



## Publicaciones Recientes

- Risso, V.A., Sanchez-Ruiz, J.M., and Ozkan, S.B. (2018). Biotechnological and protein-engineering implications of ancestral protein resurrection. *Curr. Opin. Struct. Biol.* 51, 106–115.
- Petrović, D., Risso, V.A., Kamerlin, S.C.L., and Sanchez-Ruiz, J.M. (2018). Conformational dynamics and enzyme evolution. *J. R. Soc. Interface* 15.
- Gomez-Fernandez, B.J., Garcia-Ruiz, E., Martin-Diaz, J., Gomez de Santos, P., Santos-Moriano, P., Plou, F.J., Ballesteros, A., Garcia, M., Rodriguez, M., Risso, V.A., et al. (2018). Directed -in vitro- evolution of Precambrian and extant Rubiscos. *Sci. Rep.* 8, 5532.
- Pabis, A., Risso, V.A., Sanchez-Ruiz, J.M., and Kamerlin, S.C. (2018). Cooperativity and flexibility in enzyme evolution. *Curr. Opin. Struct. Biol.* 48, 83–92.
- Betancor-Fernández, I., Timson, D.J., Salido, E., and Pey, A.L. (2017). Natural (and Unnatural) Small Molecules as Pharmacological Chaperones and Inhibitors in Cancer. (Springer, Cham), pp. 155–190.
- Clavería-Gimeno, R., Velazquez-Campoy, A., and Pey, A.L. (2017). Thermodynamics of cooperative binding of FAD to human NQO1: Implications to understanding cofactor-dependent function and stability of the flavoproteome. *Arch. Biochem. Biophys.* 636, 17–27.
- Majtan, T., Pey, A.L., Gimenez-Mascarell, P., Martínez-Cruz, L.A., Szabo, C., Kožich, V., and Kraus, J.P. (2017). Potential Pharmacological Chaperones for Cystathionine Beta-Synthase-Deficient Homocystinuria. (Springer, Cham), pp. 345–383.
- Martín-Escolano, R., Moreno-Viguri, E., Santivañez-Veliz, M., Martin-Montes, A., Medina-Carmona, E., Paucar, R., Marín, C., Azqueta, A., Cirauqui, N., Pey, A.L., et al. (2018). Second Generation of Mannich Base-Type Derivatives with in Vivo Activity against *Trypanosoma cruzi*. *J. Med. Chem.* 61, 5643–5663.
- McAuley, M., Mesa-Torres, N., McFall, A., Morris, S., Huang, M., Pey, A.L., and Timson, D.J. (2018). Improving the Activity and Stability of Human Galactokinase for Therapeutic and Biotechnological Applications. *ChemBioChem* 19, 1088–1095.

- Medina-Carmona, E., Fuchs, J.E., Gavira, J.A., Mesa-Torres, N., Neira, J.L., Salido, E., Palomino-Morales, R., Burgos, M., Timson, D.J., and Pey, A.L. (2017). Enhanced vulnerability of human proteins towards disease-associated inactivation through divergent evolution. *Hum. Mol. Genet.* 26, 3531–3544.
- Medina-Carmona, E., Betancor-Fernández, I., Santos, J., Mesa-Torres, N., Grottelli, S., Batlle, C., Naganathan, A.N., Oppici, E., Cellini, B., Ventura, S., et al. (2018a). Insight into the specificity and severity of pathogenic mechanisms associated with missense mutations through experimental and structural perturbation analyses. *Hum. Mol. Genet.*
- Medina-Carmona, E., Rizzuti, B., Martín-Escolano, R., Pacheco-García, J.L., Mesa-Torres, N., Neira, J.L., Guzzi, R., and Pey, A.L. (2018b). Phosphorylation compromises FAD binding and intracellular stability of wild-type and cancer-associated NQO1: Insights into flavo-proteome stability. *Int. J. Biol. Macromol.*
- Mesa-Torres, N., Betancor-Fernández, I., Oppici, E., Cellini, B., Salido, E., Pey, A., Mesa-Torres, N., Betancor-Fernández, I., Oppici, E., Cellini, B., et al. (2018). Evolutionary Divergent Suppressor Mutations in Conformational Diseases. *Genes (Basel)*. 9, 352.
- Muñoz, I.G., Morel, B., Medina-Carmona, E., and Pey, A.L. (2017). A mechanism for cancer-associated inactivation of NQO1 due to P187S and its reactivation by the consensus mutation H80R. *FEBS Lett.* 591, 2826–2835.
- Pey, A.L. (2018). Biophysical and functional perturbation analyses at cancer-associated P187 and K240 sites of the multifunctional NADP(H):quinone oxidoreductase 1. *Int. J. Biol. Macromol.* 118, 1912–1923.
- Santofimia-Castaño, P., Rizzuti, B., Pey, Á.L., Soubeyran, P., Vidal, M., Urrutia, R., Iovanna, J.L., and Neira, J.L. (2017). Intrinsically disordered chromatin protein NUPR1 binds to the C-terminal region of Polycomb RING1B. *Proc. Natl. Acad. Sci. U. S. A.* 114, E6332–E6341.
- Risso, V.A., Martínez-Rodríguez, S., Candel, A.M., Krüger, D.M., Pantoja-Uceda, D., Ortega-Muñoz, M., Santoyo-Gonzalez, F., Gaucher, E.A., Kamerlin, S.C.L., Bruix, M., et al. (2017). De novo active sites for resurrected Precambrian enzymes. *Nat. Commun.* 8, 16113.
- Lostao A, El Harrous M, Daouidi F, Romero A, Parody-Morreale A and Sancho J (2000). “Dissecting the energetics of the apoflavodoxin-FMN complex”. *J. Biol. Chem.* 275, 9518-26.
- Plaza del Pino IM, Ibarra-Molero B and Sanchez-Ruiz JM (2000) “Lower kinetic limit to protein thermal stability: A proposal regarding protein stability in vivo and its relation with misfolding diseases”. *Proteins: Structure, Function and Genetics* 40, 58-70.
- Ibarra-Molero B, Plaza del Pino IM, Souhail B, Hammou HO and Sanchez-Ruiz JM (2000) “The sarcosine effect on protein stability: A case of nonadditivity?”.

