CURRÍCULUM VÍTAE NORMALIZADO

Generated from: Editor CVN de FECYT

Date of document: 27/01/2019

v 1.4.0

12c42631db2fe23e3df8b31ed0bf73e2

GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

FECYT FUNDACIÓN ESPAÑOLA PARA LA CIENCIA Y LA TECNOLOGÍA

Summary of CV

This section describes briefly a summary of your career in science, academic and research; the main scientific and technological achievements and goals in your line of research in the medium -and long- term. It also includes other important aspects or peculiarities.

Dra. Ana M. Gamo received her PhD from Universidad Complutense de Madrid (UCM, Madrid, Spain) in the field of Organic Chemistry under the supervision of Prof. Mª Luz López Rodríguez. During her PhD, she developed fluorescent and biotinylated probes to study GPCRs, particularly the serotonin 5-HT1A Receptor. This work was worth two awards from two pharmaceutical companies (SEQT-Almirall-2011, finalist at Lilly-2013) and produced 3 scientific publications. She continued her research degree at Medicinal Chemistry Institute (IQM-CSIC, Madrid, Spain) with two consecutive contracts involved in two main projects: “Development of heterocyclic anti-chikungunya compounds”, under the supervision of Dr. María Jesús Pérez Pérez; and “Development of peptides and peptidomimetics to inhibit protein-protein interaction in Trypanothione Reductase of Leishmania Infantum”, under the supervision of Prof. María José Camarasa and Dr. Sonsoles Velázquez. Research that has also been published in scientific journals.

In 2015 she started her postdoctoral training at Scripps Research Institute (San Diego, CA, USA) in the laboratory of Prof. Edward Roberts, involved in a lead optimization process of kappa opioid receptor (KOR) antagonists that yielded a clinical candidate (BTRX-335140), which is currently in phase 1 clinical trials for the treatment of neuropsychiatric disorders, and which publication is in press in the Journal of Medicinal Chemistry.

Currently working as a postdoctoral researcher at Calibr (at Scripps Research, institution started by Prof. Peter Schultz), under the supervision of Dr. Arnab Chatterjee she is involved in two main programs one founded by the JDRF focused on the identification of novel treatments for type 1 diabetes and other founded by Gates Foundation aimed of developing new non nucleotide STING agonist for the treatment of autoimmune and tumor pathologies, work under provisional U.S. patent application.

ORCID: **0000-0002-7171-9878**

Current professional situation

Employing entity: The Scripps Research Institute (TSRI) **Type of entity:** R&D Centre
Department: Calibr
Professional category: Postdoctoral fellow
City employing entity: San Diego, California, United States of America
Start date: 01/12/2016
Dedication regime: Full time
Performed tasks: Development of MST1 inhibitors for the treatment of Type 1 diabetes (T1D) founded by the Juvenile Diabetes Research Foundation (JDRF). Development of new no nucleotidic STING agonists. synthesis purification and characterization of new heterocyclic compounds. Medicinal chemistry. Structure-activity relationship (SAR). Structure-based drug design (SBDD) Principal Investigator: Arnab Chatterjee

Previous positions and activities

	Employing entity	Professional category	Start date
1	The Scripps Research Institute (TSRI)	Research Associate	16/11/2015
2	Consejo Superior de Investigaciones Científicas	Bachelor	25/04/2014
3	Consejo Superior de Investigaciones Científicas	Bachelor	14/04/2013
4	Universidad Complutense de Madrid	PhD student	01/03/2009
5	Universidad Complutense de Madrid	PhD student	01/01/2009
6	Universidad Complutense de Madrid	undergraduate student fellow	07/2007
7	MINISTERIO DE EDUCACION Y CIENCIA	undergraduate student fellow	10/2006

1 **Employing entity:** The Scripps Research Institute (TSRI) **Type of entity:** R&D Centre
Department: Chemistry
City employing entity: San Diego, United States of America
Professional category: Research Associate
Start-End date: 16/11/2015 - 30/11/2016 **Duration:** 1 year - 15 days
Performed tasks: Development of new kappa opioid receptor (KOR) antagonists. Project developed in high collaboration with the industry. Hit to Lead optimization to a clinical candidate. Synthesis purification and characterization of new heterocyclic compounds. Medicinal chemistry. Structure-activity relationship (SAR). ADME evaluation. Principal Investigator: Edward Roberts

2 **Employing entity:** Consejo Superior de Investigaciones Científicas **Type of entity:** State agency
Department: Instituto de Biologia Molecular Eladio Viñuela (IBMEV)
Professional category: Bachelor
Start-End date: 25/04/2014 - 31/10/2015 **Duration:** 1 year - 6 months
Dedication regime: Full time
Primary (UNESCO code): 239001 - Design. Synthesis and study new drugs
Performed tasks: Development of new heterocyclic compounds for the regulation of the activity of transcriptional coactivator p300 in tumor, inflammation, infectious or autoimmune diseases. Principal Investigators:María Jesús Pérez Pérez (IQM-CSIC) y Yolanda Revilla (IBMEV-CSIC) Tasks: Synthesis, purification and charazterization of the new compounds. SAR. Solubility measurements.

3 **Employing entity:** Consejo Superior de Investigaciones Científicas **Type of entity:** State agency
Department: Instituto de Química Médica
Professional category: Bachelor
Start-End date: 14/04/2013 - 31/12/2013 **Duration:** 8 months - 15 days
Dedication regime: Full time
Primary (UNESCO code): 239001 - Design. Synthesis and study new drugs
Performed tasks: Inhibition of protein-protein interaction in Trypanothione Reductase of Leishmania Infantum (TryR-Li). Principal Investigator: Sonsoles Velázquez y María José Camarasa Rius. Tasks: synthesis in solid phase and purification of peptides and peptidomimetics. Proteolitic stability meassurements.

