Binding Energy and Photostability of the ɓ-cyclodextrin Encapsulates of Lornoxicam and Tenoxicam drugs:A combined Experimental and Theoretical Study

Yousra Mohamed Sabry ,Eman Youssof, Marwa Tammam, Mohamed Sabry Abdel-Mottaleb

Abstract

The lornoxicam (LRX) and tenoxicam (TNX) drugs form a stable 1:1 inclusion complex with ɒ-cyclodextrin (ɓ-CD) in aqueous solution. The experimentally determined association constants (K) of LRX- ɓ-CD and TNX- ɓ-CD are 13.4 and 10.3 M-1, 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 ɓ-CD cavity. The calculated inclusion binding energy (BE, kcal mol-1) reveals the noticeable thermal stability of LRX-ɓ-CD (-24.19 kcal/mol) over the TNX-ɓ-CD (-13.45 kcal/mol) capsulate. 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 ɓ-CD resulted in noticeable changes in the electronic characteristics of the drugs, as reflected in their reactivity indices. The fact that the water-soluble ɓ-CD formed inclusion complexes with water-insoluble LRX and TNX enables the drug delivery vehicle for oral administration.

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