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Conferencia:

Understanding ligand binding and receptor selectivity through molecular simulations

Hugo Gutiérrez de Terán

Dpto of Cell and Molecular Biology, Computational Biology and Bioinformatics, Uppsala University (Sweden)

14/07/16

Aula de Seminarios do CIQUS

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Curriculum Vitae
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Curriculum Vitae – Hugo Gutiérrez de Terán Castañón

1. ACADEMIC DEGREES.

- 2015- **Docent (Associate professor)**. Uppsala University (Sweden)
- 2004- **PhD on Experimental and Health Sciences**. Pompeu Fabra University-UPF, Barcelona (Spain). May 2004. Thesis title: *Molecular Modeling of Adenosine Receptors and Their Ligands in the Framework of Computer Aided Drug Design* (ISBN 846888524X). Supervisor: Prof. Ferran Sanz.
- 2003- **Master in Advanced Studies (MAS) on Experimental and Health Sciences**. UPF, Barcelona (Spain). May 2003.
- 1999- **M.Sc. in Pharmacy**, University of Santiago de Compostela (USC), Spain. M.Sc. Thesis project: *Conformationally Restricted Butitophenones as Potencially Atipical Antipsicotics. Synthesis of 4-oxo-4,5,6,7-tetrahydroindols from 4-oxo-4,5,6,7-tetrahydrobenzofuranes*. Supervisor: Prof. Enrique Raviña

2. PROFESIONAL EXPERIENCE.

- (6/2015 – present): ***Associate Professor*** in Computational and Systems Biology, Uppsala University.
- (8/2012 – 5/2014): ***Senior Researcher***; Department of Cell and Molecular Biology, Uppsala University.
- (8/2012 – 12/2012): ***Guest Researcher****;* Department of Cell and Molecular Biology, Uppsala University, Sweden. Funding: eSSENCE (Swedish network for e-science)
- (1/2012 – 6/2012): ***Visiting Scientist****;* The Scripps Research Institute (The Stevens lab), La Jolla (CA). Funding: *José Castillejo* (competitive fellowship), Spanish Ministry of Innovation.
- (12/2007 – 12/2012): ***Principal Scientist*** (non-Tenured fellowship); Fundación Pública Galega de Medicina Xenómica (FPGMX), Santiago de Compostela University Hospital, Spain. Funding: Autonomous Government of Galicia, Spain (competitive fellowships).
- (9/2006 – 12/2007): ***Head of data mining****;* BioFarma Group and USEF Platform for High Throughput Screening, (head: Prof. M.I. Loza), University of Santiago de Compostela, Spain. Funding: GENIUS Pharma, AIE (partnership between the Spanish Ministry of Industry and the pharmaceutical companies Almirall Prodesfarma and Laboratorios Esteve)
- (6/2004 – 8/2006): ***Postdoctoral researcher****;* Computational Chemistry lab (Prof. J. Åqvist), Department of Cell and Molecular Biology, Uppsala University, Sweden. Funding: RAPID drug discovery platform, Swedish Foundation for Strategic Research, SSF.
- (9/1999 – 5/2004): ***PhD student***, Research Group in Biomedical Informatics (GRIB), UPF (Barcelona, Spain). under the supervision of Prof. Ferran Sanz. Funding: Autonomous Government of Catalonia – Spain (competitive fellowships).

3. NATIONAL AND/OR INTERNATIONAL DISTINCTIONS AND AWARDS

- Best Scientific Trajectory, Barrie de la Maza Foundation, (International meeting of Galician researchers La Coruña, Spain, December 2015)
- Manuel Colmeiro certificate of Excellence, Autonomous Government of Galicia, Spain (May 2013).
- Several grants obtained for the attendance to conferences and workshops (see **Appendix**)

4. SCIENTIFIC OUTPUT

a) Publications (see Appendix for a complete list)

- 53 scientific articles, including 7 reviews and book chapters, with the following bibliometric indicators (as for August 2015):
  - 15 first authorships
  - 16 corresponding authorships
  - H-index = 15 (ISI WoK) / 18 (Google Scholar)
  - > 700 accumulated citations (ISI WoK and Google Scholar)
- Participation on 40 national and international conferences:
  - 8 invited lectures
  - 9 selected oral communications
  - 13 conference proceedings.
  - 22 poster presentations
- Computer programs and web servers
  - GPCR-ModSim, a toolkit for the modeling and simulation of GPCRs. (http://gpcr-modsim.org) More than 500 users worldwide. Team leader and responsible scientist of this server.
  - MIPSim: Molecular Interaction Potentials SIMilarity (IMIM / University Pompeu Fabra). Part of the development team of this program, used in Computer-Aided Drug design and computational Biochemistry.

b) Funds secured as PI: For the period 2008-2018, I have already secured funds from public sources and private foundations as principal investigator (PI), for a total of 635,000 € (~65.000€/year), and I was recipient of competitive fellowships (for a detailed list of all projects, see **Appendix**).

- (2014-2015) **Carl Trygger Foundation (Stockholm)**: 351,000 SEK (~39,000 €)
- (2014-2018) **Vetenskaprådet** (VR, Swedish Research Council, co-applicant): 4 million SEK (~423.000 €)
- (2012-2013) **Spanish National Plan for Research** (Ministry of Science): 96,000 €
- (2012) **Mobility program**, Spanish Ministry of Education (Visit to Scripps, CA): 16,000 €
- (2009-2011) **Health Research Program** (Government of Galicia, Spain): 88,300 €
- (2008-2012) **Parga Pondal Research Fellowship** (Government of Galicia, Spain): 180,000 €
- (2000-2004) **AGAUR PhD Student fellowship** (Catalan Government, Spain): 50.000 €
- (2002, 2008, 2009) **Mobility programs** (Catalan and Galician Governments): 9.000 € (3 visits to Uppsala University)

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5. COLLABORATIONS WITH THE PHARMACEUTICAL INDUSTRY AND CONSULTANCIES

- (2015-2016): with **Novo Nordisk**: *Structural understanding of PYY3-36 interaction with the NPY-family receptors* (Coordinated by Prof. Dan Larhammar, Uppsala University)
- (2012-): **Consultant** for the Unit of Pharmacological Evaluations-USEF, University of Santiago (USC) and the Galician Network for Drug Design.
- (2012-): **Consultant** for Ascidea-Computational Biology Solutions (http://www.ascidea.com/)
- (2006-2007): with **Almirall Prodesfarma** and **Laboratorios Esteve**, head of data mining at USEF-USC, as part of the GENIUS Pharma Public/private Spanish consortium
- (2004-2006): with **Medivir**, as postdoctoral researcher of the RAPID Drug Discovery center (Rational Approaches for Pathogen Inhibitor Design), at Uppsala University, funded by SSF.

