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Functionalization of eugenol as strategy to amplify the chemical space: sustainable synthesis of new thioureas and 2-aminobenzoxazoles Synthesis of thioureas and 2-aminobenzoxazoles derived from eugenol

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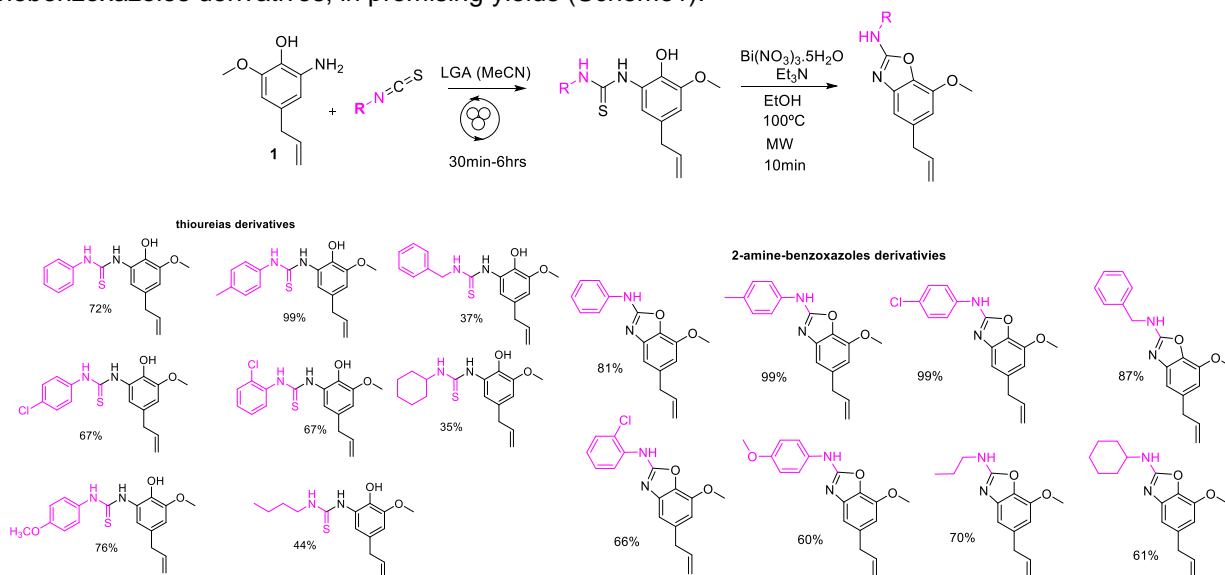
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ABSTRACT

Eugenol is a natural phenylpropenoid obtained mainly from cloves¹. It is widely used for diverse applications due to its anesthetic, cytotoxic, antifungal, and anticancer potential. Benzoxazoles are a class of heterocycles that has shown extensive chemotherapeutic activity², among these derivatives are the N-substituted benzo[d]oxazol-2-amines (2-aminobenzoxazoles) which broad pharmaceutical applications are of great importance³. An efficient and widespread method to obtain 2-aminobenzoxazoles would be a treatment of 2-aminophenols with isothiocyanates to synthesize the derivative thioureas, which subsequently undergo cyclodesulfurization with the assistance of diverse desulfurizing agents⁴. Strategies that lead expansion chemical space of natural product-based compounds is important to enable new drug discovery⁵. In this work 6-aminoeugenol (1) was obtained after a study to modify the aromatic ring of eugenol⁶, and sustainable methods as mechanochemistry and microwave were applied in view to reach thioureas and 2-aminobenzoxazoles derivatives, in promising yields (Scheme1).



Scheme 1. Synthesis of thioureas and 2-aminobenzoxazoles derived from eugenol.

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CNPQ, FAPESB, InCT energia e Ambiente, CAPES.

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