

Química Física

Áreas de conocimiento: Química Física

Director: Ana Isabel Azuaga Fortes

Secretario: Salvador Casares Atienza

Página web: <http://quimicafisica.ugr.es>

Profesorado: CU: 5, PTU: 10, PDI Contratado y Otros: 20

Tesis leídas

- Desarrollo de proteínas y compuestos terapéuticos frente a virus con máquinas de fusión de clase i / development of therapeutic proteins and compounds against viruses with class-i fusion machines

Doctorando: Cano Muñoz, Mario

Director: Francisco Conejero Lara

Fecha de lectura: 15/06/2022

Grupos de Investigación.

FQM171 BIOFISICA Y BIOTECNOLOGIA MOLECULAR

- Responsable: JOSE CRISTOBAL MARTINEZ HERRERIAS

BIO223 BIOMOLECULAS

- Responsable: JOSE MANUEL SANCHEZ RUIZ

Dirección y participación en Proyectos I+D

- 2022 Understanding general principles governing the catalytic power of the enzymes and the protein structure-function relationships, PROGRAMA RAMON Y CAJAL, 01/12/2022-30/11/2027

Investigador ENCARNACIÓN MEDINA CARMONA

- 2022 Deciphering the Molecular Basis of Enzymatic Catalysis through Resurrected Ancient Proteins:

Biotechnological Applications, Proyectos I+D+i FEDER-Andalucía, 01/01/2022-30/11/2022

Investigador ENCARNACIÓN MEDINA CARMONA

Contratos de investigación

- 2022 Production of mimetic polypeptides of the HR1 region of the S2 subunit of coronaviruses, CONTRATO ART. 83, 12/12/2022-

Responsable FRANCISCO CONEJERO LARA

Publicaciones en revistas

- 2023 Artículo: Cell Survival Enabled by Leakage of a Labile Metabolic Intermediate, Molecular Biology and Evolution, , , -

BEATRIZ IBARRA MOLERO

ENCARNACIÓN MEDINA CARMONA

- 2023 Artículo: A calorimetric and structural analysis of cooperativity in the thermal unfolding of the PDZ

tandem of human Syntenin-1, International Journal of Biological Macromolecules, 242, , 124662-

IRENE LUQUE FERNÁNDEZ

JAVIER RUIZ SANZ

JOSE CRISTOBAL MARTINEZ HERRERIAS

- 2023 Artículo: pH-driven polymorphic behaviour of the third PDZ domain of PSD95: the role of electrostatic

interactions, Crystals, 13, 2, 218-

JAVIER MURCIANO CALLES

JOSE CRISTOBAL MARTINEZ HERRERIAS

- 2022 Artículo: A single evolutionarily divergent mutation determines the different FAD-binding affinities of

human and rat NQO1 due to site-specific phosphorylation, FEBS Letters, 596, 1, 29-41

ANGEL LUIS PEY RODRÍGUEZ

NOEL MESA TORRES

- 2022 Artículo: Effect of 5-Azacytidine Treatment on Redox Status and Inflammatory Condition in MDS

Patients, Antioxidants, , , -

MARIA DEL SEÑOR LÓPEZ VÉLEZ

- 2022 Artículo: Conformational Stabilization of Gp41-Mimetic Mini-proteins Opens Up New Ways of Inhibiting

HIV-1 Fusion, International Journal of Molecular Sciences, 23, 5, 2794-

FRANCISCO CONEJERO LARA

- 2022 Artículo: Gallic acid: a natural compound exerting antitumoral activity via interaction with G-

quadruplexes, Cancers, 14, 11, -

JAVIER MURCIANO CALLES

- 2022 Artículo: New salicylic acid derivatives, double inhibitors of glycolate oxidase and lactate

