



## Publicaciones del Grupo

### Publicaciones Recientes

- Buzón, P., Ruiz-Sanz, J., Martínez, J.C. y Luque, I. "Stability, conformational plasticity, oligomerization behaviour and equilibrium unfolding intermediates of the Ebola virus matrix protein VP40" *Journal of Biomolecular Structure & Dynamics* (2020), 38: 4289-4303. doi: 10.1080/07391102.2019.1671226
- Murciano-Calles, J., Coello, A., Camara-Artigas, A., Martinez, J.C. "PDZ/PDZ interaction between PSD-95 and nNOS neuronal proteins". *Journal of Molecular Recognition* (2020), 33: e2826.
- Hermosilla, J., Pérez-Robles, R., Salmerón-García, A., Casares, S., Cabeza, J., Bones J., y Navas, N. "Comprehensive biophysical and functional study of ziv-aflibercept: characterization and forced degradation." *Scientific Reports* (2020), 10: 2675. DOI:10.1038/s41598-020-59465-7
- Beaver, SK, Mesa-Torres, N, Pey, AL "NQO1: A target for the treatment of cancer and neurological diseases, and a model to understand loss of function disease mechanisms" *Biochimica et Biophysica Acta: Proteins and Proteomics* (2020), 1867: 663-676. DOI: 10.1016/j.bbapap.2019.05.002.
- "Protein Homeostasis Diseases: Mechanisms and Novel Therapies" Ed.: Pey, AL (2020) Academic Press. ISBN: 9780128191330.
- Alburquerque-González, B., Bernabé-García, M., Montoro-García, S., Bernabé-García, A., Rodrigues, P.C., Ruiz-Sanz, J., López-Calderón, F.F., Luque, I., Nicolás, F.J., Cayuela, M.L., Salo, T., Pérez-Sánchez, H. y Conesa-Zamora, P. "New role of the antidepressant imipramine as a Fascin1 inhibitor in colorectal cancer cells." *Experimental & Molecular Medicine* (2020), 52: 281-292.
- Montoro-García S, Alburquerque-González B, Bernabé-García Á, Bernabé-García M, Rodrigues PC, den-Haan H, Luque I, Nicolás FJ, Pérez-Sánchez H, Cayuela ML, Salo T, Conesa-Zamora P.J. "Novel Anti-Invasive Properties of a Fascin1 Inhibitor on Colorectal Cancer Cells" *Journal of Molecular Medicine* (2020), 98(3):383-394. doi: 10.1007/s00109-020-01877"
- Szczepaniak, M., Iglesias-Bexiga, M., Cerminara, M., Sadqi, M., Sanchez de Medina, C., Martínez, J.C., Luque, I., Muñoz, V. "Ultrafast folding kinetics of WW

domains reveal how the amino acid sequence determines the speed limit to protein folding.” Proceedings of the National Academy of Sciences of the United States of America (2019), 116: 8137-8142.

- Iglesias-Bexiga M, Palencia A, Corbi-Verge C, Martin-Malpartida P, Blanco FJ, Macias MJ, Cobos ES, Luque I. “Binding site plasticity in viral PPxY Late domain recognition by the third WW domain of human NEDD4” Scientific Reports (2019), 9: 1-17. doi: 10.1038/s41598-019-50701-3.
- González-Magaña A, de Opakua AI, Merino N, Monteiro H, Diercks T, Murciano-Calles J, Luque I, Bernadó P, Cordeiro TN, Biasio A, Blanco FJ. “Double Monoubiquitination Modifies the Molecular Recognition Properties of p15PAF Promoting Binding to the Reader Module of Dnmt” ACS Chemical Biology (2019), 14(10):2315-2326. doi: 10.1021/acscchembio.9b00679
- Gonzalez-Magaña A, Ibáñez de Opakua A, Romano-Moreno M, Murciano-Calles J, Merino N, Luque I, Rojas AL, Onesti S, Blanco FJ, De Biasio A.J “The p12 subunit of human polymerase  $\delta$  uses an atypical PIP box for molecular recognition of proliferating cell nuclear antigen (PCNA)” The Journal of Biological Chemistry (2019), 294(11):3947-3956. doi: 0.1074/jbc.RA118.006391.
- Jurado, S., Cano-Munoz, M., Morel, B., Standoli, S., Santarossa, E., Moog, C., Schmidt, S., Laumond, G., Camara-Artigas, A., Conejero-Lara, F. “Structural and Thermodynamic Analysis of HIV-1 Fusion Inhibition Using Small gp41 Mimetic Proteins.” Journal of Molecular Biology (2019), 431(17): 3091-3106. DOI: 10.1016/j.jmb.2019.06.022
- Jabalera, Y.; Casares-Atienza, S.; Fernández-Vivas, M.A.; Peigneux, A; Azuaga-Fortes, A.I.; Jiménez-López, C.”Protein Conservation Method Affects MamC-Mediated Biomineralization of Magnetic Nanoparticles” Cryst. Growth Des. (2019), 19, 1064-1071.
- Hermosilla, J.; Sánchez-Martín, R.; Pérez-Robles, R.; Salmerón-García, A.; Casares, S.; Cabeza, J.; Cuadros-Rodríguez, L.; Navas, N. “Comparative Stability Studies of Different Infliximab and Biosimilar CT-P13 Clinical Solutions by Combined Use of Physicochemical Analytical Techniques and Enzyme-Linked Immunosorbent Assay (ELISA)” Biodrugs (2019), 33, 193-205.
- Ubago-Rodríguez, A.; Casares-Atienza, S.; Fernández-Vivas, M.A.; Peigneux, A.; Jabalera, Y.; Cuesta-Rivero, M.; Jiménez-López, C.; Azuaga-Fortes, A.I. “Structure-function of MamC loop and its effects on the in vitro precipitation of biomimetic magnetite nanoparticles” Cryst. Growth Des. (2019), DOI: 10.1021/acs.cgd.9b00150
- Peigneux, A.; Jabalera, Y.; Vivas, M.A.F.; Casares, S.; Azuaga, A.I.; Jiménez-López “Turning Properties of biomimetic magnetic nanoparticles by combining magnetosome associated proteins” C. Sci Rep (2019), 1 (1), 8804.
- Camara-Artigas, A., Murciano-Calles, J., Martinez, J.C. “Conformational changes in the third PDZ domain of the neuronal postsynaptic density protein 95”. Acta

