Claudio N. Cavasotto

Contact Information:
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Education

Ph.D. Physics, University of Buenos Aires, Argentina, 1999. Dissertation topic: *Rational Approximations to the Green Function Problem in Many Body Physics*.

Licenciado in Physics, University of Buenos Aires, Buenos Aires, Argentina, 1988.

Professional Experience

Group Leader at the IBioBA-Max Planck Society Institute, Buenos Aires, Argentina, 1/2012-present.

Member of the "Carrera del Investigador", Conicet, Argentina, 1/2012-present (Investigador Independiente).

Associate Professor, School of Biomedical Informatics, University of Texas Health Science Center at Houston (Houston, TX), and Department of Biomedical Engineering, University of Texas at Austin (Austin, TX), 3/2007 – 12/2011.

Faculty, Graduate School of Biomedical Sciences, The University of Texas at Houston, Houston, TX, 2007 – 2011.

Senior Research Scientist, MolSoft LLC, La Jolla, CA, 8/2002 – 2/2007.

Postdoctoral Fellow, Computational Chemistry and Biophysics, The Scripps Research Institute, La Jolla, CA, 2000-2002.

Assistant Professor, School of Engineering, Catholic University, Buenos Aires, Argentina, 1996-2000.

Senior Lecturer, Department of Physics, University of Buenos Aires, Argentina,1993-2000.

Director of the Petrophysics-and-Fluid Mechanics and Software-and-Calculation Divisions, INLAB, Argentina, 1990-1993.

Lecturer, School of Engineering, Catholic University, Buenos Aires, Argentina, 1989-1995.

Instructor, Department of Physics, University of Buenos Aires, Argentina,1985-1989.

Honors, Fellowships and Awards

Basel Award for the best poster at *MipTec* 2005, Basel, Switzerland.

Postdoctoral fellow, The Scripps Research Institute, La Jolla, CA, USA (2000-2002).

Fellowship from the Spanish Government for foreign researchers (2000, declined).

Fellowship from CONICET, Buenos Aires, Argentina (1990, declined).

Fellowship for graduate students (University of Buenos Aires), Argentina (1988-1989).

Honors Diploma from the University of Buenos Aires (1988).

Professional Societies

American Chemical Society.
American Physical Society.
Biophysical Society.

Professional Service

Editorial Board:

Journal of Computational and Theoretical Nanoscience (2004-2006).
Current Computer-aided Drug Design (2010 - present).
Advances and Applications in Bioinformatics and Chemistry (2008 - present).
Signal Transduction Insights (2008 - present).
Open Access Informatics (2009 - present)

Reviewer for the following journals:

Acta Biochimica et Biophysica Sinica; Archives of Biochemistry and Biophysics; Bioinformatics; Bioorganic and Medicinal Chemistry Letters; BMC Bioinformatics; Chemical Biology & Drug Discovery; Drug Discovery Today; Expert Opinion on Drug Discovery; IEEE Engineering in Medicine and Biology; IEEE Transactions on Computational Biology and Bioinformatics; Journal of Combinatorial Chemistry; Journal of Computational Chemistry; Journal of Molecular Graphics and Modelling; Journal of Chemical Information and Modeling; Journal of Chemical Theory and Computation; Journal of Computational and Theoretical Nanoscience; Journal of Computer-Aided Molecular Design; Journal of Medicinal Chemistry; Journal of Molecular Biology; Journal of the American Chemical Society; Langmuir; Proteins: Structure, Function and Bioinformatics; European Journal of Medicinal Chemistry; Journal of Physical Chemistry B.

Grant reviewer for:

Wellcome Trust (United Kingdom) (2010).
France's National Research Agency, *Agence Nationale de la Recherche*, *ANR* (2007, 2011).
Austrian Science Fund, FWF (2011).
Agencia Nacional de Promoción Científica y Tecnológica, Argentina (2011).
Fundacao para a Ciencia e a Tecnologia, Portugal (2012).
CONICET (2011-2013)

Teaching

Department of Physics, University of Buenos Aires (1985-1989; 1993-1999): Physics III (Electricity and Magnetism), Fluid Mechanics, Theoretical Physics (Electrodynamics), Molecular Physics.

School of Engineering, Catholic University, Buenos Aires, Argentina (1989-2000): Calculus (one and several variables), Modern Physics, Physics I (Mechanics, Optics and Thermodynamics), Physics II (Electricity and Magnetism).

School of Biomedical Informatics, University of Texas at Houston (2007 - 2011):
Graduate courses:
HI 5005 Essential Mathematics for Biomedicine.
HI 5312 Foundations 3 (Optimization Methods).
HI 5001 Biomolecular Modelling and Chemoinformatics in Drug Discovery.
HI 6323 Data Mining in Bioinformatics.

HI 5007 Data Strucutres and Algorithms in Biomedicine.

Research Advising

Post-doctoral Fellows
Narender Singh, Ph.D., 2007 - 2008.
Arturas Ziemys, Ph.D., 2007 - 2009.
Victor Anisimov, Ph.D., 2008 - 2011.
Martín Lavecchia, Ph.D., 2013-present.
Damián Palomba, Ph.D., 2014-present.

