



Departamento de  
Química Farmacéutica y  
Orgánica

## **Investigación y desarrollo de fármacos (Drug design and development). Grupo CTS 130**

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### **Investigadores**

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### **Líneas de investigación**

- Diseño, síntesis y evaluación de la actividad biológica de inhibidores de la interacción ácido hialurónico y CD44 como compuestos antitumorales.
- Diseño y síntesis de nuevos inhibidores de colina quinasa con actividad antitumoral.
- Diseño y síntesis de compuestos antitumorales con estructura de purinas (e isómeros) unidas a heterociclos de 6 o 7 miembros fusionados a benceno.
- Diseño y síntesis de fármacos neuroprotectores.

### **Proyectos de investigación**

1. Título: Síntesis de kinurenaminas con actividad neuroprotectora frente al daño

mitocondrial inducido por el sistema NOS/NO. Entidad Financiadora: Instituto de Salud Carlos 111. PI021181

2. Título: Evaluación de kinurenaminas sintéticas como neuroprotectores frente al daño mitocondrial inducido por el sistema NOS/NO en parkinson experimental. Entidad Financiadora: CICYT (SAF2002-01688)
3. Título: Diseño, síntesis y evaluación biológica de nuevos inhibidores selectivos de mtNOS e iNOS. Entidad Financiadora: CICYT (SAF2005-07991-C02-02)
4. Título: Anillos benzofusionados O,N-acetálicos de siete y ocho miembros, obtenidos mediante síntesis en fase sólida, con actividad anticancerosa. Entidad Financiadora: Junta de Andalucía (Código del Proyecto: 00636, Proyecto de Excelencia)
5. Título: Design, synthesis and biological studies of novel 1,4-benzoxazepines as antitumour compounds; Entidad Financiadora: Unión Europea
6. Título: Convocatoria de infraestructura científico-tecnológica (2005-2006) Entidad Financiadora: Ministerio de Educación y Ciencia y FEDER
7. Título: Nuevos derivados antitumorales, benzo o pirido fusionados a heterociclos de siete miembros O,N-acetálicos unidos a bases pirimidínicas y púricas, y compuestos relacionables. Entidad financiadora: Instituto Carlos 111, FIS PI030225
8. Título: Nuevos fármacos gemelos anticancerosos O,N-acetálicos tetrahydrobenzoxazepínicos con bases pirimidínicas o púricas. Entidad financiadora: Instituto Carlos III, FIS PI041206
9. Título: Diseño, síntesis y evaluación biológica de nuevos inhibidores selectivos de mtNOS e iNOS. Entidad financiadora: Junta de Andalucía. (P06-CTS-01941)
10. Título: Nuevos heterociclos homoquirales de alto valor añadido obtenidos a partir de bencenos disustituidos en posición orto: binomio estereoquímica-actividad antitumoral. Entidad financiadora: Instituto Carlos 111, FIS PI070227
11. Título: Choline Kinase: an important target for cancer, malaria and filariasis. Entidad financiadora: Ministerio de Ciencia e Innovación. (HD2008-0028)
12. Título: Diseño de fármacos con actividad antiproliferativa: nuevos inhibidores mejorados de colina quinasa Entidad financiadora: Junta de Andalucía (P07-CTS-

032190).