Crystallographica Section D (2019), 75: 381-391.

- Vankova, P, Salido, E, Timson, DJ, Pey AL “A Dynamic Core in Human NQO1 Controls the Functional and Stability Effects of Ligand Binding and Their Communication across the Enzyme Dimer” *Biomolecules* (2019), 9: E728. DOI: 10.3390/biom9110728.
- Razzuti, B, Bartucci, R, Pey AL “Warfarin increases thermal resistance of albumin through stabilization of the protein lobe that includes its binding site” *Archives of Biochemistry and Biophysics* (2019), 676: 108-123. doi: 10.1016/j.abb.2019.108123
- Kukreja A, Lasaro M, Cobaugh C, Forbes C, Tang JP, Gao X, Martin-Higueras C, Pey AL, Salido E, Sobolov SB, Subramanian RR. “Systemic AGT mRNA improves glyoxylate metabolism in a mouse model of Primary Hyperoxaluria Type I” *Nucleic Acid Therapeutics* (2019) DOI: 10.1089/nat.2018.0740.
- Medina-Carmona E, Rizzuti B, Martín-Escolano R, Pacheco-García JL, Mesa-Torres N, Neira JL, Guzzi R, Pey AL. “Phosphorylation compromises FAD binding and intracellular stability of wild-type and cancer-associated NQO1: Insights into flavo-proteome stability” *International Journal of Biological Macromolecules* (2019), 125: 1275-1288. DOI: 10.1016/j.ijbiomac.2018.09.108.
- Pey AL, Megarity CF, Timson DJ. “NAD(P)H quinone oxidoreductase 1 (NQO1): an enzyme which needs just enough mobility, in just the right places.” *Bioscience Reports* (2019), 39: BSR2018459. DOI: 10.1042/BSR20180459.
- Medina-Carmona E, Betancor-Fernández I, Santos J, Mesa-Torres N, Grottelli S, Batlle C, Naganathan AN, Oppici E, Cellini B, Ventura S, Salido E, Pey AL. “Insight into the specificity and severity of pathogenic mechanisms associated with missense mutations through experimental and structural perturbation analyses.” *Human Molecular Genetics* (2019), 28: 1-15. DOI: 10.1093/hmg/ddy323.
- Mateo Alarcón, P. L. (2018) “Del átomo para la guerra a Átomos para la Paz. Uso político y repercusión mediática en el franquismo (1945-1965)”. En *Entre la Alquimia y la Química*, pp. 121-155. Publicaciones de la Universidad de Granada .
- Mateo, P. L., Morente, C., Mateo-Leivas, L., Hidalgo, R. (2018) “La represión franquista contra la intelectualidad granadina: El caso de Jesús Yoldi Bereau”. *Historia Actual Online*, 46(2), 73-89
- Mateo, P.L., Conejero-Lara, F., Luque, I., Ruiz-Sanz, J., Martínez, J.C., Azuaga, A.I., Cobos, E.S. (2018) “Biocalorimetry: differential scanning calorimetry of protein solutions”, in “Enthalpy and internal energy: liquids, solutions and vapours”. Edited by Emmerich Wilhelm and Trevor M. Letcher. Royal Society of Chemistry, UK, pp. 315-335. ISBN: 978-1-78262-711-1
- Fernández-Reche, A., Cobos, E.S., Luque, I., Ruiz-Sanz, J., Martínez, J.C. (2018)

“Approaching the thermodynamic view of protein folding through the reproduction of Anfinsen’s experiment by undergraduate physical biochemistry students”. *Biochemistry and Molecular Biology Education*, 46(3): 262-269.

