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DEGREES: Master's Degree in Pharmacy "Licenciado en Farmacia" (June 1979), Universidad Complutense; "Grado de Licenciado" (September 1979), Univ. Complutense (Madrid).
Ph. D. "Doctor en Farmacia *cum laude*" (April 1987), Universidad de Alcalá (Madrid).

POSTDOC TRAINING: April 1987- September 1989, Physical Chemistry Laboratory, Oxford University, U.K.
Supervisor: Dr. W. Graham Richards.

PREVIOUS APPOINTMENTS: Lecturer of Pharmacology (1980-87)
Assistant Professor (1989-2009)
Associate Director of NFCR Center for Computational Drug Design (Oxford, 2001-06)
Member of the Editorial Advisory Board of *Journal of Medicinal Chemistry* (2006-10)

CURRENT POSITION: Full Professor of Pharmacology at University of Alcalá (since November 2009)
Member of the Editorial Advisory Board of *Anti-Cancer Agents in Medicinal Chemistry* (formerly *Current Medicinal Chemistry - Anti-Cancer Agents*), since 2001.
Editor-in-Chief of *Journal of Computer-Aided Molecular Design*, since 2001.

MEMBERSHIPS: Spanish Biophysics Society (since 1992).
Spanish Society of Medicinal Chemistry (since 1993).
Spanish Association of Cancer Researchers (since 1994).
Spanish Society of Biochemistry and Molecular Biology (since 1997).
Spanish Pharmacological Society (since 2001).
American Chemical Society (since 2006).

A. SELECTED INTERNATIONAL PUBLICATIONS

A.1. BOOK CHAPTERS

Mendoza, J.; Gago, F. (1994) Molecular recognition of dinucleotides and amino acids by artificial receptors containing a bicyclic guanidinium subunit (pp. 79-99), in *Computational Approaches in Supramolecular Chemistry*, NATO ASI Series, Kluwer Academic Publishers · ISBN 0-7923-2767-5.

Gallego, J., de Pascual, B., Ortiz, A. R., Pisabarro, M. T., Gago, F. (1995) Molecular Electrostatic Potentials of DNA Base Pairs and Drug Chromophores in Relation to DNA Conformation and Bis-Intercalation by Quinoxaline Antibiotics and Ditercalinium (pp. 274-281), in *QSAR and Molecular Modelling: Concepts, Computational Tools and Biological Applications* ed. J. R. Prous, S.A. · ISBN: 84-8124-079-6.

Ortiz, A. R., Pisabarro, M. T., Gago, F., Wade, R. C. (1995) Prediction of Drug Binding Affinities by Comparative Binding Energy Analysis: Application to Human Synovial Fluid Phospholipase A₂ Inhibitors (pp. 439-443), in *QSAR and Molecular Modelling: Concepts, Computational Tools and Biological Applications* ed. J. R. Prous, S.A. · ISBN: 84-8124-079-6.

Wade, R. C., Ortiz, A. R., Gago, F. (1998) Comparative Binding Energy Analysis (pp. 19-34), in *3D-QSAR in Drug Design, Vol. 2: Ligand-Protein Interactions and Molecular Similarity*; Kubinyi, H., Folkers, G., Martin, Y. Eds. Kluwer-ESCOM, Dordrecht · ISBN: ISBN 0-7923-4792-7.

Gago, F. & Hurley, L. H. (2002) Devising a Structural Basis for the Potent Cytotoxic Effects of Ecteinascidin 743 (pp. 643-675), in *Small Molecule DNA and RNA Binders: From Synthesis to Nucleic Acid Complexes*, Demeunynck, C. Bailly & D. Wilson, Eds., Wiley-VCH (Weinheim, Alemania) · ISBN 3-527-30595-5.

Damborsky J., Kmunicek J., Jedlicka T., Luengo S., Gago F., Ortiz A.R., Wade R.C. Rational Re-design of Haloalkane Dehalogenases Guided by Comparative Binding Energy Analysis (pp. 79-96), in *Enzyme Functionality: Design, Engineering and Screening*. Svendsen, A. (Ed.) Marcel Decker (New York) · ISBN 0-

8247-4709-7.