6. MEMBER OF INTERNATIONAL PANELS, ORGANIZATION BOARD AND SCIENTIFIC COMMITTEES

- Management Committee (Sweden) of the EU Funded Cost Action: *GLISTEN*, GPCR-Ligand Interactions, Structures, and Transmembrane Signaling.
- Member of Editorial Board: BioMed Research International.
- Reviewer of 29 journals, including: Nature Communications, Journal of Infectious Diseases, PlOS One, Journal of the American Chemical Society, etc.
- Reviewer of funding agencies:
  - National Council of Science and Research (Romania, 2010)
  - National Science Foundation-NSF (USA, 2011)
  - Agence National de la Reserche-ANR (France, 2013)
  - Catalan Agency of University Research Funding (Spain, 2013-)
  - Estonian Research Council (Estonia, 2015)
- Co-organizer of the following conferences:
  - Adenosine Receptors: Present and Future Challenges; Uppsala, 2-3/3/2015 (Conference chair)
  - eSSENCE workshop on Macromolecular structure and dynamics; Uppsala, 3-5/6/2013. (Conference chair)
  - VIII Spanish Conference on Bioinformatics; Valencia, 13-15 February 2008.
- Board member: Galician Network of Bioinformatics: (Funded with €300.000 for the period 2007-2011).
- President: Association of Spanish Researchers in Sweden (http://aces-sffs.com). Co-funder and first president, with more than 100 members.

7. TEACHING EXPERIENCE (see **Appendix** for a detailed list of achievements).

Student supervision:

- 4 PhD Students
  - David Rodríguez Díaz (USC, 2012)
  - Silvana Vasile (expected 2019)
  - Sudarsan R. Vanga (UU, expected 2018)
  - Yashmin S. Kahn (co-supervisor, expected 2016)
  - Jaka Socan(co-supervisor, expected 2019)
- 3 postdoctoral researchers
  - Mauricio Esguerra (2014-2016)
  - Alexey Siretskiy (2015-2016)
  - Jessica Salander (2014-2016)
- 3 MSc thesis
  - Carlos Vara Sánchez (USC, 2009); José Correa (UNIA, 2010); David Murphy (UL-Birkbeck)
- 1 BSc thesis/project (Miguel Pérez, USC, 2010)

Lecturing and TA on lab courses:

- Graduate courses:
  - *Coordinator and teacher*: "Structural Bioinformatics: Modeling and Simulation of Biological Molecules", USC (Editions 2008 and 2009).
- MSc courses:
  - *Lecturer*: "Introduction to Bioinformatics", MSc in Neurosciences (USC, 2007-09);
  - *Lecturer*: "Computer-aided drug design", MSc in Bioinformatics (UPF, 2005).
- BSc courses:
  - *Coordinator and Lecturer*: Molecular and Statistical Mechanics (UU, 2016-) received a 78.000 SEK (8,440 €) grant from the Faculty of Science and technology, UU.
  - *Lecturer (2014) and coordinator (2015-)* Computational and Systems Biology (UU)
  - *Lecturer (2015-)* Structural Bioinformatics (UU)
  - *TA (labs):* Molecular and Statistical Mechanics (UU, 2006)

Member of educational evaluation committees:

- 4 PhD thesis evaluated
  - Laura López Muñoz (supervisor Manuel Pastor, UPF) 2010
  - Raquel Ortega (supervisor Christian Fdez Massaguer, USC) 2011
  - Marc Brugarolas (supervisor Rafael Franco, UB) 2013
  - Xianquiang Sun (supervisor Yaoquan Tu, KTH) 2015
- Appointed as committee member for 2 PhD thesis in 2016
  - Alexandre Barrozo (supervisor Lynn Kamerlin, UU)
  - Aniroud Ranganathans (supervisor Jens Carlsson, UU)
- Committee member of 2 MSc thesis (Uppsala University) and member of the MSc thesis evaluation board in Bioinformatics, UPF (2007-2008)

Appendix to the CV

Hugo Gutiérrez de Terán Castañón

Contents

1 SCIENTIFIC OUTCOME

1.1 Scientific Publications

1.1.1 Full Articles (including reviews)

- **2016**

1. Esguerra, M.; Siretskiy, A.; Bello, X.; Sallander, J.; Gutiérrez-de-Terán, H.* (* corresponding author) GPCR-ModSim: A comprehensive web based solution for modeling G-protein coupled receptors. *Nucl. Ac. Res.* (2016) DOI:10.1093/nar/gkw403

2. Bharate,S.B.;* Singh,B.; Kachler, S.; Oliveira, A.; Kumar, V.; Bharate, S.S.; Vishwakarma, R.A.; Klotz, K.N.; Gutiérrez-de-Terán, H.* (* corresponding author). Discovery of 7-(prolinol-N-yl)-2-phenylamino-thiazolo[5,4-d]pyrimidines as novel non-nucleoside partial agonists for the A2A adenosine receptor: Prediction from molecular modeling *J Med Chem.* DOI:10.1021/acs.jmedchem.6b005

3. Salander, J.; Wallinder, C.; Hallberg, A.; Åqvist, J. Gutiérrez-de-Terán, H.* (* corresponding author) Structural Determinants of Subtype Selectivity and Functional Activity of Angiotensin II Receptors. *Bioorg. Med. Chem. Lett.* (2016) 26:1355-9

4. Gutiérrez-de-Terán, H.*; Salander, J.; Sotelo, E. (* corresponding author) Structure-Based Rational Design of Adenosine Receptor Ligands. *Curr. Top. Med. Chem.* (2016) in press

5. El Maatougui, A; Azuaje, J; González-Gómez, M; Miguez, G; Crespo, A; Carbajales, C; Escalante, L; García-Mera, X; Gutiérrez-de-Terán, H*, Sotelo E.* (* corresponding authors) Discovery of Potent and Highly Selective A2B Adenosine Receptor Antagonist Chemotypes. *J Med Chem.* (2016) 59:1967

6. Diwakarla S, Nylander E, Gronbladh A, Vanga SR, Khan YS, Gutierrez-de-Teran H, Ng L, Pham V, Savmarker J, Lundback T, Jenmalm-Jensen A, Andersson H, Engen K, Rosenstrom U, Larhed M, Aqvist J, Chai SY, Hallberg M. Binding to and Inhibition of Insulin-Regulated Aminopeptidase (IRAP) by Macrocyclic Disulfides Enhances Spine Density. *Mol Pharmacol* (2016) 89:413.

- **2015**

7. Keranen, H.; Åqvist, J. Gutiérrez-de-Terán, H.* (* corresponding author) Free energy calculations of A2A adenosine receptor mutation effects on agonist binding. *ChemComm* (2015), 51:3522.

8. Gutiérrez-de-Terán, H.,* ; Massinkc, A.* (*both authors contributed equally); Lenselink, E.B.; Zacarias, N.V.O.; Xia, L.; Heitman, L. H.; Katritch, V.; Stevens, R. C. IJzerman, A.; Sodium Ion Binding Pocket Mutations and Adenosine A2A Receptor Function. *Mol. Pharmacol.* (2015) 87:305.

9. Gutiérrez-de-Terán, H.*; Keranen, H.; Azuaje, J.; Rodríguez, D.; Åqvist, J.; Sotelo, E. (* corresponding author) Computer-Aided design of GPCR ligands. In *G-Protein Coupled Receptors (GPCR) Screening Assays* Editor: Miguel Prazeres and Sofia Martins, in the series *Methods in Molecular Biology*, (2015) 1272:271

10. Azuaje, J.; Carbajales, C.; Gonzalez-Gomez, M.; Coelho, A.; Caamaño, O.; Gutiérrez-de-Terán, H.*; Sotelo, E.* (* corresponding authors) Pyrazin-2(1H)-ones as a Novel Class of Selective A3 Adenosine Receptor Antagonists *Fut. Med. Chem.* (2015) 7:1373.

