

IV. CURRICULUM VITAE

Roberto Ricardo Gil

A. Personal Data

Title: Associate Research Professor
Director, NMR Facility
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Education

1992-1995 Postdoctoral Training. Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois at Chicago, Chicago, Illinois, USA.
1985-1989 Doctor en Ciencias Químicas (Equivalent to Ph.D. in Chemistry), Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Córdoba, ARGENTINA.
1979-1983 Licenciado en Química Orgánica (Equivalent to Bachelor of Science), Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Córdoba, ARGENTINA

Previous Appointments

July 2007 to date Associate Research Professor (CMU)*
August 2002 to date Director, NMR Facility (CMU)*
August 2002 to July 2007 Research Scientist (CMU)*
June 2001 to August 2002 Associate Professor of Chemistry (UNC)*
Feb. 2000 - Feb. 2001 Visiting Assistant Professor at the Protein NMR Group of Prof. Miguel Llinás (CMU)*
March 1995- June 2001 Assistant Professor of Chemistry (UNC)*
March 1992- March 1995 Visiting Assistant Professor of Pharmacognosy (UIC)*
1984-1991 Teaching Instructor of Natural Products Chemistry (UNC)*
1981-1983 Undergraduate Research and Teaching Assistantship (UNC)*
1981-1983 Teacher - Summer Courses of General Chemistry – College of Chemical Sciences - Córdoba National University, Argentina
1981-1983 Visiting Professor of Natural Products Chemistry – Catamarca National University - Catamarca, Argentina
Dec. 1997 – Aug 2002 Investigator of the National Research Council of Argentina
1995-2002 Manager of the NMR Laboratory of UNC.
April 2001-Aug 2002 Secretary of Science and Technology (Equivalent to Associate Dean), College of Chemical Sciences of Córdoba National University (Córdoba – Argentina)
*CMU: Department of Chemistry at Carnegie Mellon University
*UNC: Department of Organic Chemistry - College Chemical Sciences- Córdoba National University - Córdoba, Argentina
*UIC: Department of Medicinal Chemistry – College of Pharmacy – University of Illinois at Chicago – Chicago, IL

B. PUBLICATIONS and CITATIONS

1. Book Chapters

“Withanolides and Related Steroids”

Misico, R.I., Nicotra, V.E., Oberti, J.C., Barboza, G., Gil, R.R., Burton, G.

Series: Fortschritte der Chemie organischer Naturstoffe / Progress in the Chemistry of Organic Natural Products, Vol. 94. *In-press*.

Edited by: A. Douglas Kinghorn, Heinz Falk and Junichi Kobayashi.

SPRINGER WIEN NEW YORK – 2011.

“Proton and Carbon-13 NMR Studies of Steroids and Triterpenes” Pag. 281-298.

Cordell, G. A., Lin, L.-Z., Gil, R. R.

Title of the Book : SAPONINS USED IN FOOD & AGRICULTURE.

Series: *Advances In Experimental Medicine And Biology*

Edited by George R. Waller and Kazuo Yamasaki.

PLENUM PRESS - NEW YORK AND LONDON – 1996

2. Papers published or accepted for publication in recognized journals or conference proceedings that employ the review process

- 1- Qian, H.; Zhu, M.; Gayathri, C.; Gil, R.R.; Jin, R. “ Chirality in Gold Nanoclusters Probed by NMR Spectroscopy “ *ACS Nano* **2011**. ASAP Articles. DOI: 10.1021/nn203113j
- 2- Trigo-Mouriño, P.; Navarro-Vázquez, A.; Ying, J.; Gil, R. R. and Bax, A. “Structural Discrimination in Small Molecules by Accurate Measurement of Long-Range Proton-Carbon Residual Dipolar Couplings”. *Angew. Chem. Int. Ed.* **2011**, 50(33), 7576-7580.
- 3- Gil, R.R. “Constitutional, Configurational, and Conformational Analysis of Small Organic Molecules on the Basis of NMR Residual Dipolar Couplings” *Angew. Chem. Int. Ed.* **2011**, 50(32), 7222-7224. (Highlight Article by Invitation)
- 4- Abernathy, S.M.; Gil, R.R. and Akinyemi, A. “Utilizing 1H-NMR Spectroscopy to Profile Dioxin in Salmon Oil and Bacon Fat via a High-sensitivity 1 mm Microprobe”. *Atlas J. Chem. Biochem.* **2011**, 1 (1): 10-13.
- 5- Beach, E.S.; Malecky, R.T.; Gil, R.R.; Horwitz, C.P.; Collins, T.J. “ Fe-TAML/hydrogen peroxide degradation of concentrated solutions of the commercial azo dye tartrazine”. *Catalysis Science & Technology* **2011**, 1(3), 437-443.
- 6- Riveira, M.J.; Gayathri, C.; Navarro-Vazquez, A.; Tsarevsky, N.V.; Gil, R.R.; Mischne, M.P. “Unprecedented stereoselective synthesis of cyclopenta[b]benzofuran derivatives and their characterisation assisted by aligned media NMR and ¹³C chemical shift *ab-initio* predictions”. *Organic & Biomolecular Chemistry* **2011**, 9(9), 3170-3175.
- 7- Bahar, M.; Deng, Y.; Zhu, X.; He, S.; Pandharkar, T.; Drew, M. E.; Vázquez, A. N.; Anklin, C.; Gil, R. R.; Duskotch, R. W.; Werbovetz, K. A.; Kinghorn, A. D. Potent Antiprotozoal Activity of a Novel Semi-synthetic Berberine Derivative; *Bioorg. Med. Chem. Lett.* **2011**, 21, 2606-2610.
- 8- Yoon, J. A.; Gayathri, C.; Gil, R. R.; Kowalewski, T.; Matyjaszewski, K. “Comparison of the Thermoresponsive Deswelling Kinetics of Poly(2-(2-methoxyethoxy)ethyl methacrylate) Hydrogels Prepared by ATRP and FRP”. *Macromolecules* **2011**, 43, 4791-4797.
- 9- He, W.; Crawford, M.J.; Rapireddy, S.; M., M.; Gil, R.R.; Ly, D.H.; Achim, C. “The structure of a γ -modified peptide nucleic acid duplex”. *Molecular BioSystems* **2010**, 6(9), 1619-1629.
- 10- Gayathri, C.; de la Fuente, M.C.; Luy, B.; Gil, R.R.; Navarro-Vazquez, A. “Probing heterocycle conformation with residual dipolar couplings”. *Chem. Comm.* **2010**, 46(32), 5879-5881
- 11- Yeh, J.I.; Shivachev, B.; Rapireddy, S.; Crawford, M.J.; Gil, R.R.; Du, S.; Madrid, M.; Ly, D.H. “Crystal Structure of Chiral γ PNA with Complementary DNA Strand: Insights into the Stability and Specificity of Recognition and Conformational Preorganization”. *J. Am. Chem. Soc.* **2010**, 132(31), 10717-10727.
- 12- Zhu, Y.; Wu, Z.; Gayathri, C.; Qian, H.; Gil, R.R.; Jin, R. “Exploring stereoselectivity of Au₂₅ nanoparticle catalyst for hydrogenation of cyclic ketone”. *J. Catalysis*, **2010**, 271(2), 155-160.

