Edelmiro Moman, PhD
Luxembourg
+352 621 511 423 / +353 87 462 2807

miromoman@gmail.com
http://www.prosciens.com/
https://www.linkedin.com/in/edelmiro-moman-3a9979a/

Organic/medicinal/computational chemist and entrepreneur, my dream is to discover new molecules to cure disease and contribute to understand life at a molecular level.

BIOGRAPHY

I am a scientist with a highly interdisciplinary profile. All throughout my career I have demonstrated resourcefulness, a passion for learning and an ability for independent thinking and working on my own initiative.

I received a PhD in organic chemistry from the University of Santiago de Compostela, Galicia, ES (1997-2003). My keen interest in life sciences led me, through a postdoc in RCSI, IE (2004-2006), to computer-aided drug design (CADD) as a bridge between chemistry and biology with a focus on therapeutics. I next moved into integrative structural biology at IGBMC, FR (2006-2008). This learning journey has endowed me with a deep understanding of chemical reactivity, structure and intermolecular interactions, all of which are essential in modern drug discovery.

Before moving to Luxembourg to support my wife's career at the European institutions I was aware that finding a suitable scientific job in the country was going to be challenging. The rest of my professional journey proves my determination to stay on the scientific track. Thus, I accepted a position at Saarland University (DE, 2009) even if the campus was located 110 km away from our home.

A collaboration with the Laboratoire de Biologie Moléculaire et Cellulaire du Cancer (LU) to de-orphan anticancer compounds in clinical trials (Unibioscreen, BE) opened the possibility of a career as scientific consultant in Luxembourg (2010), which, in turn, led me to found the contract research organisation Prosciens SARL (2010-2013).

I then took a parental leave until February 2016, when I was offered a position at RCSI. It must be noted, however, that I have never stopped doing science in the little time left by my parental duties, as shown by my 2014 review as sole author [2] and my 2016 interdisciplinary research article as corresponding author [1]. Back at RCSI, I was keen to round out my skillsets with on-target molecular biology and cell biology, thus encompassing much of the early-stage drug discovery process.

For family reasons, I am currently interested in finding a position in Luxembourg or as close as possible.

EDUCATION

PhD in Chemistry University of Santiago de Compostela, Galicia, ES, *Cum laude*. 1997-2003.
Remote Functionalisation on the Synthesis of 1α,25-Dihydroxyvitamin D_3 Analogues.
I completed the total synthesis of four novel vitamin D analogues (collaboration with Solvay Pharmaceuticals, NE), which resulted in two publications [5,17]. Working on my own initiative, I also developed a remote functionalisation-cyclisation free radical tandem process which enabled us to access other long sought-after analogues with intricate structures. An additional publication resulted from this work [10], but most of it remains unpublished due to IP considerations. In addition to my research work, four students transitioning from industrial engineering to chemical engineering in need of support lessons were referred to me by the Dean after realising that their chemical background was inadequate for the successful completion of the transition course. I had to devise a custom-tailored 3-hours-per-week program in a very short time and, at the end of the term, all four students were successful in all of the organic chemistry-related tests.

BSc in Chemistry University of Santiago de Compostela, Galicia, ES, Honours in Advanced Organic Synthesis. 1991-1996.

PROFESSIONAL EXPERIENCE

Postdoctoral Researcher Royal College of Surgeons in Ireland (RCSI), Dublin, IE, 2016-2017 (1.5 years).
Virtual screening and biological evaluation of novel FXR modulators by means of on-target TR-FRET and cell-based assays. I have developed new technologies specifically for the current project, including a new protein-ligand binding/activity database (*Ceangal*) and a machine learning scoring function (*Scóráil*). These technologies have already shown a very promising performance and enabled the discovery of novel natural products as FXR modulators. The fact that many of this natural products are abundant in food opens the possibility for a new project in the field of functional foods / nutraceuticals.

Parental leave LU. 2014-2016 (2.5 years).
When I learned we were expecting a second child, I decided to terminate Prosciens SÀRL and go on parental leave. However, I continued coordinating the development of Prosciens' internal drug discovery portfolio.