11. Shamsudin Khan Y.;, Kazemi M.; Gutiérrez-de-Terán, H.; Åqvist J. 4. Origin of the Enigmatic Stepwise Tight-Binding Inhibition of Cyclooxygenase-1. *Biochemistry* (2015) 54:7283

12. Rodríguez, A.; Guerrero, A.; Gutiérrez-de-Terán, H.; Rodríguez, D.; Brea, J.; Loza, M.I.; Rosell, G.; Bosch, M.P. New selective A2A agonists and A3 antagonists for human adenosine receptors. Synthesis, biological activity and molecular docking studies. *Med. Chem. Comm.* (2015) 6:1178.

- **2014**

13. Gutiérrez-de-Terán, H.* The roles of computational chemistry in the ligand design of G protein-coupled receptors: how far have we come and what should we expect? (Editorial) *Fut. Med. Chem.* (2014) 6:251-54.

14. Keranen, H.; Gutiérrez-de-Terán, H.; Åqvist, J. Structural and Energetic Effects of A2A Adenosine Receptor Mutations on Agonist and Antagonist Binding. *PlOS One* (2014) 9:e108492.

15. Serra-Vinardella, J.; Díaz, L.; Gutiérrez-de-Terán, H.; Sánchez-Ollé, G.; Bujons, J.; Michelakakis, H.; Mavridou, I.; Aertsg, J.M.F.G.; Delgado, A.; Grinberg, D.; Vilageliua, L.; Casas, J. Selective chaperone effect of aminocyclitol derivatives on G202R and other mutant glucocerebrosidases causing Gaucher disease. *Int. J. Biochem. Cell Biol.* (2014) 54:245.

16. Boukharta, L.; Gutiérrez-de-Terán, H.; Åqvist, J. Computational prediction of alanine scanning and ligand binding energetics in G-protein coupled receptors. *PlOS Comp. Biol* (2014) 10:e1003585.

17. Kufareva, I.; Katritch, V.; Gutiérrez-de-Terán, H. and other Participants of GPCR Dock 2013; Stevens, R.C.; Abagyan, R. Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. *Structure* (2014) 22:1120.

18. Carbajales, C.; Prado, M.A.; Gutiérrez-de-Terán, H.; Cores, A.; Azuaje, J.; Novio, S.; Nuñez, M.J.; Fernández, B.; Sotelo, E.; García-Mera, X.; Sánchez-Lazo, P.; Freire-Garabal, M.; Coelho, A. Structure-based design of novel KSP-Eg5 inhibitors assisted by a targeted multicomponent reaction. *ChemBioChem* (2014) 15:1471.

19. Kahn, Y.; Gutiérrez-de-Terán, H.; Boukharta, L.; Åqvist, J. Towards an Optimal Docking and Free Energy Calculation Scheme in Ligand Design with Application to COX-1 Inhibitors. *J. Chem. Inf. Model.* (2014) 54:1488

- **2013**

20. Gutiérrez-de-Terán, H., ; Massinkc, A.; Rodríguez, D.; Liu, W.; Han, G.W.; Joseph, J. S.; Katritch, I.; Heitman, L. H.; Xia, L.; IJzerman, A.; Cherezov, V.; Katritch, V.; Stevens, R. C. The role of a sodium ion binding site in the allosteric modulation of the A2A adenosine G protein-coupled receptor. *Structure* (2013) 21:2175-85.

21. Xu, B.; Fällmar, H.; Boukharta, L.; Pruner, J.; Lundell, I.; Mohell, N.; Gutiérrez-de-Terán, H.; Åqvist, J.; Larhammar, D. Mutagenesis and computational modeling of the human G protein-coupled receptor Y2 for neuropeptide Y and peptide YY *Biochemistry* (2013) 52:7987-98.

22. Crespo, A.; El Maatougui, A.; Biagini, P.; Azuaje, J.; Coelho, A.; Brea, P.; Loza, M.I.; Cadavid, M.I.; García-Mera, X.; Gutiérrez-de-Terán, H. and Sotelo, E. Discovery of 3,4-Dihydropyrimidin-2(1H)-ones as a Novel Class of Potent and Selective A2B Adenosine Receptor Antagonists. *ACS Med. Chem. Lett.* (2013) 4:1031-1036.

23. Yaziji, V.; Rodríguez, D.; Coelho, A.; García-Mera, X.; Brea, J.; Loza, M.I.; Cadavid, M.I.; Gutiérrez-de-Terán, H.*; Sotelo, E.* (* corresponding authors): Selective and Potent Adenosine A3 Receptor Antagonists by Methoxyaryl Substitution on the N(2,6-Diarylpyrimidin-4-yl)acetamide scaffold. *Eur. J. Med. Chem.* (2013) 59:235-42.

24. Gutiérrez-de-Terán, H.*; Bello, X.; Rodríguez, D. (* corresponding author): Characterization of the dynamic events of GPCRs by automated computational simulations. *Biochem. Soc. Trans.* (2013), 41:205-212

25. Rodríguez, D.; Gutiérrez-de-Terán, H.* (* corresponding author) Computational Approaches for Ligand Discovery and Design in Class-A G Protein-Coupled Receptors. *Curr. Pharm. Des.* (2013), 19:2216-2236

- **2012**

26. Gutiérrez-de-Terán, H.* and Åqvist, J. (* corresponding author)LIE: Method and applications. In *Computer Aided Drug Design* Editor: Riccardo Baron, in the series *Methods in Molecular Biology*, (2012), 819:305-23.

27. Sirci, F.; Goracci, L.; Rodríguez, D.; van Muijlwijk-Koezen, J.; Gutiérrez-de-Terán, H.; Mannhold, R. Ligand-, Structure-and Pharmacophore-based Molecular Fingerprints: A Case Study on Adenosine A1, A2A, A2B, and A3 Receptor Antagonists. *J. Com. Aid. Mol. Des.* (2012), 26:1247-1266.

28. Rodríguez, D.; Gutiérrez-de-Terán, H.* (* corresponding author) Characterization of the homodimerization interface and functional hotspots of the CXCR4 chemokine receptor. *Proteins* (2012), 80:1919-1928

29. Rodríguez, D.; Bello, X.; Gutiérrez-de-Terán, H.* (* corresponding author) Molecular modelling of G Protein-Coupled Receptors through the Web. *Mol. Inf.* (2012), 31:334-341.

- **2011**

30. Pazos, E.; Pérez, M.; Gutiérrez-de-Terán, H..; Orzáez, M.; Guevara, T.; Mascareñas, J.L.; Vázquez, M.E. Rational design of a cyclin A fluorescent peptide sensor. *Org. Biomol. Chem.* (2011), 9:7629-7632

31. Fällmar, H.; Åkerberg, H.; Gutiérrez-de-Terán, H..; Lundell, I.; Mohell, N.; Larhammar, D. Identification of positions in the human neuropeptide Y/peptide YY receptor Y2 that contribute to pharmacological differences between receptor subtypes. *Neuropeptides* (2011), 45:293-300.