- 13- Gayathri, C.; Tsarevsky, N.V. and Gil, R.R. "RDCs Analysis of Small Molecules Made Easy: Fast and Tuneable Alignment by Reversible Compression / Relaxation of Reusable PMMA Gels". *Chemistry, A European Journal* **2010**, *16*(12), 3622 – 3626.
- 14- Helfer, B.M.; Balducci, Anthony; N., Aaron D.; Janjic, J.M.; Gil, R.R.; Kalinski, P.; de Vries, I. J.M.; Ahrens, E.T.; Mailliard, R.B. "Functional assessment of human dendritic cells labeled for in vivo ¹⁹F MRI cell tracking". *Cytotherapy* **2010**, *12*, 238–250.
- 15- Bencherif, S.A., Srinivasan, A., Sheehan, J.A., Walker, L.M., Gayathri, C., Gil, R.R., Hollinger, J.O., Matyjaszewski, K., Washburn N.R. "End-group effects on the properties of PEG-co-PGA hydrogels". *Acta Biomaterialia* **2009**, *5*, 1872-1883.
- 16- Garcia, M.E., Pagola, S., Navarro-Vázquez, A., Phillips, D.D., Gayathri, C., Krakauer, H., Stephens, P.W., Nicotra, V.E. and Gil, R.R. "Stereochemistry Determination by X-ray Powder Diffraction Analysis and NMR Residual Dipolar Couplings". *Angew. Chem. Int. Ed.* **2009**, *48*, 5670-5674.
- 17- Bencherif, S.A., Srinivasan, A., Sheehan, J.A., Walker, L.M., Gayathri, C., Gil, R.R., Hollinger, J.O., Matyjaszewski, K., Washburn N.R. "End-group effects on the properties of PEG-co-PGA hydrogels". *Acta Biomaterialia* **2009**, *5*, 1872-1883.
- 18- Maksymiuk, C.S., Gayathri, C., Gil, R.R. and Donahue, N.M. "Secondary Organic Aerosol Formation from Multiphase Oxidation of Limonene by Ozone: Mechanistic Constraints via Two-dimensional Heteronuclear NMR Spectroscopy". *Phys. Chem. Chem. Phys.* **2009**, *11*, 7810-7818.
- 19- Wu, Z., Gayathri, C., Gil, R.R., Jin, R. "Probing the Structure and Charge State of Glutathione-Capped Au₂₅(SG)₁₈ Clusters by NMR and Mass Spectrometry". *J. Am. Chem. Soc.* **2009**, *131*, 6535-6542.
- 20- Uriburu, M.L., Gil, R.R., Sosa, V.E. and de la Fuente, J.R. "Caffeoyl Esters of Threonic Acid and its Lactone from *Viguiera pazensis*". *J. Argentine Chem. Soc.* **2008**, *96*, 54-61
- 21- He, W., Hatcher, E., Balaeff, A., Beratan, D., Gil, R.R., Madrid, M., Achim, C. "Solution Structure of a Peptide Nucleic Acid from NMR Data: Features and Limitations". *J. Am. Chem. Soc.* **2008**, *130*, 13264-13273.
- 22- Gil, R.R., Gayathri, C., Tsarevsky, N.V., Matyjaszewski, K. "Stretched Poly(methyl methacrylate) Gel Aligns Small Organic Molecules in Chloroform. Stereochemical Analysis and Diastereotopic Proton NMR Assignment in Ludartin Using Residual Dipolar Couplings and ³J Coupling Constant Analysis". *J. Org. Chem.* **2008**, *73*, 840-848.
- 23- Silva, O.F., Fernandez, M.A., Pennie, S.L., Gil, R.R. and de Rossi, R.H. "Synthesis and Characterization of an Amphiphilic Cyclodextrin, a Micelle with Two Recognition Sites". *Langmuir* **2008**, *24*, 3718-3726.
- 24- Pacciaroni, A. del V., Gette, M.A., Derita, M., Ariza-Espinar L., Gil, R.R., Zacchino, S.A. and Silva, G.L. "Antifungal Activity of *Heterothalamus alienus* Metabolites". *Phytotherapy Research* **2008**, *22*, 524-528.
- 25- Jakubowski, W., Kirci-Denizli, B., Gil, R.R., Matyjaszewski, K. "Polystyrene with Improved Chain-End Functionality and Higher Molecular Weight by ARGET ATRP". *Macromolecular Chemistry and Physics* **2008**, *209*, 32-39.
- 26- Mario J. Simirgiotis, M.J., Adachi, S., To, S., Yang, H., Reynertson, K.A., Margaret J. Basile, M.J., Gil, R.R., Weinstein, I.B., Kennelly, E.J. "Cytotoxic chalcones and antioxidants from the fruits of a *Syzygium samarangense* (Wax Jambu)". *Food Chemistry* **2008**, *107*, 813-919.
- 27- Liendro, M.N., Uriburu, M., Viturro, C. I., Gil, R.R., Novara, L.J., de la Fuente, J.R. "Flavonoids and volatile constituents from *Achyrocline hyperchlorea*". *Biochemical Systematics and Ecology* **2007**, *35*, 720-724.
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- 29- Nicotra, V.E., Gil, R.R., Oberti, J.C., Burton, G. "Withanolides with Phytotoxic Activity from *Jaborosa caulescens* var. *caulescens* and *J. caulescens* var. *bipinnatifida*". *J. Nat. Prod.* **2007**, *70*, 808-812.