Founder & CEO Prosciens SÀRL, LU. 2010-2013 (3 years).
In Luxembourg I founded the CRO Prosciens SARL, developed novel technologies to advance our partnerts' projects – including a new reverse virtual screening protocol built *ex novo* – and coordinated several international networks of researchers to advance Prosciens' internal drug discovery portfolio. The most successful project to date has led to the discovery of a series of compounds that selectively hamper the proliferation of cancer cells by

preventing them from meeting their abnormal metabolic requirements. One compound from this series has recently been accepted by NIH's NCI-60 development programme, while different other aspects of its activity profile, such as the possibility of being developed as a non-hormonal male contraceptives, are currently under investigation. Preliminary on-target results have been reported on a 2016 article [1] .

Freelance Consultant Prosciens, LU, 2008-2010 (1 year).
I moved to Luxembourg for family reasons and established myself as a scientific consultant in the field of drug discovery. This also involved research stays in different institutions as detailed below.

Postdoctoral Researcher IGBMC, Illkirch, FR. 2006-2008 (2.5 years).
I was able to integrate information from different biochemical (site-directed mutagenesis) and biophysical (X-ray crystallography, SAXS, cryo-EM, FRET) techniques to build the first model of full-length nuclear receptor heterodimers bound to their DNA response elements. This pioneering work resulted in a highly-cited article on *Nature Structural & Molecular Biology* [4].

Postdoctoral Researcher Royal College of Surgeons in Ireland (RCSI), Dublin, IE, 2004-2006 (2.5 years).
After acquiring computer-aided drug design skills from a zero basis and on my own initiative, I led a project that allowed to gain structural insights (both computational and empirical) on the binding mode of its natural substrate, PGG_2, at the peroxidase site of the COX enzyme. This work resulted on a original article in *Biochemistry* and an Irish Health Research Board (HRB) grant valued at € 280,000. Moreover, quantum mechanics calculations shed light on the mechanistic of enzymatic catalysis and covalent inhibition at the cyclooxygenase site of the enzyme.

RESEARCH STAYS

Visiting postdoc Luxembourg Centre for Systems Biomedicine (LCSB), LU, 2010 (3 months).

Visiting postdoc Saarland University, DE, 2009 (12 months).
Design of CYP11B1 and 17-β-HSD2 inhibitors. Homology modelling and molecular dynamics of RDH1 mutants. I also supervised the MSc thesis of a foreign hearing-disabled student. He being a bioinformatician, I needed to devise a specific project tailored to match his particular set of skills. The project consisted in developing a novel methodology for the multiple alignment of proteins sequences taking advantage of the flexible structural alignment of existing crystal structures. The student was able to obtain his degree in less than a year. Furthermore, I significantly contributed to the application through which the department became part of the prestigious Helmholtz Centre for Infection Research.

Visiting postdoc CNR, Bologna, IT. 2003 (3 months).
γ-Radiolysis of nucleoside derivatives in aqueous media in order to study radiation-induced DNA damage.

Visiting scholar University of California, Berkeley, USA, 1999 (6 months).
Synthesis of nicotine fused analogues as nAChRs ligands for the treatment of neurodegenerative syndromes. Prof Rapoport offered me a postdoc in his group but that opportunity was frustrated by his sad passing away.

PUBLICATIONS

1. Masini, T., Birkaya, B., van Dijk, S., Mondal, M., Hekelaar, J., Jäger, M., Terwisscha van Scheltinga, A. C., Patel, M. S., Hirsch, A. K. H. & **Moman, E.*** Furoates and thenoates inhibit pyruvate dehydrogenase kinase 2 allosterically by binding to its pyruvate regulatory site. *J. Enzyme Inhib. Med. Chem.* 1–6 (2016).
   ROLE (Corresponding author): Project conception, coordination and supervision; computational studies; manuscript writing.
2. **Moman, E.*** Functionalization of non-activated C-H bonds in the synthesis of vitamin D metabolites and analogs. *Curr. Top. Med. Chem.* **14,** 2398–2407 (2014).
   ROLE (Corresponding author, review): Manuscript writing.
3. Bernard, E., Buckley, V., **Moman, E.**, Coleman, L., Meade, G., Kenny, D. & Devocelle, M.* Inhibition of platelet adhesion by peptidomimetics mimicking the interactive β-hairpin of glycoprotein Ibα. *Bioorg. Med. Chem. Lett.* **22,** 3323–3326 (2012).
   ROLE: Molecular dynamics simulations to optimise the design of the β-hairpin mimics.
4. Rochel, N., Ciesielski, F., Godet, J., **Moman, E.**, Roessle, M., Peluso-Iltis, C., Moulin, M., Haertlein, M., Callow, P., Mély, Y., Svergun, D. I. & Moras, D.* Common architecture of nuclear receptor heterodimers on DNA direct repeat elements with different spacings. *Nat. Struct. Mol. Biol.* **18,** 564–570 (2011).
   ROLE: Integration of the experimental information to build the first models that guided subsequent experimental studies and refinement.