4 **Employing entity:** Universidad Complutense de Madrid **Type of entity:** University
Department: Organic chemistry
Professional category: PhD student
Start-End date: 01/03/2009 - 28/02/2013 **Duration:** 4 years
Type of contract: Grant-assisted student (pre or post-doctoral, others)
Dedication regime: Full time
Primary (UNESCO code): 230291 - Chemical biological macromolecules; 230600 - Organic chemistry
Performed tasks: predoctoral fellowship name: "Contrato de Personal Investigador de apoyo de la Comunidad de Madrid (2008)" Project title: Development of chemical probes for the study of G-coupled protein receptors (GPCRs). Application to the serotoninergic receptor 5-HT1A. Principal Investigator: Mª Luz López Rodríguez, Bellinda Benhamú Salama, Mar Martín-Fontecha. Tasks: synthesis, purification and characterization (NMR, LCMS, IR) of new molecular entities. In particular synthesis of biotinilated and fluorescent probes (chemical tools). evaluation of the activity of the new compounds towards a pannel of GPCRs by radioligand binding experiments. Application of the new chemical tools in biological systems. Receptor visualization in systems of increasing complexity. Proteomic assays and data analysis. Teaching assistant of new master students

5 **Employing entity:** Universidad Complutense de Madrid **Type of entity:** University
Department: organic chemistry
Professional category: PhD student
Start-End date: 01/01/2009 - 28/02/2009 **Duration:** 2 months
Type of contract: Temporary employment contract
Primary (UNESCO code): 230291 - Chemical biological macromolecules; 230600 - Organic chemistry
Performed tasks: Development of new methodologies to study G-protein coupled receptors (GPCRs). Synthesis of fluorescent ligands with affinity for the serotoninergic receptor 5-HT1A

6 **Employing entity:** Universidad Complutense de Madrid **Type of entity:** University
Department: Organic chemistry
Professional category: undergraduate student fellow
Start-End date: 07/2007 - 12/2007
Type of contract: Grant-assisted student (pre or post-doctoral, others)
Dedication regime: Part time
Performed tasks: fellowship name: Beca de iniciación en la actividad investigadora de la UCM. Aim: Training on organic laboratory methods and techniques. Support in synthesis. curse 2007-2008.

7 **Employing entity:** MINISTERIO DE EDUCACION Y CIENCIA
Department: organic chemistry
Professional category: undergraduate student fellow
Start-End date: 10/2006 - 06/2007
Type of contract: Grant-assisted student (pre or post-doctoral, others)
Dedication regime: Part time
Performed tasks: fellowship name: Beca de Colaboración para estudiantes de licenciatura. Aim: Training on organic laboratory methods and techniques. Support in synthesis. Curse 2006-2007.

Education

University education

1st and 2nd cycle studies and pre-Bologna degrees

1 **University degree:** Higher degree
Name of qualification: Master in Organic Chemistry. Grade Point Average: 2.7 (out of 4.0) or 8.6 (out of 10)
Degree awarding entity: Universidad Complutense de Madrid **Type of entity:** University
Date of qualification: 09/2009
Average mark: Good

2 **University degree:** Higher degree
Name of qualification: Bachelor's Degree in Chemistry. Grade Point Average: 2.3 (out of 4.0)
Degree awarding entity: Universidad Complutense de Madrid **Type of entity:** University
Date of qualification: 06/2007
Average mark: Good

Doctorates

Doctorate programme: Ph.D. in Organic Chemistry
Degree awarding entity: Universidad Complutense de Madrid **Type of entity:** University
Date of degree: 13/11/2014
Thesis title: Desarrollo de sondas para el estudio de los receptores acoplados a proteína G. Aplicación al receptor serotoninérgico 5-HT1A
Thesis director: María Luz López-Rodrígez
Thesis co-director: Bellinda Benhamú; Mar Martín-Fontecha
Obtained qualification: Summa Cum Laude
Recognition of quality: Yes

Specialised, lifelong, technical, professional and refresher training (other than formal academic and healthcare studies)

1 **Type of training:** symposium
Training title: I SEQT young research symposium
Awarding entity: SEQT
End date: 09/05/2014

2 **Type of training:** scientific sesion
Training title: Sesión Científica Conmemorativa del Año Internacional de la Química de la Real Academia Nacional de Medicina "Química y Medicina: Moléculas para Terapia y Diagnóstico"
Awarding entity: Real Academia Nacional de Medicina **Type of entity:** Society

End date: 26/05/2011 **Duration in hours:** 4 hours

3 **Type of training:** Conference
Training title: IX Jornadas de la SEQT
Awarding entity: SEQT
End date: 12/11/2010

4 **Type of training:** Symposium
Training title: I Symposium of Janssen-Cilag: Application of PET Imaging in the Discovery and Development of new Drugs
Awarding entity: Pharmacy San Pablo CEU University
End date: 11/05/2010

5 **Type of training:** Course
Training title: I Escuela de Verano: Desarrollo de Nuevos Fármacos
Awarding entity: SEQT
Aims of the entity: advanced lessons of medicinal chemistry for PhD students
End date: 05/07/2009

