

CURRICULUM VITAE

Eduardo M. Sproviero

(August 2007)

Last Name: Sproviero

First and Middle Names: Eduardo Marcelo

Home Address: 1275 Chapel St, Apt 8. New Haven, CT 06511, USA.

Phone: (203)432-5911

Work Address: Department of Chemistry, School of Arts and Sciences, Yale University.
225 Prospect Street P.O. Box 208107, New Haven, CT 06520-8107, USA.

Phone: (203)432-5911. **Fax:** (203)432-6144

E-mail: eduardo.sproviero@yale.edu

. Educational History

- Postdoctoral Fellow: Yale University.
- PhD (Physics): University of Buenos Aires (*Study of conformational and structural effects in molecules. Development of methods based on orbital interactions for analyzing their electronic mechanisms*). (2003)
- University Degree (Physics): *Licenciado* in Physical Sciences from School of Exact and Natural Sciences, University of Buenos Aires (Mater's work: *Theoretical analysis of internal mobility in steroidal hormones*) (Equivalence: U.S. Master in Physics).
- High School Degree: *Bachiller* in Commercial Sciences.

. Post Graduate Courses

- **Determination of Three-dimensional Structure and Rotational Dynamics of Proteins in Solution using Nuclear Magnetic Resonance:** General techniques related with protein NMR, focused on practical applications.
- **Chemical Aspects of Environmental Pollution:** A general course that covered the subjects of chemical and physical pollution, their sources and ways of treatment. 120 hours.
- **Molecular Modeling. Structure and Dynamic:** Computational techniques related with molecular dynamics, Monte Carlo, etc., with emphasis in biological applications. The course also included a physical study of the structure of water and synthetic liposomes. 120 hours.
- **Molecular Modeling:** Usage of general molecular modeling software: Hyperchem, and PCMODEL, and the theoretical background that supports them, such as molecular mechanics force fields, and quantum mechanics (semiempirical and *ab-initio*) methods. 72 hours.
- **Nuclear Magnetic Resonance:** A general view of the subject of Nuclear Magnetic Resonance (including solids) with emphasis in two dimensional spectroscopy (analysis of the most useful sequences and chart interpretation). 30 hours.
- **Molecular Physics 1 (Theoretical Nuclear Magnetic Resonance).** Theoretical background of the NMR phenomenon especially focused on the calculation of coupling constants and their analysis in terms of contributions from localized orbitals in the propagator polarization approach. 120 hours.
- **General and Inorganic Chemistry I “A”:** The usual first university course in Chemistry, based on textbooks such as Mahan's *University Chemistry* or Gladstone's *Principles of Physical Chemistry*.
- **General and Inorganic Chemistry II:** The usual second university course in Chemistry, based on textbooks such as Mahan's *General and Inorganic Chemistry*.
- **Introduction to Gaussian. Theory and Practice:** A course on the operation of the Gaussian suite of programs. Organized by Gaussian Inc. and Silicon Graphics Computer Systems.

- **Structure of Matter: Atoms and Molecules:** A course focused on modern *ab initio* approaches to the calculation of the electronic structure and properties of molecules. 72 hours.
- **Course of Operation** of Nuclear Magnetic Resonance spectrometers Varian XL-100 (100 MHz) and Bruker AC 200 (200 MHz).
- **Organic Chemistry I:** The usual first university course in Organic Chemistry, based on textbooks such as Fessenden or Mc Murry's *Organic Chemistry*.

. Teaching Positions

Position: Teaching Assistant.

Department of Physics, School of Exact and Natural Sciences, University of Buenos Aires.

– *Period:* Since August 1990 until December 2003.

– *Signatures:*

Structure of Matter 3 (Advanced Electronic Structure applied to Atoms and Molecules, Quantum Chemistry).

Physics 4: Quantum Physics and Thermodynamics.

Laboratory 2: Geometrical and Physical Optics, and Mechanical Waves (Instrumental aspect)

Physics 2: Electricity and Magnetism.