5. Verlinden, L., Verstuyf, A., Eelen, G., Bouillon, R., Ordóñez-Morán, P., Larriba, M. J., Muñoz, A., Rochel, N., Sato, Y., Moras, D., Maestro, M., Seoane, S., Dominguez, F., Canosa, S., Nicoletti, D., **Moman, E.** & Mouriño, A.* Synthesis, structure, and biological activity of des-side chain analogues of 1α,25-dihydroxyvitamin D_3 with substituents at C18. *ChemMedChem* **6,** 788–793 (2011).
   ROLE: Design and synthesis of the reported vitamin D analogues.
6. Wangpradit, O., **Moman, E.**, Nolan, K. B., Buettner, G. R., Robertson, L. W. & Luthe, G.* Observation of an unusual electronically distorted semiquinone radical of PCB metabolites in the active site of prostaglandin H synthase-2. *Chemosphere* **81,** 1501–1508 (2010).
   ROLE: Quantum mechanics computational studies to interpret the spectra.
7. Haller, F., **Moman, E.**, Hartmann, R. W., Adamski, J. & Mindnich, R.* Molecular framework of steroid/retinoid discrimination in 17β hydroxysteroid dehydrogenase type 1 and photoreceptor-associated retinol dehydrogenase. *J. Mol. Biol.* **399,** 255–267 (2010).
   ROLE: Homology modelling and molecular dynamics studies to explain the biological results.
8. Alagha, A., **Moman, E.**, Adamo, M. F. A., Nolan, K. B. & Chubb, A. J.* Design, synthesis and evaluation of aspirin analogue having an additional carboxylate substituent for antithrombotic activity. *Bioorg. Med. Chem. Lett.* **19,** 4213–4216 (2009).
   ROLE: Project conception and computer-aided design of the compounds.
9. Neo, A. G., Carrillo, R. M., Barriga, S., **Momán, E.**, Marcaccini, S. & Marcos, C. F.* Multicomponent Synthesis of Highly Substituted 2-Pyridones. *Synlett* **2007,** 0327–0329 (2007).
   ROLE: Molecular modelling studies.
10. **Moman, E.**, Nicoletti, D. & Mouriño, A.* Strained polycycles by H^5C^{5x} free-radical cascades. *Org. Lett.* **8,** 1249–1251 (2006).
    ROLE: Project conception; development and optimisation of the free radical reactions; chemical synthesis; and manuscript writing.
11. Chubb, A. J., Fitzgerald, D. J., Nolan, K. B. & **Moman, E.*** The productive conformation of prostaglandin G_2 at the peroxidase site of prostaglandin endoperoxide H synthase: docking, molecular dynamics, and site-directed mutagenesis studies. *Biochemistry* **45,** 811–820 (2006).
    ROLE (Corresponding author): Project conception and supervision; molecular dynamics; and manuscript writing.
12. Lee, J., Chubb, A. J., **Moman, E.**, McLoughlin, B. M., Sharkey, C. T., Kelly, J. G., Nolan, K. B., Devocelle, M.* & Fitzgerald, D. J. Parallel synthesis and in vitro activity of novel anthranilic hydroxamate-based inhibitors of the prostaglandin H_2 synthase peroxidase activity. *Org. Biomol. Chem.* **3,** 3678–3685 (2005).
    ROLE: Molecular modelling studies.
13. Fernández, C., Diouf, O., **Momán, E.**, Gómez, G. & Fall, Y.* OCT Analogues Part 2. Acetylene in the Synthesis of Useful Building Blocks for Analogues of OCT Modified at C-20, C-21, and the D-Ring. S*ynthesis* **2005,** 1701–1705 (2005).
    ROLE: Synthesis of the A ring-bearing phosphonate; and studies for the installation of the side-chains.
14. Fernández, C., Gómez, G., Lago, C., **Momán, E.** & Fall, Y.* Design and Synthesis of Novel 20-*epi* Analogues of Calcitriol with Restricted Side Chain Conformation. *Synlett* **2005,** 2163–2166 (2005).
    ROLE: Synthesis of the A ring-bearing phosphonate; and studies for the installation of the side-chains.
15. **Momán, E.**, Nicoletti, D. & Mouriño, A.* Synthesis of novel analogues of 1a,25-dihydroxyvitamin D_3 with side chains at C-18. *J. Org. Chem.* **69,** 4615–4625 (2004).
    ROLE: Retrosynthetic analysis; total synthesis of several vitamin D analogues; and manuscript writing.