6 **Type of training:** symposium
Training title: XV scientific symposium Lilly foundation. Molecular Markers in Cancer Therapy: Present Use and Future Perspectives
Awarding entity: Lilly foundation
End date: 27/03/2009 **Duration in hours:** 16 hours

7 **Type of training:** Course
Training title: Curso de iniciación a la RMN
Awarding entity: Centro de asistencia a la investigación (CAI) de RMN de la UCM
End date: 01/2009 **Duration in hours:** 6 hours

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
English	B2	B2	B2	B2	B2
Spanish	C2	C2	C2	C2	C2

Teaching experience

General teaching experience

Type of teaching: Official teaching
Name of the course: Química aplicada a la biología
Type of teaching: Laboratory work
Type of subject: Core
University degree: Grado en Biología
Course given: first
Start date: 2010 **End date:** 2012

End date: 2012 **Type of hours/ ECTS credits:** Credits
Hours/ECTS credits: 2,7
Entity: Universidad Complutense de Madrid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias Biológicas

Experience supervising doctoral thesis and/or final year projects

Project title: Síntesis de ligandos marcados para el estudio de Receptores Acoplados a Proteínas G
Type of project: End of course project
Entity: Universidad Complutense de Madrid **Type of entity:** University
Student: Álvaro Lobato Fernández
Obtained qualification: with honors
Date of reading: 2012

Scientific and technological experience

Scientific or technological activities

R&D projects funded through competitive calls of public or private entities

1 **Name of the project:** Novel Beta Cell Protection Agents: TARP Program Extension. (Ref. 3-PAR-2016-241-I-X)
Entity where project took place: Calibr **Type of entity:** R&D Centre
City of entity: La Jolla, California, United States of America
Name principal investigator (PI, Co-PI....): Weijun Shen
Funding entity or bodies:
Juvenile Diavetes Research Foundation (JDRF)

Start-End date: 05/2016 - 02/2019
Total amount: 4.063.069,68 €

2 **Name of the project:** Discovery of non-addictive KOR antagonists for migraine prophylaxis. NIH Blueprint for Neuroscience Research grant 1UH2NS093030-01
Entity where project took place: The Scripps Research Institute **Type of entity:** R&D Centre
City of entity: La Jolla, California, United States of America
Name principal investigator (PI, Co-PI....): Edward Roberts
Funding entity or bodies:
National Institute of Health (NIH)

Start-End date: 09/2015 - 02/2017

3 **Name of the project:** Integration of strategies for the design and discovery of ligands with affinity for challenging targets of therapeutic interest in highly prevalent (AIDS OR CANCER) or neglected (LEISHMANIASIS) diseases. (Ref. SAF2012-39760-C02)
Entity where project took place: Instituto de Química Médica **Type of entity:** State agency
Name principal investigator (PI, Co-PI....): Maria Jose Camarasa

Funding entity or bodies:
MINECO/Plan Nacional (Programa Biomedicina)

Start-End date: 01/2013 - 12/2016
Total amount: 327.600 €

4 **Name of the project:** BIPEDD-CM. Bioinformatics Integrative Platform for structurE-based Drug Discovery 2. BIPEDD2 (ref. P2010/BMD-2457). 8 grupos + 2 laboratorios
Entity where project took place: Instituto de Química Médica **Type of entity:** State agency
Name principal investigator (PI, Co-PI....): Federico Gago Bádenas; María José Camarasa
Funding entity or bodies:
CAM- Programa de actividades de I+D entre grupos de Investigación. Edición Biociencias **Type of entity:** Consejería

Start-End date: 01/2012 - 12/2015
Total amount: 952.469 €

5 **Name of the project:** Desarrollo de compuestos para la regulación de la actividad del coactivador transcripcional p300 en patologías tumorales, inflamatorias, infecciosas o autoinmunes. Papel del sitio de fosforilación de la serina 384 (Ser384) por PKC como diana utilizada por el inhibidor viral A238L
Entity where project took place: CBM-CSIC
Name principal investigator (PI, Co-PI....): Yolanda Revilla
Nº of researchers: 8
Funding entity or bodies:
Genoma España (ahora FECYT)

Start-End date: 01/2012 - 12/2015

6 **Name of the project:** Descubrimiento y validación de nuevas dianas terapéuticas. Desarrollo de la plataforma MHit (S2010/BMD-2353)
Type of project: Research and development, including transfer **Geographical area:** Regional
Entity where project took place: Universidad Complutense de Madrid **Type of entity:** University
Nº of researchers: 15
Funding entity or bodies:
Comunidad de Madrid **Type of entity:** Consejería
City funding entity: Madrid, Community of Madrid, Spain

Start-End date: 01/2012 - 12/2015
Total amount: 741.750 €

7 **Name of the project:** Desarrollo de compuestos para la validación e identificación de dianas terapéuticas mediante química genómica directa e inversa (SAF2010-22198-C02-01)
Type of project: Research and development, including transfer **Geographical area:** National
Entity where project took place: Universidad Complutense de Madrid **Type of entity:** University
Name principal investigator (PI, Co-PI....): María Luz López-Rodríguez
Nº of researchers: 18
Funding entity or bodies:
Ministerio de Ciencia e Innovación **Type of entity:** Ministery
City funding entity: Madrid, Community of Madrid, Spain

