

## **Curriculum Vitae Dr. Carmelo García**

UPR-CUH-Chemistry

100 Road 908

Humacao, Puerto Rico 00791-4300

Phone (787) 850-0000, ext. 9054

Fax (787) 850-9422

E-mail [C\\_GARCIA@CUHAC.UPR.CLU.EDU](mailto:C_GARCIA@CUHAC.UPR.CLU.EDU)

Doctor Degree Carl Schrolemmmer Hochschule, Germany (1982)

Doctoral Thesis "Photochemical Reactions of Model-Compounds of Epoxy-Resins"  
(Advisor: Prof. Dr. H.-J. Timpe)

Post Doctoral

1982-1984 Post-doctoral Research on Quantum-Chemical Calculations on the butadiene photochemical reaction at the FU-Berlin, West Germany (Under supervision of V. Bonaci? -Kouteck? ) Photochemistry, Quantum Chemistry and Laser Photomedicine

1990-1992 Sabbatical Leave at Harvard Medical School, Research on photomedicine (under the supervision of Dr. Irene E. Kochevar) and Visiting Associate Professor at the Harvard Medical School (Boston, MA)

1990-... Visiting Chemist at Massachusetts General Hospital (Boston, MA)

## **Honors**

1972-1977 Honor registration at the University of Puerto Rico

1973 HUC medal in Chemistry and Physics

1973-1974 "Who is Who" - Certification

1974 Magna Cum Laude (Assoc. Degree - Natural Sciences)

1976 Magna Cum Laude (B.S. Chemistry)

1982 Magna Cum Laude (Ph.D. Physical Chemistry)

1987 UPR Recognition for Academic Excellence and Productivity

1999 UPR Recognition for Academic Excellence and Productivity

## **Research Interests**

Antipsychotic or neuroleptic drugs are used primarily for the treatment of schizophrenia, but also have applications in mania, anxiety, dementia and drug abuse. The major used neuroleptics belong to the general tricyclic antidepressants family (phenothiazines, dibenzazepines and dibenzodiazepines). Most of the derivatives of these drugs do also produce serious side effects, including extrapyramidal syndrome (EPS), tardative dyskinesia, parkinsonism, allergy and photosensitization. Small changes in the structure of the derivatives, change the mode of action of the drugs, the potency and the spectrum and severity of the side effects. The molecular photochemical mechanisms for their photosensitizing ability are still unknown, even through they are actually used in the United States to treat thousands and thousands of psychiatric patients annually. Recent studies on the laser flash photolysis of some phenothiazine derivatives showed that the triplet state of chlorinated phenothiazine derivatives can be efficiently quenched by the protons in the solution. The effectiveness of the quenching is

very sensitive to the structure of the drug and seems to correlate with their phototoxicity.

The goal of our project is to measure the photophysical properties of a selected group of tricyclic neuroleptics and to study their short-lived transients, especially the cation radical and the triplet. Basic UV-Vis and luminescence techniques will be employed to study their absorption/emission properties. The transients will be characterized using optical absorption measurements with a Nd-YAG laser set-up. For the triplet state of these compounds, the extinction coefficient and the quantum yield will be determined using a comparative method and the triplet-triplet energy transfer principle, respectively. Combined MM+/PM3/RHF theoretical calculations will be performed with HyperCHEM™ on the whole set of photophysical parameters. The experimental and theoretical values will be correlated with the phototoxicity of the drugs to find out if the triplet transient is directly involved in the phototoxic activity of this drug family. The major goal of this project is to find a molecular/photophysical descriptor for the phototoxic side effect of tricyclic antipsychotics.

### Recent Publications

1. C. García, G. A. Smith, W. G. McGymsey, R. Redmond, I. E. Kochevar (1995); Mechanism and solvent dependence for photoionization of promazine and chlorpromazine; *J. Am. Chem. Soc.* **117(44)**, 10871-10878
2. R. Oyola, R. Arce, A. E. Alegría, C. García (1997); Photophysical properties of gilyocalcins V and M and their binding to calf thymus DNA; *Photochem. Photobiol.* **65**, 802-810
3. I.E. Kochevar, C. García and N. Geacintov (1998); Photoaddition to DNA by Nonintercalated chlorpromazine molecules; *Photochem. Photobiol.* **68** 692-697
4. O. Cox, J. A. Dumas, L. A. Rivera, C. García and A. E. Alegría (1999) Electrochemical and Electron Spin Resonance Studies of Selected Benzazolo[3,2-*a*]quinolinium Salts;; *J. Heteroc. Chem.* **36**, 943-947
5. A. E. Alegría, C. García, G. Santiago, G. Collazo, J. Morant (2000); "Intramolecular hydrogen bonding inhibits semiquinone-Mg<sup>2+</sup> complex formation"; *J. Chem. Perkin Trans. 2*, 1569-1573
6. García, C.; Oyola, R.; Piñero, L. E.; Cruz, N.; Alejandro, F.; Arce, R. and Nieves, I. (2002); Photophysical, Electrochemical and Theoretical study of Protriptyline in several solvents; *J. Phys. Chem. B*; **106(38)**, 9794-9801
7. Arce, R.; García, C.; Oyola R.; Piñero, L.E.; Nieves, I. and Cruz, N. (2003); Photophysical and photochemical properties of amitriptyline and nortriptyline hydrochloride: A 266 nm nanosecond laser flash and theoretical study; *J. Photochem. Photobiol. A: Chem.*; **154**, 245-257