ملخص باللغة الإنجليزيه

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"تصميم وتشييد ونمذجة مركبات بنزوبيرونيه وفيوروبنزوبيرونيه ذات تأثير ضوئى كيميائى علاجى"
"Design, Synthesis and Molecular Modeling of Benzopyrone and Furobenzopyrone Analogues as Photochemotherapeutic Agents"

Abstract

This thesis concerns with design, synthesis and molecular modeling studies of certain novel benzopyrone and furobenzopyrone analogues as potential photochemotherapeutic agents. Thirtythree new intermediates and forty two final compounds in five sets of furobenzopyrone derivatives were synthesized. All the newly synthesized compounds were subjected to photosensitizing screening on the basis of their monofunctional reactivity with DNA. In addition, molecular modeling studies was performed to find structure activity relationship of the different substituents in the novel synthesized benzopyrone and furobenzopyrone derivatives and the photochemotherapeutic activity. Moreover docking of significant active antimicrobial compounds into DNA gyrase enzyme and pharmacophore search were performed.