Doctoral Students
Sharanghdar Phatak, 2008 - 2010.
Edgar Gatica, Ph. D. student, 2010 – present.

Master Students
Francisco Serna, 2010 – 2011 (director).
Edgar Gatica, 2010 – 2011 (director).
Manuel Wahle, 2008 - 2010 (co-director).

Summer Students:
Edgar Gatica, University of Houston-Downtown, 2008.
Edgar Gatica, University of Houston-Downtown, 2009.
Flavio Forti, Universitat Barcelona, 2010.

Fellowships:
Cameron Brand, Co-director (2011-2013).

Advisory Committees:
Chair, Masters Thesis Advisory Committee, UTHSC-H, Edgar Gatica, 2010 – 2011.
Chair, Masters Thesis Advisory Committee, UTHSC-H, Francisco Serna, 2010 – 2011
Member, Ph.D. Thesis Advisory Committee, MD Anderson Cancer Center, Lorenzo D'Amico, 2011.
Member, Masters Thesis Advisory Committee, UTHSC-H, Manuel Wahle, 2008 - 2010.

Thesis Tribunals
Diego Gauto (doctoral), December 2013, Department of Chemistry, Universidad de Buenos Aires.
Pablo García Risueño (doctoral), December 2011, Universidad de Zaragoza.

Service to the University

School of Health Information Sciences
- Scholarship Committee, member, 2007 - 2011.

Inter-institutional Department of Biomedical Engineering
- Graduate Studies Committee, 2009 – 2011.

Graduate School of Biological Sciences
- Admissions Committee, member, 2009 - 2011.

Gulf Coast Consortia, Chemical Genomics Chemistry Core Committee, member, 2008 – 2011.

University of Texas at Houston
- Research Conflict of Interest Committee, member, 2008 - 2011.

Research Support

Current:
PICT-2011-2778 (Cavasotto, PI) (AR$ 140,000) 27/3/2013 – 26/3/2016

Quantum mechanical scoring functions in computer-aided drug design
Role: PI

Completed:

Welch Foundation Chemistry and Biology Collaborative Grant,
Gulf Coast Consortium (Cavasotto PI) ($100,000) 12/1/08 – 11/30/09
Development of Computationally Driven Hit to Lead Optimization Strategies for BRCT inhibitors.
Role: PI.

R01 CA107039-01 (Dawson, PI) ($1,526,197) 2/04/05 – 1/31/09
Rexinoid Synergy in Prostate Cancer Apoptosis
Role: Co-PI.

Discovery Project Pilot Grant (Gulf Coast Consortium) (Loose, PI) ($70,000)1/1/08 – 12/31/08
Small Molecule Modulators of Wnt Signaling.
Role: Co-PI.

NIH 1 R01 CA109345-01 (Zhang, PI) ($1,354,543) 9/15/04 – 6/31/08
15-Deoxy-delta12,14-prostaglandin J2 as a ligand of RXR alpha.
Role: Collaborating-PI.

NIH R21 GM07768 1-01 (Piedrafita, PI) ($270,650) 11/1/06 – 8/31/08
Rational Discovery of ROR gamma Modulators.
Role: Co-PI

Tobacco-Related Disease Research Program (EEUU) ($670,085) 1/7/2004 – 30/6/2007
Vitamin A derivatives as antagonists of nicotine effects.
Role: Co-PI

Languages

Spanish, Italian, and English: fluent in reading, writing and speaking. German: intermediate knowledge (reading, writing).

Collaborations

- Dr. José Luis Alonso and Dr. Pablo Echenique, Department of Physics, Universidad de Zaragoza, Spain (Constraints in molecular simulations).
- Dr. Ignacio Borrell, IQS, Universitat Ramon Llull, Barcelona, Spain. (Drug lead optimization in protein kinases).
- Dr. Philippe Diaz, University of Montana, Missoula, MT, USA (Drug discovery and optimization for cannabinoid receptors 1 and 2).
- Dr. Maria Fillat, Department of Biochemistry, Universidad de Zaragoza, Spain (Study of FurA protein).
- Dr. Michael Garabedian, NYU School of Medicine, New York, USA (Modeling of AF-1 domain in nuclear receptors).

- Dr. David Gorenstein, Medical School, University of Texas at Houston, USA (targeting CD-44).
- Dr. F. Javier Luque, School of Pharmacy, University of Barcelona, Spain (Methodological developments in structural biology using quantum mechanical methods).
- Dr. Amarnath Natarajan, University of Nebraska, Omaha, NE, USA (study of ligand-protein interaction involving phospho-peptides).
- Dr. José Luis Neira, Universidad Miguel Hernández, Elche, Spain (targetting the HIV-1 capsid).
- Dr. F. Javier Piedrafita, Torrey Pines Institute for Molecular Science, La Jolla, CA, USA (lead discovery in RORγ and IKK protein kinase).
- Dr. Martín Ruiz de Azúa, Department of Physics, University of Buenos Aires, Argentina (electronic polarizability in biomolecular systems).

Publications (* Corresponding Author):
+1500 citations; top 5% cited author in Chemistry according to the Thompson Reuters Citation Index.