- 30- Daly, J.W., Wilham, J.M., Spande, T.F., Garraffo, H.M., Gil, R.R., Silva, G.L., Vaira, M. "Alkaloids in Bufonid Toads (*Melanophryniscus*): Temporal and Geographic Determinants for Two Argentinian Species". *Journal of Chemical Ecology* **2007**, *33*, 871-887.
- 31- Pietrasik, J., Sumerlin, B.S., Lee, H.-il, Gil, R.R., Matyjaszewski, K. "Structural mobility of molecular bottle-brushes investigated by NMR relaxation dynamics". *Polymer* **2007**, *48*, 496-501.
- 32- Reynertson, K., Wallace, A.M., Adachi, S., Gil, R.R., Hui, Y., Basile, M.J, D'Armiento, J., Weinstein, I. B., Kennelly, E.J. "Bioactive Depsides and Anthocyanins from Jaboticaba (*Myrciaria cauliflora*)". *J. Nat. Prod.* **2006**, *69*, 1228-1230.
- 33- Dragulescu-Andrasi, A., Rapireddy, S., Frezza, B.M., Gayathri, C., Gil, R.R., Ly, D.H. "A Simple γ -Backbone Modification Preorganizes Peptide Nucleic Acid into a Helical Structure". *J. Am. Chem. Soc.* **2006**, *128*, 10258-10267
- 34- Meragelman, T.L., Salido Renteria, B., Silva, G.L., Sotomayor, C., Gil, R.R. "Modified Secoiridoid from *Acicarpha tribuloides* and Inhibition of Nitric Oxide Production in LPS-Activated Macrophages". *Phytochemistry* **2006**, *67*, 1534-1538.
- 35- Nicotra, V.E., Ramacciotti, N.S., Gil, R.R., Oberti, J.C., Feresin, G.E., Guerrero, C.A., Baggio, R. F., Garland, M. T., Burton, G. "Phytotoxic Withanolides from *Jaborosa rotacea*". *J. Nat. Prod.* **2006**, *69*, 783-789.
- 36- Desmarchelier, C., Pacciaroni, A.V., Abate-Daga, D., Coussio, J., Gil, R.R., Silva, G.L. "Antioxidant and Free Radical Scavenging Activities of *Misodendrum punctulatum*, Myzodendrone and Structurally Related Phenols". *Phytotherapy Research* **2005**, *19*, 1043-1047.
- 37- Hannah, K.C., Gil, R.R., Armitage, B.A. "¹H NMR and Optical Spectroscopic Investigation of the Sequence-Dependent Dimerization of a Symmetrical Cyanine Dye in the DNA Minor Groove". *Biochemistry* **2005**, *44*, 15924-15929
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- 39- Iovu, M.C., Sheina, E.E., Gil, R.R., McCullough, R. D. "Experimental Evidence for the Quasi-"Living" Nature of the Grignard Metathesis Method for the Synthesis of Regioregular Poly(3-alkylthiophenes)". *Macromolecules* **2005**, *38*, 8649-8656.
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- 41- Braunecker, W.A., Tsarevsky, N.V., Pintauer, T., Gil, R.R., Matyjaszewski, K. "Quantifying Vinyl Monomer Coordination to CuI in Solution and the Effect of Coordination on Monomer Reactivity in Radical Copolymerization". *Macromolecules* **2005**, *38*, 4081-4088.
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- 43- Colloca, C.B., Pappano, D.B., Bustos, D.A., Sosa, V. E., Baggio, R.F., Garland, M.T., Gil, R.R. "Azorellane diterpenes from *Azorella cryptantha*". *Phytochemistry* **2004**, *65*, 2085-2089.
- 44- Díaz, O.J., Gil, R.R., Novara, L.J., Sosa, V.E. , de la Fuente, J.R. "A modified guaianolide and a noreudesmanolide from *Microliabum polymnioides*", *Phytochemistry*, **2004**, *65*, 2557-60.
- 45- Uriburu, M.L., de la Fuente, J.R., Palermo, J., Gil, R.R., Sosa, V.E. "Constituents of two *Flourensia* Species". *Phytochemistry*, **2004**, *65*, 2085-89.
- 46- Meragelman, T.L., Pedrosa, D.S., Gil R.R. "Diterpenes from *Stevia gilliesii*". *Biochemical Systematic and Ecology*, **2004**, *32*, 45-53.
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- 81- Gil, R.R., Pastoriza, J.A., Oberti, J.C., Gutierrez, A.B., Herz, W. “Guaianolides from *Stevia sanguinea*”. *Phytochemistry*, **1989**, *28*, 2841-2843.
- 82- Sosa, V.E., Oberti, J.C., Gil, R.R., Rúveda, E.A., Goedken, V.L., Gutierrez, A.B., Herz, W. “10-Epideoxicumambrin B and other constituents of *Stevia yaconensis* var. *Subeglandulosa*”. *Phytochemistry*, **1989**, *28*, 1925-1929.
- 83- Gil, R.R., Oberti, J.C., Sosa, V.E., Herz, W. “Longipinanes and a Germacranolide Carboxylic Acid from *Stevia potrerensis*”. *Phytochemistry*, **1987**, *26*, 1459-1461.
- 84- Gil, R.R., Oberti, J.C., Sosa, V.E., Herz, W. “A Guaianolide from *Stevia breviaristata*”. *Phytochemistry*, **1985**, *25*, 1479-1480.
- 85- Sosa, V.E., Gil, R.R., Oberti, J.C., Kulanthaivel, P., Herz, W. “Sesquiterpene Lactones and Flavones from *Stevia procumbens*”. *J. Nat. Prod.*, **1985**, *48*, 340-341.