- Bekri, S., Bourdely, P., Luci, C., Dereuddre, N., Su, B., Martinon, F., Braud, V.M., Luque, I., Mateo, P.L., Crespillo, S., Conejero, F., Moog, C., Le Grand, R., Anjuère, F. (2017) “Sublingual priming with a HIV gp41-based subunit vaccine elicits mucosal antibodies and persistent B memory responses in nonhuman primates”. *Frontiers in Immunology*, 8, 1-13.
- Castello, F., Paredes, J.M., Ruedas-Rama, M.J., Martín, M., Roldán, M., Casares, S., Orte, A. (2017) “Two-step amyloid aggregation: sequential lag phase intermediates”. *Scientific Reports*, 7, Art. No. 40065, 10.1038/srep40065.
- Cerón Carrasco, J.P., Coronado Parra, T., Imbernón Tudela; B., Banegas Luna, A.J., Ghasemi, F., Vegara Meseguer, J.M., Luque, I., Sikander Azam, S., Henden, S.T., Pérez Sánchez, H. (2016) “Application of Computational Drug Discovery Techniques for Designing New Drugs Against Zika” *Virus. Drug Designing: Open Access*. 5 - 2, pp. 1000e131 - 1000e131. 28/06/2016.
- García Fontana, C., Narváez Reinaldo, J.J., Castillo Correa, F., Luque Fernández, I., Manzanera, M. (2016) “A new physiological role for the DNA molecule as a protector against drying stress in desiccation-tolerant microorganisms”. *Frontiers in Microbiology*. 7, 22/12/2016. ISSN 1664-302X.
- Murciano-Calles, J., Güell-Bosh, J., Villegas, S., Martínez, J.C. (2016) “Common features in the unfolding and misfolding of PDZ domains and beyond: the modulatory effect of domain swapping and extra-elements”. *Scientific Reports*, 6, 19242.
- Zafra Ruano, A., Cilia, E., Couceiro, J. R, Ruiz Sanz, J., Schymkowitz, J., Rousseau, F., Luque, I., Lenaerts, T., (2016) “From Binding-Induced Dynamic Effects in SH3 Structures to Evolutionary Conserved Sectors”. *PLoS computational biology*, 12(5), e1004938.
- Manssour-Triedo, F., Crespillo, S., Morel, B., Casares, S., Mateo, P. L., Notka, F., Roger, M. G., Mouz, N., El-Habib, R., Conejero-Lara, F. (2016) “Molecular and physicochemical factors governing solubility of the HIV gp41 ectodomain”. *Biophysical Journal* , 111(4), 700-709.
- Martínez-Rodríguez, S., Bacarizo, J., Luque, I., Camara-Artigas, A. (2015) “Crystal structure of the first WW domain of human YAP2 isoform”. *Journal of Structural Biology*, 191(3), 381-387.
- Sánchez-Moreno, P., Buzón, P., Boulaiz, H., Peula-García, J.M., Ortega-Vinuesa, J.L., Luque, I., Salvati, A., Marchal, JA. (2015) “Balancing the effect of corona on therapeutic efficacy and macrophage uptake of lipid nanocapsules”. *Biomaterials*, 61, 266-278
- Iglesias-Bexiga, M., Castillo, F., Cobos, E. S., Oka, T., Sudol, M., Luque, I. (2015)

“WW Domains of the Yes-Kinase-Associated- Protein (YAP) Transcriptional Regulator Behave as Independent Units with Different Binding Preferences for PPxY Motif- Containing Ligands”. *PLoS One* , 10(1), 1-22.

