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MEDICINAL CHEMISTRY RESEARCH

ORIGINAL RESEARCH

Novel 2-aminopyrimidine Schiff bases as possible GABA-AT inhibitors: molecular docking, MAOS, and pharmacological screening

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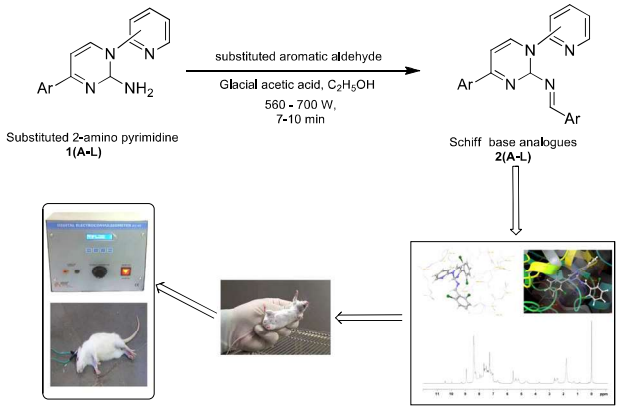
Abstract

The study aimed to design and synthesize novel 2-aminopyrimidine Schiff bases through a green chemistry approach. The compounds **2(A-L)** were synthesized through a single step reaction by reacting 2-aminopyrimidines **1(A-L)** with suitably substituted aromatic aldehydes. The synthesized compounds were characterized by physiochemical methods and spectral techniques. The compounds were tested for anticonvulsant activity using two murine models, the maximal electroshock seizure and Chemical induced seizure model. All the compounds exhibited good to moderate activity. The compounds **2C**, **2G** and **2K** were the most potent ones in the series. The molecular docking data was found to be in sync with the in-vivo experimental results. The study concludes that the compounds may act by inhibiting the enzyme, GABA-AT responsible for degradation of GABA, an inhibitory neurotransmitter. The in-silico ADMET predictions suggest the compounds to be effective and safe. The study, therefore, proposes new compounds as promising anti-convulsion agents, with a better drug profile.

Graphical abstract



Keywords Acetyl pyridine · 2-aminopyrimidine · Molecular docking · In-silico ADMET · Anticonvulsant activity · In-vivo

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