemistry	<i>Universidad Autónoma de Madrid</i>	1996

A.3. JCR articles, h Index, thesis supervised...

Number of "sexenios": 5: Investigación 4 (2019) /Transferencia 1 (2000-09)
Supervisor of Ph D thesis: 5 [(1) 2005, (1) 2006, (1) 2007, (1) 2010 (1) 2016]
Total cites: 2796 cites (Scopus)
Publications in Q1: 34
H-index (Scopus): 28

Part B. CV SUMMARY (max. 3500 characters, including spaces)

My scientific career has been focusing on the medicinal chemistry field, between academia and industry. During this time, I have been participating in several drug discovery programs, aimed at various therapeutic areas, the most significant scientific contributions coming from the area of central nervous system diseases. More specifically, I have been actively involved in the pharmaceutical development of new disease modifying drugs for treatment of Alzheimer disease.

In recent years, my scientific interests are focused on the discovery of new chemical entities that modulate proteins through allosteric mechanisms.

My academic career have been developed at the Institute of Medical Chemistry (IQM_CSIC), where I carried out my doctoral thesis (1992-1996), which I completed with a post-doctoral fellowship at the University of Oxford (1996-1999). After joining the IQM (1999), I obtained a position as tenured scientist (2002-). At the end of 2004, I became part of the biotechnology company as Medicinal Chemistry Department's Director (2004-2009).

Co-author of 80 scientific papers in the area and supervisor of five doctoral theses. Participation and management of different research projects. Involvement in R&D management (Technical Vice-Director (2010-2011) and Deputy Director of IQM (2011-2015). Participation in the organization of scientific congresses and conferences (organizing and/or scientific committees). My experience in the private sector has allowed me to have an overview of the requirements to successfully complete the processes of technology transfer; reflected in 12 patent applications, of which 4 belong to this last stage (2011-present).

In 2010, I have resumed my academic research activity at IQM, as an independent researcher, which I have been combining with management tasks as current Director of IQM since 2015.

Part C. RELEVANT MERITS

C.1. Publications (including books)

- Aledavood E, Moraes G, Lameira J, Castro A, Luque FJ, Estarellas C. Understanding the Mechanism of Direct Activation of AMP-Kinase: Toward a Fine Allosteric Tuning of the Kinase Activity. 2019 J Chem Inf Model 59(6):2859-2870.
- Bort A, Quesada S, Ramos-Torres A, Gargantilla M, Priego EM, Raynal S, Lepifre F, Gasalla JM, Rodríguez-Henche N, Castro A, Díaz-Laviada I. 2018. Identification of a novel 2-oxindole fluorinated derivative as in vivo antitumor agent for prostate cancer acting via AMPK activation. Scientific Reports, 8:4370.
- Sánchez R, Martínez J, Castro A, Pedrosa M, Quirce S, Rodríguez-Pérez R, Gasset M. The amyloid fold of Gad m 1 epitopes governs IgE binding. 2016. Scientific Reports, 6:32801.
- López-Ogalla, J., García-Palomero, E., Sánchez-Quesada, J., Rubio, L., Delgado, E., García, P., Medina, M., Castro, A., Muñoz, P. 2014. Bioactive prenylated phenyl derivatives derived from marine natural products: Novel scaffolds for the design of BACE inhibitors. MedChemComm, 5 (4), 474-488.
- Jerez MJ, Jerez M, González-García C, Ballester S, Castro A. 2013. Combined use of pharmacophoric models together with drug metabolism and genotoxicity "in silico" studies in the hit finding process. J Comput Aided Mol Des 27(1), 79- 90
- Palomo, V., Perez, D.I., Perez, C., Morales-Garcia, J.A., Soteras, I., Alonso-Gil, S., Encinas, A., Castro, A., Campillo, N.E., Perez-Castillo, A., Gil, C., Martinez, A. 2012. 5-Imino-1,2,4-thiadiazoles: First small molecules As substrate competitive inhibitors of glycogen synthase kinase 3. Journal of Medicinal Chemistry, 55 (4), 1645-1661.
- Medina M, Castro A. 2008. Glycogen synthase kinase-3 (GSK-3) inhibitors reach the clinic. Curr Opin Drug Discov Devel 533-543.
- Pérez M, Pérez DI, Martínez A, Castro A, Gómez G, Fall Y. 2009. The first enantioselective synthesis of palinurin. Chem. Commun. 3252 3254.
- Porcal W, Hernández P, González M, Ferreira A, Olea-Azar C, Cerecetto H, Castro A. 2008. Heteroarylnitrones as drugs for neurodegenerative diseases: synthesis, neuroprotective properties, and free radical scavenger properties. J Med Chem 6150-6159.

C.2. Research projects and grants

- RTI2018-095544-B-I00: Fighting chronic diseases with therapeutic approaches to modulate the endocannabinoid system. AEI. Programa estatal de I+D+i orientada a los Retos de la Sociedad. PI1: Nadine Jagerovic; PI2: Ana Castro. 2019-2021. 157.300 €
- Fundación Eugenio Rodríguez Pascual AMPK activators as treatment for vascular diseases associated with obesity. PI: Soledad Fernández-Alfonso/Ana Castro 2018. 11.375 €
- SAF2014-52661-C3-1-R: Amyloids as targets for preventing fish allergies. MINECO. Programa Estatal de I+D (Retos de la Sociedad), PI1: María Gasset; PI2: Ana Castro (2016-2017). 2015-2017. 217.800 €
- CTQ2010-19690: Synthesis of AMPK activators: A relevant kinase in metabolic processes and neuronal survival. MICINN. Plan Nacional (Programa Investigación Química Básica). PI Ana Castro. 2011-2014. 90.750 €

C.3. Contracts

- Contract: Development, synthesis and chemical characterization of IND_1316. PI Ana Castro. 2017. 8.000 €. CIBER.