Department of Organic Chemistry, School of Exact and Natural Sciences, University of Buenos Aires.

– *Period:* March 2000 - March 2001.

– *Signatures:*

Organic Chemistry 1: Spectroscopic techniques in Organic Chemistry.

. Honors and Awards

- **Fellowship Grant for undergraduate students from the University of Buenos Aires**

Period: Since September 1, 1991 to September 30, 1993.

Subject: **Theoretical study about deformation energies and flexibility of the steroid nucleus of corticoid hormones.**

Directors: Rubén H. Contreras and Gerardo Burton (senior scientists and leading professors at FCEN, UBA).

Place of work: Departments of Physics and Organic Chemistry, FCEN, UBA.

Dedication: 20 hours a week

- **Fellowship Grant for graduate students from the University of Buenos Aires**

Period: Since October 1, 1993 to February 28, 1997.

Subject: **Theoretical and experimental study of the flexibility of steroidal hormones and synthetic analogues.**

Director: Gerardo Burton.

Place of work: Department of Organic Chemistry, FCEN, UBA.

Dedication: 45 hours a week

– **Fellowship Grant for graduate student from the University of Buenos Aires**

Period: Since March 1, 1997 to August 31, 1999.

Subject: **Analysis of structure, flexibility and electronic topology of organic compounds.**

Director: Gerardo Burton.

Place of work: Department of Organic Chemistry, FCEN, UBA.

Dedication: 45 hours a week

– **Fellowship Grant** from the Fondo para el Mejoramiento de la Calidad Universitaria (FOMECA).

Period: From September 1 to November 30, 1998.

Directors: Professor Ernesto Diez Villanueva (Autonomous University of Madrid, Spain) and Professor Angel Luis Esteban Elum (University of Alicante, Spain).

Place: Department of Physical Chemistry, School of Sciences, University of Alicante, Alicante (Spain).

Subject: Theoretical and experimental study of the tautomerism in diazines using Nuclear Magnetic Resonance methods. Their correlation with structural and electronic properties using the molecular topology formalism of Bader (AIM) and the natural bond orbital methodology of Weinhold (NBO).

. Research

Undergraduate activities: During the period 1988-1990 I have made research in the Laboratory of Solids, Department of Physics, FCEN, UBA. During this period we designed, constructed and made run a non contact temperature detector. We had to design and construct some electronic circuits and we used infrared detectors (Pb S). There is a report about this work which describes the device and its construction.

Equivalent Master Work: Since March 1991 to May 1995 I have worked in a interdisciplinary project between the departments of Organic Chemistry and Physics, FCEN, UBA. The goal of this work was the study of intramolecular flexibility in steroid hormone analogues and the development of internal geometry parameters.^{1,2} During this period we developed some analytical techniques like intramolecular flexibility parameters and we use some known ones like normal mode analysis, molecular dynamics, molecular modeling, calculation of dipole-dipole

longitudinal relaxation times, coupling constants and internal correlation constants (the last three in the frame of the NMR technique). I developed all the computational programs needed for the application of these formalisms to the molecular systems of interest.

PhD activities (1995-2003): A scheme derived from the NBO formalism of localized orbitals was developed, in which the intramolecular interactions are interpreted as interactions between orbitals. The contribution of orbital interactions to any molecular property is evaluated through a perturbative type analysis. This decomposition allows interpreting the way in which a change in a region of the molecule is transmitted to other parts and determines the variation of any property. Several applications were made that include the study of how changes in molecular geometry or the addition of substituents modify, by means of molecular orbital interactions, several nuclear magnetic resonance parameters.^{4-6, 8,9} As an alternative to the previous analysis, a descriptor based on a generalization of the electronic charge density that includes canonical vacant orbitals was developed.⁷ This descriptor allows analyzing stereoelectronic interactions in direct form or through parameters associated with the charge density.

