

Jordi Mestres holds a PhD in Computational Chemistry from the University of Girona. After a post-doctoral stay at Pharmacia&Upjohn in Kalamazoo (Michigan, USA), in 1997 he joined the Molecular Design & Informatics department at N.V. Organon in Oss (The Netherlands) and in 2000 he was appointed Head of Computational Medicinal Chemistry at Organon Laboratories in Newhouse (Scotland, UK). In 2003, he took on his current position as Head of the Research Group on Systems Pharmacology, within the Research Program on Biomedical Informatics at the IMIM Hospital del Mar Medical Research Institute in Barcelona. He is also Associate Professor at the University Pompeu Fabra (UPF). In 2006, he founded Chemotargets as a spin-off company of his group. He is also the recipient of the 2006 Corwin Hansch Award from the QSAR and Modelling Society and the 2007 Technology Transfer Award from the UPF. In 2018, he was admitted as a Fellow of the Royal Society of Chemistry.

His expertise and research interests focus on the development of novel computational approaches and design of new analytics tools to predict and visualize the pharmacology and safety profiles of small molecule pharmaceuticals. He is the author of over 160 publications, 10 patents among them.

Five latest publications:

1. R. R. Tice, A. Bassan, A. Amberg, L. T. Anger, M. A. Beal, P. Bellion, R. Benigni, J. Birmingham, A. Brigo, F. Bringezu, L. Ceriani, I. Crooks, K. Cross, R. Elespuru, D. M. Faulkner, M. C. Fortin, P. Fowler, M. Frericks, H. H. J. Gerets, G. Jahnke, D. R. Jones, N. L. Kruhlack, E. Lo Piparo, J. Lopez-Belmonte, A. Luniwal, A. Luu, F. Madia, S. Manganelli, B. Manickam, **J. Mestres**, A. L. Mihalchik-Burhans, L. Neilson, A. Pandiri, M. Pavan, C. V. Rider, J. Rooney, A. Trejo-Martin, K. H. Watanabe-Sailor, A. T. White, D. Woolley, G. J. Myatt (2021) In Silico Approaches in Carcinogenicity Hazard Assessment: Current Status and Future Needs. *Computational Toxicology* 20, 100191.
2. M. J. Falaguera, **J. Mestres** (2021) Congenericity of Claimed Compounds in Patent Applications. *Molecules* 26, 5253. (Special Issue dedicated to Prof. Jurgen Bajorath).
3. N. Sánchez-Cruz, J. L. Medina-Franco, **J. Mestres**, X. Barril (2021). Extended Connectivity Interaction Features: Improving Binding Affinity Prediction through Chemical Description. *Bioinformatics* 37, 1376-1382.
4. M. J. Falaguera, **J. Mestres** (2021) Identification of the Core Chemical Structure in SureChEMBL Patents. *Journal of Chemical Information and Modeling* 61, 2241-2247.
5. M. Faria, E. Prats, J. R. Rosas Ramírez, M. Bellot, J. Bedrossiantz, M. Pagano, A. Valls, C. Gomez-Canela, J. M. Porta, **J. Mestres**, N. Garcia-Reyero, C. Faggio, L. M. Gómez Oliván, D. Raldua (2021). Androgenic Activation, Impairment of the Monoaminergic System and Altered Behaviour in Zebrafish Larvae Exposed to Environmental Concentrations of Fenitrothion. *Science of the Total Environment* 775, 145671.