- De Biasio, A., Ibañez de Opakua, A., Mortuza, G. B., Molina, R., Cordeiro, T.N., Castillo, F., Villate, M., Merino, N., Delgado, S., Gil-Carton, D., Luque, I., Diercks, T., Bernardó, P., Montoya, G., Blanco, F.J. (2015) “Structure of p15PAF-PCNA complex and implications for clamp sliding during DNA replication and repair”. *Nature Communications*, 6, 6439.
- Mateo, P. L., Gómez, M., Mateo-Leivas, L., Hidalgo. R. (2014) “Jesús Yoldi Bereau (1894-1936), el profesor de química que no se presentó a su destino”. *Anales de Química* 110(4), pp. 286-293
- Murciano-Calles, J., Marin-Argani, M., Cobos, E.S., Villegas, S., Martinez, J.C. (2014) “The impact of extra-domain structures and post-translational modifications in the folding/misfolding behaviour of the third PDZ domain of MAGUK neuronal protein PSD-95”. *Plos One*, 9, e98124.
- Murciano-Calles, J., Corbi-Verge, C., Candel, A.M., Luque, I., Martinez, J.C. (2014) “Post-translational modifications modulate ligand recognition by the third PDZ domain of the MAGUK protein PSD-95”. *Plos One*, 9, e90030.
- Murciano-Calles, J., Martinez, J.C., Marin-Argany, M., Villegas, S., Cobos, E.S. (2014) “A thermodynamic study of the third PDZ domain of MAGUK neuronal protein PSD-95 reveals a complex three-state folding behaviour.” *Biophysical Chemistry* 185, 1-7.
- Crespillo, S., Camara-Artigas, A., Casares, S., Morel, B., Cobos, E.S., Mateo, P.L., Mouz, N., Martin, C.E., Roger, M.G., El Habib, R., Sue, B., Mooge, C., Conejero-Lara, F. (2014) “Single-chain protein mimetics of the N-terminal heptad-repeat region of gp41 with potential as anti-HIV-1 drugs”. *Proceedings of the National Academy of Sciences USA* 111, 18207-18212.
- Ruzafa, D., Varela, L., Azuaga, A.I., Conejero-Lara, F., Morel, B. (2014) “Mapping the structure of amyloid nucleation precursors by protein engineering kinetic analysis”. *Physical Chemistry Chemical Physics* 16, 2989-3000.
- Crespillo, S., Casares, S., Mateo, P.L., Conejero-Lara, F. (2014) “Thermodynamic analysis of the binding of 2F5 (fab and immunoglobulin G forms) to its gp41 epitope reveals a strong influence of the immunoglobulin Fc region on affinity”. *Journal of Biological Chemistry* 289, 594-599.
- Ruzafa ,D., Conejero-Lara, F., Morel, B. (2013) “Modulation of the stability of amyloidogenic precursors by anion binding strongly influences the rate of amyloid nucleation”. *Physical Chemistry Chemical Physics* 15, 15508-15517.
- Martínez, J.C., Murciano-Calles, J., Cobos, E.S., Iglesias-Bexiga, M., Luque, I., Ruíz-Sanz, J. “Isothermal titration calorimetry: thermodynamic analysis of the binding thermograms of molecular recognition events by using equilibrium

- models". (2013). Libro: Applications of Calorimetry in a Wide Context - Differential Scanning Calorimetry, Isothermal Titration Calorimetry and Microcalorimetry, editado por Amal Ali Elkordy (ISBN: 978-953-51-0947-1), Intech, Croacia. Capítulo 4, pp 73-104.
- Corbi-Verge, C., Marinelli, F., Zafra-Ruano, A., Ruiz-Sanz, J., Luque, I., Faraldo-Gómez, J. (2013) "Two-state dynamics of the SH3-SH2 tandem of Abl kinase and the allosteric role of the N-cap". Proceedings of the National Academy of Sciences 110 (36), W3372-80.
  - Casañal, A., Zander, U., Muñoz, C., Dupeux, F., Luque, I., Botella, M.A., Schwab, W., Valpuesta, V., Marquez, J.A. (2013) "The Strawberry pathogenesis-related 10 (PR-10) Fra a proteins control flavonoid biosynthesis by binding to metabolic intermediates" Journal of Biological Chemistry 288 (49): 35322-35332.
  - Marin-Argany, M., Candel, A.M., Murciano-Calles, J., Martínez, J.C., Villegas, S. (2012) "The interconversion between a flexible beta-sheet and a fibril beta-arrangement constitutes the main conformational event during misfolding of PSD95-PDZ3 domain". Biophysical Journal 103, 738-747.
  - Martín-García, J.M., Ruiz-Sanz, J., Luque, I. (2012) "Interfacial water molecules in SH3 interactions: A revised paradigm for polyproline recognition". Biochemical Journal 442, 443-451.
  - Martín-García, J.M., Luque, I., Ruiz-Sanz, J., Cámara-Artigas, A. (2012) "The promiscuous binding of the Fyn SH3 domain to a peptide from the NS5A protein". Acta Crystallographica Section D 68, 1030-1040.
  - Zafra-Ruano, A., Luque, I. (2012) "Interfacial water molecules in SH3 interactions: getting the full picture on polyproline recognition by protein-protein interaction domains". FEBS Letters 586, 2619-2630.
  - De Biasio, A., Campos-Olivas, R., Sanchez, R., Lopez-Alonso, J.P., Pantoja-Uceda, D., Merino, N., Villate, M., Martín-García, J.M., Castillo, F., Luque, I., Blanco, F.J. (2012) "Proliferating cell nuclear antigen (PCNA) interactions in solution studied by NMR". Plos One 7, e48390 1-11.
  - Andujar-Sanchez, M., Cobos, E.S., Luque, I., Martínez, J.C. (2012) "Thermodynamic impact of embedded water molecules in the unfolding of human CD2BP2-GYF domain". Journal of Physical Chemistry B, 116, 7168-7175.
  - Ruzafa, D, Morel, B, Varela, L, Azuaga, A.I., Conejero-Lara, F. (2012) "Characterization of Oligomers of Heterogeneous Size as Precursors of Amyloid Fibril Nucleation of an SH3 Domain: An Experimental Kinetics Study" PLoS One 7(11), e49690.
  - Cámara-Artigas, A., Gavira, J.A., Casares, S., García-Ruiz, J.M., Conejero-Lara, F., Allen, J.P., Martínez, J.C. (2011) "Understanding the polymorphic behaviour of a mutant of the alpha-spectrin SH3 domain by means of two 1.1 Å resolution

structures". *Acta Crystallographica D* 67, 189-196.