1. Petrov, R.P., Wager-Miller, J., Chen, S.-R. Knight, L., McDaniel, S.W., Diaz, F., Barth, F., Pan, H.-L., Mackie, K., Cavasotto, C.N. and Diaz, P. Mastering tricyclic ring systems for desirable functional cannabinoid activity. Eur. J. Med. Chem, 69:881-907, 2013.
2. Brand, C.S., Hocker, H.J., Gorfe, A.A., Cavasotto, C.N., Dessauer, C.W. Isoform Selectivity of Adenylyl Cyclase Inhibitors: Characterization of Known and Novel Compounds. J. Pharmacol. Exp. Ther., 347:265-275, 2013.
3. Doménech, R., Hernández-Cifre, J.G.; Bacarizo, J.; Diez-Peña, A.I.; Martinez-Rodriguez, S.; Cavasotto, C.N.; García de la Torre, J.; Cámara-Artigás, A.; Velázquez-Campoy, A.; Neira, J.L. The histidine-phosphocarrier protein of the phosphoenolpyruvate: sugar phosphotransferase system of Bacillus sphaericus self-associates. PLoS ONE, 8(7):e69307, 2013.
4. He, W., Elizondo-Riojas, M., Li, X., Lokesh, G., Somasunderam, A., Thiviyanathan, V., Volk, D., Durland, R., Englehardt, J., Cavasotto, C.N., Gorenstein, D. X-Aptamers: A bead-based selection method for random incor-poration of drug-like moieties onto next-generation aptamers for enhanced binding. Biochemistry, 51:8321-8323, 2012. Erratum in: Biochemistry, 51:9592, 2012.
5. Forti, F., Cavasotto, C.N., Orozco, M., Barril, X., Luque, F.J. A multilevel strategy for the exploration of the conformational flexibility of small molecules. J. Chem. Theory Comput. 8:1808–1819, 2012.
6. Cavasotto, C.N.* Binding free energy calculation and scoring in small-molecule docking. In *Physico-Chemical and Computational Appraoches to Drug Discovery*, Royal Society of Chemistry, Eds. F. Javier Luque and Xavier Barril, 2012, pp. 195-245.
7. Dasgupta, I., Tanifum, E.A., Srivastava, M., Phatak, S.S, Cavasotto, C.N., Analoui, M., and Annapragada, A. Non inflammatory boronate based glucose-responsive insulin delivery systems. PLoS ONE 7:e29585, 2012.
8. Gatica, E.A. and Cavasotto, C.N.* Ligand and decoy sets for docking to G Protein-Coupled Receptors. J. Chem. Inf. Model., 52:1-6, 2012.
9. Cavasotto, C.N.* Normal-mode-based approaches in receptor ensemble docking. Methods Mol. Biol. 819:157-168, 2012.

10. Anisimov, V.M., Ziemys, A., Kizhake, S., Yuan, Z., Natarajan, A., Cavasotto, C.N.* Computational and experimental studies of the interaction between phospho-peptides and the C-terminal domain of BRCA1. J. Comput-aided Mol. Des. 25:1071-1084, 2011.
11. Echenique P., Cavasotto, C.N., De Marco, M., García-Risueño, P., and Alonso, J. L. An Exact Expression to Calculate the Derivatives of Position-Dependent Observables in Molecular Simulations with Flexible Constraints. PLoS ONE 6:e24563, 2011.
12. Bocanegra, R., Nevot, M., Domenech, R., López, I., Abián, O., Rodríguez-Huete, A., Cavasotto, C.N., Velázquez-Campoy, A., Gómez, J., Martínez, M.A., Neira, J.L. and Mateu, M.G. Cocktails of designed interfacial peptides abolish *in vitro* the assembly of the HIV-1 capsid and inhibit virus infection of cultured cells. PLoS ONE 6:e23877, 2011.
13. Anisimov, V.M. and Cavasotto, C.N.* Hydration free energies using semiempirical quantum mechanical Hamiltonians and a continuum solvent model with multiple atomic-type parameters. J. Phys. Chem. B 115:7896-7905, 2011.
14. Echenique P., Cavasotto, C.N., García-Risueño, P. The canonical equilibrium of constrained molecular models. Eur. Phys. J. ST, 200:5-54, 2011.
15. Anisimov, V.M. and Cavasotto, C.N.*. Quantum Mechanical Binding Free-energy Calculation for Phosphopeptide Inhibitors of the Lck SH2 Domain. J. Comput. Chem. 32:2254-2263, 2011.
16. Cavasotto, C.N.* Homology models in docking and high-throughput docking. Curr. Top. Med. Chem. 11:1528-1534, 2011.
17. Vilar, S., Ferino, G., Phatak, S.S., Berk, B., Cavasotto, C.N. and Costanzi, S. Docking-based virtual screening for GPCRs ligands: not only crystal structures but also in silico models. J. Mol. Graph. Model. 29:614-623, 2011.
18. Cavasotto, C.N.* and Phatak S.S. Docking Methods for Structure-based Library Design. Methods Mol. Biol. 685:155-174, 2011.
19. Cavasotto, C.N.* Handling protein flexibility in docking and high-throughput docking: From algorithms to applications. In *Virtual Screening. Principles, Challenges and Practical Guidelines*. WILEY-VCH Verlag. Ed. Christoph Sotriffer: 2011; Vol. 48, pp 245-262.
20. Phatak, S.S., Gatica, E.A. and Cavasotto, C.N.* Ligand-steered modeling and docking: A benchmarking study in Class A G-Protein Coupled Receptors, J. Chem. Inf. Model. 50:2119-2128, 2010.
21. Anisimov, V.M. and Cavasotto, C.N.* Quantum Mechanical Molecular Dynamics Approach to Study Charge Transfer. In *Kinetics and Dynamics*, Paneth, P.; Dybala-Defratyka, A., Eds. Springer Netherlands: 2010; Vol. 12, pp 247-266.
22. Anisimov, V.M., Bugaenko, V.L. and Cavasotto, C.N.* Quantum mechanical dynamics of charge transfer in ubiquitin in aqueous solution. ChemPhysChem 10:3194-3196, 2009.
23. Diaz, P., Phatak, S.S., Xu, J., Fronczek, F., Astruc-Diaz, F., Thompson, C., Cavasotto, C.N. and Naguib, M. 2,3-Dihydro-1-benzofuran Derivatives as a Novel Series of Potent Selective Cannabinoid Receptor 2 Agonists: Design, Synthesis, and Binding Mode Prediction through Ligand-steered Modeling, ChemMedChem 4:1615-1629, 2009. Featured on cover page.
24. Phatak, S.S., Stephan, C.C. and Cavasotto, C.N.* High-throughput and *in silico* screenings in drug discovery. Expert Opin. Drug Discov. 4:947-959, 2009.