Gago, F. (2005) Pharmacological Properties of Nimesulide: Structural Aspects of Cyclooxygenase (COX) Activity and COX-2 Inhibition by Nimesulide (pp.162-173), in *Nimesulide: Actions and Uses*. K. Rainsford (editor) Birkhäuser Verlag AG (Basel/Switzerland) · ISBN 3-7643-7068-8.

Gago, F. (2006) Computer simulations of drug-DNA interactions: A personal journey (pp. 152-189), in *Sequence-Specific DNA Binding Agents*, Michael Waring (editor), Royal Society of Chemistry (United Kingdom) · ISBN 0-85404-370-5.

Gago, F. & Moreno, S. (2009) Trabectedin, in *Encyclopedia of Cancer*. Manfred Schwab (Editor-in-Chief), Springer (Germany) · ISBN 978-3-540-36847-2.

Morreale, A. & Gago, F. (2012) COMparative BINDing Energy (COMBINE) analysis as a structure-based 3D-QSAR method (pp. 244-272), in *Physico-Chemical and Computational Approaches to Drug Discovery*, F. Javier Luque & Xavier Barril (editors), Royal Society of Chemistry (Great Britain) · ISBN-10: 1849733538.

A.2. PAPERS IN REFEREED JOURNALS (last 6 years)

108. Familiar, O.; Munier-Lehmann, H.; Negri, A.; Gago, F.; Douguet, D.; Rigouts, L.; Hernández, A.I.; Camarasa, M.J.; Pérez-Pérez, M.J. "Exploring acyclic nucleoside analogues as inhibitors of Mycobacterium tuberculosis thymidylate kinase". *ChemMedChem*, 3(7): 1083–1093 (2008).

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111. Matesanz, R.; Barasoain, I.; Yang, C.-G.; Wang, L.; Li, X.; de Inés, C.; Coderch, C.; Gago, F.; Jiménez-Barbero, J.; Andreu, J.M.; Fang, W.-S.; Díaz, J.F. "Optimization of taxane binding to microtubules. Binding affinity dissection and incremental construction of a high-affinity analogue of paclitaxel". *Chemistry & Biology*, 15(6): 573–585 (2008).

112. Pande, V. ; Ramos, M.J. ; Gago, F. "The protein kinase inhibitor balanol: structure–activity relationships and structure-based computational studies". *Anti-Cancer Agents - Medicinal Chemistry*, 8(6): 638–645 (2008).

113. Rico, E.; Alzate, J.F.; Arias, A.A.; Gago, F.; Moreno, D.; Clos, J.; Moreno, I.; Domínguez, M.; Jiménez-Ruiz, A. "*Leishmania infantum* expresses a mitochondrial nuclease homologous to EndoG that migrates to the nucleus in response to an apoptotic stimulus". *Molecular & Biochemical Parasitology*, 163(1): 28-38 (2009).

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116. Leal, J-F. M.; García-Hernández, V.; Moneo, V.; Domingo, D.; Bueren-Calabuig, J.A.; Negri, A.; Gago, F.; Guillén-Navarro, M.J.; Avilés, P.; Cuevas, C.; García-Fernández, L.F.; Galmarini, C.M. "Molecular pharmacology and antitumor activity of Zalypsis® in several human cancer cell lines". *Biochemical Pharmacology*, 78(2):162-170 (2009).

117. Bronckaers, A.; Gago, F.; Balzarini, J.; Liekens, S. "The dual role of thymidine phosphorylase in cancer development and cancer chemotherapy". *Medicinal Research Reviews*, 29(6):903-953 (2009).

118. Negri, A.; Rodríguez-Larrea, D.; Marco, E.; Jiménez-Ruiz, A.; Sánchez-Ruiz, J.M.; Gago, F. "Protein-protein interactions at an enzyme-substrate interface: characterization of transient reaction intermediates throughout a full catalytic cycle of *Escherichia coli* thioredoxin reductase". *Proteins: Structure, Function & Bioinformatics*, 78(1):36-51 (2010).
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127. Bueren-Calabuig, J.A.; Giraudon, C.; Galmarini, C.M.; Egly, J.M.; Gago, F. "Temperature-induced melting of double-stranded DNA in the absence and presence of covalently bonded antitumor drugs: insight from molecular dynamics simulations". *Nucleic Acids Research*, 39(18):8248-8257 (2011).
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129. Cortés Cabrera, A.; Gil-Redondo, R.; Perona, A.; Gago, F.; Morreale, A. "VSDMIP 1.5: an automated structure- and ligand-based virtual screening platform with a PyMOL graphical user interface". *Journal of Computer-Aided Molecular Design*, 25(9):813-824 (2011).
130. Bueren-Calabuig, J.A.; Coderch, C.; Rico, E.; Jiménez-Ruiz, A.; Gago, F. "Mechanistic insight into the catalytic activity of $\beta\beta\alpha$ -metallonucleases from computer simulations: *Vibrio vulnificus* periplasmic nuclease as a test case". *ChemBioChem*, 12(17): 2615-2622 (2011).
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10(8): 1543–1552 (2012).