- dehydrogenase, as effective agents decreasing oxalate production, *European Journal of Medicinal Chemistry*, 237, , 114396-
ANGEL LUIS PEY RODRÍGUEZ
- 2022 Review: Targeting HIF-1 α Function in Cancer through the Chaperone Action of NQO1: Implications of Genetic Diversity of NQO1, *Journal of Personalized Medicine*, 12, 5, 747-
ANGEL LUIS PEY RODRÍGUEZ
- 2022 Artículo: Allosteric Communication in the Multifunctional and Redox NQO1 Protein Studied by Cavity-Making Mutations, *Antioxidants*, 11, 6, 1110-
ANGEL LUIS PEY RODRÍGUEZ
- 2022 Artículo: Different phenotypic outcome due to site-specific phosphorylation in the cancer-associated NQO1 enzyme studied by phosphomimetic mutations, *Archives of Biochemistry and Biophysics*, 729, , 109392.-
ANGEL LUIS PEY RODRÍGUEZ
- 2022 Artículo: Loss of stability and unfolding cooperativity in hPGK1 upon gradual structural perturbation of its N-terminal domain hydrophobic core, *Scientific Reports*, 12, 1, 17200-
ANGEL LUIS PEY RODRÍGUEZ
- 2022 Artículo: Counterintuitive structural and functional effects due to naturally occurring mutations targeting the active site of the disease-associated NQO1 enzyme, *The FEBS Journal*, , , -
ANGEL LUIS PEY RODRÍGUEZ
- 2022 Artículo: Effect of naturally-occurring mutations on the stability and function of cancer-associated NQO1: Comparison of experiments and computation, *Frontiers in Molecular Biosciences*, 9, , 1063620-
ANGEL LUIS PEY RODRÍGUEZ
- 2022 Artículo: Erythrocyte Zn concentration and antioxidant response after supplementation with Zn in a postmenopausal population. A double-blind randomized trial, *Experimental Gerontology*, , , -
BARTOLOME QUINTERO OSSO
- 2022 Artículo: Structure-based discovery and in vitro validation of inhibitors of chloride intracellular channel 4 protein, *Computational and Structural Biotechnology Journal*, 21, , 688-701
ENCARNACIÓN MEDINA CARMONA
- 2022 Review: An Updated View of the *Trypanosoma cruzi* Life Cycle: Intervention Points for an Effective Treatment, *ACS Infectious Diseases*, 8, 6, 1107-1115
ENCARNACIÓN MEDINA CARMONA
- 2022 Artículo: Active site center redesign increases protein stability preserving catalysis in thioredoxin, *Protein Science*, 31, 9, e4417-
BEATRIZ IBARRA MOLERO
HECTOR GARCÍA SEISDEDOS
MARIA LUISA ROMERO ROMERO
- 2022 Book-Review: Folding free energy surfaces from differential scanning calorimetry, *Methods in Molecular Biology*, 2376, , 105-116
BEATRIZ IBARRA MOLERO
JOSE MANUEL SANCHEZ RUIZ
- 2022 Artículo: Reverse engineering analysis of the high-temperature reversible oligomerization and amyloidogenicity of PSD95-PDZ3, *Molecules*, 27, , 2813-
JOSE CRISTOBAL MARTINEZ HERRERIAS
- 2022 Artículo: Blocking PSD95-PDZ3's amyloidogenesis through point mutations that inhibit high-temperature reversible oligomerization (RO), *The FEBS Journal*, 289, , 3205-3216
JOSE CRISTOBAL MARTINEZ HERRERIAS
- 2022 Artículo: Phage display identification of nanomolar ligands for human NEDD4-WW3: energetic and dynamic implications for the development of broad-spectrum antivirals, *International Journal of Biological Macromolecules*, 207, , 308-323
CARLES CORBI VERGE
IRENE LUQUE FERNÁNDEZ
JAVIER MURCIANO CALLES
JAVIER RUIZ SANZ
JOSE CRISTOBAL MARTINEZ HERRERIAS
MANUEL IGLESIAS BEXIGA
- 2022 Artículo: Exploring Highly Conserved Regions of SARS-CoV-2 Spike S2 Subunit as Targets for Fusion Inhibition Using Chimeric Proteins, *International Journal of Molecular Sciences*, 23, , 15511-
FRANCISCO CONEJERO LARA
- 2022 Artículo: Novel chimeric proteins mimicking SARS-CoV-2 spike epitopes with broad inhibitory activity, *International Journal of Biological Macromolecules*, 222, , 2467-2478
FRANCISCO CONEJERO LARA

Capítulos de libros (con ISBN)

- 2023 Titulo Capítulo: Preparation and investigation of crucial oligomers in the early stages of Abeta40 and Abeta42 aggregation, Titulo Libro: Methods in Molecular Biology: Humana Press, a part of Springer Science + Business Media, , 2023, 978-1-0716-2597-2
BERTRAND MOREL
FRANCISCO CONEJERO LARA
- 2022 Titulo Capítulo: Understanding binding affinity and specificity of modular protein domains: A focus in ligand design for the polyproline-binding families, Titulo Libro: Protein Design and Structure. (Advances in Protein Chemistry and Structural Biology Book series; Vol 130): ELSEVIER INC., , 2022, 978-0-323-99229-9
JAVIER MURCIANO CALLES
JOSE CRISTOBAL MARTINEZ HERRERIAS
IRENE LUQUE FERNÁNDEZ
JAVIER RUIZ SANZ

