Chapter 7
The Importance of Anthraquinone and Its Analogues and Molecular Docking Calculation

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ABSTRACT

In drug-delivery systems containing nano-drug structures, targeting the tumorous tissue by anthraquinone molecules with high biological activity, and reaching and destroying tumors by their tumor-killing effect reveals remarkable results for the treatment of tumors. The various biological activities of anthraquinones and their derivatives depend on molecular conformation; hence, their intra-cell interaction mechanisms including deoxyribonucleic acid (DNA), ribonucleic acid (RNA), enzymes, and hormones. Computer-based drug design plays an important role in the design of drugs and the determination of goals for them. Molecular docking has been widely used in structure-based drug design. The effects of anthraquinone analogues in tumor cells as a result of their interaction with DNA strand has increased the number of studies done on them, and they have been shown to have a wide range of applications in chemistry, medicine, pharmacy, materials, and especially in the field of biomolecules.

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INTRODUCTION

Anthraquinone and its Common Uses

The anthraquinone molecule, which has a synthetically yellow color and has the molecular formula $C_{14}H_8O_2$, is an important organic aromatic compound with a quinone skeleton. These compounds can be obtained naturally from various plants and can also be synthesized in the laboratory environment. Anthraquinone compounds are widely used in dye production and have various applications in textile chemistry. Due to the structure of the main skeleton of the molecule, the electrochemical properties of these dyes ensure that they are resistant to sunlight, and, as a result of this property, they can be safely used for marine transportation and marine vehicles.

Anthraquinones are known to have antifungal (Agarwal et. al., 2000; Manojlovic et. al., 2005; Singh et. al., 2006; Rath et. al., 1995), anti-inflammatory (Cota et. al., 2004; Goel et. al., 1991; Chang et. al., 1996; Choi et. al., 2013), antioxidant (Chen et. al., 2004; Yen et. al., 2000; Zhang et. al., 2005), antibacterial (Demirezer et. al., 2001; Chukwujekwu et. al., 2006; Comini et. al., 2011; Yang et. al., 2012), anticancer (Zhang et. al., 2011; Abu et. al., 2013; Huang et. al., 2007; Fisher et. al., 1990; Perchellet et. al., 2000; Ge et. al., 1997), and antiviral (Lown, 1993; Schinazi et. al., 1990; Barnard et. al., 1992; Ali et. al., 2000; Cohen et. al., 1996) properties. Apart from the synthetically obtained ones, in nature, anthraquinone compounds mostly are found in many different plants, especially in Yellow Centaury and *Aloe vera*. The former, which has an active anthraquinone derivative, is considered to be a natural antidepressant. Yellow Centaury has a therapeutic effect on urinary tract infections, gastritis and ulcer-like stomach ailments, and colds and bronchitis. Moreover, various studies on these active anthraquinone derivatives have reported that the active agents are effective in prostate and breast cancers (Huang et. al., 2010).These active plants from which the anthraquinone groups are obtained by isolation, are used as alternative therapeutic agents in the treatment of ulcers, skin infections, and antidiabetic, antitumor, and immunosuppressive medications. The antioxidant properties of the anthraquinones obtained from the *Cassia* species have a therapeutic effect for many diseases and prevent degradation in food systems. These anthraquinone analogues can be used as cancer therapy drugs in important viral diseases, including polio and acquired immune deficiency syndrome (AIDS) (Dave et. al., 2012). *In vitro* studies were carried out on anthraquinone