- Murciano-Calles, J., Cobos, E.S., Mateo, P.L., Camara-Artigas, A., Martinez, J.C. (2011) "A comparative analysis of the folding and misfolding pathways of the third PDZ domain of PSD95 investigated under different pH conditions". *Biophysical Chemistry* 158, 104-110.
- Martínez, J.C., Cobos, E.S., Luque, I., Ruíz-Sanz, J. "Differential scanning calorimetry: thermodynamic analysis of the unfolding transitions in proteins, domains and peptidic fragments by using equilibrium models". (2011). Libro: *Protein folding*, editado por Eric C. Walters (ISBN: 978-1-61728-990-3), Nova Science Publishers, Inc., New York. Capítulo 10, pp 313-348.
- Luque, I. "Biophysics of Protein-Protein Interactions" (2011). Libro: *Protein Surface Recognition: Approaches for Drug Discovery*, editado por Ernest Giralt, Mark W. Peczu, Xavier Salvatella (ISBN: 9780470972137), John Wiley and Sons, Inc, United kingdom. Capítulo 2, pp 23-52.
- Pedro L. Mateo Alarcón y Manuel Cortijo Mérida. "Los dos congresos hispano-soviéticos de Biofísica". (2011). Libro: *Veinticinco Años de la Sociedad de Biofísica de España (1986-2011)*, editado por Manuel Cortijo Mérida (ISBN: 9788461553686), Comité Español de la IUPAB, España. pp 111-124.
- Palencia, A., Cámara-Artigas, A., Pisabarro, M.T., Martínez, J.C., Luque, I. (2010) "Role of interfacial water molecules in proline-rich ligand recognition by the Src homology 3 domain of Abl". *Journal of Biological Chemistry* 285, 2823-2833.
- B. Morel, B., Varela, L., Azuaga, A. I., Conejero-Lara, F. (2010) "Environmental conditions affect the kinetics of nucleation of amyloid fibrils and determine their morphology". *Biophysical Journal* 99, 3801-3810.
- Cámara-Artigas A., Murciano-Calles J., Gavira J.A., Cobos E.S., Martínez J.C. (2010) "Novel conformational aspects of the third PDZ domain of the neuronal post-synaptic density-95 protein revealed from two 1.4 Å X-ray structures". *Journal of Structural Biology* 170, 565-9.
- Murciano-Calles J., Cobos E.S., Mateo P.L., Camara-Artigas A., Martinez J.C. (2010) "An oligomeric equilibrium intermediate as the precursory nucleus of globular and fibrillar supramacromolecular assemblies in a PDZ domain". *Biophysical Journal* 99, 263-272.
- Andujar-Sánchez, M., Jara-Perez, V., Cobos, E.S., Cámara Artigas, A. (2010) "A thermodynamic characterization of the interaction of 8-anilino 1-naphthalene sulfonic acid with native globular proteins: the effect of the ligand dimerization in the analysis of the binding isotherms". *Journal of Molecular Recognition* 24, 548-556.
- Camara-Artigas, A., Andujar-Sanchez, M., Ortiz-Salmeron, E., Cuadri, C., Cobos, E.S., Martin-Garcia, J.M. (2010) "High resolution structure of alpha-spectrin SH3 domain mutant with a redesigned core". *Acta Crystallographica Section F* 66,

1023-1027.

- Morel B., Varela L., Conejero-Lara F. (2010) "The thermodynamic stability of amyloid fibrils studied by differential scanning calorimetry". *Journal of Physical Chemistry B* 114, 4010-4019.
- Lacal J., Alfonso C., Liu X., Parales R.E., Morel B., Conejero-Lara F., Rivas G., Duque E., Ramos J.L., Krell T. (2010) "Identification of a chemoreceptor for TCA cycle intermediates: differential chemotactic response towards receptor ligands". *Journal of Biological Chemistry* 285, 23126-23136.

## Publicaciones Antiguas

- Cobos ES, Iglesias-Bexiga M, Ruiz-Sanz J, Mateo PL, Luque I, Martinez JC (2009) "Thermodynamic characterization of the folding equilibrium of the human Nedd4-WW4 domain: at the frontiers of cooperative folding". *Biochemistry* 48, 8712-8720.
- Candel AM, Cobos ES, Conejero-Lara F, Martinez JC (2009) "Evaluation of folding co-operativity of a chimeric protein based on the molecular recognition between polyproline ligands and SH3 domains". *PEDS* 22, 597-606.
- Varela L, Morel B, Azuaga AI, Conejero-Lara F. (2009) "A single mutation in an SH3 domain increases amyloid aggregation by accelerating nucleation, but not by destabilizing thermodynamically the native state". *FEBS Letters* 583, 801-806.
- Ortega-Roldán JL, Ringkjøbing JM, Brutscher B, Azuaga AI, Blackledge M., van Nuland, N.A.J. (2009) "Accurate characterization of weak macromolecular interactions by titration of NMR residual dipolar couplings: application to the CD2AP SH3-C:Ubiquitin complex". *Nucleic Acid Research* 37, 1-12.
- Cobos ES, Iglesias-Bexiga M, Ruiz-Sanz J, Mateo-Alarcón PL, Luque I, Martinez JC (2009) "Thermodynamic characterization of the folding equilibrium of the human Nedd4-WW4 domain: at the frontiers of cooperative folding". *Biochemistry* 48, 8712-8720.
- Cámara-Artigas A, Martín-García JM, Morel B, Ruiz-Sanz J, Luque I (2009) "Intertwined dimeric structure for the SH3 domain of the c-Src tyrosine kinase induced by polyethylene glycol binding". *FEBS Letters* 583, 749-753.
- Candel AM, van Nuland NAJ, Martín-Sierra FM, Martinez JC, Conejero-Lara F (2008) "Analysis of the thermodynamics of binding of an SH3 domain to proline-rich peptides using a chimeric fusion protein". *Journal of Molecular Biology* 337, 117-135.
- Cobos ES, Candel AM, Martinez JC (2008) "An error analysis for two-state protein-folding kinetic parameters and f-values: progress towards precision by