32. Rodríguez, D.; Piñeiro, A; Gutiérrez-de-Terán, H.* (* corresponding author) Molecular dynamics simulations reveal insights into adenosine receptors conformational states. *Biochemistry* (2011), 50:4194-4208.

33. Díaz-Bueno, L.; Bujons, J.; Delgado, A.; Gutiérrez-de-Terán, H.*; Åqvist, J.* (* corresponding author) Computational Prediction of Structure-Activity Relationships for the Binding of Aminocyclitols to beta-Glucocerebrosidase. *J. Chem. Inf. Model.* (2011) 51:601-611.

34. Yaziji, V.; Rodríguez, D.; Gutiérrez-de-Terán, H.*; Coelho, A.; Caamaño, O.; García-Mera, X.; Brea, J.; Loza, M.I.; Cadavid, M.I.*; Sotelo, E.* (* corresponding author) Pyrimidine Derivatives as Potent and Selective A3 Adenosine Receptor Antagonists. *J. Med. Chem.* (2011) 54:457-471

- **2010**

35. Åkerberg, H.; Fällmar, H.; Sjödin, P.; Boukharta, L.; Gutiérrez-de-Terán, H.; Lundell, I.; Mohell, N.; Larhammar, D. Mutagenesis of human neuropeptide Y/peptide YY receptor Y2 reveals additional differences to Y1 in interactions with highly conserved ligand positions. *Regul. Pept.* (2010) 163:120-129

36. Areias, F.M.; Brea, J.; Gregori-Puigjané, E.; Zaki, M.E.A.; Carvalho, M.A.; Domínguez, E.; Gutiérrez-de-Terán, H.; Proença, M.F.; Loza, M.I.; Mestres, J. In silico directed chemical probing of the adenosine receptor family. *Bioorg. Med. Chem.* (2010) 18:3043-3052

37. Rodríguez-Rodríguez, C.; Rimola, A.; Rodríguez-Santiago, L.; Ugliengo, P.; Álvarez-Larena, A.; Gutiérrez-de-Terán, H.; Sodupe, M.; González-Duarte, P. Crystal structure of Thioflavin-T and its binding to Aβ 1-42 fibrils. *Chem. Commun.* (2010) 46:1156-1158

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- **2009**

39. Gutiérrez-de-Terán, H.; Correia, C.; Rodríguez, D.; Carvalho, M.A.; Brea, J.; Cadavid, M.I.; Loza, M.I.; Proença, M.F. and Areias, F. Identification of Novel Scaffolds from an Original Chemical Library as Potential Antipsychotics. *QSAR and Comb. Sci.* (2009) 28:856-860

40. Orrling, K.M.; Marzahn, M.R.; Gutiérrez-de-Terán, H.; Åqvist, J. Dunn, B.M. and Larhed, M. Alpha-Substituted Norstatines as the Transition-State Mimic in Inhibitors of Multiple Digestive Vacuole Malaria Aspartic Proteases. *Bioorg. Med. Chem.* (2009) 17:5933-5949.

41. Blanco-Arias, P.; Einholm, A.P.; Mamsa, H.; Concheiro, C.; Gutiérrez-de-Terán, H.; Romero, J.; Toustrup-Jensen, M.S.; Carracedo, A.; Jen, J.C.; Vilsen, B. and Sobrido, M.J. A C-terminal Mutation of ATP1a3 Underscores the Crucial Role of Sodium Concentration in the Pathophysiology of Rapid-Onset Dystonia-Parkinsonism. *Hum. Mol. Genet.* (2009) 18:2370-2377.

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43. Michino, M.; Abola, E.; Gutiérrez-de-Terán, H. and other GPCR Assessment Participants, Brooks III, C.L.; Dixon, J.S.; Moult, J.; Stevens, R.C. Community-wide blind assessment of methods for GPCR structure modeling and docking. *Nature Rev. Drug Discov.* (2009) 8:455-463.

- **2008**

44. Martínez, A.; Gutiérrez-de-Terán, H.; Brea, J.M.; Raviña, E.; Loza, M.I.; Cadavid, M.I.; Sanz, F.; Vidal, B. and Sotelo, E. Synthesis, Adenosine Receptor Binding and 3D-QSAR-of 4-Substituted 2-(2≠furyl)-1,2,4-triazolo[1,5-a]quinoxalines. *Bioor. Med. Chem.* (2008) 16:2103-2113.

- **2007**

45. Bjelic, S.; Nervall, M.; Gutiérrez-de-Terán, H.; Ersmark, K.; Hallberg, A.; Åqvist, J. Computational inhibitor design against malaria plasmepsins. *Cell Mol. Life Sci.* (2007) 67:2285-2305.

- **2006**

46. Gutiérrez-de-Terán, H.; Nervall, M.; Dunn, B.M.; Clemente, J.C.; Åqvist, J. Computational analysis of plasmepsin IV bound to an allophenylnorstatine inhibitor. *FEBS lett.* (2006) 580:5910-5916.

47. Gutiérrez-de-Terán, H.; Nervall, M.; Ersmark, K.; Liu, P.; Janka, L.K.; Dunn, B.M.; Hallberg, A.; Åqvist, J. Inhibitor Binding to the Plasmepsin IV Aspartic Protease from *Plasmodium Falciparum*. *Biochemistry* (2006) 45:10529-10541.

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- **2004**

49. Gutiérrez-de-Terán, H.*; Barbany, M.*; Sanz, F.; Villà-Freixa, J. Towards a MIP-based alignment and docking in computer-aided drug design. *Proteins* (2004) 56:585-594 (* these authors contributed equally)

50. Gutiérrez-de-Terán, H.; Pastor, M.; Centeno, N.B.; Åqvist, J.; Sanz, F. Comparative analysis of putative agonist binding modes in the human A_1 adenosine receptor. *Chembiochem* (2004), 5:841-849

51. Gutiérrez-de-Terán, H.; Centeno, N.B.; Pastor, M.; Sanz, F. Novel Approaches for modeling of the A_1 adenosine receptor and its agonist binding site. *Proteins* (2004), 54:705-715

- **2003**

52. Fontaine, F.; Pastor, M.; Gutiérrez-de-Terán, H.; Lozano, J.J. Sanz, F. Use of alignment-free molecular descriptors in diversity analysis and optimal sampling of molecular libraries. *Mol. Divers.* (2003), 6:135-147

53. Barbany, M.; Gutiérrez-de-Terán, H.; Sanz, F.; Villà-Freixa, J.; Warshel, A. On the generation of catalytic antibodies by transition state analogs; *ChemBioChem* (2003), 4:277-285.

- **2002**

54. Gutiérrez-de-Terán, H.; Lozano, J.J.; Segarra, V.; Sanz, F. Molecular diversity strategy on the basis of quantum mechanical computations and principal component analysis; *Comb. Chem. High T. Scr.* (2002), 5: 39-47.

55. Rodrigo, J.; Barbany, M.; Gutiérrez-de-Terán, H.; Centeno, N.B.; de-Cáceres, M.; Dezi, C.; Fontaine, F.; Lozano, J.J.; Pastor, M.; Villà, J.; Sanz, F: Comparison of biomolecules on the basis of molecular interaction potentials; *J. Brazil. Chem. Soc.* (2002), 13: 795-799.