25. Ziemys, A., Ferrari, M. and Cavasotto, C.N.* Molecular modeling of glucose diffusivity in silica nanochannels. J. Nanosci. Nanotechnol. 9:6349-6359, 2009.
26. Cavasotto, C.N* and Phatak, SS. Homology modeling in drug discovery: current trends and applications. Drug Discov. Today 14:676-683, 2009.
27. Diaz, P.; Phatak, S.; Xu, J.; Diaz, F-A.; Cavasotto, C.N. and Naguib, M. 6-Methoxy-N-alkyl Isatin Acylhydrazone Derivatives as a Novel Series of Potent Selective Cannabinoid Receptor 2 Inverse Agonists: Design, Synthesis, and Binding Mode Prediction. J. Med. Chem. 52:433-444, 2009.
28. Monti, M.C.; Casapullo, A.; Cavasotto, C.N.; Tosco, A.; Dal Piaz, F.; Ziemys, A.; Margarucci, L.; Riccio, R. The binding mode of petrosaspongiolide M to the human group IIA phospholipase A(2): exploring the role of covalent and noncovalent interactions in the inhibition process. Chem. Eur. J. 15:1155-1163, 2009.
29. Bisson, W.H.; Abagyan, R. and Cavasotto, C.N.* Molecular Basis of Agonicity and Antagonicity in the Androgen Receptor Studied by Molecular Dynamics Simulations. J. Mol. Graph. Mod. 27:452-458, 2008.
30. Cavasotto, C.N.* and Singh, N. Docking and High-Throughput Docking: Successes and the challenge of protein flexibility. Curr. Comput-Aided Drug Des. 4:221-234, 2008.
31. Pineda Torra, I.; Ismaili, N.; Feig, J.E.; Xu, C.; Cavasotto, C.N.; Pancratov R.; Rogatsky, I.; Neubert, T.A.; Fisher, E.A. and Garabedian, M.J. Phosphorylation of liver X receptor α selectively regulates target gene expression in macrophages. Mol. Cell. Biol. 28:2626-2636, 2008.
32. Chen, W.; Dang, T.; Blind, R.D.; Wang, Z.; Cavasotto, C.N.; Hittelman, A.B.; Rogatsky, I.; Logan, S.K.; Garabedian, M.J. Glucocorticoid receptor phosphorylation differentially affects target gene expression. Mol. Endocrin. 22: 1754-1766, 2008.
33. Cavasotto, C.N.*; Orry, A.J.W.; Murgolo, N.J.; Czarniecki, M.F.; Kocs, S.A.; Hawes, B.E.; O'Neill, K.A.; Hine, H.; Burton, M.S.; Voigt, J.H.; Bayne, M.L.; Monsma, F.J. Discovery of Novel Antagonist Chemotypes to a G-Protein Coupled Receptor through Ligand-steered Homology Modeling and Structure-based Virtual Screening. J. Med. Chem. 51:581-588, 2008.
34. Monti, M.C.; Casapullo, A.; Cavasotto, C.N.; Napolitano, A. and Riccio, R. Scalaradial, a dialdehyde-containing marine metabolite, exerts an unpredicted non-covalent PLA_2 inactivation. ChemBioChem 8:1585-1591, 2007.
35. Cavasotto, C.N.* and A.J.W. Orry. Ligand Docking and Structure-based Virtual Screening in Drug Discovery. Curr. Topics Med. Chem. 7:1006-1014, 2007.
36. Cavasotto, C.N.*; Ortiz, M.A.; Abagyan, R.; and Piedrafita, F.J. In silico identification of novel EGFR inhibitors with antiproliferative activity against cancer cells. Bioorg. Med. Chem. Lett. 16:1969-1974, 2006.
37. Cavasotto, C.N.* Ligand Docking and Virtual Screening in Structure-based Drug Discovery. AIP Conf. Proc. 851:34-49, 2006.
38. Orry, A.J.W.; Abagyan, R. and Cavasotto, C.N.* Structure-Based Development of Drug Target-Specific Compound libraries. Drug Discov. Today, 11:261-266, 2006.
39. Cavasotto, C.N.*; Orry, A.J.W. and Abagyan, R. Receptor Flexibility in Ligand Docking. In *Handbook of Theoretical and Computational Nanotechnology*, American Scientific Publishers. Eds. Michael Rieth and Wolfram Schommers, pp. 218-257, 2006.