- exploring pH dependencies on Leffler plots". *Biophysical Journal* 94, 4393-4404.
- Palacios A, Muñoz IG, Pantoja-Uceda D, Marcaida MJ, Torres D, Martín-García JM, Luque I, Montoya G and Blanco FJ (2008) "Molecular Basis of Histone H3K4ME3 Recognition by ING4" *Journal of Biological Chemistry* 283, 15956-15964.
  - Bemporad F, Vannocci T, Varela L, Azuaga AI, Chiti F (2008) "A model for the aggregation of the Acylphosphatase from *Sulfolobus solfataricus* in its native-like state". *Biochimica et Biophysica Acta (BBA)* 1784, 1986-1996.
  - Candel AM, Conejero-Lara F, Martinez JC, van Nuland NA, Bruix M. (2007) "The high-resolution NMR structure of a single-chain chimeric protein mimicking a SH3-peptide complex". *FEBS Letters* 581, 687-692.
  - Martín-García JM, Luque I, Mateo PL, Ruiz-Sanz J, Cámara-Artigas A. (2007) "Crystallographic structure of the SH3 domain of the human c-Yes tyrosine kinase: Loop flexibility and amyloid aggregation". *FEBS Letters* 581, 1701-1706.
  - Casares S, Ab E, Eshuis H, Lopez-Mayorga O, van Nuland NA, Conejero-Lara F. (2007) The high-resolution NMR structure of the R21A Spc-SH3:P41 complex: Understanding the determinants of binding affinity by comparison with Abl-SH3. *BMC Struct Biol.* 7(1), 22 [Epub ahead of print].
  - Ortega-Roldan JL, Romero-Romero ML, Ora A, AB E, López-Mayorga O, Azuaga AI, van Nuland NAJ (2007) "The high resolution NMR structure of the third SH3 domain of CD2AP" *J. Biomol. NMR* 39, 331-336.
  - Casares, S., López-Mayorga, O., Vega, M.C., Cámara-Artigas, A. and Conejero-Lara, F. (2007) Cooperative propagation of local stability changes from low-stability and high-stability regions in a SH3 domain. *Proteins* 67, 531-547.
  - Morel, B, Casares, S, Conejero-Lara, F (2006) "A Single Mutation Induces Amyloid Aggregation in the  $\alpha$ -Spectrin SH3 Domain: Analysis of the Early Stages of Fibril Formation" *J. Mol. Biol.* 356, 463-478.
  - Tomaselli S, Esposito V, Vangone P, Van Nuland NAJ, Bonvin AMJJ, Tancredi T, Temussi PA, Picone D (2006) "The  $\alpha$  to  $\beta$  conformational transition of Alzheimer's Ab-(1-42) peptide in aqueous media is reversible: a step by step conformational analysis suggests the location of the  $\beta$  conformation seeding " *ChemBioChem* 7, 257-267.
  - Sibille N, Favier A, Azuaga AI, Ganshaw G, Bott R, Bonvin AMJJ, Boelens R, Van Nuland NAJ (2006) "Comparative NMR study on the impact of point mutations on protein stability of *Pseudomonas mendocina* lipase" *Protein Sci.* 15, 1915-1927.
  - Duarte AM, Wolfs CJ, Van Nuland NAJ, Harrison MA, Findlay JB, Van Mierlo CP, Hemminga MA (2006) "Structure and localization of an essential transmembrane segment of the proton translocation channel of yeast H(+)-V-ATPase" *Biochim Biophys Acta. Biomembranes* 1768(2), 218-227.

