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A One-pot Rapid Synthesis, Docking Study and Biological Evaluation of Some Tetrahydropyrimidine-5-carboxylates

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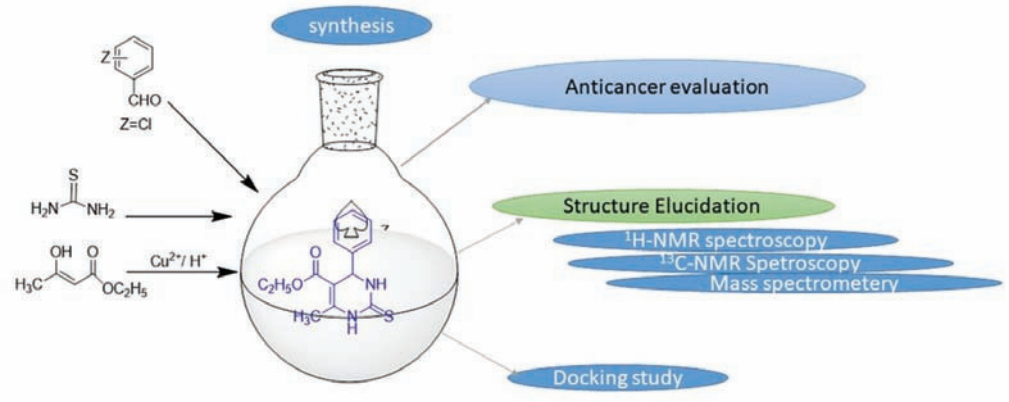
ABSTRACT Three tetrahydropyrimidine derivatives, namely, ethyl 6-methyl-2-thioxo-4-phenyl-1,3,4-tetrahydropyrimidine-5-carboxylate (**17a**), ethyl 4-(3-chlorophenyl)-6-methyl-2-thioxo-4-phenyl-1,3,4-tetrahydropyrimidine-5-carboxylate (**17b**), and ethyl 4-(4-chlorophenyl)-6-methyl-2-thioxo-4-phenyl-1,3,4-tetrahydropyrimidine-5-carboxylate (**17c**) were prepared through one-pot multicomponent and environment-friendly modified Biginelli condensation reaction among thiourea, substituted benzaldehydes, and ethyl acetoacetate in the presence of cupric chloride as a cheap catalyst. The synthesized compounds were analyzed by ^{1}H NMR, ^{13}C NMR, and mass spectral data. Furthermore, these compounds (**17a-c**) were screened for antifungal and anticancer activity against human HepG2 liver cell lines. Biological evaluation revealed that all three analogs showed no antifungal activity against (*Aspergillus niger* and *Colletotrichum gloeosporioides*) fungal strains while 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assays to **17a-c** showed excellent anticancer activity against HepG2 cancer cell lines. All the synthesized compounds (**17a-c**) were studied to measure the interactions by docking study.



KEYWORDS Grindstone, Human HepG2 liver cell Lines, Mass spectrometry, 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assays, Nuclear magnetic resonance analysis, Pyrimidine derivatives.