The combined application of the effect of orbital interactions on molecular properties and of the latter on macroscopic properties can be used to individualize which are the intramolecular interactions that determine a particular macroscopic response. Oriented to the study of the biological activity, the method of the polarization propagator (that allows evaluating of orbital contributions to molecular properties) was combined with the GAPT scheme of partitioning of molecular properties into atomic contributions (usually important to study biological effects), at RPA-INDO level. In addition, parameters of intramolecular geometry and flexibility were identified, and were used to interpret the biological activity of steroidal compounds.¹⁰ The results of these studies gave rise to publications (published and in preparation) included in item C and presentations included in item G.

The results of this work has been published and reported therein (see Publications, Reports and Presentations).

Postdoctoral Activities (2004-Present): The main focus of my postdoctoral activities involve the computational study of macromolecules and oxomanganese complexes. In the macromolecule field, recent breakthroughs in X-ray crystallography and advances in quantum mechanics /molecular mechanics (QM/MM) hybrid methods have allowed the construction of chemically sensible models of enzymatic active sites, and other regions of interest within proteins. Following this direction, I applied QM/MM techniques to study structural and electronic properties of two systems that participate in the conversion of light into chemical energy: rhodopsin and photosystem II (PSII). Both systems involve delicate mechanisms that include small regions of the protein. These regions need to be analyzed at a high level of theory to understand the mechanisms in which they are involved. In the case of rhodopsin, I studied the

effect of the protein environment over the electronic properties of the retinylidene chromophore, with especial emphasis in charge redistributions, and NMR parameters. In the case of PSII, I studied the oxygen evolving center (OEC) of PSII. I prepared some models that include complete ligation of the catalytic center by amino acid residues, water, hydroxide and chloride as determined by the intrinsic electronic properties of the oxomanganese core and the perturbational influence of the surrounding protein environment. Starting from this model, I also proposed structures along the Kok cycle that represent a mechanistic proposal for water oxidation based on QM/MM models. The structures were validated by comparison of their simulated EXAFS spectra with experimental data. The resulting QM/MM structural models are consistent with available mechanistic data and also compatible with X-ray diffraction models and EPR spectroscopy. Each step of the cycle includes a detailed analysis of changes in bond-distances, manganese oxidation states, rearrangement of water molecules around the OEC, and protonation states of manganese ligands and nearby residues, among other atomistic details.

. Skills

My research work involved mainly the application and modification of molecular physics techniques to organic chemistry molecules, with the aim of studying chemical properties and analyzing biological problems. During the last years I studied several NMR parameters in organic molecules and their relation with stereoelectronic properties. I also developed a method related with NBO localized orbitals to evaluate quantitatively which is the effect of selected intra/inter-molecular interactions (delocalization, steric and electrostatic) over molecular properties, *e.g.* atomic charges, NMR coupling constants, NMR shieldings, etc. (this method could be applied also to all molecular properties that depend on molecular orbitals, either in the DFT or HF context). I have worked too in a formalism that include the space spanned by the manifold of vacant orbitals to study properties that involve these kind of orbitals, like hyperconjugation, anomeric effect, etc. I also have some experience in molecular dynamics simulations of small molecules, harmonic dynamics, evaluation of dynamical NMR parameters (T1, T2) (included in the master's work), reaction mechanisms in compounds that include lithium, etc. I have a good experience in FORTRAN source codes as I write several in-house computational programs. I also have experience with UNIX systems, and Windows platforms.

I also developed skills in the use of specialized software to manipulate macromolecules, especially for interconversion between different formats and/or visualization. I am also able to translate electronic wave functions between different computational packages (*e.g.* Gaussian and Jaguar). Other capabilities include the ability to compute electronic properties of selected regions within proteins, even when the computation of those magnitudes are not included in the standard

computational packages. I also have a good experience in calculating NMR, EXAFS, and IR parameters, as well as pkas, redox potentials, electrostatic potentials, atomic charges, etc.