1.1.2 Books and Book Chapters

1. Hardy, B.; Affentranger, R.; Contini, A.; Gutiérrez-de-Terán, H.; Spitzner, J.; Papoian, R.; Seibel, W.; Nelson, S.; Wisenman, J.; Bryant, S. and Doreig, C. Collaborative Drug Design of Plasmodium Kinase Inhibitors. In *IProtein phosphorylation in Parasites: Novel targets for Antiparasitic intervention* Editors: Christian Doerig, Gerald Spaeth and Martin Wiese. Wiley-VCH Verlag GmbH & Co. 2013 (ISBN: 978-3-527-33235-9)

2. Gutiérrez-de-Terán, H. and Åqvist, J. The linear response approximation and linear interaction energy methods. In *A course on biomolecular simulations* Editor: Jordi Villà-Freixa. Ed. Huygens, Barcelona. 2011 (under edition)

1.1.3 Conference Proceedings

1. Gutiérrez-de-Terán, H.*; Bello, X.; Rodríguez, D. (* corresponding author): Characterization of the dynamic events of GPCRs by automated computational simulations. *Biochem. Soc Trans* (see article 1), Vol 41, issue on: *G-protein-coupled-receptors: from structural insights to functional mechanisms*.

2. Gutiérrez-de-Terán, H.; Boukarta, L.; Keranen, H. *et al*: Integration of computational modeling, site-directed mutagenesis and ligand binding assays in GPCRs: An exploration of receptor architecture and ligand binding in neuropeptide Y receptors. *Abstracts of Papers of the Am. Chem. Soc.*, (2012) 243:xxx-COMP

3. Rodríguez D., Gutiérrez-de-Terán H.; Bender, A. . *et al*: Discovery of potent and selective adenosine receptor ligands via multi-objective design. *Abstracts of Papers of the Am. Chem. Soc.*, (2012) 243:xxx-COMP

4. Gutiérrez-de-Terán, H.; Rodríguez, D; Bello, X.; Development and applications of a structural bioinformatics platform for the characterization of G protein-coupled receptors. *Abstracts of Papers of the Am. Chem. Soc.*, (2011) 241:116-COMP

5. Rodríguez, D; Gutiérrez-de-Terán, H.; Influence of protonation states, single point mutations and ligands in the dynamics of adenosine receptors *Abstracts of Papers of the Am. Chem. Soc.*, (2011) 241:20-COMP

6. Rodríguez, D; Yaziji, V; Sotelo, E and Gutiérrez-de-Terán, H.: Mutually complementary ligand and and structure-based computational studies on a novel series of potent and selective A_3 adenosine receptor antagonists. *Drugs of the Future* (2010), 35, suppl A:PC.107

7. Gutiérrez-de-Terán, H and Åqvist, J.: A comprehensive computational study of aspartic proteases in drug design. *Drugs of the Future* (2010), 35, suppl A:PC.167

8. Rodriguez AM, Rosell G, Bujons J, Gutiérrez-de-Terán, H., Rodriguez D, Brea JM, Loza MI, Guerrero A, Bosch MP.: Synthesis, biological activity and molecular docking analysis of new A2A adenosine receptor agonists. *Purinergic Signalling* (2010), 6, suppl 1:41-42

9. Gutiérrez-de-Terán, H.; Correia, C.; Rodríguez, D.; Carvalho, M.A.; Brea, J.; Cadavid, M.I.; Loza, M.I.; Proença, M.F. and Areias, F. Identification of Novel Scaffolds from an Original Chemical Library as Potential Antipsychotics. *QSAR and Comb. Sci.* (see article 16) issue on *EuroQSAR-2008*.

10. Orrling, K.; Marzahn, M.R.; Gutiérrez-de-Terán, H.; Åqvist, J.; Dunn, B.M. and Mats Larhed, M. Novel aspartyl protease inhibitors in the quest against malaria. *Drugs of the Future* (2008), 33, suppl A, 41

11. Gutiérrez-de-Terán, H., H; Åqvist J; Sanz F. Comparative analysis of putative agonist binding modes in the human A1 adenosine receptor. *Abstracts of papers of the ACS 229* (2005):U778

12. Carotti A, Cadavid MI, Centeno NB, Esteve C, Fontaine F, Gutiérrez-de-Terán, H., Loza MI, Martínez A, Nicoletti O, Nieto R, Pastor M, Raviña E, Sanz F, Segarra V, Sotelo E, Stefanachi A, Vidal B. 9-Deazaxanthines as selective A2B AR ligands: design, synthesis and SAFIR studies. *Drugs of the future*, (2004) 29, suppl. A

13. Gutiérrez-de-Terán, H.; Centeno, N.B.; Pastor, M; Sanz, F.: Agonist binding modes in human A_1 adenosine receptor. Molecular dynamics and docking studies; *Drugs of the future* (2002) 27, suppl. A

1.2 Conferences and Invited Lectures

Presenting author is indicated in bold.

1.2.1 Organising committee

1. Adenosine Receptors: Present and Future Challenges; Uppsala, 2-3 March 2015 (co-organizer and chair of the conference).

2. *XV SMI conference on Advances and Progress in Drug Design*, London, UK, 16-17 February 2015 (chair of the conference).

3. eSSENCE workshop on Macromolecular structure and dynamics; Uppsala, 3-5 June 2013 (co-organizer and chair of the conference).

4. I Xornadas Galegas de Bioinformatica; A Coruña, 4 April 2008; II Xornadas Galegas de Bioinformatica; Santiago de Compostela, 1 December 2009 (Member of the Steering and Scientific Commitees)

5. VIII Spanish Conference on Bioinformatics; Valencia, 13-15 February 2008 (Member of the Steering and Scientific Commitees)

6. XVII International Symposium on Medicinal Chemistry; Barcelona, 1-5 September 2002 (Member of the local committee)

1.2.2 Invited lectures

1. *IV workshop in New Trends in Computational Chemistry for Industry Applications*, Barcelona, Spain, 2-3 October 2015.
Gutiérrez-de-Terán: *Understanding ligand binding, receptor selectivity and pharmacological profiles on GPCRs from computer simulations*

2. *XV SMI conference on Advances and Progress in Drug Design*, London, UK, 16-17 February 2015.
Gutiérrez-de-Terán: Predicting protein structure, ligand binding and receptor selectivity on GPCRs

3. *Drug Discovery and Development*, Online Event, Select Biosciences, 17-18 June 2014.
Gutiérrez-de-Terán: Computational Modeling and Simulation of GPCRs in Structure-Based Drug Design

4. *XIV SMI conference on Advances and Progress in Drug Design*, London, UK, 17-18 February 2014.
Gutiérrez-de-Terán: Modeling and simulation of GPCRs: applications to structure based drug design

5. *XIII annual Structure-Based Drug Design conference*, Boston, MA, 19-21 June 2013.
Gutiérrez-de-Terán: An Automated Pipeline for the Modeling and Simulation of GPCRs: Applications to Structure-Based Drug Design

6. *GLISTEN MC/WG meeting and workshop: GPCR Ligand Design*, Warsaw, Poland, 7-9 October 2013.
Gutiérrez-de-Terán: Molecular dynamics simulations and Free Energy Calculations can contribute to the structural and functional characterization of GPCRs

7. *XIII annual Structure-Based Drug Design conference*, Boston, MA, 19-21 June 2013.
Gutiérrez-de-Terán: An Automated Pipeline for the Modeling and Simulation of GPCRs: Applications to Structure-Based Drug Design.

