

Francisco Javier González Fernández

Curriculum vitae

Dr. en Ciencias Químicas por la Universidad de Oviedo, 1989.

Profesor Titular de Química Orgánica, 1993 – presente.

Especialización y Líneas de Investigación:

Química Computacional y Estudio de mecanismos de reacción.

Síntesis asimétrica de β -Lactamas, β -Aminoácidos y β -Péptidos y β -Sultamas

Inhibidores enzimáticos y Antibióticos: mecanismos de acción de β -Lactamas y β -Sultamas.

Lista de Publicaciones:

AUTORES: J. Barluenga, F.J. González, S. Fustero, V. Gotor

TITULO: Diels-Alder Cycloaddition Reaction of unactivated 2-aza-1,3-dienes with dialkyl azodicarboxylates and heterocumulenes.

REF. REVISTA: *J. Chem. Soc., Chem. Commun.* 1179, 1986 CLAVE: A

AUTORES: J. Barluenga, F.J. González, V. Gotor, S. Fustero

TITULO: Cycloaddition of unactivated 2-aza-1,3-dienes with heterocumulenes: A convenient route to the synthesis of 1,3-difunctionalized compounds

REF. REVISTA: *J. Chem. Soc., Perkin Trans. I* 1988, 1739-1744 CLAVE: A

AUTORES: J. Barluenga, J. Joglar, F.J. González, V. Gotor, S. Fustero

TITULO: A simple regiospecific synthesis of substituted pyridines from 2-aza-1,3-dienes

REF. REVISTA: *J. Org. Chem.* 1988, 53, 5960-5963 CLAVE: A

AUTORES: J. Barluenga, F. Palacios, F.J. González, S. Fustero

TITULO: An efficient and general strategy for the synthesis of 1,4-dihydro- λ^3 - and - λ^5 -azaphosphinines from 2-aza-1,3-dienes

REF. REVISTA: *J. Chem. Soc., Chem Comm.* 1988, 1596-1597 CLAVE: A

AUTORES: J. Barluenga, F.J. González, S. Fustero, M.C. Foces-Foces, F. Hernandez Cano, A. San Feliciano

TITULO: Diels-Alder reaction of unactivated 2-aza-1,3-dienes with azodienophiles and tetracyanoethyl ene.

Crystal structure of 1,2-bis(ethoxycarbonyl)-3-ethyl-6-methyl-3,5-diphenyl-1,2,3,6-tetrahydro-1,2,4-triazine

REF. REVISTA: *J. Chem. Res. (S)* 1989, 66-67 CLAVE: A

AUTORES: J. Barluenga, J. Joglar, F.J. González, S. Fustero

TITULO: Reduction of 5,6-dihydro-2H-1,3-oxazines. A simple approach to 1,3-aminoalcohols

REF. REVISTA: *Tetrahedron Lett.* 1989, 2001-2004 CLAVE: A

AUTORES: J. Barluenga, F.J. González, S. Fustero
TITULO: Diels-Alder reaction of unactivated 2-aza-1,3-dienes with diethyl ketomalonate: A carbon dioxide equivalent
REF. REVISTA: *Tetrahedron Lett.* **1989**, 2685-2688 CLAVE: A

AUTORES: J. Barluenga, F.J. González, S. Fustero
TITULO: Unactivated 2-aza-1,3-dienes: Halogenation and face selectivity in Diels-Alder reactions
REF. REVISTA: *Tetrahedron Lett.* **1990**, 397-398 CLAVE: A

AUTORES: J. Barluenga, J. Joglar, F.J. González, S. Fustero
TITULO: Electronically neutral 2-aza-1,3-dienes: Are they useful intermediates in Organic Synthesis?
REF. REVISTA: *Synlett.* **1990**, 1, 129-138 CLAVE: R

AUTORES: J. Barluenga, F.J. González, S. Fustero, X. Solans, M.V. Domenech
TITULO: An exceptionally simple and unexpected 'one-pot' synthesis of new 4,6-diazasemibullvalenes
REF. REVISTA: *J. Chem. Soc., Chem Comm.* **1990**, 1057-1059 CLAVE: A

AUTORES: J. Barluenga, R. Pérez Carlón, F.J. González, S. Fustero
TITULO: Synthesis of 4(1H)-pyridones by carbonylation of 2-aza-1,3-dienes
REF. REVISTA: *Tetrahedron Lett.* **1990**, 3793-3796 CLAVE: A