Start-End date: 01/2011 - 06/2014
Total amount: 695.750 €

8 **Name of the project:** Desarrollo de nuevos agentes terapéuticos para el tratamiento de enfermedades neurodegenerativas y oncológicas (GR35/10-A, 2011)
Type of project: Research and development, including transfer
Entity where project took place: Universidad Complutense de Madrid **Type of entity:** University
Name principal investigator (PI, Co-PI....): Bellinda Benhamú Salama
Nº of researchers: 20
Funding entity or bodies:
Universidad Complutense de Madrid **Type of entity:** University
City funding entity: Madrid, Community of Madrid, Spain

Start-End date: 01/2011 - 12/2011
Total amount: 7.724 €

9 **Name of the project:** Aproximación multidimensional a la identificación y caracterización de nuevas dianas terapéuticas y al desarrollo de nuevos fármacos mediante el empleo de Química modular, nanocristales y semiconductores (quantum dots) y proteómica (S SAL-0249/2006; 2007-2010)
Entity where project took place: Universidad Complutense de Madrid **Type of entity:** University
Nº of researchers: 19
Funding entity or bodies:
Comunidad Autonoma de Madrid

Start-End date: 01/2007 - 12/2010

10 **Name of the project:** Desarrollo de nuevas metodologías de diseño molecular en el descubrimiento de fármacos e integración de nuevas técnicas para la identificación y validación de nuevas dianas terapéuticas (SAF2007-67008-C02-01)
Type of project: Research and development, including transfer **Geographical area:** National
Entity where project took place: Universidad Complutense de Madrid **Type of entity:** University
Name principal investigator (PI, Co-PI....): María Luz López-Rodríguez
Nº of researchers: 16
Funding entity or bodies:
Ministerio de ciencia y tecnología

Start-End date: 01/2008 - 10/2010
Total amount: 445.280 €

Results

Industrial and intellectual property

Title registered industrial property: AGONISTS OF STIMULATOR OF INTERFERON GENES STING
Inventors/authors/obtainers: Emili Chin; Luke Lairson; Arnab Chatterjee; Manoj Kumar; Ana M. Gamo
Entity holder of rights: California Institute for Biomedical Research (Calibr), a public benefit, not-for-profit corporation of California
Nº of application: U.S. Provisional Patent Application No. 62/633,409
Country of inscription: United States of America
Date of register: 21/02/2018

Scientific and technological activities

Scientific production

Publications, scientific and technical documents

1 Miguel Guerrero; Mariangela Urbano; Eun-Kyong Kim; Ana M. Gamo; Sean Riley; Lusine Abgaryan; Nora Leaf; Lori Jean Van Orden; Steven J. Brown; Jennifer Y. Xie; Frank Porreca; Michael Cameron; Hugh Rosen; Edward Roberts. Design and synthesis of clinical candidate BTRX-335140: a novel and selective kappa opioid receptor (KOR) antagonist. Journal of Medicinal Chemistry. In press. 2019.
Type of production: Scientific paper
Position of signature: 4
Total no. authors: 14

2 Alejandro Revuelto; Marta Ruiz-Santaquiteria; Hector de Lucio; Ana M. Gamo; Alejandra Carriles; Kilian Gutierrez; Pedro Sánchez-Murcia; Juan Hermoso; Federico Gago; María-José Camarasa; Antonio Jiménez-Ruiz; Sonsoles Velazquez. From peptidic to non-peptidic dimerization inhibitors of Leishmania infantum trypanothione reductase: pyrrolopyrimidine vs imidazole-phenyl-thiazole scaffolds. ACS Infectious Diseases. In revision. 2019.
Type of production: Scientific paper
Position of signature: 4
Total no. authors: 12

3 Federico Camicia; Ana M. Celentano; Malcolm E. Johns; John D. Chan; Lucas Maldonado; Hugo Vaca; Nicolás Di Siervi; Laura Kamentezky; Ana M. Gamo; Silvia Ortega-Gutierrez; Mar Martin-Fontecha; Carlos Davio; Jonathan S. Marchant. Unique pharmacological properties of serotonergic G-protein coupled receptors from cestodes. PLOS Neglected Tropical Diseases. 09/02/2018.
Type of production: Scientific paper
Position of signature: 9
Total no. authors: 13
Relevant results: Cestodes are a diverse group of parasites, some of them being agents of neglected diseases. In cestodes, little is known about the functional properties of G protein coupled receptors (GPCRs) which have proved to be highly druggable targets in other organisms. Notably, serotoninergic G-protein coupled receptors (5-HT GPCRs) play major roles in key functions like movement, development and reproduction in parasites.

4 Asier Gómez-SanJuan; Ana M. Gamo; Leen Delang; Alfonso Pérez-Sánchez; Siti Naqiah Amrun; Rana Abdelnabi; Sofie Jacobs; Eva-María Priego; María-José Camarasa; Dirk Jochmans; Pieter Leyssen; Lisa F P Ng; Guilles Querat; Johan Neyts; María-Jesús Pérez-Pérez. Inhibition of the replication of different strains of chikungunya virus by 3-aryl-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-ones. ACS Infectious Diseases. 4 - 4, pp. 605 - 619. 06/02/2018.

Type of production: Scientific paper

Position of signature: 2

Total no. authors: 15

Relevant results: The re-emergence of chikungunya virus (CHIKV) is a serious global health threat. CHIKV is an alphavirus that is transmitted to humans by Aedes mosquitoes; therefore, their wide distribution significantly contributes to the globalization of the disease. Unfortunately, no effective antiviral drugs are available. We have identified a series of 3-aryl-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-ones as selective inhibitors of CHIKV replication. New series of compounds have now been synthesized with the aim to improve their physicochemical properties and to potentiate the inhibitory activity against different CHIKV strains. Among these newly synthesized compounds modified at position 3 of the aryl ring, tetrahydropyranyl and N-t-butylpiperidine carboxamide derivatives have shown to elicit potent antiviral activity against different clinically relevant CHIKV isolates with 50% effective concentration (EC50) values ranging from 0.30 to 4.5 μM in Vero cells, as well as anti-CHIKV activity in human skin fibroblasts (EC50 = 0.1 μM), a clinically relevant cell system for CHIKV infection.