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134. Coderch, C.; Klett, J.; Morreale, A.; Díaz, J.F.; Gago, F. "Comparative Binding Energy (COMBINE) analysis supports a proposal for the binding mode of epothilones to β -tubulin". *ChemMedChem*. 7(5):836-843 (2012).

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141. Gago, F. "Molecular simulations of drug-receptor complexes in anticancer research". *Future Medicinal Chemistry*, 4(15) 1961-1970 (2012).

142. Peón, A.; Coderch, C.; Gago, F.; González-Bello, C. "Comparative Binding Energy (COMBINE) Analysis for Understanding the Binding Determinants of Type II Dehydroquinase Inhibitors". *ChemMedChem*, 8(5) 740–747 (2013).

143. Coderch, C.; Tang, Y.; Klett, J.; Zhang, S.-E.; Ma, Y.-T.; Shaorong, W.; Matesanz, R.; Pera, B.; Canales, A.; Jiménez-Barbero, J.; Morreale, A.; Díaz, J.F.; Fang, W.-S.; Gago, F. "A structure-based design of new C2- and C13-substituted taxanes: tubulin binding affinities and quantitative structure-activity relationships using Comparative Binding Energy (COMBINE) analysis". *Organic & Biomolecular Chemistry*, 11 (18) 3046 - 3056 (2013).

144. Casanova, E.; Moreno, D.; Gigante, A.; Rico, E.; Oliva, C.; Camarasa, M.-J.; Gago, F.; Jiménez-Ruiz, A.; Pérez-Pérez, M.-J. "5'-trityl-substituted thymidine derivatives as a novel class of antileishmanial agents: *Leishmania infantum* EndoG as a potential target". *ChemMedChem*, 8(7):1161-1174 (2013).

145. Toro, M. A.; Sánchez-Murcia, P.A.; Moreno, D.; Ruiz Santa Quiteria, M.; Alzate, J.F.; Negri, A.; Camarasa, M.J.; Gago, F.; Velázquez, S.; Jiménez-Ruiz, A. "Probing the dimerization interface of *Leishmania infantum* trypanothione reductase with site-directed mutagenesis and short peptides". *ChemBioChem*, 14(10):1212-1217 (2013).

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149. Parayil, A.; Gago, F. "New horizons in pharmaceutical biotechnology by melding biology and engineering". *Current Opinion in Biotechnology*, 24(6):1069–1071 (2013).
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Resumé

Federico Gago studied Pharmacy at Complutense University, Madrid, and followed post-doctoral studies at the Physical Chemistry Laboratory, Oxford University, under the supervision of Prof. W. Graham Richards. He teaches Pharmacology at the Schools of Pharmacy and Medicine in the University of Alcalá (Madrid), one of the oldest European universities, where he is a Full Professor in the Department of Biomedical Sciences. He was Associate Director of the NFCR Center for Computational Drug Design (Oxford) from 2001 to 2006 and a member of the Editorial Advisory Board of *Journal of Medicinal Chemistry* from 2006 to 2010. Since 2001 he has been serving as an Editor-in-Chief for *Journal of Computer-Aided Molecular Design* and as a member of the Editorial Advisory Board for *Anti-Cancer Agents in Medicinal Chemistry* (formerly *Current Medicinal Chemistry - Anti-Cancer Agents*).

Prof. Gago has authored more than 150 research papers in specialized scientific journals and has published several reviews and book chapters. His research interests are in the areas of structure-based drug design, receptor-based structure-activity relationships, and computer simulations of drug-targeted biomolecular systems including DNA, enzymes and pharmacological receptors.