. References

1. Professor Victor S. Batista, Chemistry Department, Yale University, New Haven, CT. victor.batista@yale.edu
2. Professor Gary W. Brudvig, Chemistry Department, Yale University, New Haven, CT. gary.brudvig@yale.edu
3. Professor Gerardo Burton, Department of Organic Chemistry, School of Exact and Natural Sciences, University of Buenos Aires, Argentina. burton@go.fcen.ub.ar
4. Professor Rubén H. Contreras, Department of Physics, School of Exact and Natural Sciences, University of Buenos Aires, Argentina. contrera@df.uba.ar

. Publications

1. G. Burton, M. Galigniana, S. de Lavallaz, A. L. Brachet-Cota, E. M. Sproviero, A. A. Ghini, C. P. Lantos and M. C. Damasco., **Sodium-Retaining Activity of Some Natural and Synthetic 21-Deoxysteroids**, *Molecular Pharmacology*, **47**, 535-543 (1995).
2. Eduardo M. Sproviero, Andrés Ferrara, Rubén H. Contreras and Gerardo Burton, **^1H - ^1H Long Range Couplings in Fused Cyclopropanes. NMR Spectral Assignment and Conformation of 17,18-Cyclosteroids**, *J. Chem. Soc., Perkin Trans. 2*, 933-937 (1996).
3. G. A. Aucar, E. Botek, S. Gomez, E. M. Sproviero and R. H. Contreras **RPA AM1 calculations of NMR spin-spin coupling constants: geminal ^{119}Sn - ^{119}Sn couplings**, *Journal of Organometallic Chemistry*, **524**, 1-7 (1996).
4. Eduardo M. Sproviero, Gerardo Burton, **Stereoelectronic Contributions to ^1H - ^1H Coupling Constants**, *Molecules*, **5**, 539-540 (2000).
5. Sproviero, E. M.; Burton, G.; **Stereoelectronic Contributions to long range ^1H - ^1H Coupling Constants**, *J. Phys. Chem. A*, **106**, 7834 (2002).
6. Sproviero, E. M.; Burton, G.; **Stereoelectronic Interactions and Molecular Properties. A NBO Based Study of Uracil**, *J. Phys. Chem. A*, **107**, 5544 - 5554 (2003).
7. James P. McEvoy, Jose A. Gascon, Eduardo M. Sproviero, Victor S. Batista and Gary W. Brudvig; **Computational Structural Model of the Oxygen Evolving Complex in Photosystem II: Complete Ligation by Protein, Water and Chloride**, *Photosynthesis: Fundamental Aspects to Global Perspectives, vol. 1*, (D. Bruce and A. van der Est, ed.) Allen Press Inc., Lawrence, Kansas, 278-280, 2005.