40. Hernández, J.A.; Meier, J.; Barrera, F.N.; Ruiz de los Paños, O.; Hurtado-Gómez, E.; Bes, M.T.; Fillat, M.T.; Peleato, M.L.; Cavasotto, C.N.* and Neira, J.L.* The conformational stability and thermodynamics of Fur A (ferric uptake regulator) from Anabaena sp. PCC 7119. Biophys. J. 89:4188-4200, 2005.

41. Kovacs J.A., Cavasotto, C.N.*; and Abagyan, R.A. Conformational Sampling of Protein Flexibility in Generalized Coordinates: Aplication to ligand docking, J. Comp. Theor. Nanosci. 2:354-361, 2005.

42. Cavasotto, C.N.*; Kovacs J.A. and Abagyan, R.A. Representing Receptor Flexibility in Ligand Docking through Relevant Normal Modes, J. Am. Chem. Soc. 127:9632-9640, 2005.

43. Cavasotto, C.N.*; Orry, A.J.W. and Abagyan, R. The Challenge of Considering Rreceptor Flexibility in Ligand Docking and Virtual Screening. Curr. Comput.-Aided Drug Des. 1:423-440, 2005.

44. Li, W.; Cavasotto, C.N.; Cardozo, T.; Ha, S.; Dang, T.; Taneja, S.S.; Logan, S.K. and Garabedian, M.J. Androgen receptor mutations identified in prostate cancer and androgen insensitivity syndrome display aberrant ART-27 coactivator function. Mol. Endocrinol, 19: 2273-2282, 2005. (Featured on cover page of issue).

45. Cavasotto, C.N.* and Abagyan, R. Protein Flexibility in Ligand Docking and Virtual Screening to Protein Kinases. J. Mol. Biol. 337:209-225, 2004.

46. Cavasotto, C.N.; Liu, G.; James, S. Y.; Hobbs, P. J.; Peterson, V. J.; Bhattacharya, A. A.; Kolluri, S. K.; Zhang, X.-K.; Leid, M.; Abagyan, R.; Liddington, R. C. and Dawson, M. I. Determinants of Retinoid X Receptor Transcriptional Antagonism. J. Med. Chem. 47:4360-4372, 2004.

47. Bordner, A.J.; Cavasotto, C.N. and Abagyan, R.A. Direct Derivation of Van der Waals Force Field Parameters from Quantum Mechanical Interaction Energies. J. Phys. Chem. B. 107: 9601-9609, 2003

48. Cavasotto, C.N.; Orry, A.J.W. and Abagyan, R.A. Structure-Based Identification of Binding Sites, Native Ligands and Potential Inhibitors for G-Protein Coupled Receptors. Proteins: Structure, Function and Genetics, 51:423-433, 2003.

49. Giribet, C.G.; Ruiz de Azúa, M.C.; Vizioli, C.V. and Cavasotto, C.N. Electronic mechanisms of intra and intermolecular J couplings in systems with C-H…O interactions. Int. J. Mol. Sci. 4: 203-217, 2003.

50. Bordner, A.J.; Cavasotto, C.N. and Abagyan, R.A. Calculation of water, n-octanol and n-hexadecane solvation free energies using a continuum electrostatics model. J. Phys. Chem. B, 106:11009-11015, 2002.

51. Cavasotto, C.N.* Finite expansion of the inverse matrix in the polarization propagator method. Theor. Chem. Acc. 104: 491-498, 2000.

52. Cavasotto, C.N. and Grinberg H. A Liouville-space method for the decoupling of the polarization propagator equation of motion. Chem. Phys. Lett. 303: 558-566, 1999.

53. Bochicchio, R.; Ferraro, M.; Grinberg, H. and Cavasotto, C. Self-energies for the particle-hole propagator from Feynman-Dyson equations. J. Mol. Struct. (THEOCHEM) 335: 1-9, 1995.

54. Cavasotto, C.N.; Giribet, C.G.; Ruiz de Azúa, M.C. and Contreras, R.H. Exo-exo and endo-endo vicinal proton spin-spin coupling constants in norbornane and norbornene. An IPPP-CLOPPA

analysis. J. Comp. Chem. 12: 141-146, 1991.

