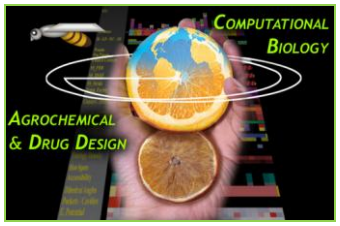

ELECTRONIC STRUCTURE AND ANTIOXIDANT ACTIVITY OF ISOCOUMARINS

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Isocoumarins are natural polyphenols that can be found in a variety of plant species and present antioxidant properties. Paepalantine, a naturally occurring isocoumarin first isolated from the Brazilian plant *Paepalanthus bromelioides*, has been previously pointed to have several functions, as inhibition of serine and cysteineproteases, antimicrobial and anti-inflammatory activities, some of them related to its antioxidant activity.

Our study focuses on paepalantine, its glycosylated forms paepalantine 9-*O*-β-D-glucopyranoside and paepalantine 9-*O*-β-D-allopyranosyl(1->6) glucopyranoside, 8,8-paepalantine dimer, vioxanthin; and also on two paepalantine semi-synthetic analogues of paepalantine, 9,10-acylated compound and 9-OH-10-methylated compound. Our aim is to establish a relation between their chemical structures and their properties, correlationing the structural differences between all these analogues to alterations on antioxidant activity.

For this purpose, we will design and submit these compounds to high-level quantum calculations based on Density Functional Theory (DFT) in different pH ranges, in order to propose mechanisms for their antioxidant activity, and to PM6 semiempirical calculations in order to determine their pK_a. We intend to analyze electronic affinity, ionization potential, bond dissociated energies, stabilization energies and spin density distribution of these molecules. The antioxidant potentials and pK_a values of these analogues will also be experimentally determined for comparison and validation purposes, using DPPH method and titration.

Our preliminary PM6 results showed that the pK_a value for paepalantine is close to physiological pH; and the anionic forms of paepalantine, its dimer and vioxanthin have lower heat of formation than their respective neutral forms. Their higher stability indicates that the anionic forms of these compounds may have a more important role on the antioxidant activity than the neutral molecules. Further calculations are being performed.

Keywords: isocoumarins, antioxidant activity, DFT calculations.