- Patent licensed: Heterocyclic inhibitors of glycogen synthase kinase GSK-3 (ES-200001185, WO01/85685). Company: Neuropharma/Noscira. 21/07/2000 to 11/05/2020. Royalties: 138.706,69 €

C.4. Patents

- Sánchez Herreros Rosa, Martínez Fernández Javier, Castro Morera Ana, Gasset Vega María, Rodríguez Pérez Rosa, Pedrosa Delgado María, Quirce Gancedo Santiago, Food allergen extracts and methods of producing and using the same. Application Number: EP16382413.9. Date of Receipt 06. 09. 2016. Entity: CSIC, Fundación para la Investigación Biomédica del Hospital Universitario la Paz

- Castro Morera Ana, Quesada Sánchez Sergio, Díaz-Lavidada Marturet Inés, Rodríguez Henche Nieves, Ramos Torres Agata, Bort Bueno Alicia. Indolin-2-one derivatives and their therapeutic use. P201630826. Country ES. Priority date: 17.06.2016. Entity: CSIC, UAH.

- Castro Morera Ana, Sanz Bigorra Pascual, Quesada Sánchez Sergio, Garcia Gimeno María Adelaida, Luque Garriga, Francisco Javier, Bidón-Chanal Badia, Axel. Spiric compounds derived from oxindol-pyrazol [3,4-b] pyridone and their therapeutic uses. P201531786. Country ES. Priority date: 10.12.2015. Extended countries: WO/2017/098073. PCT/ES2016/070868 Date: 09.12.2016. Entity: CSIC, CIBER, UB

- Castro Morera Ana, Sanz Bigorra Pascual, Vela Ruiz Marta, Garcia Gimeno María Adelaida. Derivatives of indol for the prevention and/or treatment of diabetes and related disorders. P201431364. Country ES. Priority date: 19.09.2014. Extended countries: WO 2016042194 A1. US 20170283378 A1. PCT/ES2015/070677. Entity: CSIC, CIBER

- Medina Padilla, Miguel; Castro Morera, Ana; (+2) Substituted phenanthroline derivatives for the treatment of neurodegenerative or haematological diseases or conditions, or cáncer. PCT/EP2009/066817 Country: ES Priority date: 17.06.2010 Entity: Noscira Extended countries: PCT WO/2010/066832. Use of Patent: Noscira

- Martinez Gil, Ana; Castro Morera, Ana; (+5). Heterocyclic inhibitors of Glycogen Synthase Kinase GSK-3 ES200001185 and GB0030284.4 PCT (WO01/85685): ES, GB. Priority date: 11.05.2000. Entity: CSIC-UAM. Licensed patent: Europe (EP 1286964 B1, Spain, United Kingdom, Belgium, Switzerland, Cyprus, Germany, Denmark, Finland, France, Greece, Croatia, Ireland, Italy, Liechtenstein, Lithuania, Luxembourg, Austria, Latvia, Monaco, Macedonia, Holland, Portugal, Romania, Sweden, Slovenia and Turkey), USA (US 7,781,643), Australia (AU2006200668), and Republic of Korea. DESIGNATED COUNTRIES: Canada, Japan, China, Israel, Mexico (MX2002/011079), Brazil, Hungary (HU0302002), Poland, Czech Republic (CZ296087) and Russia (RU2002133222). Use of Patent: Noscira

C.5, C.6, C.7... (e. g., Institutional responsibilities, memberships of scientific societies...)

C.5 Doctoral Theses supervised

- **2016** Exploring AMPK as a therapeutic target through the discovery of new modulators. Sergio Quesada Sánchez. Faculty of Chemistry. UCM. Papers: 1

- **2010** BACE-1 inhibitors for the treatment of Alzheimer's disease: Synthesis and biological evaluation of new derivatives of marine prototypes. Javier López-Ogalla. Faculty of Chemistry. UNED. Papers: 1

- **2007** Research and development of nitrones as oxidative stress modulating agents. Williams Porcal. Faculty of Chemistry. University of the Republic. Montevideo. Uruguay. Papers: 8

C6. Experience in the organization of R&D activities organization

- Participation in the Organizing Committee of the Spanish Italian Medicinal Chemistry Congress. Barcelona. **2015**
- Participation in the Organizing Committee of the XI Conference of the Spanish Society of Therapeutic Chemistry. Malaga. **2014**
- Participation in the Organizing Committee of the IV Summer School of the Spanish Society of Therapeutic Chemistry. Tres Cantos. Madrid. **2014**
- Participation in the Organizing Committee of the XVII Congress of the Spanish Society of Therapeutic Chemistry. Madrid. **2013**
- Participation in the Scientific Committee of the X Conference of the Spanish Society of Therapeutic Chemistry. Segovia. **2012**

C7. R&D management experience

- President of the Board of the Organic Chemistry Centre "Lora Tamayo" (CSIC) **2016-2018**
- Director of Medicinal Chemistry Institute (IQM_CSIC) **2015-present**
- Deputy Director of Medicinal Chemistry Institute (IQM_CSIC). **2011-2015**
- Technical Vice-Director of Medicinal Chemistry Institute (IQM_CSIC). **2009-2011**
- Secretary of the Spanish Society of Therapeutic Chemistry. **2011-2015**
- Member of the Spanish Society of Therapeutic Chemistry. **2008-2010**
- Treasurer of the Spanish Society of Therapeutic Chemistry. **2003-2007**