55. Cavasotto, C.N.; Giribet, C.G.; and Contreras, R.H. Localization method for semiempirical molecular orbitals based of the Boys-Foster criterion. J. Mol. Struct. (THEOCHEM) 210: 107-110, 1990.
56. Contreras, R.H.; Giribet, C.G.; Ruiz de Azúa, M.C.; Cavasotto, C.N.; Aucar, G.A. and Krivdin L.B. Quantum chemical analysis of the orientational lone-pair effect on spin-spin coupling constants. J. Mol. Struct. (THEOCHEM) 210: 175-186, 1990.
57. Cavasotto, C.N.; Giribet, C.G.; Ruiz de Azúa, M.C.; Contreras, R.H. and Pérez, J. ^{2}J(Se-Se) couplings in diseleno-substituted alkenylic compounds: A CLOPPA-IPPP analysis. J. Magn. Res. 87: 209-219, 1990.

Submitted manuscripts:

1. Rossi, M.; Rotblat, B.; Ansell, K.; Caraglia, M.; Bernassola, F., Cavasotto, C.N., Knight, R.A., Ciechanover, A., Melino, G. High throughput screening for inhibitors of the HECT ubiquitin E3 ligase ITCH identifies antidepressant drugs as regulators of autophagy.

In preparation:

1. Cavasotto, C.N.* Algorithms for considering target flexibility in small molecule docking. Drug Discov. Today, invited review.

Organization of Scientific Events

1. *FOCEM Course: Introduction to Structural Biology and Bioinformatics*, Pasteur Institut-IBioBA-MPSP, Montevideo, Uruguay, November 11-15, 2013.

Oral presentations:

1. Comparative modelling, *FOCEM Course: Introduction to Structural Biology and Bioinformatics*, Pasteur Institut, Montevideo, Uruguay, November 11-15, 2013.
2. Computer-aided Drug Discovery and Design, *FOCEM Course: Introduction to Structural Biology and Bioinformatics*, Pasteur Institut, Montevideo, Uruguay, November 11-15, 2013.
3. Design of Ligand and Small-Molecule Decoy Libraries for Docking to G Protein-Coupled Receptors. *4to. Congreso Argentino de Bioinformática y Biología Computacional (4CAB2C) y 4ta. Conferencia Internacional de la Sociedad Iberoamericana de Bioinformática (SolBio)*, Rosario, Santa Fe, Argentina, October 29-31, 2013.
4. Computer-aided structure based drug discovery in GPCRs. *Novartis Symposium on GPCRs - 6th Brazilian Symposium on Medicinal Chemistry*, Canela-RS, Brazil, October 28-31, 2012.
5. *In silico* characterization of molecular interactions in biological systems. *3er. Congreso Argentino de Bioinformática y Biología Computacional*, Oro Verde, Entre Ríos, Argentina, September 26-28, 2012.

6. *In silico* characterization of molecular interactions in biological systems. *"Frontiers in Science" – A Joint Symposium of the Max Planck Society and the Polo Cientifico*, Buenos Aires, Argentina, April 22-25, 2012.
7. *In silico* characterization of molecular interactions in biological systems. Department of Physics, University of Texas at San Antonio, San Antonio, TX, October 21, 2011.
8. Ligand-steered homology modelling and high-throughput docking: Successful evaluation in GPCRs. *New trends in Computational Chemistry for Industry Application*, May 27, 2011, Barcelona, Spain.
9. *In silico* characterization of molecular interactions in biological systems. Department of Biological Chemistry, University of Buenos Aires, Buenos Aires, Argentina, May 16, 2011.
10. Modeling ligand-protein interaction. BIFI and University of Zaragoza, Zaragoza, Spain, November 18, 2010.
11. Ligand-steered homology modeling and high-throughput docking: Successful evaluation in GPCRs. School of Pharmacy, University of Barcelona, November 4, 2010.
12. Cavasotto, C.N. and Phatak, S.S. Ligand-steered homology modeling and high-throughput docking: Successful evaluation in aminergic GPCRs. *240th Meeting of the American Chemical Society*, August 22-26, 2010, Boston, MA.
13. Anisimov, V.M, Bugaenko, V.L. and Cavasotto, C.N. Quantum-mechanical simulation of biological macromolecules and its application in structure-based drug design. *238th Meeting of the American Chemical Society*, August 16-20, 2009, Washington DC.
14. Coupling ligand-steered homology modeling and structure-based virtual screening: Discovery of novel antagonist chemotypes to the melanin concentrating hormone receptor, a class A GPCR. *Johns Hopkins Medical School*, August 22, 2009, Baltimore, MD.
15. High-throughput docking in Drug Discovery. *Workshop on High Throughput Screening Large Scale Data Sets*. John S. Dunn Gulf Coast Consortium for Chemical Genomics, October 31, 2008, Houston, TX.
16. Coupling ligand-steered homology modeling and structure-based virtual screening: Discovery of novel antagonist chemotypes to the melanin concentrating hormone receptor, a class A GPCR. *236st Meeting of the American Chemical Society*, August 17-21, 2008, Philadelphia, PA.
17. Computer-aided Protein Modeling and Structure-Based Drug Discovery. *Advances in Oncology Institutional Grand Rounds*, MD Anderson Cancer Center, June 20, 2008, Houston, TX, USA.
18. Novel Chemotypes to Melanin-Concentrating Hormone Receptor 1 Discovered Through Ligand-Steered Homology Modeling and Virtual Screening. Drug Discovery Chemistry 2008, *Cambridge Healthtech Institute*, April 29-30, 2008, San Diego, CA, USA.
19. Ligand and structure based screening, *Workshop on High Throughput / High Content Screening and its application to Target-based Drug Discovery Research*, John S. Dunn Gulf Coast Consortium for Chemical Genomics, November 8, 2007, Houston, TX.
20. Physics and Computers in the Aid of Drug Discovery, *Keck Annual Research Conference,* October 11-12, 2007, League City, TX.
21. Protein Modeling and Computer-aided Drug Discovery, University Miguel Hernandez, Elche, Spain, September 11, 2007.