AUTORES: J. Barluenga, J. Joglar, F.J. González, S. Fustero, C. Krüger, Y.-H. Tsay
TITULO: Synthesis of 1,3-aminoalcohols from 2-aza-1,3-dienes by reduction of 5,6-dihydro-2H-1,3-oxazines
REF. REVISTA: *Synthesis* **1991**, 387-393 CLAVE: A

AUTORES: J. Barluenga, F.J. González, S. Fustero, S. García-Granda, E. Pérez-Carreño
TITULO: Synthesis and diastereofacial selectivity in Diels-Alder reactions of halogenated 2-aza-1,3-dienes.
REF. REVISTA: *J. Org. Chem.* **1991**, 56, 4459-4463 CLAVE: A

AUTORES: J. Barluenga, F.J. González, R. Pérez Carlón, S. Fustero
TITULO: 2-Aza-1,3-dienes: A new and simple method for the synthesis of functionalized pyridine derivatives
REF. REVISTA: *J. Org. Chem.* **1991**, 56, 6751-6754 CLAVE: A

AUTORES: J. Barluenga, R. Pérez Carlón, F.J. González, F. López Ortiz, S. Fustero
TITULO: Tandem cycloaddition-rearrangement of 2-aza-1,3-dienes. A simple and efficient synthesis of 1,4-diazepin-7(1H, 6H)-thiones
REF. REVISTA: *J. Chem. Soc., Chem Comm.* **1991**, 1704-1705 CLAVE: A

AUTORES: F.J. González, K.N. Houk
TITULO: Ab initio transition structures for Diels-Alder reactions of 2-azabutadienes with alkenes and alkynes: Effects of the substituents, the aza group and catalysis on reactivity
REF. REVISTA: *J. Org. Chem.* **1992**, 57, 3031 CLAVE: A

AUTORES: L. Raimondi, F.K. Brown, J. González, K.N. Houk
TITULO: Empirical force field models for the transition states of intramolecular Diels-Alder reactions based upon ab initio transition structures.
REF. REVISTA: *J. Am. Chem. Soc.* **1992**, 114, 4796 CLAVE: A

AUTORES: J.A. Sordo, J. González, T.L. Sordo
TITULO: An ab initio study on the mechanism of the ketene-imine cycloaddition reaction.
REF. REVISTA: *J. Am. Chem. Soc.* **1992**, 114, 6249 CLAVE: A

AUTORES: F.J. González, K.N. Houk
TITULO: Why are isoxazoles unreactive in Diels-Alder reactions? An ab initio computational study
REF. REVISTA: *J. Org. Chem.* **1992**, 57, 3753 CLAVE: A

AUTORES: J. Barluenga, R. Pérez Carlón, J. González, J. Joglar, F. López Ortiz, S. Fustero
TITULO: A simple preparation of 1H-1,4-diazepine-7(6H)-thiones and their ring contraction to 1-vinyl-2,3-dihydro-1H-imidazole-2-thiones by thermal rearrangement reaction.
REF. REVISTA: *Bull. Soc. Chim. Fr* **1992**, 129, 566 CLAVE: A

AUTORES: X. Assfeld, J.A. Sordo, J. González, M.F. Ruiz-López, T.L. Sordo
TITULO: Electrostatic solvent effect on the ketene-imine cycloaddition reaction.
REF. REVISTA: *J. of Mol. Structure (THEOCHEM)*, **1993**, 287, 193 CLAVE: A

AUTORES: R. López, T.L. Sordo, J.A. Sordo, J. González
TITULO: Torquoelectronic effect in the control of the stereoselectivity of ketene-imine cycloaddition reactions.
REF. REVISTA: *J. of Organic Chemistry*, **1993**, 58, 7036 CLAVE: A

AUTORES: X. Assfeld, M.F. Ruiz-López, J. González, R. López, J.A. Sordo, T.L. Sordo
TITULO: Theoretical analysis of the role of the solvent on the reaction mechanisms: one-step versus two-step ketene-cycloaddition reaction.
REF. REVISTA: *J. of Comput. Chem.*, **1994**, 15, 479-487 CLAVE: A

AUTORES: M.I. Menéndez, J. González, J.A. Sordo, T.L. Sordo
TITULO: Theoretical analysis of the effect of Lewis acid catalysts on reactivity in the Diels-Alder reaction of 2-azabutadiene with ethylene.
REF. REVISTA: *J. of Mol. Structure (THEOCHEM)*, **1994**, 309, 295-299 CLAVE: A