- Palencia A, Martinez JC, Mateo PL, Luque I, Camara-Artigas A (2006) Structure of human TSG101 UEV domain. *Acta Crystallogr D Biol Crystallogr.* 62(Pt 4), 458-64.
- Cuadri-Tome C, Baron C, Jara-Perez V, Parody-Morreale A, Martinez JC, Camara-Artigas A (2006) "Kinetic analysis and modelling of the allosteric behaviour of liver and muscle glycogen phosphorylases" *J. Mol. Recognit.* 19, 451-457.
- Cámara-Artigas A, Palencia A, Martínez JC, Luque I, Gavira JA, García-Ruiz JM (2006) "Crystallization by capillary counter-diffusion and structure determination of the N114A mutant of the SH3 domain of Abl tyrosine kinase complexed with a high-affinity peptide ligand" *Acta Crystallographica D* D63, 646-52.
- Lange C, Luque I, Hervas M, Ruiz-Sanz J, Mateo PL, De la Rosa MA (2005) "Role of the surface charges D72 and K8 in the function and structural stability of the cytochrome c(6) from *Nostoc* sp PCC 7119" *FEBS J.* 272, 3317-3327.
- Martinez JC, Lopez-Mayorga O, Parody-Morreale A, Gavira JA (2005) "Binding curves by continuous gradient flow-mix calorimetry" *Thermochimica Acta* 437, 140-144.
- Azuaga AI, Neira JL, van Nuland NAJ (2005) "HPr as a model protein in structure, interaction, folding and stability studies " *Protein and Peptide Letters* 12, 123-137.
- Ekkelenkamp MB, Hanssen M, Hsu STD, de Jong A, Milatovic D, Verhoef J, van Nuland NAJ (2005) "Isolation and structural characterization of epilancin 15X, a novel lantibiotic from a clinical strain of *Staphylococcus epidermidis*" *FEBS Lett.* 579, 1917-1922.
- Bernard C, Houben K, Derix NM, Marks D, van der Horst MA, Hellingwerf KJ, Boelens R, Kaptein R, van Nuland NAJ (2005) "The solution structure of a transient photoreceptor intermediate: Delta 25 photoactive yellow protein" *Structure* 13, 953-962.
- Palencia A, Cobos ES, Mateo PL, Martinez JC, Luque I. (2004) "Thermodynamic Dissection of the Binding Energetics of Proline-rich Peptides to the Abl-SH3 Domain: Implications for Rational Ligand Design." *J Mol Biol.* 336, 527-537.
- Casares S, Sadqi M, López-Mayorga O, Conejero-Lara F, van Nuland NA.J. (2004) Detection and characterization of partially unfolded oligomers of the SH3 domain of alpha-spectrin". *Biophys J.* 86, 2403-2413.
- Cobos ES, Pisabarro MT, Vega MC, Lacroix E, Serrano L, Ruiz-Sanz J, Martinez JC (2004) "A miniprotein scaffold used to assemble the polyproline II binding epitope recognized by SH3 domains" *J. Mol. Biol.* 342, 355-365.
- Ruiz-Sanz J, Filimonov VV, Christodoulou E, Vorgias CE, Mateo PL (2004) "Thermodynamic analysis of the unfolding and stability of the dimeric DNA-binding protein HU from the hyperthermophilic eubacterium *Thermotoga*

maritima and its E34D mutant" Eur J Biochem. 271,1497-1507.

- Cobos ES, Filimonov VV, Vega MC, Mateo PL, Serrano L, Martinez JC. (2003) "A thermodynamic and kinetic analysis of the folding pathway of an SH3 domain entropically stabilised by a redesigned hydrophobic core". J. Mol. Biol. 328, 221-233.
- Azuaga AI, Canet D, Smeenk G, Berends R, Titgemeijer F, Durkens R, Mateo PL, Scheek RM, Robillard GT, Dobson CM, van Nuland NA. (2003) "Characterization of single-tryptophan mutants of histidine-containing phosphocarrier protein: evidence for local rearrangements during folding from high concentrations of denaturant". Biochemistry 42, 4883-95.
- Casares S, Sadqi M, Lopez-Mayorga O, Martinez JC, Conejero-Lara F. (2003) "Structural cooperativity in the SH3 domain studied by site-directed mutagenesis and amide hydrogen exchange". FEBS Lett. 539, 125-30.
- Casares S, Sadqi M, Lopez-Mayorga O, Martinez JC, Conejero-Lara F. (2003) "Structural cooperativity in the SH3 domain studied by site-directed mutagenesis and amide hydrogen exchange". FEBS Lett. 539, 125-30.
- Martin-Sierra FM, Candel AM, Casares S, Filimonov VV, Martinez JC, Conejero-Lara F. (2003) "A binding event converted into a folding event". FEBS Lett. 553, 328-32.
- Sadqi, M., Casares, S., López-Mayorga, O., Martínez, J. C. and Conejero-Lara F. (2002) "pH dependence of the hydrogen exchange in the SH3 domain of alpha-spectrin". FEBS Lett. 514, 295-299.
- Cobos ES, Filimonov VV, Galvez A, Valdivia E, Maqueda M, Martinez JC, & Mateo PL. (2002) "The denaturation of circular enterocin AS-48 by urea and guanidinium hydrochloride". Biochim. Biophys. Acta 1598, 98-107.
- Nezami A, Luque I, Kimura T, Kiso Y, & Freire E. (2002) "Identification and characterization of allophenylnorstatine-based inhibitors of plasmepsin II, an antimalarial target". Biochemistry 41, 2273-2280
- Luque I, Leavitt SA, & Freire E. (2002) "The linkage between protein folding and functional cooperativity: two sides of the same coin?" Annu. Rev. Biophys. Biomol. Struct. 31, 235-256.
- Luque I, & Freire E. (2002) "Structural parameterization of the binding enthalpy of small ligands". Proteins 49, 181-90.
- Azuaga AI, Dobson CM, Mateo PL, & Conejero-Lara F. (2002) "Unfolding and aggregation during the thermal denaturation of streptokinase". Eur. J. Biochem. 269, 4121-4133.
- Sadqi M, Casares S, Lopez-Mayorga O, & Conejero-Lara F. (2002) "The temperature dependence of the hydrogen exchange in the SH3 domain of

