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THESIS ABSTRACT

Quinones as synthon for construction of heterocyclic systems with anticipated bioactivity

Alaa E. Hassanien

Chemistry Department, Faculty of Science, Mansoura University, Mansoura, Egypt
Basic Science Department, Higher Future institute of Technology and Engineering, Mansoura, Egypt

Background: Lawsone (2-hydroxynaphthalene-1,4-dione) is a natural product that shows significant biological activity. The National Cancer Institute (NIH, United State) disclosed the lawsone skeleton that contains the quinone moiety as a precursor for clinically cytotoxic activity. **Aim**: Lawsone has interesting pharmacological performance, particularly as antitumor, antimicrobial, anti-parasite (*Trypanosoma cruzi*), and Leishmanicidal activity, anti-lung cancer. **Materials and Methods:** Three different approaches were taken in the synthetic approach. The first approach was based on the synthesis of naphthoquinone annulation that was synthesized from the reaction of 2 with different bi-nucleophilic reagents via Michael addition followed by intramolecular condensation. The second approach was based on the synthesis of new α-lapachone analogs during the cyclo-condensation reaction of 1 with α,β-unsaturated ketones. The third approach was based on the synthesis of novel spiro lawsone-ring skeletons, which focuses on the synthesis of spiro lawsone ring skeletons by Claisen-Schmidt condensation of 1 with some selected advanced reagents. **Results**: Pharmacological studies of the synthetic compounds provided an indication of biological activities, including effects against hepatocellular carcinoma (HePG-7) and mammary gland breast cancer (MCF-7). The molecular structures of some molecules were examined by using DFT calculations. **Conclusion**: The synthetic compounds possess significant anti-tumor capabilities.

Keywords: Alpha Lapachone; Anti-Oxidant; Anti-Tumor; Geometrical optimization; Lawsone

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