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Data article

Influence of piperidine ring on stability and reactivity of piperine

Christiane P.O. Aguiar[a], Dielly C.F. Lopes[b], Rosivaldo S. Borges[a,*]

[a] Núcleo de Estudos e Seleção de Moléculas Bioativas, Instituto de Ciências da Saúde, Universidade Federal do Pará, 66075-110 Belém, PA, Brazil

[b] Laboratório de Neuropatologia Experimental, Hospital Universitário João de Barros Barreto, Universidade Federal do Pará, Belém, PA, Brazil

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ABSTRACT

The influence of piperidine ring on chemical reactivity and stability of piperine (PPN) was elucidated using quantum chemistry calculations with Density Functional Theory at DFT/B3LYP/6-31G(d,p) level of theory. Conformational analysis and electronic properties for PPN were compared to piperic acid (PPA). Piperidine ring has displayed great influence on steric-electronic properties of PPN, especially among aromatic ring, carbonyl moiety and alkenes system, respectively. All s-trans conformers showed higher stability when compared to s-cis conformers. The lower Gap^{L-H} for PPA showed that it is more reactive than PPN, providing that PPN is more nucleophilic than PPA and PPA is more electrophilic than PPN. In conclusion, piperidine ring is related to the chemical stability of PPN, through steric and electronic properties.

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Specifications table

Subject area	*Bioorganic chemistry*
Compounds	*Piperine*
Data category	*Theoretical data*
Data acquisition format	*Theoretical calculation*
Data type	*Analyzed*
Procedure	*A conformational study using molecular modeling for chemical stability and reactivity of the piperine and related derivative was done. Piperidine ring has great influence on double bond and carbonyl moieties. The strains among these groups are responsible for all chemical properties of piperine.*
Data accessibility	*The data are in this article*

1. Rationale

Piperine (PPN) is the major component of Piper nigrum Linn, belonging to Piperaceae family, popularly known as black pepper [1]. Its several biological effects are known, among them antibacterial, insecticide, antiparasitic, antioxidant, anti-inflammatory, antipyretic, antidiarrheal, digestive, hepatoprotective, anti-spermatogenic, antidepressant, antispasmodic, antimutagenic, antimetastatic, anti-apoptotic, antithyroid, anticonvulsant [2–4]. It also plays a functional and nutraceutical role,

* Corresponding author.
E-mail address: rosborg@ufpa.br (R.S. Borges).

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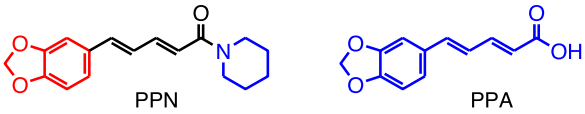

Fig. 1. Chemical structure for all compounds studied here.

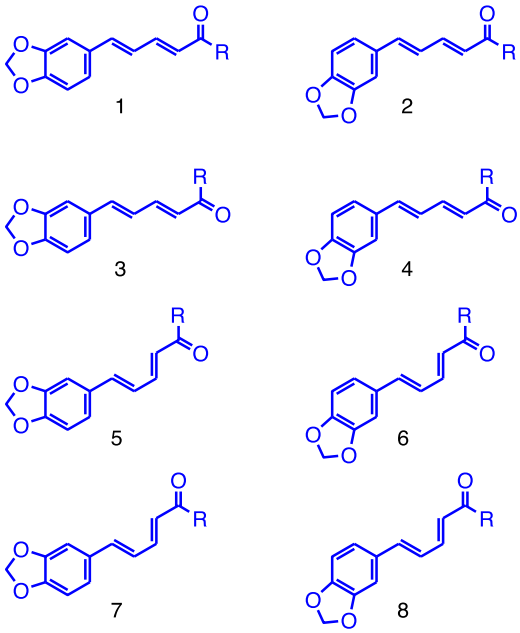

Fig. 2. Preferential structures of low energy.

improving the functionality of organs, preventing pathologies or enhancing the biological action of drugs and other compounds [3,5–7].

Furthermore, PPN is a trans stereoisomeric derivative, also known as (E,E)−1-[5-(1,3-*benzodioxol*-5-*yl*)−1-*oxo*-2,4-*pentyldenyl*]-piperidine [8], and together with its isomer chavicine are responsible for the pungency of P. nigrum L. [9]. PPN structure is composed of three subunits, i.e. a 1,3-benzodioxole group, also called piperonal nucleus (subunit A in red); a butadiene chain (subunit B in black), and; an amide function constituted by a piperidine ring with α-β-unsaturated carbonyl moiety (subunit C in blue) [10]. It is biosynthesized from the reaction between piperidine and piperic acid (PPA) as a piperoyl-CoA [11].

For these reasons, PPN has a great potential for the production of new drugs or for the increase of the bioavailability of drugs already produced by the pharmaceutical industry [2], either for the prevention or treatment of different pathologies. Therefore, the aim of this study was to understand the structural characteristics of PPN and the influence of the piperidine ring on the stability and reactivity of PPN by theoretical calculations, through comparison of its chemical structure with its analogous PPA (Fig. 1).

2. Procedure

The molecular modeling using DFT/B3LYP/6-31G(d,p) method [12–15] was performed to establish the relationship between chemical structure and the possible conformer of low energy. Each conformer was obtained on single point after the most stable structure, followed by optimization [16]. Eight preferential structures (1–8) of low energy were selected for conformational study of both compounds studied here, i.e. PPN and PPA, where R can be piperidine ring or hydroxyl moiety, preferentially as s-trans or s-cis forms, among aromatic ring, carbonyl moiety, and alkenes system, respectively (Fig. 2).

The geometry of all the molecules was calculated by the PM3 semiempirical method [17]. In addition, the geometric optimizations in the structures for eight conformations of piperine (PPN) and piperic acid (PPA) were carried out by using the theory of density functional (DFT) due to the good compromise between the description of the electronic correlation and the computational time [18]. The methods of theoretical studies by computational calculations were performed using Gaussian 09 program. Structural and electronic properties were obtained by highest occupied molecular orbital (HOMO) energy and lowest unoccupied molecular orbital (LUMO) energy as parameters, related to nucleophilicity and electrophilicity, respectively. [19]. In order to analyze the reactivity of the compounds, the HOMO-LUMO $Gap^{L\text{-}H}$ was calculated (Eq. 1)

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