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TOPIC(s): (Chemo)enzymatic strategies

Chemo-enzymatic Synthesis and Biological Activity Evaluation of Propenylbenzene Derivatives

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PURPOSE OF THE ABSTRACT

Propenylbenzenes, such as isosafrole, anethol, isoeugenol, and their derivatives, are widely found in essential oils from plants such as the aniseed tree, liquorice, and the cananga tree [1]. Compounds of this group are economically important and are used in the flavour and fragrance industries as well as the pharmaceutical and cosmetic industries, and as intermediates in the synthesis of more complex products [2]. Propenylbenzenes have broad biological activities, such as antioxidant, antimicrobial, anti-inflammatory, and antiproliferative. In view of the different biological activities of propenylbenzenes and their widespread use in industry, it is worth looking for derivatives of these compounds [3]. As the interest in compounds obtained via environmentally friendly methods is currently growing, the necessity for the development of new methods for producing propenylbenzene derivatives such as diols and hydroxy ketones has increased in recent years.

The aim of presented study was to develop an efficient process for synthesising oxygenated derivatives of these compounds and evaluate their potential biological activities. In this research, we propose a two-step biocatalytic method. The first step involves the chemo-enzymatic synthesis of corresponding diols 1b–5b from propenylbenzenes 1a–5a via enzymatic epoxidation followed by epoxide hydrolysis (Figure 1.). The second step involves the microbial oxidation of a diasteroisomeric mixture of diols 1b–5b to yield the corresponding hydroxy ketones 1c–4c, which in this study was carried out on a preparative scale using Dietzia sp. DSM44016, Rhodococcus erythropolis DSM44534, R. erythropolis PCM2150, and Rhodococcus ruber PCM2166. The propenylbenzene derivatives thus obtained and the starting compounds were tested for various biological activities, including antimicrobial, antioxidant, haemolytic, and anticancer activities, and their impact on membrane fluidity. The results indicate the potential utility of these compounds as fungistatics, antioxidants, and proliferation



inhibitors of selected cell lines.

FIGURES

FIGURE 1

Figure 1. Two-step synthesis of propenylbenzene derivatives: diols 1b?5b and hydroxy ketones 1c?4c.

1. aq. H2O2, Novozym 435, EtOAc, 30 ?C, 18 h, KOH, MeOH; 2. PCM medium, 23 ?C, 3?11 days.

KEYWORDS

Biotransformation | fragrances | oxidation | biological activity

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FIGURE 2

[3] F. Bruna, Arabian Journal of Chemistry, 2022, 15, 104271.