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## Experimental and quantum mechanical studies on the ion-pair of levocetirizine and bromocresol green in aqueous solutions

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### Abstract

In the present work, levocetirizine dihydrochloride (LEV) was found to interact with bromocresol green (BCG) via ion-pair formation. UV-vis and FTIR spectroscopy were used to validate the data obtained from quantum mechanical calculations (QMC). The electrostatic potential maps show that the reaction is preferred through the interaction of the sulfonic acid group of BCG and the quaternary ammonium group of LEV. The optimized geometry of the product shows that there are six different intermolecular hydrogen bonds between the studied molecules resulting from the ionic attraction between the oppositely charged groups. The UV-vis spectra suggest the formation of an ion-pair. This finding is contradicting with the previous charge-transfer hypothesis. (C) 2016 Elsevier B.V. All rights reserved.

### Keywords

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