Contribuciones en congresos

- 2023 Poster en Congreso: Chimeric miniproteins targeting the highly conserved heptad repeat 2 (HR2) region of the SARS-CoV-2 spike protein, 2nd. MOSBRI Scientific Conference, 05/06/2023, - Zaragoza, España, Congreso
FRANCISCO CONEJERO LARA
- 2023 Poster en Congreso: Hyperstable gp41-mimetic miniprotein with strong anti-HIV activity, 2nd. MOSBRI Scientific Conference, 05/06/2023, - Zaragoza, España, Congreso
FRANCISCO CONEJERO LARA
- 2022 Poster en Congreso: Understanding the phosphorylation effects in the antioxidant NQO1 enzyme., Iberian Biophysics Congress, 20/06/2022, - Bilbao, Congreso
ANGEL LUIS PEY RODRÍGUEZ
- 2022 Poster en Congreso: Site-specific phosphorylation determines NQO1 stability and activity, 44 Congreso de la Sociedad de Bioquímica y Biología Molecular Española, 06/09/2022, Málaga, Congreso
ANGEL LUIS PEY RODRÍGUEZ
- 2022 Poster en Congreso: Structure-based discovery and in vitro validation of inhibitors of chloride intracellular channel 4 protein, 8th International IBERIAN BIOPHYSICS CONGRESS, 20/06/2022, - Bilbao, PAIS VASCO, Congreso
ENCARNACIÓN MEDINA CARMONA
- 2022 Poster en Congreso: Identification of TSG101-UEV ligands of interest as broad-spectrum antivirals, 8th International IBERIAN BIOPHYSICS CONGRESS, 20/06/2022, - Bilbao, PAIS VASCO, Congreso
JAVIER MURCIANO CALLES
IRENE LUQUE FERNÁNDEZ
MANUEL IGLESIAS BEXIGA
ANDRÉS PALENCIA CARRILERO
JOSE CRISTOBAL MARTINEZ HERRERIAS
- 2022 Poster en Congreso: Exploring the druggability of the ALIX-V domain for the identification of broad-spectrum antivirals, 8th International IBERIAN BIOPHYSICS CONGRESS, 20/06/2022, - Bilbao, PAIS VASCO, Congreso
JAVIER MURCIANO CALLES
JAVIER RUIZ SANZ
IRENE LUQUE FERNÁNDEZ
JOSE CRISTOBAL MARTINEZ HERRERIAS
- 2022 Poster en Congreso: Specificity and thermodynamics of the interaction between four human PDZ domains and eight host, viral and designed ligands, XXXVIII Reunión Bienal de la Real Sociedad Española de Química, 27/06/2022, Granada, España, Congreso
EVA SANCHEZ COBOS
JOSE CRISTOBAL MARTINEZ HERRERIAS
JAVIER MURCIANO CALLES
- 2022 Poster en Congreso: The quantitative evaluation of kinetic effect on PSD95-PDZ3's reversible oligomerization at high temperature, The 60th Annual Meeting of the Biophysical Society of Japan, 28/09/2022, Hakodate, Japón, Congreso
JOSE CRISTOBAL MARTINEZ HERRERIAS
- 2022 Poster en Congreso: Reverse engineering analysis of the high-temperature reversible oligomerization and amyloidogenicity of PSD95-PDZ3, The 60th Annual Meeting of the Biophysical Society of Japan, 28/09/2022, Hakodate, Japón, Congreso
JOSE CRISTOBAL MARTINEZ HERRERIAS
- 2022 Poster en Congreso: Computational and biophysical approaches to identify Fascin allosteric



inhibitors as novel antimetastatic drugs, XIV Spanish Drug Discovery Network Meeting 2022, 24/11/2022, Granada, Congreso

JOSE CRISTOBAL MARTINEZ HERRERIAS

IRENE LUQUE FERNÁNDEZ

JAVIER RUIZ SANZ

- 2022 Poster en Congreso: A multidisciplinary approach for the identification of TSG101-UEV ligands with potential as novel broad-spectrum antivirals, XIV Spanish Drug Discovery Network Meeting 2022, 24/11/2022, Granada, Congreso

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- 2022 Poster en Congreso: Identification of ALIX-V domain ligands of interest as broad-spectrum antivirals using phage display, XIV Spanish Drug Discovery Network Meeting 2022, 24/11/2022, Granada, Congreso

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