Journal of Molecular Liquids 346 (2022) 117862

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Synthesis, characterization, biological and DFT studies of charge-transfer complexes of antihyperlipidemic drug atorvastatin calcium with Iodine, Chloranil, and DDQ

S. Niranjani [a], C.B. Nirmala [b], P. Rajkumar [c], Goncagül Serdaroğlu [d], N. Jayaprakash [e], K. Venkatachalam [f,*]

[a] Department of Chemistry, Shrimathi Devkunvar Nanalal Bhatt Vaishnav College for Women, Chennai 600 044, Tamil Nadu, India
[b] Department of Plant Biology and Plant Biotechnology, Shrimathi Devkunvar Nanalal Bhatt Vaishnav College for Women, Chennai 600 044, Tamil Nadu, India
[c] PG Department of Physics, King Nandhivarman College of Arts and Science, Thellar-604 406, Affiliated to Thiruvalluvar University, Serkkadu, Vellore-632 115, Tamil Nadu, India
[d] Sivas Cumhuriyet University, Department of Science Education, 58140 Sivas, Turkey
[e] Department of Chemistry, SRM Valliammai Engineering College (Autonomous), Chennai 603 203, Tamil Nadu, India
[f] Department of Analytical Chemistry, University of Madras, Guindy Campus, Chennai 600 025, Tamil Nadu, India

ARTICLE INFO

Article history:
Received 11 July 2021
Revised 9 October 2021
Accepted 15 October 2021
Available online 9 November 2021

Keywords:
Atorvastatin calcium
Iodine
Chloranil
DDQ
Charge-transfer complexes
DFT
Antibacterial activity

ABSTRACT

Extremely coloured charge-transfer complexes (CTCs) of antihyperlipidemic drug, atorvastatin calcium (ATC) acting as n-electron donor with the electron acceptors, namely, iodine as σ-acceptor, 2,3,4,6-tetra chloro-1,4-benzoquinone (chloranil, CHL), 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) as π-acceptors have been explored. Elemental analysis, thermal analysis, FTIR spectroscopy, Raman spectroscopy, NMR spectroscopy, and mass spectroscopy techniques were used to explain the chemical mechanism of the synthesized ATC-CTCs. It has been found that the stoichiometry of the complexes was to be 1:1 ratio in ATC-iodine and 1:2 ratio in ATC-CHL; ATC-DDQ. Elemental and mass analysis were confirmed the above ratio of ATC-CTCs which was $[(ATC)I]I_3$, $[(ATC)(CHL)_2]$, and $[(ATC)(DDQ)_2]$ respectively. The biological activities of the formed ATC-CTCs were also tested against various bacterial strains. In addition, the frontier molecular orbitals (FMO) of the title compound was performed at the HF/6-311G** level to display the favourable reactivity tendency and the best suitable site for the electrophilic and nucleophilic attacks. The natural bond orbital (NBO) analysis was employed to predict the possible non-covalent interactions and its result disclosed that the $n \rightarrow \Pi^*$ and $\Pi \rightarrow \Pi^*$ interactions had a critical role in the enlightening of the stabilization of the compound. The achieved results are more appropriate for the estimation of antihyperlipidemic drug, ATC in pharmaceutical dosage forms.

1. Introduction

Mulliken and his co-workers had introduced a new concept, which is known as charge-transfer complex (CTC). An attraction between a donor and an acceptor forms CTC having weak bonds in it [1]. Colored CTC, which is formed by the molecular interactions between donor and acceptor can generally be absorbed easily in apparent visible region [2]. The rate control, specificity and a lot of biochemical reversible reactions could be mainly administrated by this type of formation of CTC. This could make prominent role in biomolecules [3,4]. The potential antimicrobial properties of CTC discloses against Gram-positive, Gram-negative bacteria and also against fungi [5–10].

Atorvastatin calcium (ATC) shown in Fig. 1, is a second generation, synthetic, statin category, 3-hydroxy-3-methylglutaryl-coen zyme A (HMG-CoA) reductase inhibitor [11]. This ATC is highly competent, effective antihyperlipidemic drug used for hyper cholesterolaemia [12]. The HMG-CoA reductase is held responsible for the rate determination step in the mevalonate pathway of synthesis of cholesterol [13]. HMG-CoA inhibition employs to reduce cholesterol in human blood stream and enhance low density lipoprotein (LDL) receptors formation [14]. ATC is officially confirmed in United States Pharmacopoeia 34 (USP), Indian Pharmacopoeia (IP) [15,16]. Some antibacterial activities of ATC and other statins have been reported in the literatures [17,18].

ATC, atorvastatin calcium; CHL, 2,3,4,6-tetrachloro-1,4-benzoquinone; DDQ, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone; CTC, charge-transfer complex; DFT, density functional theory.

* Corresponding author.
E-mail address: venkatachalam@unom.ac.in (K. Venkatachalam).

https://doi.org/10.1016/j.molliq.2021.117862
0167-7322/