

# Binding Energy and Photostability of the $\beta$ -cyclodextrin Encapsulates of Lornoxicam and Tenoxicam drugs: A combined Experimental and Theoretical Study

*Yousra Mohamed Sabry, Eman Youssef, Marwa Tammam, Mohamed Sabry Abdel-Mottaleb*

## Abstract

The lornoxicam (LRX) and tenoxicam (TNX) drugs form a stable 1:1 inclusion complex with  $\beta$ -cyclodextrin ( $\beta$ -CD) in aqueous solution. The experimentally determined association constants ( $K$ ) of LRX- $\beta$ -CD and TNX- $\beta$ -CD are 13.4 and 10.3 M<sup>-1</sup>, respectively. Quantum chemical computations simulated the preferred orientation of guest molecules in the host. Geometry optimized results using the ONIOM technique provided more in-depth insights and identified the structure and showed that both drugs were partially encapsulated within the  $\beta$ -CD cavity. The calculated inclusion binding energy (BE, kcal mol<sup>-1</sup>) reveals the noticeable thermal stability of LRX- $\beta$ -CD (-24.19 kcal/mol) over the TNX- $\beta$ -CD (-13.45 kcal/mol) capsule. Furthermore, the photostabilities of the encapsulated drugs were tested. Drug encapsulation did not result in any additional photostability. Moreover, encapsulation of the drugs in the  $\beta$ -CD resulted in noticeable changes in the electronic characteristics of the drugs, as reflected in their reactivity indices. The fact that the water-soluble  $\beta$ -CD formed inclusion complexes with water-insoluble LRX and TNX enables the drug delivery vehicle for oral administration.

*Egyptian journal of chemistry 2021, January*