3. Papers published in recognized journals or conference proceedings that do not employ the peer-review process

- 86- Yoon, J. A.; Gayathri, C.; Gil, R. R.; Bencherif, S. A.; Aksak, B.; Kim, E. K.; Oh, J. K.; Matyjaszewski, K.; Kowalewski, T. “Structured responsive hydrogels prepared by ATRP”. *PMSE Preprints* **2011**.
- 87- Abernathy, S.M., Gil, R.R., Ainyemi, A. “Profiling dioxin in salmon oil and bacon using a high-sensitivity 1 mm microprobe via ¹H-NMR”. Preprints of Extended Abstracts presented at the

ACS National Meeting, American Chemical Society, Division of Environmental Chemistry
2007, *47*, 197-202.

- 88- Braunecker, W.A., Tsarevsky, N.V., Pintauer, T., Gil, R.R., Matyjaszewski, K. "Exploring the consequences of monomer coordination in radical polymerization". *Polymer Preprints* **2005**, *46*, 237-238.
- 89- Huang, J., Gil, R.R., Matyjaszewski, K. "Atom transfer radical copolymerization of 5,6-benzo-2-methylene-1,3-dioxepane and n-butyl acrylate". *Polymer Preprints* **2005**, *46*, 150-151.
- 90- Iovu, M.C., Simplaceanu, V., Gil, R.R., Matyjaszewski, K. "¹³C DEPT NMR study of poly(vinyl acetate) synthesized by degenerative transfer polymerization with alkyl iodides". *Polymer Preprints* (American Chemical Society, Division of Polymer Chemistry) **2004**, *45*, 988-989.

3. Citations

- After publication of Ref. 21, I was interviewed by Chemical & Engineer News for the article on Residual Dipolar Couplings in small molecules: "NMR Method Downsizes" Technique favored for determining macromolecular structures zooms in on small molecules. March 17, 2008
Volume 86, Number 11 pp. 44-45. Article Location:
http://pubs.acs.org/cen/email/html/cen_86_i11_8611sci1.html
- Ref. 24 was selected in 2008 among the 9 best articles (out of ca. 1200 articles) that have been published in the Wiley-VCH Macromolecular Journals within the previous 18 months. The article was published in the special reprint volume "Best of Macro 2008".

C. Information reflecting external reputation

1. Citations and awards

- Top Ten Youngsters of the Year. **1996**. Granted by the Stock Exchange Market of Córdoba. Córdoba. Argentina.
- Top Twelve Outstanding Citizens and/or Institutions of the Year of Catamarca Province - Argentina **1996**. Sponsored by the City of Catamarca and Catamarca Province Governments.
- CATAMARCA 96. Given to the best of the twelve candidates above. Sponsored by the City of Catamarca and Catamarca Province Governments.

2. Invited talks and selected presentations to conferences

Selected Presentations (last 5 years).

- "Exploring the consequences of monomer coordination in radical polymerization". Braunecker, Wade A., Tsarevsky, Nicolay V., Pintauer, Tomislav, Gil, Roberto R., Matyjaszewski, Krzysztof. 230th ACS National Meeting, Washington, DC, United States, Aug. 28-Sept. 1, **2005**.
- "Atom transfer radical copolymerization of 5,6-benzo-2-methylene-1,3-dioxepane and n-butyl acrylate". Huang, Jinyu, Gil, Roberto, Matyjaszewski, Krzysztof. 230th ACS National Meeting, Washington, DC, United States, Aug. 28-Sept. 1, **2005**.
- "Binding mode of DiSC2(5) with duplex DNA determined by two-dimensional NMR". Hannah, Kristen C., Gil, Roberto R., Armitage, Bruce. 229th ACS National Meeting, San Diego, CA, United States, March 13-17, **2005**.
- "Flavonoids without substitution in the B ring from *Achyrocline hyperclhora*". de la Fuente, J.R., Liendro, N., Uriburu, M.L. and Gil, R.R. XV National Symposium of Organic Chemistry – Argentine Organic Chemistry Society. Mar del Plata, Buenos Aires, Argentina. Nov. 6-8, **2005**.
- "5-Deoxyxflavonoids from the genus *Flourensia*". Uriburu, M.L., Gil, R.R., Sosa, V.E. and de la Fuente, J.R. XV National Symposium of Organic Chemistry – Argentine Organic Chemistry Society. Mar del Plata, Buenos Aires, Argentina. November 6-8, **2005**.
- "NMR study of solution aggregates of a molecular lollipop β -cyclodextrin". Silva, O. F., Hoyos de Rossi, R., Pennie, S.L. and Gil, R.R. XV National Symposium of Organic Chemistry – Argentine Organic Chemistry Society. Mar del Plata, Buenos Aires, Argentina Nov. 6-8, **2005**.

