Applications of molecular modeling methods to host-guest supramolecular chemistry

FakhrEldin O. Suliman

Department of Chemistry, College of Science, Sultan Qaboos University, Al-Khod 123, Oman. Email: fsuliman@squ.edu.om /sulimanfo@gmail.com

Recently, there has been an increase in interest in molecular modeling studies on the formation and stability of inclusion complexes of a variety of molecules and other aspects of supramolecular chemistry. Various theoretical approaches have been applied in these studies such as molecular mechanics, molecular dynamics, semiempirical methods, as well as hybrid techniques such as quantum-mechanics–molecular mechanics (QM–MM) techniques [1-8]. Hartree–Fock (HF) and density functional theory (DFT) calculations especially using the popular B3LYP functional combined with different standard basis set have been used reliably to describe host guest interactions of CDs with several molecules [9–12]. Despite this rapid development and use of *ab initio* and DFT semiempirical methods still attract great deal of attention owing to their less computational demands. The recently introduced semiempirical PM7 and PM6 methods has been found to give accurate estimates of molecular properties comparable to those obtained by HF and DFT methods at even lower computational cost, making them attractive methods for the description of inclusion complexes [13]. Our interest in molecular modeling studies is associated with the investigation of non-covalent interactions especially those affecting chiral separations by supramolcular assemblies. In these studies we aimed at rationalizing and predicting the experimental results obtained using different experimental techniques such as capillary electrophoresis, gas chromatography and liquid chromatography, nuclear magnetic resonance (NMR) spectroscopy, fluorescence and absorption spectroscopy, etc.

The present study represents a tutorial review on our experience with molecular modeling techniques [4, 5, 8, 14-18]. Furthermore, here we presents examples of investigation on spuramolecular systems involving various host molecules such as cyclodextrins,

cucurbit[n]urils, and crown ethers. Theoretical calculations were used to model the mechanism of host-guest interactions and to predict their stabilities through calculation of thermodynamic properties of the respective inclusion complexes. Using molecular dynamic calculations enantiodifferentiation of different chiral mixtures has been investigated. The obtained theoretical results corroborated the experimental findings and in many instances predicted the separation parameters efficiently. We also employed molecular dynamic simulation in aqueous media to further investigate the hydrogen bonding patterns and other intermolecular interactions involved in these complexes in order to understand the mechanisms of separation.

References

(1) S. Chaudhuri, S. Chakraborty, P.K. Sengupta, J. Mol. Struct. 975 (2010) 160.

(2) S. Chakraborty, S. Basu, A. Lahiri, S. Basak, J. Mol. Struct. 977 (2010) 180.

(3) M.-J. Huang, Z. Quan, Y.-M. Liu, Int. J. Quantum Chem. 109 (2009) 81.

(4) A.A. Elbashir, F.E.O. Suliman, B. Saad, H.Y. Aboul-Enein, Talanta 77 (2009) 1388.

(5) A.A. Elbashir, F.E.O. Suliman, B. Saad, H. Aboul-Enein, Biomed. Chromatogr. 24 (2009) 393.

(6) C. Yan, Z. Xiu, X. Li, C. Hao, J. Mol. Graph. Model. 26 (2007) 420.

(7) C. Jullian, V. Brossard, I. Gonzalez, M. Alfaro, C. Olea-Azar, J. Solut. Chem. (2011) 727.

(8) A.A. Elbashir, F.O. Suliman, J. Chromatogr. A 1218 (2011) 5344.

(9) Z. Li, E.P.A. Couzijn, X. Zhang, J. Phys. Chem. B 116 (2012) 943.

(10) W. Li, B. Lu, F. Chen, F. Yang, Z. Wang, J. Mol. Struct. 990 (2011) 244.

(11) P. Liu, D. Zhang, J. Zhan, J. Phys. Chem. A 114 (2010) 13122.

(12) J.K. Khedkar, V.V. Gobre, R.V. Pinjari, S.P. Gejji, J. Phys. Chem. A 114 (2010) 7725.

(13) J.J.P. Stewart, J. Mol. Model. 13 (2007) 1173.

(14) B. Varghese, S.N. Al-Busafi, F.O. Suliman, S.M.Z. Al-Kindy, Spectrochim. Acta Part A (2017) 173, 383-389.

(15) F.O. Suliman, AA Elbashir, OJ Schmitz, J. Incl. Phenom. Macrocycl. Chem. (2015) 83 (1-2), 119-129.

(16) B. Varghese, S.N. Al-Busafi, F.O. Suliman, SMZ Al-Kindy, Spectrochimica Acta Part A (2015) 136, 661-671.

(17) S.K. Al-Burtomani, F.O. Suliman, RSC Adv, (2017) *submitted*.

(18) B. Varghese, F.O. Suliman, N. S. S. Al Bishri, N. Al-Rwashda, Carbohydrate Polymer, (2017) *submitted*.