8. Jose A. Gascon, Eduardo M. Sproviero and Victor S. Batista, **QM/MM Study of the NMR Spectroscopy of the Retinylidene Chromophore in Visual Rhodopsin**, *J. Chem. Theor. Comput.*, **1**, 674-685, 2005.
9. Jose A. Gascon, Eduardo M. Sproviero and Victor S. Batista, **Computational Studies of the Primary Photo-Transduction Event in Visual Rhodopsin**, *Acc. Chem. Res.*, **39**, 184-193, 2006.
10. Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig, and Victor S. Batista, **An idealized Mn₄CaO₄ cluster as a model of the OEC of Photosystem II. A DFT/B3LYP Structural and Electronic Characterization of Mixed-Valence Multinuclear Oxomanganese Cluster Ions**, *J. Inorg. Biochem.*, **100**, 786-800, 2006.
11. Kevin Leung, Susan B. Rempe, Peter A. Schultz, Eduardo M. Sproviero, Victor S. Batista, Michael E. Chandross, and Craig J. Medforth, **Density functional theory and DFT+U study of transition metal porphine adsorbed on Au(111) surfaces and effects of applied electric fields**, *J. Am. Chem. Soc.*, **128**, 3659-3668, 2006.
12. E. M Sproviero, J. A. Gascon, J. P. McEvoy, G. W. Brudvig, and V. S. Batista,, **QM/MM Model of the Oxygen Evolving Complex of Photosystem II**, *J. Chem. Theor. Comput.*, **4**, 1119-1134, 2006.
13. Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig and Victor S. Batista. **Structural Models of the Oxygen-Evolving Complex of Photosystem II**, *Current Opinion Struct. Biol.*, **17**, 173-180, 2007.
14. Eduardo M. Sproviero, Katherine Shinopoulos, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig and Victor S. Batista. **QM/MM computational studies of substrate water binding to the oxygen evolving complex of Photosystem II**, *Phil. Trans. R. Soc. London B*, in press, 2007.
15. Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig and Victor S. Batista. **QM/MM Study of the Catalytic Cycle of Water Splitting in Photosystem II**, *J. Am. Chem. Soc.*, submitted, 2007.
16. Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig and Victor S. Batista. **Computational studies of the O₂-evolving complex of photosystem II and biomimetic oxomanganese complexes**, *Coord. Chem. Rev.*, in press, 2007.
17. Eduardo M. Sproviero, James P. McEvoy, Jose A. Gascon, Gary W. Brudvig and Victor S. Batista. **Computational Insights into the O₂-evolving complex of photosystem II**, *Photosynthesis Research*, submitted, 2007.

In preparation:

18. Eduardo M. Sproviero, José A. Gascón, Malcolm H. Levitt, and Victor S. Batista, **QM/MM- and NMR-based electronic structure analysis of the Rhodopsin Chromophore.**
19. Eduardo M. Sproviero, Gerardo Burton and Rubén H. Contreras, **Topological analysis of stereoelectronic interactions.**
20. Eduardo M. Sproviero, Gerardo Burton and Rubén H. Contreras, **^{17}O NMR Chemical Shifts and Electron Delocalizations. DFT-GIAO and NBO Studies of their Angular Dependences in Conjugated Carbonyls.**
21. Eduardo M. Sproviero, Gerardo Burton and Rubén H. Contreras, **Electron Delocalizations in Amide Groups. Applications to 5-substituted Uracils and their Relationships with ^{17}O NMR Chemical Shifts.**
22. Eduardo M. Sproviero and Gerardo Burton, **Intramolecular Flexibility Analysis. An Application to Δ^4 -3-ketosteroids.**

. Reports

PhD thesis: Study of conformational and structural effects in molecules. Development of methods based on orbital interactions for analyzing their electronic mechanisms.

Master's work: Theoretical analysis of internal mobility in steroidal hormones

Undergraduate work: Non contact temperature detector

. Presentations

- **An algorithm for structural refinement based on *ab initio* simulations of EXAFS spectra: Applications to studies of metalloproteins.** Eduardo M. Sproviero, and Victor S. Batista.
234th ACS National Meeting, American Chemical Society, Boston, MA, August 19-23, 2007.
- **QM/MM structural determination of the oxygen evolving complex of photosystem II.** Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig, and Victor S. Batista.
234th ACS National Meeting, American Chemical Society, Boston, MA, August 19-23, 2007.
- **Ligation of the C-terminus of the D1-polypeptide of photosystem II to the Oxygen Evolving Complex of Photosystem II.** Jose A. Gascon, Eduardo M. Sproviero, James P. McEvoy, Gary W. Brudvig and Victor S. Batista.
Proceeding of the 14th International conference on Photosynthesis, Glasgow, U.K., submitted, 2007.

