

Área: FIS

Flavonoids (Kaempferol, Quercetin and Myricetin) from *C. ternatea*: Computational (*in silico*) Study of their Potential as Natural Sunscreen Agents

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Highlights

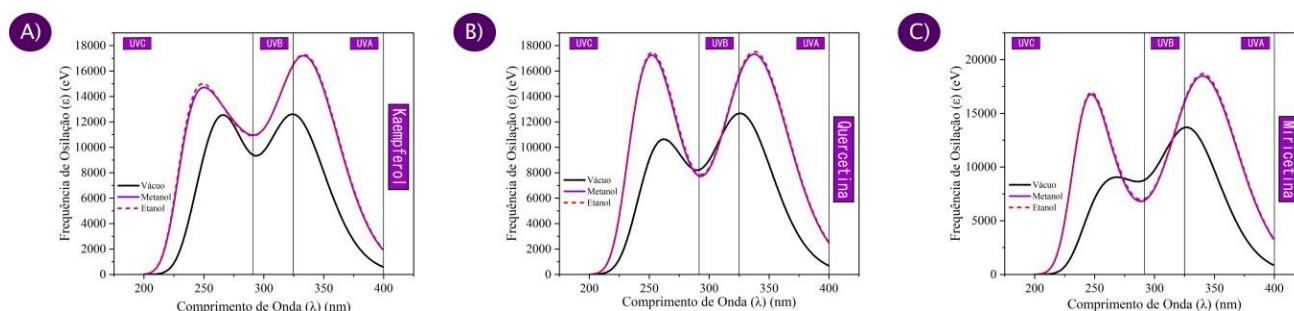
Flavonoids absorb UV radiation and exhibit photoprotective properties.

These natural and biodegradable molecules can be used to enhance synthetic filters in organic sunscreens.

Resumo/Abstract

The greatest diversity of natural products is found in the plant kingdom and is called phytochemicals. These phytochemicals exhibit unique biological properties and, in addition to their function in plants, confer beneficial effects on human health. Industries make extensive use of these molecules, including in the development of pharmaceuticals, sustainable cosmetics, dyes, food additives, and agrochemicals. However, developing new products requires extensive experimental testing (*in vitro/in vivo*), with high costs and long execution times. Therefore, theoretical studies (*in silico*) are gaining prominence, like those performed using Density Functional Theory (DFT) for the evaluation of molecular properties^{1,2}. In this work the DFT and TD-DFT at the level of theory B3LYP/6-31G(d) were applied for the ground and excited states of the flavonoids Kaempferol, Quercetin and Myricetin found in the plant *Clitoria ternatea linn* (Fabaceae family). In the ground state interaction models (PCM) with protic polar solvents (water, ethanol, and 1,2-propanediol) thermochemical parameters demonstrated spontaneous interactions of the molecules with all solvents. To evaluate the photoprotective activity of these molecules, UV absorption spectra were simulated. The spectra showed strong absorption in the UVA and UVC regions, and weak absorption in the UVB region with the typical two absorption bands of flavonoids and λ_{MAX} values closely matching experimental data (methanol/ethanol). Therefore, the application of these three molecules in sunscreen formulations is promising, potentially acting synergistically with synthetic filters to broaden the absorption spectrum and enhance product performance on the skin (SPF).

Figure 1: UV absorption spectra of (a) Kaempferol, (b) Quercetin and (c) Myricetin at gas phase and solvents methanol/ethanol, B3LYP, 6-31G(d), electronic singlet configuration.



Source: The Author.

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