alpha-spectrin". FEBS Lett. 527, 86-90.

- Cobos ES, Filimonov VV, Galvez A, Maqueda M, Valdivia E, Martinez JC & Mateo PL. (2001) "AS-48: a circular protein with an extremely stable globular structure". FEBS Lett. 505, 379-82.
- Todd MJ, Luque I, Velazquez-Campoy A, Freire E. (2000) "Thermodynamic basis of resistance to HIV-1 protease inhibition: calorimetric analysis of the V82F/I84V active site resistant mutant". Biochemistry 39, 11876-83.
- Luque I, Freire E. (2000) "Structural stability of binding sites: consequences for binding affinity and allosteric effects". Proteins, Suppl 4, 63-71.
- Velazquez-Campoy A, Luque I, Todd MJ, Milutinovich M, Kiso Y, Freire E. (2000) "Thermodynamic dissection of the binding energetics of KNI-272, a potent HIV-1 protease inhibitor". Protein Sci. 9, 1801-9.
- Lambeir, A.M., Backmann, J., Ruiz-Sanz, J., Filimonov, V. Nielsen, J.E., Kursula, I., Norledge, B.V. & Wierenga, R.K. (2000) "The Ionization of a Buried Glutamic-Acid Is Thermodynamically Linked to the Stability of Leishmania-Mexicana Triose Phosphate Isomerase". Eur. J. Biochem. 267, 2516-2524.
- Fernandez, A.M., Villegas, V., Martínez, J.C., van Nuland, N.A.J., Conejero-Lara, F., Avilés, F.X., Serrano, L., Filimonov, V.V. & Mateo, P.L. (2000) "Thermodynamic Analysis of Helix-Engineered Forms of the Activation Domain of Human Procarboxypeptidase A2". Eur. J. Biochem. 267, 5891-5899.
- Vega MC, Martinez JC, Serrano L. (2000) "Thermodynamic and structural characterization of Asn and Ala residues in the disallowed II' region of the Ramachandran plot". Protein Sci. 9, 2322-8.
- Azuaga AI, Woodruff ND, Conejero-Lara F, Cox VF, Smith RA, Dobson CM. (1999) "Expression and characterization of the intact N-terminal domain of streptokinase". Protein Sci. 8, 443-6.
- Mohana-Borges R, Silva JL, Ruiz-Sanz J, de Prat-Gay G. (1999) "Folding of a pressure-denatured model protein". Proc. Natl. Acad. Sci. USA 96, 7888-93.
- Martinez JC & Serrano L. (1999) "The folding transition state between SH3 domains is conformationally restricted and evolutionarily conserved". Nat. Struct. Biol. 6, 1010-6.
- Ruiz-Sanz J, Simoncsits A, Toro I, Pongor S, Mateo PL, Filimonov VV. (1999) "A thermodynamic study of the 434-repressor N-terminal domain and of its covalently linked dimers". Eur. J. Biochem. 263, 246-53.
- van den Berg B, Chung EW, Robinson CV, Mateo PL, Dobson CM. (1999) "The oxidative refolding of hen lysozyme and its catalysis by protein disulfide isomerase" EMBO J. 18, 4794-803.
- Filimonov VV, Azuaga AI, Viguera AR, Serrano L, Mateo PL. (1999) "A

thermodynamic analysis of a family of small globular proteins: SH3 domains”  
Biophys Chem. 77, 195-208.

- Martinez JC, Viguera AR, Berisio R, Wilmanns M, Mateo PL, Filimonov VV & Serrano L. (1999) “Thermodynamic analysis of alpha-spectrin SH3 and two of its circular permutants with different loop lengths: discerning the reasons for rapid folding in proteins”. Biochemistry 38, 549-59.
- Sadqi M, Casares S, Abril MA, Lopez-Mayorga O, Conejero-Lara F & Freire E. (1999) “The native state conformational ensemble of the SH3 domain from alpha-spectrin” Biochemistry 38, 8899-906.
- Padmanabhan S, Laurents DV, Fernandez AM, Elias-Arnanz M, Ruiz-Sanz J, Mateo PL, Rico M & Filimonov VV. (1999) “Thermodynamic analysis of the structural stability of phage 434 Cro protein” Biochemistry 38, 15536-47.