- **Density functional theory (DFT) studies of structures and properties for high-valent intermediates Q in methane monooxygenase (MMO) and X in ribonucleotide reductase (RNR).** Louis Noodleman, Wen-Ge Han, Eduardo M. Sproviero and Victor S. Batista.
233rd ACS National Meeting, American Chemical Society, Chicago, IL, March 25-29, 2007.
- **DFT-QM/MM Models of the oxygen-evolving complex of photosystem II and characterization of synthetic oxomanganese complexes.** Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig, and Victor S. Batista.
232nd ACS National Meeting, American Chemical Society, San Francisco, CA, September 10-14, 2006.
- **DFT-QM/MM Study of the Mechanism of Photosynthetic Water Splitting.** Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig, and Victor S. Batista.
Gordon Research Conference in Photosynthesis, Bryant University, Smithfield, RI, July 2-7, 2006.
- **QM/MM model of the O₂-evolving complex of photosystem II.** Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig, and Victor S. Batista.
231st ACS National Meeting, American Chemical Society, Atlanta, GA, March 26-30, 2006.
- **Density functional theory and DFT+U study of transition metal porphine adsorbed on Au(111) surfaces and effects of applied electric fields.** Kevin Leung, Susan B. Rempe, Peter A. Schultz, Eduardo M. Sproviero, Victor S. Batista, Michael E. Chandross, and Craig J. Medforth.
231st ACS National Meeting, American Chemical Society, Atlanta, GA, March 26-30, 2006.
- **Green chemistry based on TiO₂ functionalized with oxo-manganese catalysts.** Sabas G. Abuabara, Clyde W. Cady, Jim M. Schleicher, Jason Baxter, Eduardo M. Sproviero, Gary W. Brudvig, Robert H. Crabtree, Charles A. Schmuttenmaer, and Victor S. Batista.
231st ACS National Meeting, American Chemical Society, Atlanta, GA, March 26-30, 2006.
- **QM/MM Structural Model of the Oxygen Evolving Complex in Photosystem II.** Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig, Victor S. Batista.
50th Biophysical Society Annual Meeting, Salt Lake City, UT, February 18-22, 2006.
- **Density functional theory study of transition metal porphyrins deposited on a gold substrate.** Kevin Leung, Peter A. Schultz, Michael E. Chandross, Eduardo M. Sproviero, Victor S. Batista.
230th ACS National Meeting, American Chemical Society, Washington, DC, August 28-September 1, 2005.
- **Computational Structural Studies of the Oxygen-Evolving Complex of Photosystem II.** James P. McEvoy, Eduardo M. Sproviero, Jose A. Gascon, Victor S. Batista, and Gary W. Brudvig.

International Conference on Biological Inorganic Chemistry, Ann Arbor, MI, July 31st to August 5th, 2005.

- **Structural and Electronic Properties of the Oxygen Evolving Complex in Photosystem II: QM/MM Study of the Complete Ligation by Protein, Water and Chloride.** Eduardo M. Sproviero, Jose A. Gascon, Victor S. Batista.
Quantum Chemistry Applied: From H₃ to Biocatalysis. An international conference to celebrate the 60th birthday of Prof. Per E.M. Siegbahn, 18 - 22 June, 2005.
- **Structural and electronic properties of the oxygen evolving complex in photosystem II: QM/MM study of the complete ligation by protein, water and chloride.** Eduardo M. Sproviero, Jose A. Gascon, James P. McEvoy, Gary W. Brudvig, and Victor S. Batista.
229th ACS National Meeting, American Chemical Society, San Diego, CA, March 13-17, 2005.
- **NBO Analysis of NMR Chemical Shifts in Rhodopsin using QM/MM Hybrid Methods.** Eduardo M. Sproviero, Jose A. Gascon, Victor S. Batista.
49th Biophysical Society Annual Meeting, Long Beach, CA, February 12-16, 2005.
- **Ozone-water clusters: NBO analysis of stereoelectronic interactions.** Eduardo M. Sproviero, Devon M. M. Philip, Sergio D. Dalosto, and Victor S. Batista.
227th ACS National Meeting, American Chemical Society, Anaheim, CA, March 28-April 1, 2004.
- **Study of substituents effects by means of electronic delocalizations. Its relation with Hammett parameters.** Eduardo M. Sproviero and Gerardo Burton
XIV Argentine Symposium of Organic Chemistry, Argentine Research Society in Organic Chemistry (SAIQO), Rosario, Argentine, November 9-12, 2003.
- **Decomposition of molecular properties in terms of interactions between NBO orbitals.** Eduardo M. Sproviero and Gerardo Burton
88^a Argentine Symposium of Physics, Argentine Physical Society (AFA). September 22-25, 2003. San Carlos de Bariloche. Argentine.
- **How interactions between orbitals contribute to molecular properties.** Eduardo M. Sproviero, Rubén H. Contreras and Gerardo Burton.
College on Biophysics: From Molecular Genetics to Structural Biology, Abdus Salam International Centre for Theoretical Physics, Miramare Trieste, Italy, October 1-12, 2001.
- **Electronic delocalizations in substituted uracils. Their relation with ¹⁷O chemical shifts and other related properties.** Eduardo M. Sproviero, Rubén H. Contreras and Gerardo Burton.