- “Primary investigation of peptide nucleic acid (PNA) duplex structure by NMR spectroscopy”. He, Wei; Madrid, Marcela; Gil, Roberto R.; Achim, Catalina. 233rd ACS National Meeting, Chicago, IL, United States, March 25-29, **2007**.
- “Profiling dioxin in salmon oil and bacon using a high-sensitivity 1 mm capillary microprobe via ¹H-NMR”. Abernathy, Shawn M.; Gil, Roberto R.; Akinyemi, Akintunde. 233rd ACS National Meeting, Chicago, IL, United States, March 25-29, **2007**.
- “Butirolactones from *Viguiera pazensis*”. Uriburu, Maria L.; Gil, Roberto R.; Novara, Lazaro J.; Sosa, Virginia E.; de la Fuente, Juana R., XVI National Symp. Organic Chemistry – Argentine Organic Chemistry Society. Mar del Plata, Buenos Aires, Argentina. Nov. 11-14, **2007**.
- “Probing Heterocycle Conformation with Residual Dipolar Couplings”. Gayathri, Chakicherla; de la Fuente, M. Carmen; Luy, Burkhard; Gil, Roberto R.; Armando Navarro-Vázquez. 50th Experimental Nuclear Magnetic Resonance Conference, Asilomar Conference Grounds, Pacific Grove, California, USA. March 29 - April 3, **2009**.
- “Exploiting Pseudo-Symmetry Relationships in Conformational Analysis using Residual Dipolar Couplings”. Armando Navarro-Vázquez; Raquel Santamaria-Fernandez; Marcos Battistel; Victor Sanchez-Pedregal; Roberto R. Gil. 51th Experimental NMR Conference, Daytona Beach, FL, USA. April 18-23, **2010**.
- “Origin of conformational organization of .gamma.-peptide nucleic acids (PNAs)”. Crawford, Matthew J.; Gil, Roberto; Ly, Danith H. 240th ACS National Meeting, Boston, MA, United States, August 22-26, **2010**.
- “Characterization of Cyclopentahydrobenzofuranes Through NMR in Aligned Media and Ab-initio Chemical Shift Computation”. Riveira MJ, Gayathri C, Navarro-Vázquez A, Gil RR, Mischne MP. SIBEAQO-II (Segundo Simposio Iberoamericano de Química Orgánica). Santiago de Compostela, Spain. September 8-12, **2010**.
- “Structured responsive hydrogels prepared by ATRP”. Yoon, Jeong Ae; Gayathri, Chakicherla; Gil, Roberto R.; Bencherif, Sidi A.; Aksak, Burak; Kim, Eun Kyung; Oh, Jung Kwon; Matyjaszewski, Krzysztof; Kowalewski, Tomasz. Abstracts of Papers, 241st ACS National Meeting & Exposition, Anaheim, CA, United States, March 27-31, **2011**.
- “Conformation in Water of the Anti-Obesity Drug Lorcaserin”. Pablo Trigo-Mouriño, M. Carmen de la Fuente, Víctor Sánchez-Pedregal, Armando Navarro-Vázquez, Roberto R. Gil. 52nd Experimental Nuclear Magnetic Resonance Conference. Asilomar Conference Grounds. Pacific Grove, CA, USA. April 10-15, **2011**.

Invited Talks.

- “Bioactive Natural Products”. Department of Organic Chemistry, College of Chemical Sciences, Córdoba National University. Córdoba - Argentina. March **1996**.
- “Sesquiterpene Lactones: Chemistry, Chemotaxonomy and Biochemistry”. Department of Organic Chemistry, College of Science and Natural History, University of Buenos Aires. Buenos Aires. Argentina. March **1997**.
- “Sesquiterpene Lactones: Chemistry, Chemotaxonomy and Biochemistry”. College of Sciences, University of La Plata. La Plata. Argentina. September **1997**.
- “Plant-Derived Aromatase Inhibitors”. Department of Chemistry, Florida International University, Miami, Florida, USA. July **1998**.
- “Natural Inhibitors of the Aromatase Enzyme”. Invited Speaker. “XII National Symposium of Organic Chemistry” organized by the Argentinean Society of Organic Chemistry (SAIQO). Los Cocos, Córdoba, Argentina. November 14-17, **1999**.
- “Nuclear Magnetic Resonance of Proteins”. Invited Speaker. “XIII Meeting of the Biology Society of Córdoba”. Córdoba, Argentina. August **2001**.
- “New Bruker Technologies: LC-NMR-MS of Natural Products”. Invited Speaker. Joint presentation with Mr. Sylvain Meguellatni from Bruker Analytik GMBH – Germany. “XIII National Symposium of Organic Chemistry” organized by the Argentinean Society of Organic Chemistry (SAIQO). Huerta Grande, Córdoba, Argentina. November **2001**.

- “Isolation and Structure Elucidation of Bioactive Natural Products”. Department of Chemistry – Carnegie Mellon University – Pittsburgh (PA). April 17th, **2002**.
- “NMR Studies of the Interaction of DNA Duplexes with Cyaning Dyes”. College of Chemistry – Córdoba National University – Córdoba – Argentina. November 17th, **2004**.
- “Partial Alignment of Small Molecules in Organic Solvents Using Stretched Poly(Methyl Metacrylate) Gels. Use of Residual Dipolar Couplings for the Determination of Relative Stereochemistry of Remotely Located Stereocenters”. XVI National Simposium of Organic Chemistry – Argentine Organic Chemistry Society. Mar del Plata, Buenos Aires, Argentina. November 11-14, **2005**.
- “Residual Dipolar Couplings in Small Organic Molecules. A Powerful Tool to Determine the Relative Stereochemistry of Remotely Located Stereocenters”. Presentation given to the undergraduate students of the MBRS/RICE and MARC Program at Hunter College, City University of New York, Manhattan, New York City. December **2007**.
- “Residual Dipolar Couplings in Small Organic Molecules. A Powerful Tool to Determine the Relative Stereochemistry of Remotely Located Stereocenters”. Department of Chemistry Annual Retreat, Pittsburgh, PA, USA. September **2008**.
- “Residual Dipolar Couplings in Small Organic Molecules. A Powerful Tool to Determine the Relative Stereochemistry of Remotely Located Stereocenters”. Rapid Structure Characterization Laboratory, Pharmaceutical Sciences, Schering-Plough Research Institute. Summit, NJ, USA. October 17, **2008**.
- “The ACD/Labs Online Experience at Carnegie Mellon”. ACD/Labs NMR Software Symposium at 50th Experimental NMR Conference. Asilomar, Pacific Grove, California, USA. March 29, **2009**.
- “NMR Spectroscopy in Anisotropic Media. Applications to the Determination of Configuration and Conformation of Small Molecules”. Plextronics Inc. Pittsburgh, PA. March 9, **2010**.
- “Stereochemistry Determination of Natural Products by NMR Residual Dipolar Couplings and Powder X-Ray Diffraction Analysis”. Invited Speaker at the 51th Experimental NMR Conference (ENC). Daytona Beach, Florida, USA. April 21, **2010**.
- “Aplicación de Acomplamientos Dipolares Residuales al Análisis Estructural de Productos Naturales” (Talk in Spanish). Departamento de Química Orgánica, Universidade de Vigo, Vigo, Spain. May 18, **2010**.
- “Revisiting Quantitative Nuclear Overhauser Effect in Small Molecules”. Departamento de Química Orgánica, Universidade de Vigo, Vigo, Spain. May 19, **2010**.
- “RDCs Analysis of Small Molecules Made Easy: Fast and Tunable Alignment By Reversible Compression/Relaxation of Reusable PMMA Gels”. Clemens-Schöpf-Institute for Organic Chemistry and Biochemistry, Technical University, Darmstadt, Germany. May **2010**.
- “Applications of Residual Dipolar Couplings to the Configurational and Conformational Analysis of Natural and Synthetic Small Organic Molecules”. Spring Washington Area NMR Group Meeting. Washington, DC, USA. June 11, **2010**.
- “NMR Spectroscopy in Anisotropic Media: A Powerful Tool for the Configurational, Conformational and Constitutional Analysis of Small Organic Molecules”. Department of Chemistry, Southern Methodist University, Dallas, Texas, USA. February 18, **2011**.
- “Structural Discrimination by Accurate Measurement of Long-Range Proton-Carbon Residual Dipolar Couplings, a Powerful NMR Tool for the Constitutional, Configurational, and Conformational Analysis of Small Organic Molecules” Invited Speaker at the XXXIII Reunión Bional de la Real Sociedad Española de Química (XXXIII Bional Meeting of the Spanish Royal Society of Chemistry), Valencia, Spain. July 25-28, **2011**.
- “NMR Spectroscopy in Anisotropic Media: A Powerful Tool for the Configurational, Conformational and Constitutional Analysis of Small Organic Molecules”. Department of