8. Invited seminar, GRIB - Pompeu Fabra University, Barcelona, 18 April 2005
Gutiérrez-de-Terán: Computational studies on plasmepsin IV inhibitors: applications to antimalarial drug design.

1.2.3 Selected oral communications

1. *G-protein-coupled-receptors: from structural insights to functional mechanisms - co-organized by the Biochemical Society and Monash University*, Prato, Italy, 12-14 September 2012.

Gutiérrez-de-Terán, H.; Katritch, S.; Cherezov, V.; IJzerman, A.; Heitman, L.; Stevens, R.C.: The impact of endogenous allosteric binders on Adenosine A2A receptor structure and function.

2. *243^{th} ACS National Meeting*, San Diego (CA), 13-17 March 2016.
Gutiérrez-de-Terán, H.; Sotelo, E.: Combining Ligand-Based and Structure-Based Ligand Design Towards the Development of Potent and Selective Antagonists for the Adenosine Receptors.

3. *243^{th} ACS National Meeting*, San Diego (CA), 25-29 March 2012.

   - **Gutiérrez-de-Terán**, H.; Boukarta, L.; Keranen, H. *et al*: Integration of computational modeling, site-directed mutagenesis and ligand binding assays in GPCRs: An exploration of receptor architecture and ligand binding in neuropeptide Y receptors.
   - **Rodríguez D.**, Gutiérrez-de-Terán H.; Bender, A. . *et al*: Discovery of potent and selective adenosine receptor ligands via multi-objective design

4. *241^{th} ACS National Meeting*, Anaheim (CA), 27-31 March 2011.:

   - Gutiérrez-de-Terán, H.; Rodríguez, D.; Bello, X: Developmentand applications of a structural bioinformatics platform for thecharacterization of G protein-coupled receptors.
   - **Rodríguez D.**, Gutiérrez-de-Terán H.: Influence of protonation states, single point mutations and ligands in the dynamics of adenosine receptors.

5. *VIIth ERA Chemistry Flash Conference: Bioinspired Chemistry*: Santiago de compostela, 24-27 October 2010.
Gutiérrez-de-Terán, H: A Structural bioinformatics platform for the study of GPCRs.

6. *XIII Congress of the Spanish Society of Medicinal Chemistry (SEQT)* organized by the SEQT, Valencia, 18-21 September 2011.
Gutiérrez-de-Terán, H.: Structure-Based Ligand Design on Adenosine Receptors.

7. *VIII Jornadas Nacionales de Bioinformática*: Valencia, 13-15 February 2008. Gutiérrez-de-Terán, H.; Orrling, K.; Dunn, B.M.; Åqvist J. Investigating Promiscuous Inhibition of Proteases by Computational Methods.

8. *XIII Congress of the Spanish Society of Medicinal Chemistry (SEQT)* organized by the SEQT; Santiago de Compostela, 9-12 september 2003.
Gutiérrez-de-Terán, H; Åqvist J; Sanz F. Definition of the agonist binding mode on the A_1 adenosine receptor: binding free energy prediction on a series of agonists.

9. *I Meeting of the Catalan Network of Molecular Modeling*; Barcelona, 24-25 January 2002.
Gutiérrez-de-Terán, H; Dezi, C; Pastor, M; Sanz, F.: Developement of a systematic protocol for modeling GPCRs.

10. *Annual meeting of the Theoretical Chemistry Network of Generalitat de Catalunya*; Barcelona, 13-14 july 2000.
Gutiérrez-de-Terán, H; Lozano, JJ; Segarra, V; Sanz, F.: Molecular diversity study on the basis of quantum-mechanical computations.

1.2.4 Poster presentations

Presentation of my work in more than 20 posters on 15 different conferences worldwide.

1. *Gordon Research Conference on Molecular Pharmacology*, Lucca (Barga), Italy, 28 April - 3 May 2013.
   Gutiérrez-de-Terán, H.; Massink, A.; Lessenik, B.; Katritch, S.; Stevens, R.C. Allosteric modulation of the A2A receptor by sodium ions and amilorides.

2. *9th WATOC conference*, Santiago de Compostela, 17-22 July 2011.
   Rodríguez D.; Mokarzel-Falcón, L.; Gutiérrez-de-Terán H.: Molecular Dynamics Simulations OF G Pprotein-Coupled Receptor Dimers.

3. *XXIth International Symposium of Medicinal Chemistry*: Brussels, 1-5 September 2010.

   - **Rodríguez, D**; Yaziji, V; Sotelo, E and Gutiérrez-de-Terán, H: Mutually complementary ligand and structure-based computational studies on a novel series of potent and selective A_3 adenosine receptor antagonists.
   - **Gutiérrez-de-Terán**, H and Åqvist, J.: A comprehensive computational study of aspartic proteases in drug design.
     Publication: Drugs of the future, 35, suppl. A (2010)

4. *ISQBP President's Meeting*: Cetraro, Italy, 14-16 June 2010.
   Rodríguez, D.; Bello, X.; Piñeiro, A.; Brocos, P.; Gutiérrez-de-Terán, H.: A Structural Bioinformatics Platform FOR G-Protein Coupled Receptors

5. *IX Jornadas Nacionales de Bioinformatica*: Lisbon, 3-6 November 2009.
   Rodríguez, D.; Piñeiro, A.; Brocos, P.; Gutiérrez-de-Terán, H.: Adenosine receptors: A systematic structural study based on the crystal structure of hA_2A receptor

6. *Int. Workshop in memoriam of Angel R. Ortiz*: Madrid, 25-28 January 2009.

   - Gutiérrez-de-Terán, H.; Rodríguez, D.: Adenosine receptors: A systematic structural study of ligand binding based on the crystal structure of hA_2A receptor.
   - Rodríguez D., GutiÃl'rrez-de-TerÃąn H., Dunn B.M.: Investigation of the binding site of plasmepsins with peptidomimetic inhibitors.

7. *Euro QSAR 2008*: Uppsala, 21-26 September 2008.
   Gutiérrez-de-Terán, H.; Areias, F.; Rodríguez, D.; Brea, J.; Proenca, M.F.; Loza, M.I.: Identification of novel scaffolds from an original chemical library as potential antipsychotics.

8. *XXth International Symposium of Medicinal Chemistry*: Viena, 29 september 2008.
   Orrling, K.; Marzahn, M.R.; Gutiérrez-de-Terán, H.; Åqvist, J.; Dunn, B.M. and Mats Larhed, M. Novel aspartyl protease inhibitors in the quest against malaria.

9. *VIII Jornadas Nacionales de Bioinformática*: Valencia, 13-15 February 2008.
   Gutiérrez-de-Terán, H; Brea, J.; Loza, M.I. Pharmacological profiling using HTS: Design and analysis of HTS campaigns.