22. Protein Modeling and Computer-aided Drug Discovery, University of Zaragoza, Zaragoza, Spain, September 6, 2007.
23. Protein Modeling and Drug Discovery, MD Anderson Cancer Center, Houston, TX, July 5, 2007.
24. Computer-based Methods in Structural Biology and Drug Discovery. Rice University, Houston, TX, June 7, 2007.
25. Computational Methods in Structural Biology and Drug Discovery. University of Texas Health Science Center at Houston, Medical School, Houston, TX, June 4, 2007.
26. Docking and Virtual Screening to Protein Kinases. *Fourth Annual Conference on Protein Kinase Targets, Cambridge Healthtech Institute*, June 12-14, 2006, Boston, MA, USA.
27. Ligand docking and virtual screening in structure-based drug discovery. *BIFI 2006 - II International Conference: From Physics to Biology: the interface between experiment and computation*, February 8-11, 2006, Zaragoza, Spain.
28. Computation and Simulation in Structural Biology and Drug Discovery, *National Center of Oncology Research (CNIO)*, February 28, 2005, Madrid, Spain.
29. Structure-based development of drug target-specific compound libraries. *IBC 2nd Annual Target-Based Compound Libraries*, December 6-8, 2004, San Diego, CA, USA.

Contributions to scientific meetings:

1. Brand, C.S. Hocker, H.J., Gorfe, A.A., Cavasotto, C.N., and Dessauer C.W. Isoform Selectivity of Adenylyl Cyclase Inhibitors and Identification of Novel Compounds. Experimental Biology 2013, April 20-24, 2013, Boston, MA.
2. Brand, C.S., Malik, S., Smrcka, A.V., Cavasotto, C.N., Dessauer, C.W. Targeting of Adenylyl Cyclase for Inhibition by Peptides and Novel Small Molecule Inhibitors, 21st Keck Annual Research Conference, October 8, 2011, Houston, TX.
3. Petrov, R.R., Astruc-Diaz, F.; Cavasotto, C.N. and Diaz, P. Novel series of cannabinoid modulators for thetreatment of obesity associated disorders. *241st Meeting of the American Chemical Society*, March 27-31, 2011, Anaheim, CA.
4. Petrov, R.R., Astruc-Diaz, F.; Cavasotto, C.N. and Diaz, P. Novel series of CB2 selective agonists for the treatment of neuropathic pain. *241st Meeting of the American Chemical Society*, March 27-31, 2011, Anaheim, CA.
5. Neira, J.L., Doménech, R., Bocanegra, R., Abián, O., Correa, J., Sousa-Hervés, A., Bueno, M., Velázquez-Campoy, A., Cavasotto, C.N., Riguera, R., Sancho, J., Fernández, E. and Mateu, M.G. Designing inhibitors against the capsid protein of HIV-1. *V National Conference BIFI 2011*, February 2-4, 2011, Zaragoza, Spain.
6. Dasgupta, I., Srivastava, M., Tanifum, E.A., Phatak, S.S.,Cavasotto, C.N., and Annapragada, A. Boronic Acid Based Microparticulate Insulin Delivery System. *BMES 2010*, October 6-9, 2010, Austin, Texas.

7. Echenique, P., Cavasotto, C.N., García-Risueño, P. and Alonso, J.L. The canonical equilibrium of constrained molecular models. *Constraints in Molecular Simulation*, Zaragoza, Spain, September 2-4, 2010.

8. Petrov, R.R., Phatak, S.S.; Diaz, F-A.; Cavasotto, C.N. and Diaz, P. Novel series of CB2 selective antagonists for the treatment of autoimmune disorders: Synthesis, functional evaluation and ligand-steered modeling. *240th Meeting of the American Chemical Society*, August 22-26, 2010, Boston, MA.

9. Costanzi, S., Vilar, S., Ferino, G., Phatak, S.S., Berk, B., Cavasotto, C.N. Assessment and optimization of docking-based virtual screening for GPCR ligands: Not only crystal structures but also homology models. *240th Meeting of the American Chemical Society*, August 22-26, 2010, Boston, MA.

10. Cavasotto, C.N., Phatak, S.S., and Gatica, E.A. High-quality ligand-steered modeling and docking evaluation of class A G protein-coupled receptors. *240th Meeting of the American Chemical Society*, August 22-26, 2010, Boston, MA.

11. Phatak, S.S.; Diaz, P.; Xu, J.; Diaz, F-A.; Naguib, M and Cavasotto, C.N. Ligand-steered modeling of the cannabinoid receptor 2: Successful applications to rationalize SAR data of selective CB2 inverse agonist and agonist compounds. *240th Meeting of the American Chemical Society*, August 22-26, 2010, Boston, MA.

