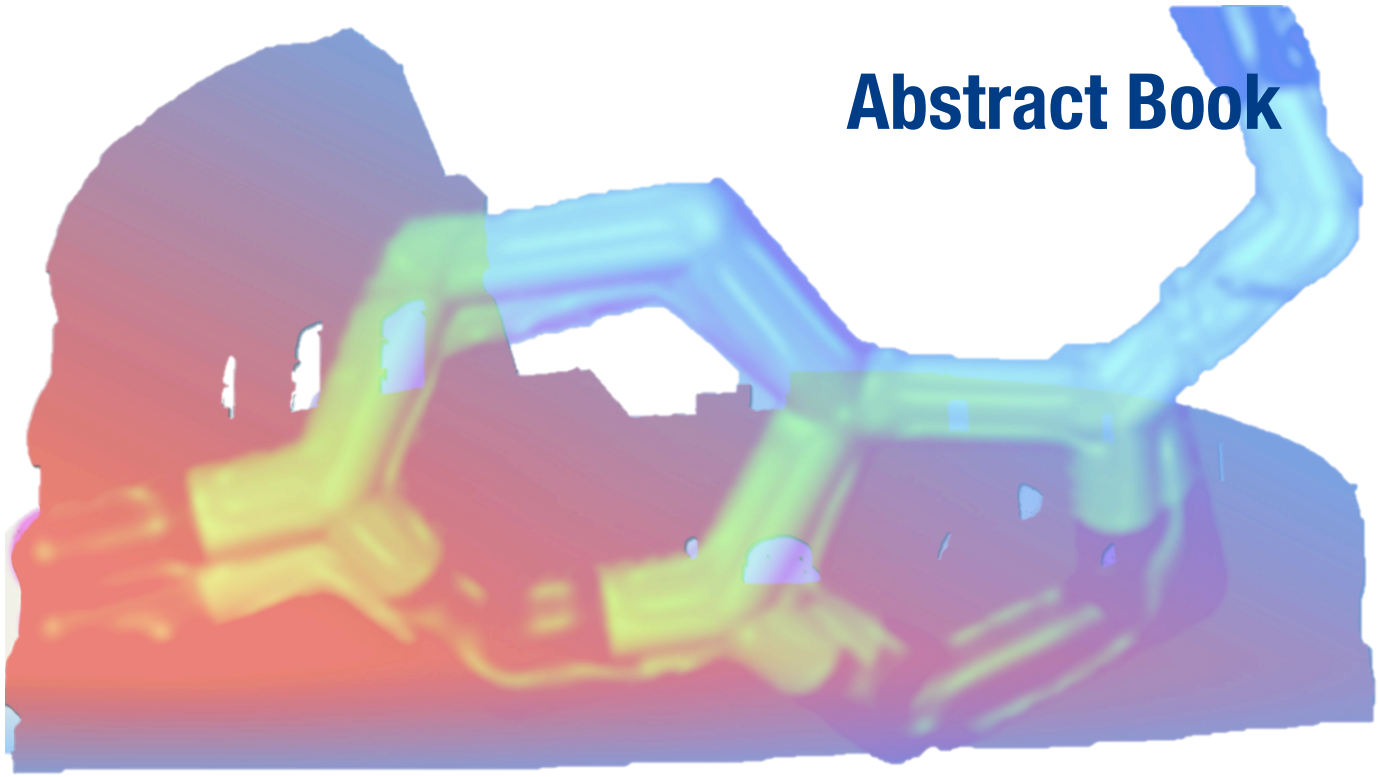
Italian Chemical Society
Division of Medicinal Chemistry

European Federation
for Medicinal Chemistry

NMMC Roma 2013

# XXII National Meeting on Medicinal Chemistry

**September 10-13, Roma - Italy**



## Abstract Book

**Under the Patronage of**

SAPIENZA
UNIVERSITÀ DI ROMA

ISTITUTO PASTEUR
FONDAZ. CENCI BOLOGNETTI

DIPARTIMENTO DI CHIMICA
E TECNOLOGIE DEL FARMACO

REGIONE LAZIO

PROVINCIA
DI ROMA

w3.uniroma1.it/nmmc2013

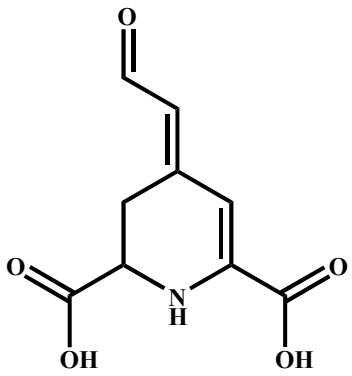
# THEORETICAL DETERMINATION OF THE $pK_a$s OF BETALAMIC ACID RELATED TO THE FREE-RADICAL SCAVENGER CAPACITY: COMPARISON BETWEEN SEMI-EMPIRICAL AND *AB INITIO* METHODS

Anna Maria Almerico,* Marco Tutone, Antonino Lauria

*Dipartimento di Scienze e Tecnologie Biologiche Chimiche e Farmaceutiche (STEBICEF) Università di Palermo, Via Archirafi 32, 90123 Palermo, Italy*

annamaria.almerico@unipa.it

Health benefits of dietary phytochemicals have been suggested in recent years. Among thousands of different compounds, Betalains, which occur in a number of vegetables of the *Cariophyllalae* order with cactus pear fruits and red beet as the principal dietary sources, have been considered because of reducing power and potential to affect redox-modulated cellular processes[1-3]. The antioxidant power of Betalains is strictly due to the dissociation rate of the acidic moieties present in all the molecules of this family of phytochemicals. Experimentally, only the $pK_a$s of Betanin have been determined, and recently, it was evidenced as the acid dissociation, at different environmental pHs, affects on its electron donating capacity, and further on its free-radical scavenging power[4]. The same correlation was studied on another betalain family compound, Betalamic Acid, but no $pK_a$s values were experimentally measured [5].




With the aim to justify its behaviour as free-radical scavenger, we calculated *in silico* the $pK_a$s of Betalamic Acid by means different approaches. Starting from the known experimental $pK_a$s of a number of acid compounds, both phytochemicals and small organic, we compared two semi-empirical approaches and DFT calculation to give a realistic prediction of the $pK_a$s of Betalamic Acid. Obtained results by means these computational approaches are concordant with the experimental results of Gandia-Herrero[5] who showed that the free-radical scavenging capacity drastically decrease at pH>5 in stable solution of the free radical $ABTS^{\circ+}$. In fact as showed by us *in silico*, at the experimental pH>5, in solution, the dianionic species is predominant exploiting the high electron donating capability (HOMO energy) to decrease the concentration of the colorant. Therefore the computational calculated $pK_a$s values of Betalamic Acid resulted very reliable

**References**

1) Scalbert, A. *et al*. *Am*. *J*. *Clin*. *Nutr*. **2005**, 81, 215S-217S.
2) Raederstorff, D. *Int*. *J*. *Vitam*. *Nutr*. *Res*. **2009**, 79, 152-165.
3) Herr, I. *et al*. *Cancer Treat*. *Rev*. **2010**, 36, 377-383.
4) Glyszczynska, A. *et al*. *Food Add*. *& Contam*. **2006**, 23, 1079-1087.
5) Gandìa-Herrero, F. *et al*. *J*. *Nat*. *Prod*. **2012**, 75, 1030-1036.