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Density Functional Theory Based Investigation of (2E)-1-(Anthracen-9-yl)-3-(3,4-Dichlorophenyl)Prop-2-En-1-One

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ABSTRACT

DFT/B3LYP method has been employed to study recently synthesized (2E)-1-(Anthracen-9-yl)-3-(3,4-dichlorophenyl)prop-2-en-1-one. In the present work, the calculated values, i.e. geometric parameters, mulliken charges, frontier orbital analysis, dipole moments and QSAR properties are reported.
Keywords: DFT, B3LYP, QSAR

I. INTRODUCTION

Chalcones are an important class of natural compounds and have been broadly applied as synthons in synthetic organic chemistry. Synthetic analogues of chalcones are being investigated worldwide for the development of more potent and efficient drugs for the treatment of a number of diseases such as cancer, diabetes, HIV, tuberculosis,malaria etc[1-8]. The nonlinear optical [NLO] properties of the different chalcone derivatives have also been reported [9-12]. The density functional theory provides the ground state properties of a system, and the electron density plays a key role. DFT predicts a great variety of molecular properties molecular structures, ionization energies, electric and magnetic properties.

II. COMPUTATIONAL STUDY

The structure of recently synthesized[13] (2E)-1-(Anthracen-9-yl)-3-(3,4-dichlorophenyl)prop-2-en-1-one. was optimized (RMS gradient = 0.0005994) with Density Functional Theory (DFT) using B3LYP method with 6-31G(d,p) basis set in GAMESS package[14]. Initial geometry of the compound was generated using Chem Bio3D Ultra 14.0. Geometry optimization was carried out without any geometrical constraints. The calculation of QSAR properties are performed by Chem Bio3D Ultra 14.0.

III. RESULTS AND DISCUSSIONS

3.1 DFT structural parameters

The DFT calculations were carried out with B3LYP/6-31G (d,p). The geometry parameter viz. Calculated bond distances, bond angle and torsion angles of compound is given Table 1

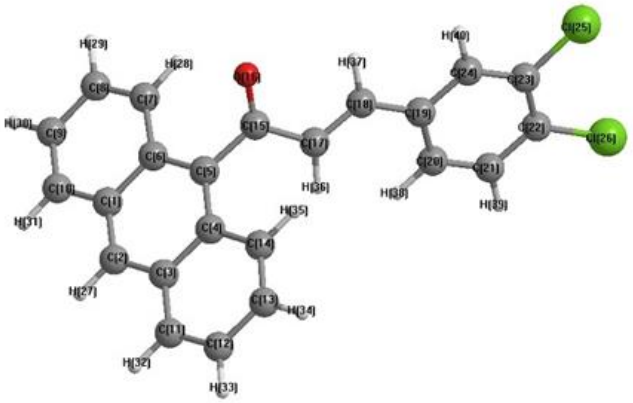

Figure 1. DFT / B3LYP optimized structure of the compound.

Table 1. Selected structure parameters

Bond distances		Bond angles		Torsion angles	
C15-O16	1.229	C4-C5-C15	119.827	C4-C5-C15-O16	-122.213
C5-C15	1.509	C6-C5-C15	119.091	C6-C5-C15-O16	61.327
C15-C17	1.487	C5-C4-C14	122.821	C5-C15-C17-C18	174.478
C17-C18	1.346	O16-C15-C17	121.893	C6-C5-C15-C17	-114.136
C18-C19	1.462	C5-C15-O16	121.958	C4-C5-C15-C17	62.324
C22-Cl26	1.745	C21-C22-Cl26	118.841	C17-C18-C19-C24	-169.019
C23-Cl25	1.748	C24-C23-Cl25	118.801	Cl25-C23-C24-C19	-179.885

3.2 Frontier Orbital Energy Analysis

According to the frontier molecular orbital theory, HOMO and LUMO are the most important factors that affect the bioactivity. HOMO has the priority to provide electrons, while LUMO can accept electrons first [15]. The energies of HOMO-2 to LUMO +2 orbitals are given in Table 2. HOMO – LUMO energy gap is 2.9823 eV (0.1096 a.u.).

Table 2. Energy levels (a.u.) of MOs calculated in their ground state in the gas phase.

HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2
-0.2427	-0.2393	-0.1973	-0.0877	-0.0636	-0.0290

3.3 Mulliken Atomic Charges

Table 3 exhibits the calculated Mulliken atomic charges except for atoms H. C_{15} is the most positively charged one, which can interact with the negative charged part of the receptor easily. The negative charges is mainly located on atom O_{16}, so it can interact easily with the positive part of the receptor. C_{15} being most positive and O_{16} most negative therefore C_{15}-O_{16} bond polarity plays a key role. Longer the C_{15}-O_{16} bond, more is C–O polarity and the biological activity must be the strong.

Table 3. Mulliken atomic charges except for atoms H (e) using DFT.

Atom No.	Charge
C1	0.105876
C2	-0.201911
C3	0.108796
C4	0.083506
C5	-0.054081
C6	0.086334
C7	-0.122284
C8	-0.094692
C9	-0.09225
C10	-0.12209
C11	-0.121815
C12	-0.09354
C13	-0.09432
C14	-0.136398
C15	0.31722

O16	-0.473207
C17	-0.139154
C18	-0.081395
C19	0.124539
C20	-0.101601
C21	-0.071268
C22	-0.0889
C23	-0.094678
C24	-0.10585
Cl25	0.024011
Cl26	0.026779

QSAR properties

QSAR studies facilitate to be acquainted with and calculate the physico chemical properties of a drug and its effect on biological activity. The common physico chemical properties include hydrophilic, electronic and steric nature. Hydrophobic character of a drug is important in recognizing its effortlessness in crossing the cell membrane and its interaction with the receptor.

Table 4. QSAR properties

Dipole Moment(Debye)	**LogP**	**Molar Refractivity (cm^3 / mol)**	**Partition Coefficient (Octanol/water)**
3.366	6.688	110.826	8.184

IV. CONCLUSION

DFT calculations reveal that small HOMO-LUMO gap of 2.9823 eV, location of HOMO on C15-O16 bond and bond polarity of C15-O16 bond as seen from Mulliken charge analysis will be key factors deciding biological activity of the molecule. QSAR properties generated show good penetrating capacity of the molecule into cell membrane.

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