

Área: ORG

## Dihydropyrimidinone–Chalcone Molecular Hybrids: Design, Synthesis, and Characterization

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Palavras Chave: Chalcones; DHPMs; Biginelli reaction; molecular hybridization; Michael acceptor.

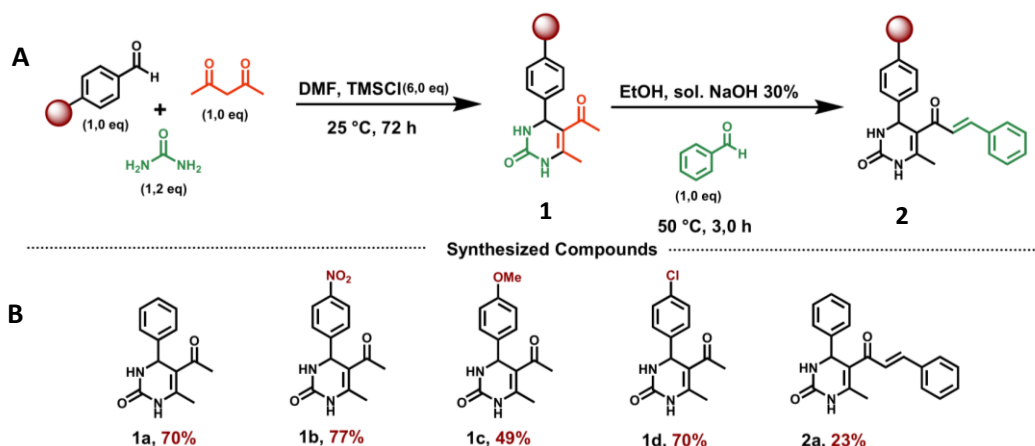
### Highlights

Molecular hybridization of chalcone and DHPM scaffolds affords novel candidates for biological evaluation

### Abstract

Chalcones, simple aromatic  $\alpha,\beta$ -unsaturated enones broadly found in plants, are classic Michael acceptors and display diverse biological activities across multiple molecular targets [1]. Dihydropyrimidinones (DHPMs), typically accessed via the Biginelli one-pot multicomponent condensation (aldehyde, 1,3-dicarbonyl compound, urea), likewise exhibit a wide pharmacological profile, acting through ion-channel modulation, enzyme inhibition, receptor engagement, and signaling-pathway blockade, with reported anti-inflammatory, antitumor, and anti-HIV relevance [2].

Motivated by these complementary properties, our work adopts a molecular-hybridization strategy to fuse the chalcone and DHPM pharmacophores and probe potential synergistic bioactivity [3]. We are synthesizing chalcone motifs appended to distinct DHPM cores (Scheme 1-A). To date, four DHPMs (1a–1d) and one DHPM–chalcone hybrid have been obtained (Scheme 1-B). All compounds were characterized by 1D/2D NMR and GC–MS, or by HPLC for thermolabile samples. In the next steps, we intend to optimize yields, synthesize new hybrids from DHPMs (1a-1d) and forward DHPM-Chalcones for biological tests in partnership with UFPR.



**Scheme 1.** Biginelli synthesis of DHPM cores and subsequent construction of a DHPM–chalcone hybrid.

[1] DHALI WAL, Jagjit Singh et al. *Molecules*, v. 27, n. 20, p. 7062, 2022.

[2] SARVAIYA, Bhavesh H. et al. *Journal of Heterocyclic Chemistry*, v. 61, n. 8, p. 1325-1348, 2024.

[3] GONTIJO, Vanessa S. et al. *Current neuropharmacology*, v. 18, n. 5, p. 348-407, 2020.

### Acknowledgments



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