5 Ana M. Gamo; Hector de Lucio; Marta Ruiz-Santaquiteria; Sonia de Castro; Pedro A. Sánchez-Murcia; Miguel A. Toro; Kilian Jesús Gutiérrez; Federico Gago; Antonio Jiménez-Ruiz; María-José Camarasa; Sonsoles Velázquez. Improved proteolytic stability and potent activity against Leishmania infantum trypanothione reductase of α/β-peptide foldamers conjugated to cell-penetrating peptides. European Journal of Medicinal Chemistry. 140, pp. 615 - 623. 18/09/2017.

Type of production: Scientific paper **Format:** Journal

Position of signature: 1

Total no. authors: 11

Impact source: WOS

Impact index in year of publication: 4.816

Relevant results: The objective of the current study was to enhance the proteolytic stability of peptide-based inhibitors that target critical protein-protein interactions at the dimerization interface of Leishmania infantum trypanothione reductase (Li-TryR) using a backbone modification strategy. To achieve this goal we carried out the synthesis, proteolytic stability studies and biological evaluation of a small library of a/b3-peptide foldamers of different length (from 9-mers to 13-mers) and different a/b substitution patterns related to prototype linear a-peptides.We show that several 13-residue a/b3-peptide foldamers retain inhibitory potency against the enzyme (in both activity and dimerization assays) while they are far less susceptible to proteolytic degradation than an analogous a-peptide. The strong dependence of the binding affinities for Li-TryR on the length of the a,b-peptides is supported by theoretical calculations on conformational ensembles of the resulting complexes. The conjugation of the most proteolytically stable a/b-peptide with oligoarginines results in a molecule with potent activity against L. infantum promastigotes and amastigotes.

6 Alba Gigante; Asier Gómez-SanJuan; Leen Delang; Li Changqing; Oskía Bueno; Ana M. Gamo; Eva-María Priego; María-José Camarasa; Dirk Jochmans; Pieter Leyssen; Etienne Decroly; Bruno Coutard; Guilles Querat; Johan Neyts; María-Jesús Pérez-Pérez. Antiviral activity of [1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-ones against chikungunya virus targeting the viral capping nsP1. Antiviral Research. 144, pp. 216 - 222. 12/06/2017.

Type of production: Scientific paper

Position of signature: 6

Total no. authors: 15

Impact source: WOS

Impact index in year of publication: 4.307

Relevant results: Chikungunya virus (CHIKV) is a re-emerging alphavirus transmitted to humans by Aedes mosquitoes. Since 2005, CHIKV has been spreading worldwide resulting in epidemics in Africa, the Indian Ocean islands, Asia and more recently in the Americas. CHIKV is thus considered as a global health concern. There is no specific vaccine or drug available for the treatment of this incapacitating viral infection. We previously identified 3-aryl-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-ones as selective inhibitors of CHIKV replication and proposed the viral

capping enzyme nsP1 as a target. This work describes the synthesis of novel series of related compounds carrying at the aryl moiety a methylketone and related oximes combined with an ethyl or an ethyl-mimic at 5-position of the triazolopyrimidinone. These compounds have shown antiviral activity against different CHIKV isolates in the very low mM range based on both virus yield reduction and virus-induced cell-killing inhibition assays. Moreover, these antivirals inhibit the in vitro guanylylation of alphavirus nsP1, as determined by Western blot using an anti-cap antibody. Thus, the data obtained seem to indicate that the anti-CHIKV activity might be related to the inhibition of this crucial step in the viral RNA capping machinery.

7 Ana M. Gamo; Juan A. González-Vera; Ainoa Rueda-Zubiaurre; Dulce Alonso; Henar Vázquez-Villa; Lidia Martín-Couce; Óscar Palomares; Juan A. López; Mar Martín-Fontecha; Bellinda Benhamú; María L. López-Rodríguez; Silvia Ortega-Gutiérrez. Chemoproteomic approach to explore the target profile of GPCR ligands. Application to 5-HT1A and 5-HT6 receptors.Chemistry - A European Journal. 22 - 4, pp. 1313 - 1321. 12/11/2015.

Type of production: Scientific paper
Position of signature: 1
Total no. authors: 12
Impact source: WOS
Impact index in year of publication: 5.771

Relevant results: Determination of the targets of a compound remains an essential aspect in drug discovery. A complete understanding of all binding interactions is critical to recognize in advance both therapeutic effects and undesired consequences. However, the complete polypharmacology of many drugs currently in clinical development is still unknown, especially in the case of G protein-coupled receptor (GPCR) ligands. In this work we have developed a chemoproteomic platform based on the use of chemical probes to explore the target profile of a compound in biological systems. As proof of concept, this methodology has been applied to selected ligands of the therapeutically relevant serotonin 5- HT1A and 5-HT6 receptors, and we have identified and validated some of their off-targets. This approach could be extended to other drugs of interest to study the targeted proteome in disease-relevant systems.

