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Curcumin derivatives: Anti-inflammatory, analgesic, ulcerogenic, cyclooxygenase-2 inhibition and molecular docking studies

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Curcumin has shown pharmacological properties against different phenotypes of various disease models. Different synthetic routes have been employed to develop its numerous derivatives for diverse and improved therapeutic roles. In present study, we have synthesized curcumin derivatives containing isoxazole, pyrazoles and pyrimidines then the synthesized molecules were evaluated for their anti-inflammatory and antinociceptive activities in experimental animal models. Acute toxicity of synthesized molecules was evaluated in albino mice by oral administration. Any behavioral and neurological changes were observed at dose of 10mg/kg body weight. Additionally, cyclooxygenase-2 (COX-2) enzyme inhibition studies were performed through *in vitro* assays. *In vivo* anti-inflammatory studies showed that curcumin with pyrimidines were most potent anti-inflammatory agents which inhibited induced edema from 74.7-75.9%. Compound 7, 9 and 12 exhibited relatively higher prevention of writhing episodes than any other compound with antinociceptive activity of 73.2, 74.9 and 71.8% respectively. This was better than diclofenac sodium (reference drug, 67.1% inhibition). Similarly, COX-2 *in vitro* inhibition assays results revealed that compound 12 (75.3% inhibition) was the most potent compound. Molecular docking studies of 10, 11 and 12 compounds in human COX-2 binding site revealed the similar binding mode as that of other COX-2 selective inhibitors.

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