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Molecular Docking Studies, Structural and Vibrational Features on 2 -Methylcyclopentane-1, 3-Dione Using DFT Methods

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ABSTRACT

The structural analysis of the molecule 2-Methylcyclopentane-1,3-dione was carried out using DFT/B3LYP method and their fundamental modes of vibrations are studied using FT-IR and FT-Raman spectroscopic techniques, recording the spectra in the range of 4000-400 cm^{-1}. Variation in the frequencies is correlated with the change in structural parameters. Including UV-Visible spectrum was recorded in range of 200-400 nm to explore possible electronic transitions, in combination with NBO and HOMO-LUMO contributions and also NBO analysis which helps to locate the intermolecular electronic interactions and their stabilization energy were discussed. The ^{13}C NMR and ^{1}H NMR chemical shifts are calculated using the gauge -independent atomic orbital (GIAO) method, with the B3LYP functional. The ESP map predicts surface extremes and ELF evaluates electron hole distribution i.e., charge transfer with in the title compound. The mulliken population analysis and natural charge analysis were carried out. Further, RDG analysis and anti-bacterial activity of these molecules were studies using molecular docking.

Keywords:— *FT-IR, FR-Raman, NBO, UV analysis, HOMO, LUMO, Docking analysis, etc.,*

I. INTRODUCTION

The cyclopentane structural unit is presented in various bioactive compounds, such as neutokinin-1, glycosidase inhibitors, prostaglandins, and natural lipid analogues. These compounds are mostly used as building block in the carbocyclic nucleoside analogues, which can exhibit activity against a variety of dieseses (HIV, HSC, Cancer and hepatitis). There were so many studies have been carried and reported [1-5], but spectroscopic studies with the special comparison the quantum computational methods have not yet been reported so far. This present study is aimed at making analytical comparison of the spectroscopic data with the theoretical studies.

Experimental details

The sample of 2-Methylcyclopentane-1, 3-dione is purchased from the Sigma-Aldrich chemicals, with 98% of purity. The sample is used as such without any purification for recording the spectra. The FT-RAMAN spectrum is recorded in the range of 3500-50 cm^{-1} with spectral width of 2 cm^{-1} spectra were recorded on a perkinelmer spectrum 1 FT-IR instrument and Bruker RFS 27 spectrophotometer, respectively. The spectrum of FT-IR was recorded in the range of 4000-400 cm^{-1} in the same instrument at a resolution of ±1 cm^{-1}.All band frequencies are found to be accurate at ±1cm^{-1}. The UV spectrum is recorded range from 700-200 n using a perkin elmer lambda 35 spectrophotometer with 1 nm resolution.

Quantum Chemical Calculations

In this work, the entire computational calculations were performed using the GAUSSIAN 09 software [5]. The geometry of the titled compound was first optimized using B3LYP functional in combination with 6-311++G (d,p) basis set. Vibrational wavenumbers were also calculated with the same functional and basis set.^{1}H and ^{13}C NMR chemical shifts were calculated using the GIAO functional along withB3LYP and 6-311++G (d,p) combination. The electronic properties such as NBO and HOMO-LUMO were calculated using time dependent TD-SCF-B3LYP method under same basis set. The dipole moment, linear polarizability and hyperpolarizabilities of the titled compound were obtained from molecular polarizabilities based on theoretical calculations. The reactive site of the title compound was evaluated at MEP surface analysis. In addition to that, the changes in the thermodynamic functions (heat capacity, entropy, and enthalpy) were also investigated for the different temperatures of the title molecule, using same B3LYP functional and 6-311++G (d,p) basis set.

II. Result and Discussion

Molecular Geometry

The molecular geometry known as the molecular structure is the arrangement of atoms in a molecule. Knowing the molecular structure of a compound can help determine the reactivity, polarity, magnetism and also the biological activity [6]. The theoretically possible optimized geometrical structure of the molecule is shown in Fig. 1 having minimum energy. The optimized geometrical bond lengths and bond angles of the compound calculated by DFT method with 6-311++G (d,p) basis set are given in Table 1.

In the present compound the bond lengths C1-C2, C2-C3, C3-C4, C4-C9, C9-C10 shows 1.53Å, 1.52Å, 1.54Å, 1.53Å, 1.52Å and 1.52Å. Which are in good agreement with the literature values. The average computed bond length of C-H gives the expected value 1.09 Å [7]. In the present compound the bond lengthsC2-H5,C3-H6, C2-H15, C3-H16, C10-H11, C10-H12 and C10-H13 shows 1.09 Å which are in good agreement with the literature value whereas the bond lengths C9-H14show a value 1.10 Å which may be due to the attachment of substitution at C9 atom.