AUTORES: M.I. Menéndez, J. González, J.A. Sordo, T.L. Sordo
TITULO: Theoretical analysis of the thermal and Lewis acid catalyzed reactions of butadiene with ethylene.
REF. REVISTA: *J. of Mol. Structure (THEOCHEM)*, **1994**, 309, 295-299 CLAVE: A

AUTORES: D. Suárez, X. Assfeld, J. González, M.F. Ruiz-López, T.L. Sordo, J.A. Sordo
TITULO: Solvent effects on hetero Diels-Alder reactions of sulfur dioxide with 1,3-dienes.
REF. REVISTA: *J. of Chem. Soc., Chem. Commun.* **1994**, 1683-1684 CLAVE: A

AUTORES: D. Suárez, J. González, T.L. Sordo, J.A. Sordo
TITULO: Ab initio study of the thermal and Lewis acid-catalyzed hetero Diels-Alder reaction of 1,3-butadiene and isoprene with sulfur dioxide.
REF. REVISTA: *J. of Org. Chem.*, **1994**, 59, 8058-8064 CLAVE: A

AUTORES: J. Barluenga, T.L. Sordo, J.A. Sordo, S. Fustero, J. González
TITULO: An AM1 study on π -facial selectivity in Diels-Alder reactions of 2-aza-1,3-dienes with azodienophiles.
REF. REVISTA: *J. of Mol. Structure (THEOCHEM)*, **1994**, 315, 63-69 CLAVE: A

AUTORES: K.N. Houk, J. González, Y. Li
TITULO: Pericyclic reaction transition states: Passions and punctilios, 1935-1995.
REF. REVISTA: *Acc. Chem. Res.*, **1995**, 28, 81-90 CLAVE: R

AUTORES: B. de Pascual-Teresa, J. González, A. Asensio, K.N. Houk
TITULO: Ab initio based force field modeling of the transition states and stereoselectivities of Lewis acid catalyzed asymmetric Diels-Alder reactions.
REF. REVISTA: *J. Am. Chem. Soc.* **1995**, 117, 4347-4356 CLAVE: A

AUTORES: R. López, D. Suárez, M.F. Ruiz-López, J. González, J.A. Sordo, T.L. Sordo
TITULO: Solvent effects on the stereoselectivity of ketene-imine cycloaddition reactions.
REF. REVISTA: *J. of Chem. Soc., Chem. Commun.* **1995**, 1677-1678 CLAVE: A

AUTORES: J. González, T.L. Sordo, J.A. Sordo
TITULO: The role of hard Lewis acids in the tuning of the exo/endo stereoselectivity in Diels-Alder reactions: Ab initio calculations.
REF. REVISTA: *J. of Mol. Structure (THEOCHEM)*, **1996**, 358, 23-27 CLAVE: A

AUTORES: D. Suárez, R. López, J. González, T.L. Sordo, J.A. Sordo
TITULO: Ab initio study of the effect of CH...O hydrogen bonding on the exo/endo stereoselectivity of Diels-Alder reactions of 2-substituted-1,3-dienes with sulfur dioxide.
REF. REVISTA: *Int. J. of Quantum Chemistry*, **1996**, 57, 493-499 CLAVE: A

AUTORES: A. Venturini, J. Joglar, S. Fustero, J. González
TITULO: Diels-Alder Reactions of 2-Azabutadienes with Aldehydes: Ab Initio and Density Functional Theoretical Study of the Reaction Mechanism, Regioselectivity, Acid Catalysis, and Stereoselectivity.
REF. REVISTA: *J. of Org. Chem.*, **1997**, 62, 3919-3926 CLAVE: A

AUTORES: J. González, J.A. Sordo

TITULO: Theoretical results on Hetero-Diels-Alder Reactions.

REF. REVISTA: *Recent Res. Dev. in Organic Chem., Trans. Res. Net.* 1997, vol. 1 CLAVE: CL

AUTORES: A. Venturini, F. López-Ortiz, J.M. Alvarez, J. González

TITULO: Theoretical Proposal of a Catalytic Mechanism for the HIV-1 Protease Involving an Enzyme-Bound Tetrahedral Intermediate.