Chemistry and Biochemistry, University of North Carolina at Greensboro. Greensboro, NC, October 7th, 2011.

- "Resonancia Magnética Nuclear en Medios Anisotrópicos. Una Herramienta Poderosa en el Análisis Configuracional, Conformacional y Constitucional de Moléculas Orgánicas". Invited Speaker at XVII Simposio Argentino de Química Orgánica (XVII Argentine Symposium of Organic Chemistry). Villa Carlos Paz, Córdoba, Argentina. November 13-16, 2011.

Short stays

- Institute of Organic Synthetic Chemistry (IQUIOS), Rosario, Argentina. Sponsored by the National Research Council of Argentina to work in Structural Modifications of Sesquiterpene Lactones under the supervision of Prof. Edmundo A. Rúveda. September-November 1987.
- Bruker Analytik GMBH, Rheinstetten, Germany. Sponsored by Bruker to perform studies of Natural Product by LC-NMR-MS. August 24th – September 5th, 2001. The results were presented at the XIII Symposium of the Argentinian Organic Chemistry Society in November 2001 (See above in Invited Talks).

3. Memberships and offices held in professional societies

- American Chemical Society
- Spectroscopy Society of Pittsburgh

4. Committee work outside the university

- Member of the Advisory Board of the Secretary of Science and Technologies - Universidad Nacional de Córdoba - Córdoba - ARGENTINA - Duties: Evaluate Grants and Fellowship Applications in the Field of Biological Science. 1999-2001.
- Co-organizer / Co-Chair of the Natural Products Drug Discovery Symposium at the First Pharmaceutical Congress of the Americas. Organized by the American Society of Pharmaceutical Scientists (AAPS), Orlando - Florida - USA - March 2001.
- Coordinator of the Area Pharmacology of Natural Products of the Montevideo Group. 1999-2002.
- Co-Chair with Professor Burkhard Luy from the Karlsruhe Institute of Technology (Karlsruhe, Germany) of the Workshop "Residual Dipolar Couplings: From Sample Preparation to Stereochemistry" at the SMASH 2010 Conference in Portland, Oregon. September 26-29, 2010. (SMASH: Small Molecules Are Still Hot).
- Program Chair for SMASH 2012 to be held in Providence, Rhode Island. September 2012.

5. Consulting

- Consultant for different Argentinean Companies in Structure Elucidation using Spectroscopic Techniques (NMR, IR, MS). 1995-2002.
- Pressure Chemicals Co., Pittsburgh, PA. 2003 to date.
 - Neo Solutions, INC. Pittsburgh, PA, 2005.
 - North Haven Chemicals, Pittsburgh, PA. 2006.
 - Plextronics INC. Pittsburgh, PA, 2008 to date.
 - Valspar Corporation, Pittsburgh Research Branch. Pittsburgh, PA. 2009 to date.

6. Contract and grant support, including funding that the candidate has had in the past, current funding, and currently submitted proposals

Current Funding:

Source: US National Science Foundation

Title: "MRI: Acquisition of a New 500 MHz NMR Console and Accessories to Support Research and Education at Carnegie Mellon University"

Period: 2010-2013

Amount: \$243,530

Source: US National Science Foundation

Title: “Collaborative Research: Development of New Methodologies in NMR Spectroscopy of Small Organic Molecules in Anisotropic Media”

Period: Sept 2011- Sept 2014

Amount: \$ 330,000

Past Funding (USA):

- Berkman Faculty Development Fund – Carnegie Mellon University (\$ 7,000). 2005-2006. Research Topic: “Development of an NMR Spectroscopic Method for Simultaneous Observation of Both Liquid Phases in Two-Liquid-Phase System”. Joint application with Dr. Colin P. Horwitz.
- Hispanic-Serving Institutions Education Grants Program – USDA. (\$ 350,000). 2005-2009 “Leveraging a Research University Partnership to Enhance Minority Students' Laboratory Skills. Joint application Department of Biology (Dr. Edward Kennelly, PI), Lehman College – CUNY and Departments of Biology and Chemistry (Drs. Roberto R. Gil and Colin P. Horwitz, Co-PI's), Carnegie Mellon University.

Past Funding (Argentina):

- Reentry Grant. Fundación Antorchas. Argentina. 1995. Research Topic: Plant-Derived Regulator of Steroidogenic Enzymes .
- Grants for Medical Research. Fundación Alberto P. Roemmer. 1996-1997. Research Topic: Plant-Derived Regulator of Steroidogenic Enzymes . Joint application with Professor Alfredo Flury of Biochemistry Department.
- Research Grant. Fundación Antorchas. Argentina. 1997. Research Topic: Plant-Derived Regulator of Steroidogenic Enzymes .
- Support to Young Scientists. Research Council of Córdoba Province. 1997. Research Topic: Plant-Derived Regulator of Steroidogenic Enzymes .
- Research Grant. Fundación Antorchas. Argentina. 1998 and 2001. Research Topic: Bioactive Natural Products from Plants. Joint application with Dr. Gloria L. Silva.
- Research Grant. Secretary of Science and Technology - Universidad Nacional de Córdoba - Córdoba - Argentina. 1999-2001. Research Topic: Bioactive Natural Products from Plants. Joint application with Dr. Gloria L. Silva.
- Research Grant. Research Council of Córdoba Province, Argentina, 1999. Research Topic: Plant-Derived Antioxidant, Cytotoxic Metabolites and Aromatase Inhibitors. Joint application with Dr. Gloria L. Silva.