The values of bond angle within the this ring varies form 103-125 º [8]. This implies that the bond angle is not uniform as expected to be 120º. So, the structure of the this ring is not regular hexagonal the CCC bond angle are reported values are not agreeing with the expected value which may be due to the attachment of substitutional group. In the substituent attached to the ring the bond angles CCC, CCO, CCH all shows value shown in the Table. 1. Next CCO bond angles get 125º

which is also good agreement with the expected value. The dihedral angles between cyclopentane and methyl group C2 -C1-C9-C10 and C3-C4-C9-C10 are 151º which is evident from the torsional angles .

Natural bond orbital analysis (NBO) Analysis

The NBO analyses are most important method for studying the various possible donors and acceptors in the molecule with their occupancy value in each position. similarly the various possible transitions among these donors and acceptors are provided. The inter and intra molecular interaction and especially charge transfer from electron donor to electron acceptor. This overall stabilization energy from the second-order micro disturbance theory is reported [9]. The energy of E(2) are due to molecular interaction between the electron is high intensive and more extent of conjugation of the hole system. The NBO occupied orbital is Lewis-type (bond or lone pair) and unoccupied orbital is non-Lewis type (anti-bond or Rydgberg). NBO analysis was performed on the title molecule at the B3LYP/6-311++G(d,p) basis set level can be elucidate the molecule. The fock matrix was elucidating in the donor-acceptor interactions in the NBO analysis [10].

$$E_2 = \Delta E_{ij} = q_i \frac{F(i,j)^2}{E_i - E_j}$$

Where q_i is the donor orbital occupancy, are ε_i and ε_j diagonal; elements and *F(i,j)* is the off diagonal NBO Fock matrix element reported [11].The high stabilization energy of the transitions gives a measure of the probabilities of the transitions; which indicate the highly probable in this molecule are O7 to C1-C2 (n-σ*, 10.99 Kcal/mol), O8 to C3-C4 (n-σ*, 10.99 Kcal/ mol),O7 to C1-C9 (n-σ*, 10.95 Kcal/mol). So, NBO analysis clearly explains the evidences of the formation of intra molecular hydrogen bonding interaction between lone pair O to C anti-bonding orbitals. The stabilization energy E(2) associated with the hydrogen bonding interaction (C 9 - H 14) σ → σ* (C 10 - H 11) is obtained as 1.27Kcal/mol.

Natural Population Analysis

The atomic charges exhibit direct influence on the dipole moment, molecular polarization, electronic structure, molecular reactivity, vibrational frequency of the system [12] and so on. The charges on the atoms of the molecule 2-Methylcyclopentane-1,3-dione was computed by Natural atomic charge (NAC) method using B3LYP functional with 6-311++G (d, p) basis set and are presented in Table .3 and graphically in Fig. 2. The Natural charge show that all carbon atoms are in this ring is expected to be negative charge. The C1& C4 carbon atom which is attached to Carboxylic acid group (C=O) atoms is predicted with maximum positive charge 0.6021&0.6021inNPA method respectively. Electronegative atoms attached with the carbon atoms pull out the partial charges from these atoms and hence these carbon atoms become positive. All hydrogen atoms clarifies normally positive range.

Spectral Analysis

The FT-IR and FT-Raman vibrations absolute readings were deducted using DFT quantum mechanical method. The experimental and theoretical vibrational results are presented in table.4 and the corresponding spectrums are depicted in Figure 3 & 4. The observed IR and Raman spectra of 2-Methylcyclopentane-1, 3-dione respectively. The Harmonic vibrational frequencies, calculated IR and Raman Intensities of entire molecular system diagnosed by PED analysis using popular VEDA program. The 2-Methylcyclopentane

-1,3-dione molecule give rise to 8 CH, 6 CC&2 CO modes.

CH vibration

Basically C-H stretching vibration of title compounds occur between 3100 – 3000 cm^{-1} [13]. The CH stretching vibrations in this derivatives arises from degenerate theoretical mode 3079-2911 cm^{-1}. In the title compound, the density studies experimentally observed vibrational wave numbers for the medium C-H stretching vibrations is 3080 &2948 cm^{-1} in FT-IR and 3080 & 3019 cm^{-1} for FT- Raman. And in-plane/out plane mode of vibrations are occur at the ranges are normally lies in the expected ranges. So vibrations not affected much more substitution atom the PED contribution of CH symmetric and asymmetric all mode vibrations are contribution was good.