13. Título: Diseño y síntesis de nuevos inhibidores mejorados de colina quinasa como potenciales fármacos con actividad antiproliferativa Entidad financiadora: Ministerio de Ciencia e Innovación (SAF2009-11955).
14. Título: Diseño y síntesis de nuevos heterociclos oxigenados de siete y ocho miembros benzofusionados como fármacos con actividad antiproliferativa frente a cáncer de mama. Entidad financiadora: Ministerio de Ciencia e Innovación (SAF2010-18263).
15. Título: nuevos heterociclos homoquirales de alto valor añadido obtenidos a partir de bencenos disustituídos en posición orto: binomio estereoquímica-actividad antitumoral. Instituto Carlos III, FIS PI070227.
16. TITULO: CHOLINE KINASE: AN IMPORTANT TARGET FOR CANCER, MALARIA AND FILARIASIS. ACCIONES INTEGRADAS HISPANO-ALEMANAS, CONVOCATORIA 2008. MINISTERIO DE CIENCIA E INNOVACIÓN. Código del Proyecto: HD2008-0028.
17. TITULO: IX JORNADAS DE LA SOCIEDAD ESPAÑOLA DE QUÍMICA TERAPÉUTICA. ACCIONES COMPLEMENTARIAS DENTRO DEL SUBPROGRAMA DE ACCIONES COMPLEMENTARIAS A PROYECTOS DE INVESTIGACIÓN FUNDAMENTAL NO ORIENTADA. CONVOCATORIA 2010. MINISTERIO DE CIENCIA E INNOVACIÓN. Referencia: SAF2010-08941-E (subprograma).
18. TITULO: INNOVADORES O,N-ACETALES ACÍCLICOS DE 5-FLUOROURACILO Y DERIVADOS PURÍNICOS DI- Y TRI-SUSTITUIDOS COMO HERRAMIENTAS FARMACOLÓGICAS PARA EL TRATAMIENTO DE CÉLULAS MADRE CANCEROSAS. INSTITUTO CARLOS III, FIS PI10/00592.
19. TITULO: IX JORNADAS DE LA SOCIEDAD ESPAÑOLA DE QUÍMICA TERAPÉUTICA. ACTIVIDAD CIENTÍFICA DE LA JUNTA DE ANDALUCÍA (La Resolución corresponde a la Secretaría General de Universidades, Investigación y Tecnología de 10 de marzo de 2011 (BOJA de 5 de abril de 2011). Referencia: fecha 5 de abril de 2011 y referencia /905/11 del Vicerrectorado de Política Científica e Investigación, Servicio de Gestión de Investigación.
20. TITULO: PROGRAMA CIÊNCIA SEM FRONTEIRAS - BOLSAS NO PAÍS MODALIDADE. PESQUISADOR VISITANTE ESPECIAL - PVE. CHAMADA DE PROJETOS Nº 03/2014. COVERED AREA: Drugs. MEC/MCTI/CAPES/CNPq/FAPs

(Brasil).

21. TITULO: Desarrollo de fármacos frente a células madre tumorales (CSCs) mediante cribado de librerías sintéticas utilizando GPCRs, quinasas y la interacción calcineurina-NFAT como dianas. SECRETARÍA DE ESTADO DE INVESTIGACIÓN, DESARROLLO E INNOVACIÓN SECRETARÍA GENERAL DE CIENCIA, TECNOLOGÍA E INNOVACIÓN DIRECCIÓN GENERAL DE INNOVACIÓN Y COMPETITIVIDAD SUBDIRECCIÓN GENERAL DE COLABORACIÓN PÚBLICO-PRIVADA. ( RTC-2015-3386-1).
22. TITULO: Mejora de la actividad anticancerosa del bozepinib, bozinib y derivados, mediante la introducción del grupo trifluorometilo . Junta de Andalucía . (CS2016.1).
23. TITULO: Small molecules with anti-angiogenic effect. The Granada Research of Excellence Initiative on BioHealth (GREIB)\_START-UP PROJECTS FOR YOUNG RESEARCHERS. the Campus of International Excellence of the Ministry of Science and Innovation (Class B, R+D+I - Top ResearchAreas) GREIB.PYR\_2011\_15. (2011 HASTA 2012)
24. TITULO: “Búsqueda de nuevos fármacos antimaláricos: Diseño, Síntesis y Evaluación Biológica de nuevos compuestos como potenciales inhibidores de la colina quinasa en Plasmodium falciparum”. CEI-Biotic UGR-Granada(22/05/2013 HASTA 31/12/2013).
25. TITULO: Pequeñas moléculas con actividad antiprolifertiva y antiangiogénica . Consejería de Innovación Ciencia y Empleo de la Junta de Andalucía Proyectos de Excelencia. (2014 HASTA /2017).