8 Mario Fuente Revenga; Concepción Pérez; José A. Morales-García; Sandra Alonso-Gil; Ana Pérez-Castillo; Daniel-Henri Caignard; Matilde Yáñez; Ana M. Gamo; María Isabel Rodríguez-Franco. New insights on the pharmacology of 6-methoxy-1,2,3,4-tetrahydro-beta-carboline (pinoline) and melatonin – pinoline hybrids, displaying potent neurogenic properties. ACS Chemical Neuroscience (Journal cover). 6, pp. 800 - 810. 27/03/2015.

Type of production: Scientific paper **Format:** Journal
Position of signature: 8
Total no. authors: 9
Impact source: WOS
Impact index in year of publication: 4.348

Relevant results: 6-Methoxy-1,2,3,4-tetrahydro-beta-carboline (pinoline) and N-acetyl-5-methoxytryptamine (melatonin) are both structurally related to 5-hydroxytryptamine (serotonin). Here we describe the design, synthesis and characterization of a series of melatonin rigid analogues resulting from the hybridization of both pinoline and melatonin structures. The pharmacological evaluation of melatonin – pinoline hybrids comprises serotonergic and melatonergic receptors, metabolic enzymes (monoaminoxidases), antioxidant potential, the in vitro blood-brain barrier permeability, and neurogenic studies. Pinoline at trace concentrations and 2-acetyl-6-methoxy-1,2,3,4-tetrahydro-beta-carboline (2) were able to stimulate early neurogenesis and neuronal maturation in an in vitro model of neural stem cells isolated from the adult rat subventricular zone. Such effects are presumably mediated via serotonergic and melatonergic stimulation respectively

9 Dulce Alonso; Henar Vázquez-Villa; Ana M. Gamo; María Fernanda Martínez-Esperón; Mariola Tortosa; Alma Viso; Roberto Fernández de la Pradilla; Elena Junquera; Emilio Aicart; Mar Martín-Fontecha; Bellinda Benhamú; María Luz López-Rodríguez; Silvia Ortega-Gutiérrez. Development of fluorescent ligands for the human 5-HT1A receptor. ACS Medicinal Chemistry Letters. 1 - 6, pp. 249 - 253. WASHINGTON(United States of America): ACS, 14/05/2010. Available on-line at: <http://dx.doi.org/10.1021/ml100053y>. ISSN 1948-5875

Type of production: Scientific paper **Format:** Journal

Position of signature: 3
Total no. authors: 13
Relevant results: In this work, we report the design and synthesis of a set of fluorescent probes targeting the human 5-HT1A receptor (h5-HT1AR). Among the synthesized compounds, derivative 4 deserves special attention as being a high-affinity ligand (Ki = 2 nM) with good fluorescent properties (Iem > 1000 au and a fluorescence quantum yield of 0.26), which enables direct observation of the h5-HT1AR in cells. Thus, it represents the first efficacious fluorescent probe for the specific labeling of h5-HT1AR in cells. Our results provide the basis for the introduction of a variety of tags in scaffolds of G protein-coupled receptor (GPCR) ligands that enable visualization, covalent binding, or affinity pull-down of receptors. These strategies should contribute to the optimization of the therapeutic exploitation of known or new members of the GPCR superfamily by providing valuable information about their location or level of expression.

Works submitted to national or international conferences

1 **Title of the work:** DISCOVERY OF A NOVEL SMALL MOLECULE STING AGONIST AS A NEW CANCER IMMUNOTHERAPY
Name of the conference: 25th Biennial Congress of the European Association for Cancer Research
Type of participation: 'Participatory - poster
City of event: Amsterdam,
Date of event: 30/06/2018
End date: 03/07/2018
Organising entity: European Association for Cancer Research (EACR)
Emily Chin; Manoj Kumar; Ana M. Gamo Albero; Arnab Chatterjee; Luke Lairson. ESMO Open Cancer Horizons. 10.1136/esmoopen-2018-EACR25.450,

2 **Title of the work:** New MST1 inhibitors for the treatment of diabetes
Name of the conference: Calibr Symposium
Type of event: symposium
Type of participation: Participatory - oral communication
City of event: United States of America
Date of event: 26/04/2018
Organising entity: Calibr
City organizing entity: San Diego, United States of America
Ana Maria Gamo Albero Ana Maria Albero; Siying Zhu; Manoj Kumar; Taylor Baguley; Murali Surakattula; Nicky Rogers; Van Nguyen-Tran; Sean Joseph; Victor Chi; Arnab Chatterjee; Michael Petrassi; Weijun Shen; Mathew Tremblay.

3 **Title of the work:** POTENT LEISHMANICIDAL ACTIVITY OF PEPTIDES TARGETING THE DIMERIZATION INTERFACE OF TRIPANOTHIONE REDUCTASE BY USING CELL-PENETRATING PEPTIDES (CPPs)
Name of the conference: III SEQT young research symposium
Type of participation: 'Participatory - poster
City of event: Barcelona,
Date of event: 17/06/2016
Organising entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Marta Ruiz-Santaquiteria; Ana M. Gamo; Miguel Toro; Héctor de Lucio; Pedro Sánchez-Murcia; Federico Gago; Antonio Jiménez; María José Camarasa; Sonsoles Velázquez.

4 **Title of the work:** PYRROLOPYRIMIDINE-BASED α-HELIX MIMETICS TO INHIBIT THE DIMERIZATION INTERFACE OF TRYPANOTHIONE REDUCTASE OF LEISHMANIA INFANTUM
Name of the conference: III SEQT young research symposium
Type of participation: 'Participatory - poster

City of event: Barcelona,
Date of event: 17/06/2016
Organising entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Marina de Anabitarte; Marta Ruiz-Santaquiteria; Ana M. Gamo; Miguel Toro; Héctor de Lucio; Pedro Sánchez-Murcia; Federico Gago; Antonio Jiménez; María José Camarasa; Sonsoles Velázquez.