Protein Science 9, 820-826.

- Georgescu RE, Garcia-Mira MM, Tasayco ML and Sanchez-Ruiz JM (2001) "Heat capacity analysis of oxidized Escherichia coli thioredoxin fragments (1--73, 74--108) and their noncovalent complex. Evidence for the burial of apolar surface in protein unfolded states." *Eur. J. Biochem.* 268, 1477-85.
- Irún MP, Garcia-Mira MM, Sanchez-Ruiz JM and Sancho J (2001) "Native hydrogen bonds in a molten globule: the apoflavodoxin thermal intermediate." *J. Mol. Biol.* 306, 877-88.
- Garcia-Mira MM and Sanchez-Ruiz JM (2001) "pH corrections and protein ionization in water/guanidinium chloride." *Biophys. J.* 81, 3489-502.
- Gribenko AV, Guzman-Casado M, Lopez MM and Makhatadze GI (2002) "Conformational and thermodynamic properties of peptide binding to the human S100P protein". *Protein Science* 11, 1367-1375.
- Acevedo O, Guzman-Casado M, Garcia-Mira MM, Ibarra-Molero B and Sanchez-Ruiz JM (2002) "pH corrections in chemical denaturant solutions." *Anal. Biochem.* 306, 158-61.
- Garcia-Mira MM, Sadqi M, Fischer N, Sanchez-Ruiz JM and Muñoz V (2002) "Experimental identification of downhill protein folding." *Science* 298, 2191-5.
- Guzmán-Casado M, García-Mira MM, Sánchez-Ruiz JM, Giménez-Gallego G and Parody-Morreale A (2002) "Energetics of heparin binding to human acidic fibroblast growth factor." *Int. J. Biol. Macromol.* 31, 45-54.
- Guzman-Casado M, Parody-Morreale A, Robic S, Marqusee S and Sanchez-Ruiz JM (2003) "Energetic evidence for formation of a pH-dependent hydrophobic cluster in the denatured state of *Thermus thermophilus* ribonuclease H". *J. Mol. Biol.* 329, 731-43.
- Robic S, Guzman-Casado M, Sanchez-Ruiz JM and Marqusee S (2003) "Role of residual structure in the unfolded state of a thermophilic protein". *Proceedings of the National Academy of Sciences of USA* 100, 11345-9.
- Guzmán-Casado M., Garcia-Mira, MM, Cano-Soldado P, Gimenez-Gallego G, Sanchez-Ruiz JM and Parody-Morreale A (2004) "Energetics of the Interaction of Human Acidic Fibroblast Growth Factor with Heparin and the Functional Analog Myo-inositol hexasulfate". In *Biocalorimetry 2. Applications of calorimetry in the biological sciences*. J.E. Ladbury, M.Doyle eds. Wiley, (2004), 133-150.
- Garcia-Mira MM, Boehringer D and Schmid FX (2004) "The folding transition state of the cold shock protein is strongly polarized" *J Mol Biol.* 339,555-69.
- Campos LA, Garcia-Mira MM, Godoy-Ruiz R, Sanchez-Ruiz JM and Sancho J (2004) "Do proteins always benefit from a stability increase? Relevant and residual stabilisation in a three-state protein by charge optimisation" *J. Mol.*

Biol. 344, 223-37.

- Godoy-Ruiz R, Perez-Jimenez R, Garcia-Mira MM, Plaza del Pino IM and Sanchez-Ruiz JM (2005) "Empirical parametrization of pK values for carboxylic acids in proteins using a genetic algorithm." *Biophys. Chem.* 115, 263-6.
- Perez-Jimenez R, Godoy-Ruiz R, Parody-Morreale A, Ibarra-Molero B and Sanchez-Ruiz JM (2006). "A simple tool to explore the distance distribution of correlated mutations in proteins". *Biophysical Chemistry* 119, 240-6.
- Garcia-Mira MM and Schmid FX (2006) "Key role of coulombic interactions for the folding transition state of the cold shock protein" *J. Mol. Biol.* 364, 458-68.
- Pey AL, Rodriguez-Larrea D, Bomke S, Dammers S, Godoy-Ruiz R, Garcia-Mira MM and Sanchez-Ruiz JM (2008) "Engineering proteins with tunable thermodynamics and kinetic stabilities" *Proteins* 71, 165-74.
- Suarez M., Tortosa P., Garcia-Mira M.M., Rodriguez-Larrea D., Godoy-Ruiz R., Ibarra-Molero B., Jaramillo A., Sanchez-Ruiz J. (2010). Using multi-objective computational design to extend protein promiscuity. *Biophysical Chemistry* 147, 13-19.
- Casares-Atienza S, Weininger U, Camara-Artigas A, Balbach J and Garcia-Mira MM "Re-examination of onconase thermal unfolding mechanism". Enviado a publicar.
- Casares-Atienza S, Weininger U, Camara-Artigas A, Balbach J and Garcia-Mira MM (2010). Alpha-helix 1 plays key role in onconase thermal unfolding mechanism. *Proteins* (submitted).