## Patentes

1. Autores: Juan Carlos Lacal; Joaquín María Campos Rosa; Miguel Ángel Gallo Mezo; Antonio Espinosa Úbeda; Título: Derivados de piridinio y quinolinio. Patente solicitud nº: P200400072 (14/01/2004)
2. Autores: Juan Carlos Lacal; Joaquín María Campos Rosa; Miguel Ángel Gallo Mezo; Antonio Espinosa Úbeda; Título: Derivados de piridinio y quinolinio. Patente solicitud nº: W0506842A 1 (28/07/2005)
3. Autores: Antonio Espinosa Úbeda; Darío Acuña Castroviejo; Miguel Ángel Gallo Mezo; Antonio José Entrena Guadix; Encarnación Camacho Quesada; Germaine

Escames Rosa; María Dora Carrión Peregrina; Luisa Carlota López Cara: Título: Inhibidores de la óxido nítrico sintasa (NOS) con actividad neuroprotectora. Patente solicitud nº: P200601917 (07/07/2006)

4. Autores: Antonio Espinosa Ubeda; Darío Acuña Castroviejo; Miguel Ángel Gallo Mezo; Antonio José Entrena Guadix; Encarnación Camacho Quesada; Germaine Escames Rosa; María Dora Carrión Peregrina; Luisa Carlota López Cara: Título: 3-Benzoilpirazoles inhibidores de la óxido nítrico sintasa (NOS) con actividad neuroprotectora. Patente solicitud nº: P200702478 (07/07/2006)
5. Autores: Joaquín María Campos Rosa; Antonio Espinosa Ubeda; Miguel Ángel Gallo Mezo; José Antonio Gómez Vidal; María Del Carmen Núñez Carretero; Antonia Aránega Jiménez; Título: (2,3-Dihidro-5H-1 ,4-benzodiheteroepin-3-il)purinas con actividad antitumoral; Patente solicitud nº: P0601538 (24/05/2006)
6. Autores: Ana Conejo García; Luisa Carlota López Cara; Juan Antonio Marchal Corrales; Fernando Rodríguez Serrano; Miguel Ángel Gallo Mezo; Houria Boulaiz ; Antonio Espinosa Ubeda; Joaquín María Campos Rosa; Antonia Aránega Jiménez; Título: Nuevas (RS)-7- ó 9-(1 ,2,3,5-tetrahidro-4, 1-benzoxazepin-3-il)-7H ó 9H-purinas con actividad antitumoral; Patente solicitud nº: P200802431 (07/08/2008).
7. Autores: Marchal Corrales, Juan Antonio; Aránega Jiménez, Antonia; Conejo García, Ana; García Chaves, María Ángeles; Cruz López, Olga; Boulaiz, Houria; Rodríguez Serrano, Fernando; Cativiela Marín, Carlos; Perán Quesada, Macarena; Jiménez Sanz, Ana Isabel; García Ruiz, Juan Manuel; Choquesillo Lazarte, Duane; Campos Rosa, Joaquín María. TITULO: Enantiómeros de derivados benzoheteroepínicos y su uso como agentes anticancerígenos. Patente solicitud nº: P201030415, (22/03/2010).
8. AUTORES: Gamarro Conde, Francisco; Campos Rosa, Joaquín María; Castanys Cuello, Santiago; Gómez Pérez, Verónica; García Hernández, Raquel; Manzano González, José Ignacio. TITULO: Derivados ciclofánicos de bis-piridinio como fármacos antiprotozoarios. Nº DE REGISTRO: P201231534, 5 de octubre de 2012.
9. AUTORES: Campos Rosa, Joaquín M.; Conejo García, Ana; Marchal Corrales, Juan Antonio; Morales Marín, Fátima; Morata Tarifa, Cynthia; Ramírez Rivera, Alberto. TÍTULO: Sulfonamidas derivadas de aminas secundarias con grupos 1,3-dioxolanilalquílicos y fenilmetilpurínicos, y su utilización como agentes

anticancerígenos. Nº DE REGISTRO: P201430048, 20 de enero de 2014.