REF. REVISTA: *J. Am. Chem. Soc.* **1998**, 120, 1110-1111 CLAVE: A

AUTORES: M.I. Konaklieva, X.-F. Ren, H. Shi, S. Dickey, D. V. Lim, J. González, E. Turos

TITULO: Studies on Nonconventionally Fused Bicyclic β -Lactams.

REF. REVISTA: *J. Org. Chem.* **1998**, 63, 8898-8917 CLAVE: A

AUTORES: X.-F. Ren, M.I. Konaklieva, H. Shi, J. González, S. Dickey, D. V. Lim, , E. Turos

TITULO: N-Thiolated Bicyclic and monocyclic β -Lactams.

REF. REVISTA: *Tetrahedron.* **2000**, 56, 5571 CLAVE: A

AUTORES: C. del Pozo, E. Alonso, F. López-Ortiz, F. Fernández-Marí, M. Bayod, J. González

TITULO: Synthesis of 1,1-Dioxopenicillanoyloxymethyl 6-[D- α -(benzylideneaminophenylacetamido)]penicillanate and analogs. New Intermediates in the Preparation of Sultamicillin.

REF. REVISTA: *Tetrahedron* **2001**, 57, 6209-6214. CLAVE: A

Autores (p.o. de firma): E. Alonso, F. López-Ortiz, C. del Pozo, E. Peralta, A. Macías, J. González

Título: Spiro β -Lactams as β -Turn Mimetics. Design, Synthesis, and NMR Conformational Analysis.

Ref. X revista: *J. Org. Chem.*

Clave: A Volumen: 66 Páginas, inicial: 6333 final: 6338 Fecha: 2001

Autores (p.o. de firma): E. Alonso, C. del Pozo, J. González

Título: Staudinger reactions of unsymmetrical cyclic ketenes: A synthetically useful approach to spiro β -Lactams and derivatives. Reaction mechanism and theoretical studies.

Ref. X revista: *J. Chem. Soc., Perkin Trans. I*

Clave: A Volumen: Páginas, inicial: 571 final: 576 Fecha: 2002

Autores (p.o. de firma): E. Alonso, C. del Pozo, J. González

Título: Synthesis of α,α -disubstituted- β -Amino Esters and Peptide Derivatives.

Ref. X revista: *Synlett*

Clave: A Volumen: Páginas, inicial: 69 final: 72 Fecha: 2002

Autores (p.o. de firma): Ignacio Fernández, Julia María Álvarez Gutiérrez, Nikolaus Kocher, Dirk Leusser, Dietmar Stalke, Javier González, Fernando López Ortiz

Título: [Li{CH(Me)P(Ph)₂(NCO₂Me)}₂(THF)₂]: Crystal, Solution and Calculated Structure of a *N*-Delocalized Lithium Phosphazene.

Ref. X revista: *J. Am. Chem. Soc.*

Clave: A Volumen: 124 Páginas, inicial: 15184 final: 15185 Fecha: 2002

Autores (p.o. de firma): A. Venturini, J. González

Título: A CASPT2 and CASSCF Approach to the Cycloaddition of Ketene and Imine: A New Mechanistic Scheme of the Staudinger Reaction.

Ref. X revista: *J. Org. Chem.*

Clave: A Volumen: 67 Páginas, inicial: 9089 final: 9092 Fecha: 2002

Autores (p.o. de firma): Carlos del Pozo, Alberto Macías, Fernando López-Ortiz, Miguel Ángel Maestro, Eduardo Alonso, Javier González

Título: Diastereo- and Enantioselective Synthesis of Novel β -Lactam-Containing 1,4-Benzodiazepines through a Ketene-Imine Cycloaddition Reaction.

Ref. X revista: *Eur. J. Org. Chem.*

Clave: A Volumen: 3 Páginas, inicial: 535 final: 545 Fecha: 2004

Autores (p.o. de firma): Alberto Macías, Eduardo Alonso, Carlos del Pozo, Javier González

Título: Unusual rearrangement of spiro β -lactams to 1,4-diazabicyclo[4.4.0] and 1,4-diazabicyclo[4.3.0]nonanes. Synthesis of conformationally restricted σ -receptor ligands.

Ref. X revista: *Tetrahedron Letters*

Clave: A Volumen: 45 Páginas, inicial: 4657 final: 4660 Fecha: 2004

Autores (p.o. de firma): Antonio Morán Ramallal, Fernando López Ortiz, Javier González

Título: Ionic vs. Pericyclic transition states for the cyclization reactions of C_{α} -N anions derived from amides and phosphinamides.