CO vibration

The CO vibrational frequency range at 1715 -1680 cm^{-1} is corresponding to the C=O stretching vibration mode [14]. In the present study the calculated C=O stretching vibration modes are found at 1809 and 1768 cm^{-1} while the recorded frequency reading for C=O is 1717 cm^{-1} in IR spectrum is assigned with 88% of PED contribution and FT-Raman at 1712 cm^{-1}. The standard deformation modes of Carbonyl group are lying in the range of 700 to 400cm^{-1} [15] for the present case experimental deformation mode for C=O presented at 552 and 468cm^{-1} in observed spectra. The carbonyl group (C=O) in plane bending vibration for the title molecule are experimentally found at 533 cm^{-1} in Infrared spectrum.

C-C vibration

The CC stretching vibrations are very much important in the spectrum to form symmetric and asymmetric stretching vibrations. In present bands between 1500-1400 cm^{-1} [16] in the ranges are usually assigned to the CC modes. However the CC bond is found at having the observed calculated spectrum value. To attributed the C-C stretching vibration 1474 -1298 cm^{-1} and recorded FT-IR spectrum 1461, 1435, 1414 and 1336 cm^{-1} recorded FT-Raman spectrum 1452 and 1244 cm^{-1}. The in-plane bending vibrations are generally appearing in the 1300-1000 cm^{-1}. The CH in-plane bending vibrations are observed at 1298-1182 cm^{-1} . The Simultaneous activation of the CC single stretching mode spectra provides evidence for the charge transfer interaction between the donor and acceptor groups through the π system and enhances bioactivity of the title molecule. This vibrations is in good agreement with the observed spectrum.

Electronic absorption spectrum Analysis

The UV-Vis absorption spectrum of the titled compound is recorded in the range 200-400 nm are shown in Fig 7. Theoretical calculation shave been investigated in Gas phase and in organic solvent (ethanol) by TD-DFT method in order to get a deeper insight into the possible electronic excitations, wavelengths, oscillator strength sand major orbital contributions of various excitations of the titled compound [17].The electronic transitions and the corresponding excitation energies for the set wo phases are presented Table 5. The spectrum depicts three absorption peaks for title molecules which are intense primary absorption wavelength at 228 nm, secondary absorption at 358 nm, tertiary absorption at 259 nm, those are all absorption is due to the $n \rightarrow \pi^*$ transition in this ring. Here the hypsochromic shift was observed in the experimental absorption wavelength is duo to the solvent effect.

Frontier molecular orbital analysis

According to the frontier molecular ortial (FMO) theory, highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are vital elements that reflect the bioactivity of the compounds. The energy gap between HOMO and LUMO is used to find the chemical behavior, high reactivity, low kinetic stability of the compound. Using B3LYP method, the calculated HOMO and LUMO energies of the titled molecule is 0.0574and 0.0628eV, respectively, and the energy gap between them is -0.0054eV.The HOMO-LUMO energy gap and different reactivity descriptors of molecule in both levels are presented in Table 6. The negative surface was represented as red and the positive charges were represented by green color. The low HOMO-LUMO energy gap reveals the ultimate possible charge transfer within the molecule and hence there is the possibility of high chemical and biological reactivity [18].These values denoted good stability having this compound.

MEP (Molecular Electrostatic Potential) Analysis

Molecular electrostatic potential surface is denoted for the charge distribution around the molecule. In this surface analyzed charge distribution on the molecular interaction which determines the reactive sites in the molecules. The relation between electrostatic potential energy and charge distribution is [19],

$$\text{Potential energy}=K\frac{q1q2}{r}$$

Where this equation get clear indicates higher electrostatic potential energy surface i.e., positive charge (blue) and lower electrostatic potential energy surface i.e., negative charge of an electron. As per Molecular electrostatic potential mapped surface potential order red < orange < yellow < green < blue. In present study, MEP surface mapped using B3LYP/6-311++G(d, p) method. The 2-Methylcyclopentane-1, 3-dione compound view red and yellow regions are observed on top of oxygen atoms which are strong sites for electrophilic reactivity. Therefore MEP ascertains the electronegativity of oxygen atoms. It is concluded that there are significant difference in electron density in different regions of the molecule.

Molecular Docking

Based on the structure of the compound PASS is an online tool [20] which is used for the prediction of the various types of activities. Molecular docking has become an increasingly significant tool for drug discovery. The main application lies in the structure based virtual screening for indentifying new actively compounds towards a particular target protein. For docking study AutoDock 4 software package [21] was utilized to perform docking simulation. Autodock Tools Graphical user interface was utilized to find the protein structures of the ligand. Atomic charges were calculated by Kollman method and Lamarckian genetic Algorithm (LGA) was utilized for molecular docking calculation.