10. *High Content Analysis, Spain*: Madrid, 26-27 March 2007. Presentation of the poster:
    Gutiérrez-de-Terán, H; Brea, J.; Loza, M.I. Pharmacological profiling using HTS: Design and analysis of HTS campaigns.

11. *Screening and Medicinal Chemistry Europe, Select Biosciences*: Barcelona, 20-21 February 2007

12. *ISQBP President's Meeting*; Strasbourg, 24-27 June 2006.
Gutiérrez-de-Terán, H Nervall, M.; Ersmark, K.; Liu, P.; Janka, L.K.; Dunn, B.M.; Hallberg, A.; Åqvist, J. Inhibitor binding to the plasmepsin IV aspartic protease from *P. falciparum*

13. *8th International Symposium on Adenosine and Adenine Nucleotides*; Ferrara, 24-28 May 2006.
A. Stefanachi, A. Carotti, J.M. Brea, M.I. Cadavid, N.B. Centeno, C. Esteve, F. Fontaine, **Gutiérrez-de-Terán, H**, M. Isabel Loza, A. Martinez, S. Moro, O. Nicolotti, R. Nieto, M. Pastor, E. Ravina, F. Sanz, V. Segarra, E. Sotelo, B. Vidal. Structural insights into hA_2B affnity and selectivity of 9-deazaxanthines from combined ligand and structure-based approaches.

14. *229^{th} ACS National Meeting*; San Diego (CA), 13-17 March 2005.
Gutiérrez-de-Terán, H; Åqvist J; Sanz F. Comparative analysis of putative agonist binding modes in the human A_1 adenosine receptor.

15. *Bioinformatics: Present Applications and Future Challenges*; Barcelona, 19-21 mayo 2003.

16. *XVIII International Symposium on Medicinal Chemistry*; Copenhagen-Malmö, September 2002.
Carotti A, Cadavid MI, Centeno NB, Esteve C, Fontaine F, Gutierrez de Teran H, Loza MI, Martínez A, Nicoletti O, Nieto R, Pastor M, Raviña E, Sanz F, Segarra V, Sotelo E, Stefanachi A, Vidal B. 9-Deazaxanthines as selective A2B AR ligands: design, synthesis and SAFIR studies.

17. *Theoretical Biophisics Symposium*; Donostia, 5-7 March 2003.
Barbany, M; **Gutiérrez-de-Terán, H** Sanz, F; Villá-Freixa, J. Similarity between TSA and TS in the framework of the Langevin Dipoles solvation method.

18. *XVII International Symposium on Medicinal Chemistry*; Barcelona, 1-5 September 2002.
Gutiérrez-de-Terán, H; Centeno, N.B.; Pastor, M; Sanz, F.: Agonist binding modes in human A_1 adenosine receptor. Molecular dynamics and docking studies.

19. *I National Meeting on Molecular Modeling and Chemoinformatics*; Barcelona, 22 marzo 2002

20. 3rd Workshop on Chemical Structure and Biological Activity: Perspectives in QSAR; Sao Paulo, September 2001. Conferences (Prof. Ferran Sanz):

    - Sanz, F.; Barbany, M.; Villá, J.; Gutiérrez-de-Terán, H.; Centeno, N.B.; Segarra, V. MIP-based alignement of biomolecules
    - Sanz, F.; Gutiérrez-de-Terán, H.; Lozano, J.J.; Segarra, V. Diversity Studies in Parallel Synthesis Planning
    - Sanz, F.; Carrieri, A.; Centeno, N.B.; Dezi, C.; Gutiérrez-de-Terán, H.; Pastor, M.; Rodrigo, J. Modelling of ligand-GPCR interactions

21. *XII Congress of the Spanish Society of Medicinal Chemistry (SEQT)* organized by the SEQT; Sevilla, 10-14 de september 2001.
Gutiérrez-de-Terán, H; Centeno, NB; Segarra, V; and Sanz, F.: Non-evident structural superpositions under the basis of MEP. Application on antagonists of adenosine receptor A_{2A}.

22. *Computational Byophisics 2000*; Nice, 13-15 june 2000.
Gutiérrez-de-Terán, H; Lozano, JJ; Segarra, V; Sanz, F.: Molecular diversity study on the basis of quantum mechanical computations.

1.3 Research projects

- Quantitative Structure-Based Models for Ligand Interactions with G-Protein Coupled Receptors.
Funding: Swedish Research Council (VR) period 2014-2018
PI: Johan Åqvist and Hugo Gutiérrez de Terán
Role: Co-applicant and sharing the coordination of the project with Prof. Åqvist (4M SEK / €420.000Funding)

- Development of the GPCR-ModSim computational platform for the structural characterisation of G-protein coupled receptors.
Funding: Carl Tryggers Fundation (Stockholm) period 2014-2015 PI: Hugo Gutiérrez de Terán
Role: Principal Investigator (590.000 SEK / €62.000 Funding)

- Elucidation of GPCR structures and interactions with their ligands:Applications to structure-based drug design.
Funding: Spanish Ministry of Science and Innovation (MICINN) period 2012-2013
PI: Hugo Gutiérrez de Terán
Role: Principal Investigator (€96.000 Funding)

- A Structural Bioinformatics plataform for the study of GPCRs: Applications the study of mutations and novel approaches for virtual screening.
Funding: Xunta de Galicia (Autonomous Governmnet) period 2009-2011
PI: Hugo Gutiérrez de Terán
Role: Principal Investigator (€88.300 Funding)

- DIANA programme of Pharmacogenetics:
Funding: Fundación Barrié de la Maza, 2008-2010
Role: Senior researcher (full period). Subproject: Study of the response to antipsychotic tratment and appearance of side effects in psychotic patients.

- ComBioMed Network
Funding: Spanish Ministry of Health (ISCIII, RETICS programme). Starting in 2007
PI (Coordinator):Fernando Martín (ISCIII)
Role: member of the network (2007-2008)

- Hit and Lead Generation from an original chemical library through virtual screening and high throughput screening
Funding:Xunta de Galicia (Autonomous goverment), period 2007-2010
PI: Maria Isabel Cadavid Torres (USC)
Role: Assistant researcher (2007-2008).

- Galician Bioinformatics Network
  Fiunding: Xunta de Galicia (Autonomous goverment), period 2007-2011
  PI: Alejandro Pazos Sierra (UC) and David Posada (UVigo)
  Role: Board member, coordinator of infrastructures of the network (300.000 €Funding)

- Galician Drug Design Network
  Funding: Xunta de Galicia (Autonomous goverment), period 2007-2009
  PI: Maria Isabel Loza (USC)
  Role: member of the network (full period) and currently consultant.