- XII Argentine Symposium of Physical Chemistry and Inorganic Chemistry. Argentine Research Society in Physical Chemistry, San Martín de Los Andes, Neuquén, Argentine, April 23-27, 2001.
- **Stereoelectronic contributions to ^1H - ^1H coupling constants.** Eduardo M. Sproviero, Rubén H. Contreras and Gerardo Burton.
XII Argentine Symposium of Organic Chemistry "Dr. Eduardo Guerreiro", Argentine Research Society in Organic Chemistry (SAIQO), Los Cocos, Córdoba, Argentine, November 14-17, 1999.
 - **^{17}O Nuclear magnetic shieldings and electronic delocalizations. Theoretical study of their angular dependence in carbonyls.** Eduardo M. Sproviero, Gerardo Burton and Rubén H. Contreras.
83° Argentine Symposium of Physics, Argentine Physical Society (AFA), September 21-25, 1998.
 - **Stereoelectronic interaction contributions to four bond coupling constants.** Eduardo M. Sproviero, Rubén H. Contreras and Gerardo Burton.
XI Argentine Symposium of Organic Chemistry, Argentine Research Society in Organic Chemistry (SAIQO), Villa Giardino, Córdoba, November 16-19, 1997.
 - **Intramolecular interactions that affect the Karplus curve.** Eduardo M. Sproviero, Gerardo Burton, Claudia G. Giribet, Rubén H. Contreras and Nélica M. Peruchena.
82° Argentine Symposium of Physics, Argentine Physical Society (AFA), Complejo Ferial San Luis, San Luis, September 21-26, 1997.
 - **Structural analysis, intramolecular flexibility analysis, and electronic topology of organic compounds.** Eduardo M. Sproviero and Gerardo Burton.
Meeting of Grant's Honorees from University of Buenos Aires, September 23-25, 1997, Escuela Superior de Comercio "Carlos Pellegrini", UBA.
 - **Topological analysis of stereoelectronic interactions.** Eduardo M. Sproviero, Gerardo Burton and Rubén H. Contreras.
Structural and Mechanistic Organic Chemistry, University of Georgia, Athens, Georgia, United States, June 3-7, 1997.
 - **Topological study of intramolecular interactions that involve virtual orbitals.** Eduardo M. Sproviero, Gerardo Burton and Rubén H. Contreras.
81° Argentine Symposium of Physics, Argentine Physical Society (AFA), Tandil, Buenos Aires, September 16-20, 1996.
 - **Theoretical and experimental studies of the molecular flexibility of steroidal hormones and synthetic analogues.** Eduardo M. Sproviero and Gerardo Burton.

Meeting of Grant's Honorees from University of Buenos Aires, November 28 to December 1, 1995, Facultad de Derecho, UBA.