12. Costanzi, S., Ferino, G., Vilar, S., Berk, B., Engel, S., Tikhonova, I., Gershengorn, M.C., Harden, T.K., Jacobson, K.A., Cavasotto, C. Identification of GPCR Ligands through Docking-based Virtual Screening: Not only Crystal Structures but also Homology Models. *28th Camerino-Cyprus-Noordwijkerhout Symposium "Trekking through Receptor Chemistry"*, May 16-20, 2010, Camerino, Italy.

13. Phatak, S.S.; Diaz, P.; Xu, J.; Diaz, F-A.; Naguib, M and Cavasotto, C.N. Ligand-steered Modeling of the Cannabinoid Receptor 2: Successful Applications to Rationalize SAR Data of Selective CB2 Inverse Agonist and Agonist Compounds. *15th Annual Structural Biology Symposium*, March 19, 2010, Galveston, TX.

14. Phatak, S.S.; Diaz, P.; Xu, J.; Diaz, F-A.; Naguib, M and Cavasotto, C.N. Ligand-steered Modeling of the Cannabinoid Receptor 2: Successful Applications to Rationalize SAR Data of Selective CB2 Inverse Agonist and Agonist Compounds. *UTHSC-H Research Day "Engines of Discovery"*, November 20, 2009, Houston, TX.

15. Gatica, E.A and Cavasotto, C.N. Validation of Novel *in silico* Methodologies. *Annual Biomedical Research Conference for Minority Students (ABRCMS),* November 5, 2009, Phoenix, AZ.

16. Phatak, S.S.; Diaz, P.; Xu, J.; Diaz, F-A.; Naguib, M and Cavasotto, C.N. Ligand-steered Modeling of the Cannabinoid Receptor 2: Successful Applications to Rationalize SAR Data of Selective CB2 Inverse Agonist and Agonist Compounds. *19th Keck Center Annual Research Conference "Computation in Biology: from Gene to Neuron"*, October 29-30, 2009, Houston, TX.

17. Anisimov, V.M, Bugaenko, V.L. and Cavasotto, C.N. Quantum-mechanical simulation of biological macromolecules and its application in structure-based drug design. *238th Meeting of the American Chemical Society*, August 16-20, 2009, Washington DC.

18. Anisimov, V.M and Cavasotto, C.N. QM method development for structure-based drug design. *238th Meeting of the American Chemical Society*, August 16-20, 2009, Washington DC.

19. Cavasotto, C.N. and Anisimov, V.M. Study of Charge Transfer in Ubiquitin in Aqueous Solution. *XXVth Anniversary of the Theoretical Chemistry network of Catalunya*, June 29-July 3, 2009, Barcelona, Spain.

20. Bocanegra, R., Rodríguez-Huete, A., Fuertes, M.A., Cavasotto, C.N., Neira, J.L and Mateu, M.G. *In vitro inhibition of the immunodeficiency virus by a peptide which mimics the dimerization interface*. 10th National Meeting of Virology, June 21-24, 2009, Salamanca, Spain.

21. Gatica, E.A and Cavasotto, C.N. Incorporating Protein Flexibility in Virtual Screening. *Annual Biomedical Research Conference for Minority Students (ABRCMS),* November 6, 2008, Orlando, FL.

22. Gatica, E.A and Cavasotto, C.N. Incorporating Protein Flexibility in Virtual Screening. *Graduate School and Internship Fair*, University of Houston-Downtown, October 24, 2008, Houston, TX.

23. Bisson, W.H., Abagyan, R. and Cavasotto, C.N. Role of point mutations causing antiandrogen withdrawal syndrome studied by molecular simulations and computational prediction approaches. *231st Meeting of the American Chemical Society*, March 25-30, 2006, Atlanta, GA.

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25. Orry, A.J.W. and Cavasotto, C.N. Ligand-docking-based homology model of the Melanin-Concentrating Hormone 1 receptor. *231st Meeting of the American Chemical Society*, March 25-30, 2006, Atlanta, GA.

26. Monti, M.C., Cavasotto, C.N., Tosco, A., Dal Piaz, F., Leone, A., Casapullo, A., Riccio, R., Abagyan, R.A. and Gomez-Paloma, L. Inhibition of human group IIA Phospholipase A_2 by Petrosaspongiolide M through a mechanism of protein-protein trans-inactivation. *231st Meeting of the American Chemical Society*, March 25-30, 2006, Atlanta, GA.

27. Abagyan, R., An, J., Cavasotto, C., Fernandez-Recio, J., Kufareva, I., Totrov, M. Predicting Molecular Association. *J. Biomol. Struct. Dynam.*, 22, 823:824, 2005. *Albany 2005. The 14th Conversation*, June 14-18 2005, Albany, NY.

28. Bisson, W.H., Cavasotto, C.N. and Abagyan, R. The role of point mutations causing antiandrogen withdrawal syndrome studied by molecular simulations and computational prediction approaches. *MipTec*, May 9-12 2005, Basel, Switzerland.

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32. Cavasotto, C.N.*; Kovacs J.; Totrov M. and Abagyan, R.A. Incorporating receptor flexibility in ligand docking and virtual screening through a normal mode analysis-based procedure. *48th Meeting of the Biophysical Society*, February 14-18, 2004, Baltimore, MD.

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