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TOPIC(s): Clean reactions / Biomass conversion

Rapid and Green Synthesis of Bio-Based Organic UV Filters with Antibacterial Activity

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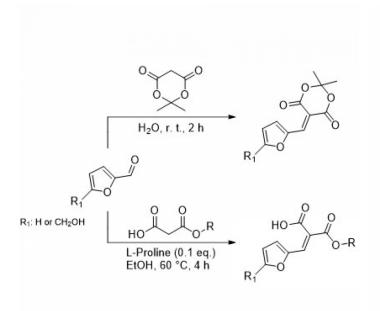
PURPOSE OF THE ABSTRACT

While crucial for life on Earth, significant exposure to solar light can have negative effects on human skin[1]. It has been widely shown that UV-B (290-320 nm) and UV-A (320-400 nm) radiations penetrate most of the skin barriers, leading to the formation of reactive oxygen species (ROS), which in turn, induce oxidative damage such as lipid membrane alteration[2] or DNA mutation[3]. In order to protect oneself against the harmful effect of those radiations, a wide range of sunscreens is available, some of them containing organic filters (i.e., octinoxate or avobenzone) increasingly criticized due to their impact on environment (i.e., coral bleaching, formation of toxic degradation products and endocrine disruption). In response to this problem, some countries have started to ban such organic filters, Hawaii recently issued a bill against the use and sale of sunscreens avobenzone- or octinoxate-containing from January 1st, 2021[4]. Consequently, offering a bio-based alternative, with reduced environmental and public health risks, is essential to protect humans against harmful radiations.

Conjugated and aromatic compounds (i.e., phenolic or furfural derivatives) are known to exhibit the ability to absorb wavelengths in the ultraviolet spectrum (200-400 nm)[5]. Furfural is a renewable bio-based chemical produced from a variety of agricultural byproducts (i.e., wheat bran, oat, corncobs or sawdust), and has a wide range of use, from solvent to aroma[6]. Recently, lignin-derived phenols (p-hydroxybenzaldehydes) were used as starting materials to engineer new organic UV filters with great potential but only partially covering the UV-B region [7]. Replacing phenols by furfural - that offers a hypsochromic shift of absorbance - would lead to a better fit to substitute octinoxate.

In regard to the aforementioned considerations, we synthesized several furfural derivatives via a Knoevenagel condensation, with a set of green conditions to minimize the impact on environment: use of water or ethanol as solvent, L-proline as catalyst, moderate heating and short reaction time. Under such conditions, we were able to synthesize a wide range of furfural derivatives exhibiting both an extended conjugation throughout their backbone and high steric hinderance on the ? position, two factors shown as important parameters in recent studies to obtain anti-UV properties[5]. The investigation of their absorbance properties and their photostability, benchmarked against that of octinoxate, proved them to be suitable as potential sustainable alternatives. Moreover, furfural being known to exhibit antibacterial activities[8], the synthesized compounds were tested against three different strains (i.e., Escherichia coli, Candida albicans and Bacillus subtilis) and benchmarked against phenoxyethanol. Finally, In Silico and In Vitro assays for endrocrine disruption were conducted to determine potential health risks associated to these compounds.

FIGURES



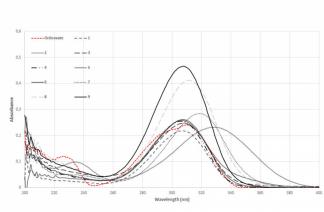


FIGURE 1

Reactions

Knoevenagel reactions for the synthesis of antibacterial UV-B filters.

FIGURE 2

UV-Vis spectra

KEYWORDS

UV Filters | Green chemistry | Antibacterial | Bio-based

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