Ref. X revista: *Organic Letters*

Clave: A Volumen: 6 Páginas: 2141 inicial, final: 2144 Fecha: 2004

Autores (p.o. de firma): Ignacio Fernández, Javier González, Fernando López Ortiz

Título: Deuterium-labeling and NMR study of the dearomatization of N-Alkyl-N-benzylidiphenylphosphinamides through anionic cyclization: ortho and benzylic lithiation directed by complex-induced proximity effects.

Ref. X revista: *Journal of American Chemical Society*

Clave: A Volumen: 126 Páginas, inicial: 12551 final: 12564 Fecha: 2004

Autores (p.o. de firma): Alberto Macías, Eduardo Alonso, Carlos del Pozo, Alessandro Venturini, Javier González

Título: Diastereoselective [2+2]-cycloaddition reactions of unsymmetrical cyclic ketenes with imines: synthesis of modified prolines and theoretical study of the reaction mechanism.

Ref. X revista: *Journal of Organic Chemistry*

Clave: A Volumen: 69 Páginas, inicial: 7004 final: 7012 Fecha: 2004

Autores (p.o. de firma): Carlos del Pozo, Alberto Macías, Eduardo Alonso, Javier González

Título: Reactions of 1,4-benzodiazepinic N-nitrosoamidines with tosylmethyl Isocyanide: a novel síntesis of Midazolam.

Ref. X revista: *Synthesis*

Clave: A Volumen: Páginas, inicial: 2697 final: 2703 Fecha: 2004

Autores (p.o. de firma): Antonio Morán Ramallal, Ignacio Fernández, Fernando López Ortiz, Javier González

Título: Mechanism of anionic dearomatizing reactions of diphenylphosphinamide derivatives: A theoretical and experimental study.

Ref. X revista: *Chemistry. A European Journal*

Clave: A Volumen: 11 Páginas, inicial: 3022 final: 3031 Fecha: 2005

Autores (p.o. de firma): Edward Turos, Cristina Coates, Jeung-Yeop Shim, Yang Wang, J. Michelle Leslie, Timothy E. Long, G. Zurrés Kumar Reddy, Alex Ortiz, Marci Culbreath, Sonja Dickey, Daniel V. Lim, Eduardo Alonso, Javier González

Título: N-Methylthio β -lactam antibacterials: Effects of the C3/C4 ring substituents on anti-MRSA activity.

Ref. X revista: *Bioorganic & Medicinal Chemistry*

Clave: A Volumen: 13 Páginas, inicial: 6289 final: 6308 Fecha: 2005

Autores (p.o. de firma): Alberto Macías, Antonio Morán Ramallal, Eduardo Alonso, Carlos del Pozo, Javier González

Título: Synthesis of Enantiopure Pyrrolidine-Derived Peptidomimetics and Oligo- β -peptides via Nucleophilic Ring-opening of β -lactams.

Ref. X revista: *Journal of Organic Chemistry*

Clave: A Volumen: 71 Páginas, inicial: 7721 final: 7730 Fecha: 2006

Autores (p.o. de firma): Alessandro Venturini, Javier González

Título: Mechanistic aspects of the Ketene-Imine Cycloaddition reactions

Ref. X revista: Mini-Reviews in Organic Chemistry

Clave: R Volumen: 3 Páginas, inicial: 185 final: 194 Fecha: 2006

Autores (p.o. de firma): Santos Fustero, Javier González, Carlos del Pozo

Título: 1,4-benzodiazepine N-nitrosoamidines. Useful intermediates in the synthesis of tricyclic benzodiazepines.

Ref. X revista: Molecules

Clave: A Volumen: 11 Páginas, inicial: 583 final: 588 Fecha: 2006

Autores (p.o. de firma): Santos Fustero, Gema Chiva, Julio Piera, Alessandro Volonterio, Matteo Zanda, Javier González, Antonio Morán Ramallal

Título: The Role of Fluorine in the Stereoselective Tandem Aza-Michael Addition to Acrylamide Acceptors: An Experimental and Theoretical Mechanistic Study

Ref. X revista: Chemistry. A European Journal

Clave: A Volumen: 13 Páginas, inicial: 8530 final: 8542 Fecha: 2007