7. Fellowships

- Granted by Córdoba National University, while undergraduate student, in order to do research at the Natural Products Laboratory - Organic Chemistry Department. 4/1/83 to 12/31/83.
- Granted by The Air Force of Argentina to work at the laboratories of the Air Force in Córdoba. Field: UV-Vis and Infrared Spectroscopy. 7/1/83 to 11/1/83.
- Granted by the National Research Council of Argentina (CONICET):
 - a) Four-year fellowship to support the Graduate Studies at Córdoba National University. 1985-1988. Supervisor: Prof. Juan C. Oberti.
 - b) One-year fellowship to support postdoctoral studies at Córdoba National University. 1989. Supervisor: Prof. Juan C. Oberti.
 - c) Two-year external fellowship to support postdoctoral training at College of Pharmacy - University of Illinois at Chicago - Chicago - USA. Supervisor: G. A. Cordell. 1992-1994.

8. Reviews of publications and research proposals

- Invited to review manuscripts for the following peer-reviewed journals:
Angewandte Chemie Int. Ed.; Bioorganic & Medicinal Chemistry Letters; Chirality; Chemistry – A European Journal; European Polymer Journal; J. Am. Chem. Soc.; Journal

of the Brazilian Chemical Society; Journal of Heterocyclic Chemistry; Journal of Natural Products; Journal of Magnetic Resonance; Journal of Organic Chemistry; Journal of Molecular Structure; Langmuir; Magnetic Resonance in Chemistry; Phytochemistry; Tetrahedron

- Invited to evaluate grant proposals for:
 - Agencia Nacional de Promoción Científica y Tecnológica de Argentina (National Agency for the Promotion of Science and Technology of Argentina, equivalent to US NSF)
 - The PSC-CUNY Research Award Program - City University of New York - Bronx - NY.
 - National Research Council of Argentina (CONICET).

9. Editorial Work

- Guest Editor for Special Issue – Spring 2012
Magnetic Resonance in Chemistry
Topic: "NMR of Small Molecules in Anisotropic Media"

D. Service and committee work within the University

- Department Committees (Chemistry)
 - Instrumentation Committee
 - Diversity Committee
 - Graduate Recruiting Committee
- College Committees
 - MCS Ad-Hoc Committee on Appointments with Indefinite Tenure (1 yr)
- University Committees
 - President's Diversity Advisory Council (DAC) (2004 to date)
 - Graduate Workgroup of DAC (2004 to date)
 - Graduate Recruiting Sub-Committee of the DAC (2004 to date)
 - Strategic Plan 2008 Committee: Community Success Subcommittee (2007-2008)
- Other service
 - Faculty mentor of the Mellon College of Sciences mentoring program COMPASS (Coaching Minority Progress and Academic Success in Science)
 - Coordinator of the CUNY-Carnegie Mellon Summer Research Program.
 - <http://www.chem.cmu.edu/ccsrp>
 - Co-Chaired with Emeritus Professor Joseph Dadok (CMU) and Dr. Istvan Pelczer (Princeton University) the Organizing Committee of the "NMR Symposium Honoring Aksel A. Bothner-By" on March 26-27th, 2009 at the Mellon Institute Building.
 - <http://www.chem.cmu.edu/nmr-symposium/index.html>
- Diversity Activities
 - Working on building diversity recruiting pipelines with Lehman College, Hunter College and Brooklyn College of the City University of New York (joint efforts with Dr. Rea Freeland and Dr. Colin Horwitz).
 - Developed recruiting pipelines with the Chemistry Department at Howard University thru Prof. Shawn Abernathy, Director of the NMR Facility at Chemistry Department.
 - The main objectives of the USDA Grant with CUNY include: enhancing the biology and chemistry curriculum at Lehman College using NMR and mass spectrometry expertise at Carnegie Mellon and hiring a dedicated technician to assist with the operation and maintenance of Lehman's NMR facility; creating a three-year pilot summer internship program (2006-2008) for CUNY undergraduate students, with special emphasis from groups currently underrepresented in the sciences, to work at Carnegie Mellon in biology and chemistry laboratories; identifying in either Chemistry or Biological Sciences at

Carnegie Mellon, and receive a \$50,000 USDA graduate fellowship; and upgrading the nuclear magnetic resonance (NMR) facilities at Lehman and Carnegie Mellon by enhancing the sensitivity of existing NMR spectrometers and providing access to state-of-the-art inverted detected NMR experiments.

- To strengthen our bonds with CUNY, I traveled to New York in April 2004 and helped Prof. Edward Kennelly at Lehman College to setup and optimize NMR Experiments on their new Bruker Avance AV-300 NMR Spectrometer. I also trained students from underrepresented groups in science to work in NMR Spectroscopy. Since then I visited CUNY in a yearly basis.
- Attended together with Emily Stark from Biology Department as exhibitors to the Annual Biomedical Research Conference for Minority Students (ABRCMS – <http://abrcms.org>) in Atlanta 2005 and Anaheim 2006. The Chemistry and Biology Departments rented a booth at the conference to promote our graduate and summer research programs.

V. INFORMATION ON CONTRIBUTIONS TO EDUCATION

A. Courses and seminars taught by the candidate

Taught NMR Spectroscopy at the “II Escuela Andina de Espectroscopía” (2nd Andean School of Spectroscopy) organized by SPECTRA 2009, Lima-Peru, March 2-6, 2009. The school was attended by university students (graduate and undergraduate) and faculty members from Bolivia, Peru, Venezuela and Colombia.