- **Partition of molecular properties into atomic contributions within the Green function formalism.** Eduardo M. Sproviero and Gerardo Burton.
80° Argentine Symposium of Physics, Argentine Physical Society (AFA), San Carlos de Bariloche, Río Negro, October 2-6, 1995.
- **RPA-AM1 theoretical calculation of ${}^2J(\text{Sn-Sn})$ couplings: several factors that affect them.** E. Botek, S. Gomez, E. Sproviero. 80° Argentine Symposium of Physics, Argentine Physical Society (AFA), San Carlos de Bariloche, Río Negro, October 2-6, 1995.
- **Conformational interconversion of Δ^4 -3-cetosteroids. Calculation of the intrinsic reaction coordinate.** Eduardo M. Sproviero and Gerardo Burton.
X Argentine Symposium of Organic Chemistry, Argentine Research Society in Organic Chemistry (SAIQO), Los Cocos, Córdoba, Argentine, November 12-15, 1995.
- **Atomic Polar Tensors in the polarization propagator Approach. Applications to atomic properties.** Eduardo M. Sproviero and Gerardo Burton.
XX Argentine Symposium of Chemistry. Argentine Chemistry Association. Córdoba, Argentine, November 14 to 18, 1994.
- **Theoretical and Experimental Study about flexibility of steroid hormones and synthetic analogues.** Eduardo M. Sproviero and Gerardo Burton.
Meeting of Grant's Honorees from University of Buenos Aires, October 4-7, 1994.
- 1) **Intramolecular flexibility parameters in the model free approach.** Eduardo M. Sproviero and Gerardo Burton.
2) **Modified pregnanes conformations analyzed by 2D-NMR and semiempirical methods.** Andrés Ferrara, Eduardo M. Sproviero and Gerardo Burton.
IX Argentine Symposium of Organic Chemistry, Argentine Research Society in Organic Chemistry.
- **Theoretical and Experimental Study of the flexibility of steroid hormones and synthetic analogues.** Eduardo M. Sproviero and Gerardo Burton.
Meeting of Grant's Honorees from University de Buenos Aires, October 4-7, 1993.
- **Harmonic analysis of internal flexibility in Steroid hormone analogues.** Eduardo M. Sproviero and Gerardo Burton.
VIII Argentine Symposium of Physical Chemistry.
- **Theoretical Study about deformation energies and flexibility of the steroid nucleus in hormones with corticoid action.** Eduardo M. Sproviero and Gerardo Burton.
Meeting of Grant's Honorees from University of Buenos Aires, October 26-28, 1992.

- **Theoretical and computational analysis of internal mobility in steroid hormone analogues.** Eduardo M. Sproviero y Gerardo Burton.
Third academic and technological meeting, IBM of Argentine. University of La Plata, La Plata, Buenos Aires, September 23-25, 1992. This work was nominee among the ten better works in the event.
- **Theoretical Study of deformation energies and flexibility of the steroid nucleus in hormones with corticoid action.** Eduardo M. Sproviero and Gerardo Burton.
Meeting of Grant's Honorees from University of Buenos Aires, October 28-30, 1991.
- **Theoretical study of conformational flexibility in steroidal hormone analogues.** Eduardo M. Sproviero and Gerardo Burton.
VIII Argentine Symposium of Organic Chemistry, Argentine Research Society in Organic Chemistry (SAIQO). Huerta Grande, Córdoba, Argentine, November 6-8, 1991.

. Professional Activities

- System manager of the computational network of the Organic Chemistry Department, FCEN, UBA, since September 1999 until December 2003.

. Refereeing

- Journal: *Anales de la Asociación Química Argentina*.

. Membership in Professional Societies

- Argentine Physical Society (AFA).
- Argentine Research Society in Organic Chemistry (SAIQO).
- American Chemical Society (ACS).
- Biophysical Society.

. Languages

- English: Reading, writing and conversation.
- French: Reading.