10. AUTORES: Campos Rosa, Joaquín M; Marchal Corrales, Juan A., García Rubiño, M<sup>ª</sup> Eugenia, Morata Tarifa, Cynthia, Ramírez Rivera, Alberto. TÍTULO: BENZO-HETEROCICLOS DE SEIS MIEMBROS CON ÁTOMOS DE OXÍGENO Y NITRÓGENO CON ACTIVIDAD ANTITUMORAL. P201630714. 31/05/2016.
11. Autores: Molina Pineda de las Infantas, Ignacio; Torres Rusillo, Sara; Fernández Rubio, Pablo; Pineda de las Infantas y Villatoro, Maria José; Diaz Mochón Juan José y Unciti-Broceta, Asier. Título: Derivados de purina como inhibidores de DAPK-1. N. de solicitud: P201400229

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1. A. Unciti-Broceta, M. J. Pineda de las Infantas, J. J. Díaz-Mochón, R. Romagnoli, P. G. Baraldi, M. A. Gallo, A. Espinosa. Regioselective one-pot synthesis of 9-alkyl-6 chloropyrido[3,2-e][1,2,4]triazolo[4,3-a]pyrazines. Reactivity of aliphatic and aromatic hydrazides. *J. Org. Chem.*, 2005, 70, 2878-2880.
2. G. Costantino, A. Entrena Guadix, A. Macchiarulo, A. Gioiello, R. Pellicciari; Molecular Dynamics Simulation of the Ligand Binding of Farnesoid X Receptor. Insights into Helix-12 Stability and Coactivator Peptide Stabilization in Response to Agonist Binding. *J. Med. Chem.*, 2005, 48, 3251-3259.
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4. J. M. Campos, E. Saniger, J. A. Marchal, S. Aiello, I. Suárez, H. Boulaiz, M. A. Gallo, A. Espinosa; New Medium Oxacyclic O,N-Acetals and Related Open Analogues: Biological Activities. *Curr. Med. Chem.*, 2005, 12, 1423-1438
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6. A. Entrena, M. E. Camacho, M. D. Carrión, L. C. López Cara, G. Velasco, J. León, G. Escames, D. Acuña-Castroviejo, V. Tapias, M. A. Gallo, A. Vivó, A. Espinosa. Kynurenamines as Neural Nitric Oxide Synthase Inhibitors. *J. Med. Chem.*, 2005,

7. J. M. Campos, R. M. Sánchez-Martín, A. Conejo-García, A. Entrena, M. A. Gallo, A. Espinosa. (Q)SAR Studies to Design New Human Choline Kinase Inhibitors as Antiproliferative Drugs. *Curr. Med. Chem.*, 2006, 13, 1231-1248
8. L. Milanese, A. Espinosa, J. M. Campos, M. A. Gallo, A. Entrena. Insight into the Inhibition of Choline Kinase by Ca<sup>2+</sup> Ion: Homology Modeling and Molecular Dynamics Simulations. *Chem. Med. Chem.*, 2006, 1, 1216-1228
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10. L. C. López-Cara, M. E. Camacho, M. D. Carrión, M. A. Gallo, A. Espinosa, A. Entrena; An unexpected aromatization during the N-alkylation reaction of 3,4-dihydro-1H-pyrazole derivatives: Insight into the reaction mechanism. *Tetrahedron Lett.*, 2006, 47, 6239-6242.
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12. R. Romagnolli, P. G. Baraldi, V. Remusat, M. D. Carrión, L. C. López Cara, L. C.; et al. Synthesis and biological evaluation of 2-(3,4,5-trimethoxybenzoyl)-3-amino 5-aryl thiophenes as a new class of tubulin inhibitors. *J. Med. Chem.*, 2006, 49, 6425-6428
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14. P. G. Baraldi, D. Preti, M. A. Tabrizi, F. Fruttarolo, R. Romagnoli, M. D. Carrión, L. C. López, et al. Synthesis and Biological Evaluation of Novel 1-Deoxy-1-[6-(hetero)arylcarbonyl]hydrazino]-9H-purin-9-yl]-N-ethyl-beta-D-ribofuranuronamide Derivatives as Useful Templates for the Development of

A2B Adenosine Receptor Agonists. *J. Med. Chem.*, 2007, 50, 374-380

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