<http://postgrado.uni.edu.pe/espectroscopia/contenido/programaEAE.html>

Taught four lectures at the 2nd Latin American NMR School. Universidad Industrial de Santander, Bucaramanga, Colombia. November 8-12, 2010.

http://www.yo-que.ch/nmrlab/mediawiki-1.15.1/index.php/LANMR_2

At Carnegie Mellon: Laboratory IV (09-322) - NMR Laboratory. Fall 2004 and 2005.

As Professor of the Organic Chemistry Department of the College of Chemical Science at Córdoba National University (Córdoba – Argentina) participated in the following courses:

Undergraduate:

- Spectroscopic Techniques in Organic Chemistry
- Advanced Analytical Chemistry
- Bioorganic Chemistry
- Organic Chemistry

Graduate:

- Phytochemistry: Occurrence and Biosynthesis of Natural Products
- Advanced Nuclear Magnetic Resonance: Modern multinuclear and multidimensional NMR Spectroscopy and its application to structural studies of organic molecules, peptides and proteins

B. Advising and mentoring of undergraduate students

- Stephen M. Greenwald (Graduated 2005)

Spring Semester 2003: Independent Research for credit

Summer 2003: Summer Fellowship and Small Undergraduate Research Grant from the Undergraduate Research Initiative at CMU

Fall Semester 2003: Independent Research for credit

Spring Semester and Summer 2004: Supported by the Howard Hughes Medical Institute Program for Undergraduate Research

Steve was the recipient of the 2004 Undergraduate Award from the Society for Applied Spectroscopy (Pittsburgh Section) for his Undergraduate Research in NMR Spectroscopy.

He has successfully completed a dissertation for his BS/MS Degree from Carnegie Mellon in 2006. Steve is currently a graduate student with Prof. Jeffrey A. Reimer in the College of Chemistry at UC Berkeley

- Ben Naman (Graduated 2006)

Summer Research 2005 funded by Peter C. Dozzi Pittsburgh Internship Initiative Grant Fall Semester 2005 funded by Berkman Faculty Development Fund

“Development of an NMR Spectroscopic Method for Simultaneous Observation of Both Liquid Phases in Two-Liquid-Phase System”

Ben was the recipient of the 2006 Undergraduate Award from the Society for Applied Spectroscopy (Pittsburgh Section) for his Undergraduate Research in NMR Spectroscopy.

Ben graduated in 2006 and his training in NMR spectroscopy played a key role when hired by Givaudan, a leading Ohio company in the fragrance and flavors industry.

- Grisel Perez (Graduated 2007)

Fall Semester 2006 – Research for Credit

“Identification of Antioxidant Phenolic Glycosides from the seed of the West African fruit *Blighia Sapida* (Akee)”

- Sarah Pennie (Graduated 2007)

Summer Undergraduate Research Program 2005 – Merk Computational Fund - CMU

Summer Undergraduate Research Grant from Undergraduate Research Office – CMU

“NMR Study of Solution Aggregates of a Molecular Lollipop β -Cyclodextrin”

Fall Semester 2006 – Spring Semester 2007 – Research for Credit 3 Units

Research for Credit “Study of a Functional Polymer by NMR Diffusion Ordered Spectroscopy (DOSY)”

- Sage Bowser (Graduated 2007)

Spring Semester 2007 – Research for Credit 12 Units

“Development of 2D NMR Methods for the Quantification of the Ratio *trans/cis* Fatty acids in Margarines”

Right after graduation, Sage was hired as the assistant of the NMR Laboratory Manager of the Department of Chemistry at the University of Pittsburgh.

- Dami Phillips (Graduated 2010)

Summer Undergraduate Research 2007– HHMI

Fall Semester 2007 – Research for Credit 9 units

“Structure Elucidation of a Steroidal Lactone Using NMR Residual Dipolar Couplings”

- Americo Fraboni (Graduated 2010)

Summer Undergraduate Research 2009

Fall Semester 2009 – Research for Credit 3 units

“Structure Elucidation of a Benzazepine Derivatives by NMR Spectroscopy in Anisotropic Media”

- Supervised, during the years 2006 to 2008, the NMR work of two excellent undergraduate students from Prof. Neil Donahue (Chemistry and Chemical Engineering). These two students, Mr. Joshua E. Tischuk and Ms. Christina S. Maksymiuk graduated from CMU with the combined MS/BS Degree in 2007 and 2008, respectively.

C. Graduate degree candidates and postdoctoral collaborators

Advisor/Co-Advisor:

- Ph. D.: Tamara L. Meragelman – Córdoba National University - Argentina. 1999-2002.
- M.Sc. (Co-Advisor): Viviana E. Nicotra. Comahue National University. Argentina. 1998
- Mr. Pablo Trigo-Mouriño, graduate student from the University of Santiago de Compostela (Spain) has spent three months performing research in my laboratory from 09/2010 to 12/2010.

Member of Advisory Committees at CMU:

- Soumitra Ghosh. Department of Chemical Engineering. Advisor: Michael Domach Co-advisor: Ignacio Grossmann. Graduated 2007.
- Kristen C. Hannah. Advisor: Bruce Armitage. Graduated 2007.
- Wade Braunecker. Advisor: Krzysztof Matyjaszewski. Graduated in 2008.

- Wei He. Advisor: Catalina Achim. Graduated 2009.
- Marcos Battistel (Chair). Advisor: Miguel Llinas. Graduated 2010.
- Soumen Kundu. Advisor: Terry Collins.
- Brendan McGee. Advisor: Terry Collins.

Member of Thesis Advisory Committee at Córdoba National University, Córdoba, Argentina

a) 3 Ph.D. Thesis: Mrs. Gabriela Díaz, Mrs. Paola Pucci and Ms. Natalia Soledad Ramacciotti

b) 3 M.Sc. Thesis: Gabriela Gioino (Grad. 2001), María C. Luján (Grad. 2001), Ana Paula Vilchez

Member of Thesis Evaluation Committee: one Ph.D. Student. 1999. Rosario National University - Rosario - Santa Fe Province – Argentina

Postdoctoral Collaborator and NMR Assistant: Dr. Gayathri Withers (2006 to date)