

**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 computational approaches and analytics tools to predict and visualize the pharmacology and safety profiles of small molecule pharmaceuticals and cosmeceuticals. More recently, he has developed a particular interest in pursuing a fundamental understanding of the nature, composition and biological role of the human metabolome. He is the author of over 150 publications, 10 patents among them.

Some recent publications:

1. A. Bofill, X. Jalencas, T. I. Oprea, **J. Mestres** (2019). The Human Endogenous Metabolome as a Pharmacology Baseline for Drug Discovery. *Drug Discovery Today*, in press. (Highlighted in the Editorial of the September issue in *Drug Discovery Today* in the August issue of *Nature Reviews Drug Discovery*).
2. J. Olivés, **J. Mestres** (2019). Closing the Gap between Therapeutic Use and Mode of Action in Remedial Herbs. *Frontiers in Pharmacology*, accepted.
3. S. Dyballa, R. Miñana, M. Rubio, C. Cornet, T. Pederzani, G. Escaramis, R. Garcia-Serna, **J. Mestres**, J. Terriente (2019). Comparison of Zebrafish Larvae and hiPSC Cardiomyocytes for Predicting Drug Induced Cardiotoxicity in Humans. *Toxicological Sciences* 171, accepted.
4. F. Sanz, F. Pognan, T. Steger-Hartmann, C. Díaz, M. Cases, M. Pastor, P. Marc, J. Wichard, K. Briggs, D. Watson, T. Kleinöder, C. Yang, A. Amberg, M. Beaumont, A. Brookes, S. Brunak, M. T. D. Cronin, G. F. Ecker, S. Escher, N. Greene, A. Guzmán, A. Hersey, P. Jacques, L. Lammens, **J. Mestres**, W. Muster, H. Northeved, M. Pinches, J. Saiz, N. Sajot, A. Valencia, J. van der Lei, N. P. E. Vermeulen, E. Vock, G. Wolber, I. Zamora (2017). Legacy Data Sharing to Improve Drug Safety Assessment: the eTOX Project. *Nature Reviews Drug Discovery* 16, 811-812.
5. R. Garcia-Serna, D. Vidal, N. Remez, **J. Mestres** (2015). Large-Scale Predictive Drug Safety: From Structural Alerts to Biological Mechanisms. *Chemical Research in Toxicology* 28, 1875-1887. (Journal cover of Volume 28, Issue 10, October 2015).