- GENIUS Pharma, AIE
  Funding: Spanish Ministry of Industry, Laboratotios Almirall Prodesfarma, Laboratorios Esteve. Period 2006-2009.
  PIs: Maria Isabel Loza, Maria Isabel Cadavid (USC)
  Role: Head of data mining (2007-2008)

- Rational Approaches to Pathogen Inhibitor Discovery (RAPID)
  Funding: Swedish Fundation for Strategic Research (SSF). Period: 2003-2008
  PI: Alwyn Jones (UU)
  Role: Postdoctoral researcher (2004-2006)

- Development of methods and software for the analysis of the tree-dimensional similarity between molecules with biological relevance.
  Funding: Spanish Ministry of Health (FIS). Period: 2001-2003
  PI: Ferran Sanz Carreras (UPF)
  Role: Predoctoral researcher (full period)

- New mechanisms of action in antiallergic therapeutics. Design, synthesis and pharmachology of new molecules with dualactivity H1/NK1.
  Funding: CICYT (Spanish Science & Technology Comitee). Period: 1998-2001
  PI: Ferran Sanz Carreras (UPF)
  Role: Predoctoral researcher (1999-2001)

1.4 Distinctions, awards and personal grants

- *Manuel Colmeiro* Certificate, from the Autonomous government of Galicia, for the consolidation of young researchers (Second stage of the tenure track program)

- Sabbatical research stay, The Scripps Research Institute, La Jolla (CA). 6 month stay. Working at the Stevens lab in the collaborative project *Exploration of the conformational equilibrium of GPCRs with a combination of molecular dynamics, computational chemistry and X-ray crystallography* (January-July 2012). Funded by the Spanish Ministry of Education, Jose Castillejo program (15,000 €).

- Research stay, Uppsala University. 1 month stay, as part of the activities of my funded project *A Structural Bioinformatics plataform for the study of GPCRs*, Xunta de Galicia (June 2011)

- Research stay, Uppsala University. 2 months stay to work on the project *A Comprehensive study of aspartic proteases* (August-September 2009). Funded by Xunta de Galicia, Mobility program (3,000 €)

- Research stay, Uppsala University. 2 months stay to work on the project *Computational prediction of ligand binding to GPCRs* (August-September 2008). Funded by Xunta de Galicia, Mobility program (3,000 €)

- Mobility program, Barcelona Supercomputing Centre. (financed by Spanish Ministry of Education). Two weeks stay to work on the project: *High-throughput LIE: Large-scale computational prediction of ligand binding affinities.* (November 2007)

- Post-doctoral fellowship from the *Swedish Science Fundation*. Institute of Cell and Molecular Biology, Uppsala University. (june 2004 - september 2006)

- Guest researcher at Padova University, Molecular Simulation Group, invited by Prof. Stefano Moro (1 week, january 2006)

- Conference grants:

  - Spanish Society for Medicinal chemistry. Awarded grant to attend the XII and the XIII National meetings (see below)
  - Chemical Computing group. Awarded a grant to attend the e-Chaminfo Training Workshop (Oxford, 2007, see below)
  - Regional Government of Galicia. Awarded a grant to attend the Euro QSAR 2008 meeting, Uppsala (see below)

- Pre-doctoral fellowship from *Fundació IMIM* (january - may 2004). Research Grup on Biomedical Informatics, Pompeu Fabra University, Barcelona.

- Pre-doctoral short stay fellowship from *Generalitat de Catalunya* (september-november 2002). Uppsala University.

- Pre-doctoral fellowship from *Generalitat de Catalunya* (Catalonian goverment); 2000-2004. Research Grup on Biomedical Informatics Pompeu Fabra University, Barcelona.

- Pre-doctoral fellowship from *Fundaci'o IMIM* (october - december 1999). Research Group on Biomedical Informatics Pompeu Fabra University, Barcelona.

- Undergraduate Fellowship from the Spanish Ministry of Education (academic course 1998-99): Student in the Department of Organic Chemistry, University of Santiago de Compostela.

2 TEACHING EXPERIENCE

2.1 Student supervision

- *Phd thesis supervisor*, Universidade de Santiago de Compostela - FPGMX. (2008-2012).
  Title: Computational Approaches for the Characterization of the Structure and Dynamics of G Protein-Coupled Receptors: Applications to Drug Design.
  Student: David Rodríguez Díaz. Examined on date 9th November 2012 (qualification: *Cum laudem*)

- *Master's thesis supervisor*, M.Sc. Bioinformatics, International University of Andalucía (UNIA) (2009-2010)
  Project: Structural Analysis of HIV-1 Integrase: Towards the Design of New Inhibitors.
  Student: José Correa Barsuto. Defended on 14th July 2011 (max. qualification)

- *End of Course Project supervisor*, BS Biology, University of Santiago de Compostela (UNIA) (2009-2010)
  Project: Molecular modeling of the interaction sensor-ciclin A/CDK. Applications to the design of new chemical sensors.
  Student: Miguel Perez. Defended on 2nd July 2010 (max. qualification)

- *Master's thesis supervisor*, University o Santiago de Compostela - FPGMX. (2007-2009).
  Project: Application of computational techniques to GPCR drug design.
  Student: David Rodríguez Díaz.
  Defended on 30th june 2009 (max. qualification)

- *Master's thesis supervisor*, M.Sc. Neurosciences, University of Santiago de Compostela (academic sourse 2008-2009)
  Project: Molecular Modeling of GPCRs Heterodimerization: Study of the A_2A/D_2 Heterodimer.
  Student: Carlos Vara Sanchez.
  Defended on 22th july 2009 (max. qualification)

2.2 Lecturing and Course coordination

- *Coordinator and Teacher*, Faculty of Natural Sciences, MSc course (2014 -).
  Course: Computational and Systems Biology.
  Lecturer in the 2014 edition, from the 2015 edition also coordinator of the course.

- *Coordinator and Teacher*, Faculty of Natural Sciences, MSc course (2015 -).
  Course: Molecular and Statistical Mechanics.
  Lecturer and coordinator of the course from the 2015/16 edition??

  Recipient of a **78.000 SEK grant from the Faculty of Science and Technology, UU** for the elaboration of this course.

- *Teacher*, Faculty of Natural Sciences, BSc course (2015 -).
  Course: Structural Bioinformatics.
  Lecturer from the 2014/15 edition

- *Coordinator and teacher*, "Course on Structural Bioinformatics: Modeling and Simulation of Biological Molecules", Universidade Santiago de Compostela. 2 anual editions (1-4 December 2008 / 30 November-3 December 2009) Development of original material for the course.

- *Teacher*, M.Sc. Neurosciences, Universidade Santiago de Compostela. Editions 2007, 2008 and 2009.
  Course: Introduction to Bioinformatics (Theory and lab sessions). Development of original material for the course.

- *Teacher*, Summer Course on Bioinformatics, Universidade Santiago de Compostela. Editions 2008 and 2009
  Course: Introduction to Structural Bioinformatics and Computer Aided Drug Design (Theory and lab sessions).

- *Invited teacher*, M.Sc. Bioinformatics for Health Sciences, Pompeu Fabra University (Barcelona). 1st Eddition, April 2005

Course: Computer Assisted Drug Design (lab sessions). Development of original material for the course.
Referee in the master degree candidate's evaluation. 3rd and 4th editions of the M.Sc., 2007 and 2008.

- *Teacher*, Uppsala University. Winter 2005.
  Course: Molecular and Statistical Mechanics (lab sessions).

2.3 Teaching training courses

- *Supervising PhD students*, Uppsala University (Spring 2015). 3 weeks on a full-time basis.
- *Doctoral Supervision Training within the Faculty of Science and Technology*, Uppsala University (Autumn 2014). 2 days on a full-time basis.
- *Academic Teaching Training Course*, Uppsala University (Spring 2014). 5 weeks on a full-time basis.