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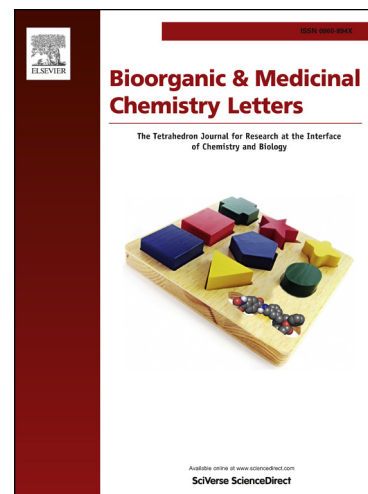
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# Synthesis, Biological activity evaluation and Molecular Docking studies of novel Coumarin substituted thiazolyl-3-aryl-pyrazole-4-carbaldehydes

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## ABSTRACT

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A novel series of coumarin substituted thiazolyl-3-aryl-pyrazole-4-carbaldehydes (**4a-o**) were synthesized via an efficient, one-pot multicomponent approach involving 3-(2-bromoacetyl)coumarins (**1a-g**), thiosemicarbazide (**2**) and substituted acetophenones (**3a-c**) utilizing Vielsmeier-Haack reaction condition with good yields. The title compounds structure was elucidated by spectroscopic data (IR, NMR and Mass) and elemental analysis. All the synthesized compounds were screened for their in vitro cytotoxic activity against MCF-7, DU-145 and Hela cell lines and studied detailed about molecular interaction of probable target protein human microsomal cytochrome CYP450 2A6 using docking simulation. These coumarin derivatives were exhibiting moderate to appreciable cytotoxic activities. The compounds **4m** and **4n** exhibited significant cytotoxic activity with IC<sub>50</sub> values having 5.75 and 6.25  $\mu$ M against Hela cell line. Similarly compound **4n** also exhibiting good anti cancer property and antibacterial activity against DU-145 cell line and gram negative bacterial strains.

According to World Health Organization (WHO), cancer is the second leading cause of death in humans after cardiovascular disease across the globe. Breast cancer and Prostate cancer are among the most notorious cancer types in women and men respectively and a threat for both the developed and developing countries. Numerous cancer therapeutic reports and literature reveal that there is no anticancer agent showing 100% efficacy without side effects. Therefore, across the globe, there is a huge thrust among the researchers to develop

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