5 **Title of the work:** Chemoproteomic Approach to Explore the Target Profile of GPCR Ligands: Application to 5-HT1A and 5-HT6 Receptors
Name of the conference: III BIENNIAL MEETING OF THE CHEMICAL BIOLOGY GROUP / XII CARBOHYDRATE SYMPOSIUM
Date of event: 14/03/2016
End date: 16/03/2016
Organising entity: Centro de Investigaciones Biológicas **Type of entity:** State agency
Ana M. Gamo; Juan A. González-Vera; Ainoa Rueda-Zubiaurre; Dulce Alonso; Henar Vázquez-Villa; Lidia Martín-Couce; Oscar Palomares; Juan A. López; Mar Martín-Fontecha; Bellinda Benhamú; María Luz López-Rodríguez; Silvia Ortega-Gutiérrez.

6 **Title of the work:** α/β3-Peptide foldamers: potent dimerization inhibitors of Leishmania Infantum Trypanothione Reductase with improved proteolytic stability
Name of the conference: II SEQT young research symposium
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Madrid, Spain
Date of event: 12/06/2015
Organising entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Ana M. Gamo; Marta Ruiz-Santaquiteria; Pedro Sánchez-Murcia; Miguel A. Toro; Héctor de Lucio; Federico Gago; Antonio Jiménez-Ruiz; María José Camarasa; Sonsoles Velázquez.

7 **Title of the work:** Re-emerging viruses: [1,2,3]triazolo[4,5-D]pyrimidin-7(6H)-ones as potent and selective inhibitors of chikungunya virus replication
Name of the conference: II SEQT young research symposium
Type of participation: 'Participatory - poster
City of event: Madrid, Spain
Date of event: 12/06/2015
Organising entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Asier Gómez-SanJuan; Ana M. Gamo; Oskía Bueno; Alfonso Pérez-Sánchez; Alba Gigante; Susana Herrero; Pieter Leyssen; Johan Neyts; María José Camarasa; María-Jesús Pérez-Pérez.

8 **Title of the work:** Merging of pineal neurochemicals. Pharmacological profiles and neurogenic potential
Name of the conference: XVII SEQT Congress
Type of event: Conference
Type of participation: 'Participatory - poster
City of event: Madrid, Community of Madrid, Spain
Date of event: 02/10/2013
End date: 04/10/2013
Organising entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Mario Fuente Revenga; Nerea Fernández Sáez; Concepción Pérez; José A. Morales-García; Sandra Alonso-Gil; Ana Pérez-Castillo; Daniel-Henri Caignard; Dolores Viña; Matilde Yáñez; Ana M. Gamo; López-Rodríguez María Luz; Rodríguez-Franco María Isabel.

9 **Title of the work:** Development of molecular probes for the study of 5-HT1A receptor
Name of the conference: XI edition (2013) of Lilly Awards for PhD Students
Type of participation: 'Participatory - poster
City of event: Alcobendas, Spain
Date of event: 27/09/2013
Organising entity: Lilly España **Type of entity:** Business
Ana M. Gamo; Dulce Alonso; Henar Vázquez-Villa; Mar Martín-Fontecha; Bellinda Benhamú; María Luz López-Rodríguez; Silvia Ortega-Gutiérrez.

10 **Title of the work:** Development of chemical probes for the study of G protein-coupled receptors
Name of the conference: XXII International Symposium on medicinal chemistry
Type of participation: 'Participatory - poster
City of event: Berlín, Germany
Date of event: 02/09/2012
End date: 06/09/2012
Organising entity: European Federation for Medicinal Chemistry (EFMC)
Silvia Ortega-Gutiérrez; Ana M. Gamo; Lidia Martín-Couce; Dulce Alonso; Juan A. González-Vera; Henar Vázquez-Villa; Mar Martín-Fontecha; Bellinda Benhamú; María Luz López-Rodríguez.

11 **Title of the work:** Chemical probes for the study of G protein-coupled receptors
Name of the conference: XXIV Biennial Meeting of Organic Chemistry (RSEQ)
Type of participation: Participatory - oral communication
City of event: San Sebastián, Basque Country, Spain
Date of event: 11/07/2012
End date: 13/07/2012
Organising entity: Real Sociedad Española de Química **Type of entity:** Society
María Luz López-Rodríguez; Bellinda Benhamú; Mar Martín-Fontecha; Ana M. Gamo; Henar Vázquez-Villa; Juan A. González-Vera; Ainoa Rueda-Zubiaurre; Silvia Ortega-Gutiérrez.

12 **Title of the work:** Development of Chemical Probes for the Study of G Protein-Coupled Receptors
Name of the conference: I Reunión Bienal del Grupo Especializado de Química Biológica (GEQB) de la Real Sociedad Española de Química (RSEQ)
Type of participation: Participatory - oral communication
City of event: Santiago, Galicia, Spain
Date of event: 08/03/2012
End date: 09/03/2012
Organising entity: Real Sociedad Española de Química **Type of entity:** Sociedad
Silvia Ortega-Gutiérrez; Mar Martín-Fontecha; Ana M. Gamo; Henar Vázquez-Villa; Juan A. González-Vera; Bellinda Benhamú; María Luz López-Rodríguez.

