Title:	Design and synthesis of sulfur cross-linked 1,3,4-oxadiazole-nitro(furan/thiophene)-propenones as dual inhibitors of inflammation and tuberculosis: molecular docking and Hirshfeld surface analysis
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Abstract:	A series of 3-[5-nitro(furan/thiophene)-2-yl]-1-aryl-3-(5-aryl-1,3,4-oxadiazol-2-ylthio)prop-2-en-1-one derivatives was synthesized and studied with the aim of developing dual inhibitors of multidrug-resistant tuberculosis and inflammation. The in vivo anti-inflammatory activity results showed excellent inhibition of rat paw edema. The methoxybenzene/nitrofuryl derivative of title compounds showed 83% inhibition of inflammation during 2–6 h after carrageenan injection. All compounds showed anti-tuberculosis activity at MIC of 50 µg/cm3. The molecular docking studies revealed that the oxadiazole and nitrofuran groups played a significant role in the inhibiting site of the enzymes COX1, COX2, 5-LOs, and InhA by forming hydrogen bonding with Tyr 385, Ser 530, Tyr 467, and Tyr 158 amino acid residues, respectively. The novel compounds are active antibacterial agents with potential inhibition on E. coli bacteria. The toxicity results showed good percentage viability of human kidney cell lines with IC50 value greater than 100 µg/cm3 concentration. The Hirshfeld surface analysis and electrostatic potential map of compound showed good intermolecular contacts and hydrogen bonding donor and acceptor potential.
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