DIPARTIMENTO DI FARMACIA E BIOTECNOLOGIE

Life & Chemical Sciences Seminars

Electrochemistry meets Medicinal Chemistry: Successful Examples

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(Prof.ssa Maria Laura Bolognesi)

Abstract

There is a beneficial interface between electrochemistry and life sciences, useful for the design, development and characterization of redox-selective molecules and their molecular mechanism of action [1,2]. The ever-increasing interest in biologically active quinones has resulted in new strategies to decrease toxicity, modulate activity, and direct the compound to the target. As such, it is pertinent to continue to explore their synthesis, biological activities and redox mechanisms through a combined theoretical and experimental approach.

In the present case, several successful examples of the use of electrochemical techniques in medicinal chemistry is shown, concerning multiple redox-centered hybrid quinones, like pterocarpanequinones [3], chalcogenated [4], halogenated, and fluorescent ones [5], using cyclic voltammetry, spectroelectrochemistry, computational chemistry [6] and electrochemical-based macromolecular interaction studies [7] (Figure 1). Electrochemical studies play, indeed, a beneficial role in biomedicine and as perspectives, more adequate cell models and interaction among areas of research are urgently required. It is time to rationalize the synthesis of quinones and better work the question of selectivity, activity modulation, in situ drug delivery, among other strategies, to have a more realistic and applied action.

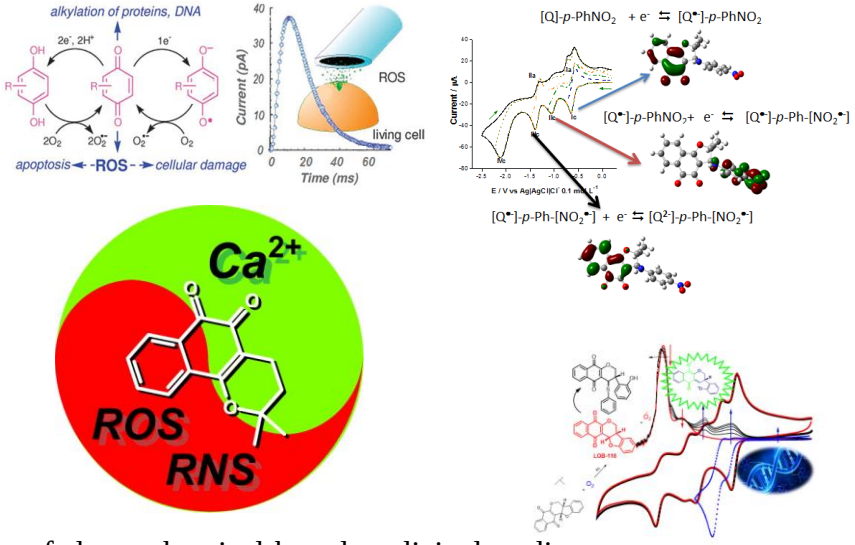

Figure 1**.** Examples of electrochemical-based medicinal studies

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References: [1] Hillard E.A. et al., Chem. Commun. **2008**, 2612-2628; [2] Paiva, Y.G. et al., Curr. Top. Med. Chem. **2015**, 15, 136-162. [3] Silva, T. L. et al. ChemElectroChem. **2016**, 3, 1-13. [4] Jardim et al. **2015**. RSC Advances 5, 78047-78060. [5] Gontijo et al. Chem. Commun **2016,** 52, 13281–13284. [6] ArmendárizVidales et al., J. Org. Chem. **2014**, 79, 5201-5208, [7] De Vasconcellos et al.,J. Electroanal. Chem. **2016**, 765, 168-178.

Biosketch

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H index: 34 (Scopus) >3500 citations; 33 (ISI)

EDUCATION: Pharmacist (1975) Faculty of Pharmacy, Federal University of Minas Gerais (UFMG), Belo Horizonte, MG, Brazil, PhD (13/10/1983): Chemistry Department, Federal University of Minas Gerais, Brazil, under the supervision of Alaíde Braga de Oliveira. Post doctoral 09/1985 – 08/1987: Queen Mary and Westfield College, University of London, with Prof. James Utley. Synthesis and Electrochemistry of quinonemethides and their behavior as pro-bases; 04/1992 –10/1992: Organisch-Chemisches Institüt, Münster, Germany, with Prof. Hans-J. Schäffer. Diastereoselective Kolbe reactions. Visiting professor 10/2004 – 04/2005; 03/2007-04/2007; 09/2008: Ecole Normale Supérieure. Département de Chimie. UMR CNRS 8640 PASTEUR, with Prof. Christian Amatore.

RESEARCH ACTIVITIES
Organic Electrochemistry: investigation of the reduction/oxidation mechanisms of natural products, organic halides, compounds of mixed functionality and several other classes of biologically active compounds (quinones, N-oxides, NO donors, phenols, nitroaromatics, etc), and correlation of thermodynamic and kinetic parameters (E_{redox} and others) with biological activities, helping in the investigation of molecular mechanism of action. Organic electrosynthesis: electrochemical modification of natural products by reduction and oxidation. **Bioelectrochemistry/ Electroanalysis**: DNA biosensors, chemical sensors for quantification and analysis of compounds of biomedical importance. Electron transfer/Oxidative Stress studies: clinical and animal models investigation on diseases based on oxidative stress, quantification of biomarkers of oxidative stress and their relationship with diseases (cardiovascular, diabetes, gastrointestinal ones, metabolic syndrome), amperometric monitoring of oxidative bursts at single cells level, in the presence of quinones. Boron dopped diamond electrodes. **Food Chemistry**: determination of antioxidant and pro-oxidant activities of nutraceuticals and residues from the food industry, development of new methodologies. Carbonylic Stress.

PUBLICATIONS/SUMMARY
Publications: 166; Patents: 4; Book Chapters: 12
Master Science under my supervision: 29 + 4 in co-supervision; under way: 04
PhD under my supervision: 30 + 5 in co-supervision); under way: 10
Post-doctoral supervision: 08; under way: 02
Awards: 12
AWARDS & HONORS:

- **1984. "YOUNG SCIENTIST AWARD"** – National Brazilian Award. First place. Category: graduate - CNPq, Fundação Roberto Marinho, Grupo Ultra.
- **1997. "FOREIGN YOUNG CHEMIST AWARD"** - International Symposium-Electroorganic Synthesis'97, Kurashiki, Japan - IS-EOS'97, September 1997.
- **2011. National Award Marie Curie.** Distinguished Women on Chemistry. Sociedade Brasileira de Química (Brazilian Society of Chemistry)
- **2012. Jabuti Award** "**Química Medicinal: Novas Estratégias em Planejamento Racional de Fármacos, 2010,** p. 186-229**. EDUSP.** ISBN: 9788531412660
- **2013. XIX SIBEE Honoured Professor** (Simpósio Brasileira de Eletroquímica e Eletroanalítica, Brazilian Symposium on Electrochemistry and Electroanalysis)

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