13 **Title of the work:** Development of molecular probes for the study of 5-HT1A receptor
Name of the conference: XVI Congreso de la SEQT
Type of participation: 'Participatory - poster
City of event: Valencia, Valencian Community, Spain
Date of event: 18/09/2011
End date: 21/09/2011
Organising entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Ana M. Gamo; Dulce Alonso; Henar Vázquez-Villa; Mar Martín-Fontecha; Bellinda Benhamú; María Luz López-Rodríguez; Silvia Ortega-Gutiérrez.

14 **Title of the work:** Development of molecular probes for the study of 5-HT1A receptor
Name of the conference: II SEQT Summer School. Medicinal Chemistry in Drug Discovery: The Pharma Perspective
Type of participation: 'Participatory - poster
City of event: San Lorenzo del Escorial, Community of Madrid, Spain
Date of event: 26/06/2011
End date: 29/06/2011
Organising entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Ana M. Gamo; Dulce Alonso; Henar Vázquez-Villa; Mar Martín-Fontecha; Bellinda Benhamú; María Luz López-Rodriguez; Silvia Ortega-Gutiérrez.

15 **Title of the work:** Development of chemical probes for the study of G protein coupled receptors
Name of the conference: Frontiers in Medicinal Chemistry: Emerging Targets, Novel Candidates and Innovative Strategies
Type of participation: 'Participatory - poster
City of event: Estocolmo, Sweden
Date of event: 19/06/2011
End date: 21/06/2011
Organising entity: European Federation for Medicinal Chemistry (EFMC)
Bellinda Benhamú; Ana M. Gamo; Lidia Martín-Couce; Dulce Alonso; Juan A. González-Vera; Henar Vázquez-Villa; Mar Martín-Fontecha; Silvia Ortega-Gutiérrez; María Luz López-Rodríguez.

16 **Title of the work:** Development of chemical probes for the study of G protein-coupled receptors
Name of the conference: Second National Meeting on Medicinal Chemistry
Type of participation: Participatory - oral communication
City of event: Coimbra, Portugal
Date of event: 28/11/2010
End date: 30/11/2010
Organising entity: Sociedad Portuguesa de Química
Mar Martín-Fontecha; Dulce Alonso; Ana M. Gamo; Lidia Martín-Couce; Juan A. González-Vera; Henar Vázquez-Villa; Bellinda Benhamú; Silvia Ortega-Gutiérrez; Maria luz López-Rodríguez.

17 **Title of the work:** Synthesis of chemical probes for the study of serotonin 5-HT1A and 5-HT6 receptors
Name of the conference: XXIst International Symposium on Medicinal Chemistry
Type of participation: 'Participatory - poster
City of event: Bruselas, Belgium
Date of event: 05/09/2010
End date: 09/09/2010
Organising entity: European Federation for Medicinal Chemistry (EFMC)
Henar Vázquez-Villa; Mar Martín-Fontecha; Dulce Alonso; Ana M. Gamo; Juan A. González-Vera; María Fernanda Martínez-Esperón; Mariola Tortosa; Alma Viso; Roberto Fernández de la Pradilla; Elena Junquera; Emilio Aicart; Bellinda Benhamú; María Luz López-Rodríguez; Silvia Ortega-Gutiérrez.

Other dissemination activities

Title of the work: Taller de la aspirina, dentro de las actividades programadas en las Jornadas de Puertas Abiertas del CSIC
Name of the event: Semana de la ciencia y la tecnología en el CSIC 2013
Type of event: Fairs and exhibitions
City of event: Madrid, 2013, Spain
Date of event: 2013
Organising entity: Consejo Superior de Investigaciones Científicas
Type of entity: State agency

Other achievements

Obtained grants and scholarships

1 **Name of the grant:** Contrato de personal investigador de apoyo 2008
Aims: Pre-doctoral
Awarding entity: Comunidad de Madrid
Type of entity: Consejería de Educación
Conferral date: 01/03/2009
Duration: 4 years
End date: 28/02/2013

2 **Name of the grant:** Beca de iniciación en la actividad investigadora curso 2007-2008
Aims: laboratory training for undergraduate students
Awarding entity: Universidad Complutense de Madrid
Type of entity: University
Conferral date: 07/2007
End date: 12/2007

3 **Name of the grant:** Beca de Colaboración Curso 2006-2007
Aims: laboratory training for undergraduate students
Awarding entity: MINISTERIO DE EDUCACION Y CIENCIA
Conferral date: 10/2006
Duration: 1 year
End date: 06/2007

4 **Name of the grant:** grant to attend: IX JORNADAS DE LA SEQT
Aims: attend to scientific meeting
Awarding entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Duration: 3 days

5 **Name of the grant:** grant to attend: SEQT Second Summer School on Medicinal Chemistry: The pharma perspective
Aims: attend to scientific meeting
Awarding entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Duration: 4 days

Scientific societies and professional associations

1 **Name of the society:** Real Sociedad Española de Química (RSEQ)
Start date: 2015

2 **Name of the society:** Sociedad Española de Química Terapéutica (SEQT)
Start date: 2009

Prizes, mentions and distinctions

1 **Description:** finalist in the XI Lilly edition (2013) of PhD students awards
Awarding entity: Lilly España **Type of entity:** Business
Conferral date: 2013

2 **Description:** Almirall award in the XV young researchers SEQT awards
Awarding entity: SOCIEDAD ESPAÑOLA DE QUIMICA TERAPEUTICA
Conferral date: 2011