BOOK CHAPTERS

1. Buckley, V., Bernard, E., Moman, E., Coleman, L., Kenny, D. & Devocelle, M. in *Understanding Biology Using Peptides* (ed. Blondelle, S. E.) 451–452 (Springer New York, 2006).
2. Moman, E., Chubb, A. J. & Nolan, K. B. in *Metal Ions in Biology and Medicine: Les Ions Métalliques en Biologie et en Médecine* (eds. Alpoim, M. C., Morais, M. V. & Santos, M.-A.) 122-128 (John Libbey Eurotext, 2006).

PATENTS

Devocelle, M., Kenny, D., Foley, V. & Moman, E. Peptidomimetics and Uses Thereof. (2005).
https://patentscope.wipo.int/search/en/detail.jsf?docId=WO2005035568

INVITED PRESENTATIONS

15th IUPAB & 5th EBSA International Biophysics Congress, 27 August 2005, Montpellier, FR. Moman, E. *et al.* Molecular Docking and Dynamics Studies on the Peroxidase Site of Prostaglandin Endoperoxide Synthase. *Eur. Biophys. J.* **34**, 827 (2005).

ORGANISATION OF CONFERENCES

Organising committee of the Molecular Graphics & Modelling Society International Meeting, Trinity College Dublin, IE, 2005

RESEARCH SUPERVISION

1. Supervision of an MSc thesis in bioinformatics, Saarland University, DE, 2009.
2. Supervision of a final-year student and a TREO student, RCSI, Dublin, IE, 2005.

TEACHING

1. Qualified Teacher Status (QTS), National College for Teaching and Leadership, UK, 2017.
2. Organiser and lecturer at the Molecular Modelling Workshop, University of Extremadura, ES, 2008/2009.
3. Undergraduate chemistry laboratory assistant, RCSI, Dublin, IE, 2004-2005.
4. Advanced Organic Chemistry support lessons, USC, Galicia, ES, 2000-2001.
5. Chemistry undergraduate laboratory assistant, USC, Galicia, ES, 1998-2001.
6. Certificate of Pedagogical Aptitude (CAP), USC, Galicia, ES, 1997. It involved teaching a trimester of organic chemistry to International Baccalaureate students at the Multilingual IES Rosalia de Castro.

VARIA

1. TIDA/SFI Get Started Technology Venture Programme, DCU Ryan Academy for Entrepreneurs, Dublin, IE, 2016.
2. Codify Programming Workshops, TCD, Dublin, IE, 2016.
3. Reviewer for international scientific journals (*ChemBioChem*, *J. Steroid Biochem. Mol. Biol., Eur. J. Pharm. Sci.*).
4. Member of a PhD Thesis jury, organic chemistry, University of Vigo, Galicia, ES, 2007.

SKILLS

Organic synthesis (retrosynthetic analysis, handling of air, light and moisture-sensitive compounds, NMR, HPLC), **medicinal chemistry**, **computational chemistry** (GAMESS-US, MOPAC), **CADD** (MOE, Sybyl, Maestro, Pharmer), **computational structural biology** (NAMD, Desmond, Modeller), **integrative structural biology** (Situs, NMFF), **chemoinformatics** (OpenBabel, Filter-It), **biophysics** (TR-FRET), advanced Linux administration, advanced Bash scripting, Python.

LANGUAGES

English (full professional proficiency), **French** (professional proficiency), **Galician** Portuguese (native), **German** (B1), **Italian** (good comprehension, basic expression), **Portuguese** (full professional proficiency), **Slovak** (basic), **Spanish** (native).