The AutoDock Bonded distance, bonded residue and number of hydrogen bond are shown in table. The 3D crystal structure of Endolysin from bacillus anthracis was obtained from Protein Data Bank. 3HMC has a good resolution 1.4 Å and attached co -crystallized inhibitors were used to identify the active site. Here the receptor is the protein and the compound under investigation acts as the ligand which binds to the receptor. PDB files have various potential problems such as added waters, missing atoms, chain breaks etc. that should be rectified to be used before in ADT which

is a built on Python Molecular Viewer [22] to solve all these problems.

The optimized molecular structure of the compound obtained using Gaussian 09 using B3LYP/6-3++G(d,p) level was docked to the protein through ADT. The active site of the enzyme was defined to add residues of the active site with the use of grid size90Å x90Å x90Åusing Autogrid. The analysis shows that the MET 129 with bond length of 1.8 and TRY with bond length of 2.0 implies ligand protein interaction. Role of net charge on catalytic domain and influence of cell wall binding domain on bactericidal activity, specificity, and host range of phage lysins.

III. Figures and Tables

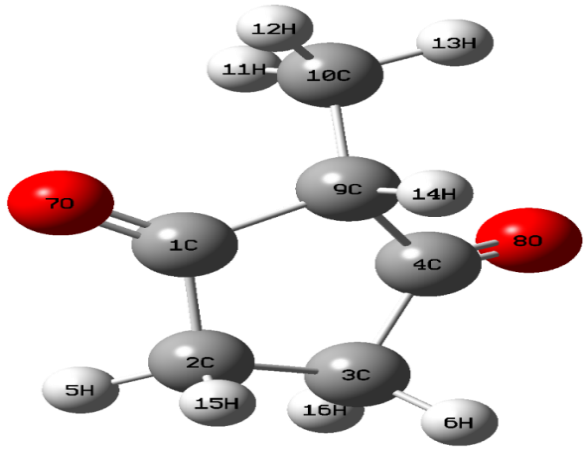

Figure 1: Optimized structure of 2-Methylcyclopentane-1, 3-dione

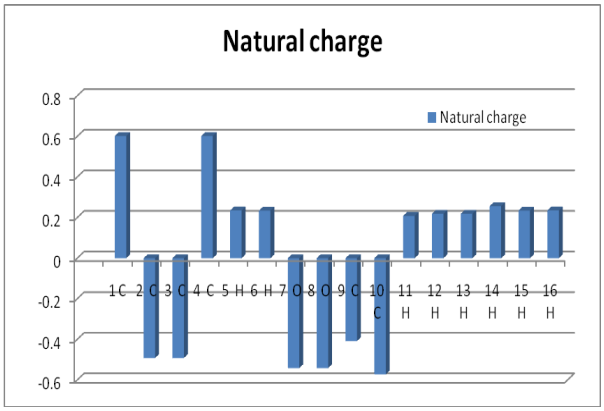

Figure 2: Plot of atomic charges of 2-Methylcyclopentane-1, 3-dione

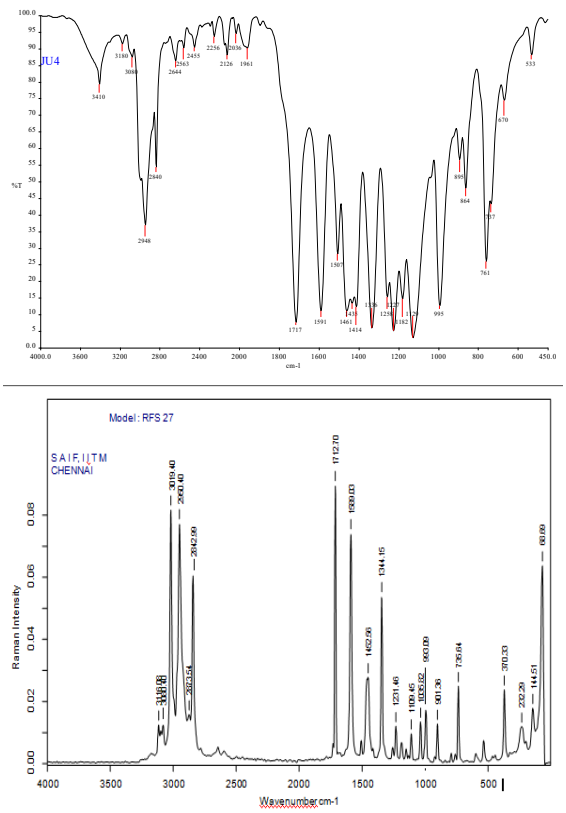

Figure 3: Simulated FT-IR & FT-Raman spectra of the 2-Methylcyclopentane-1,3-dione

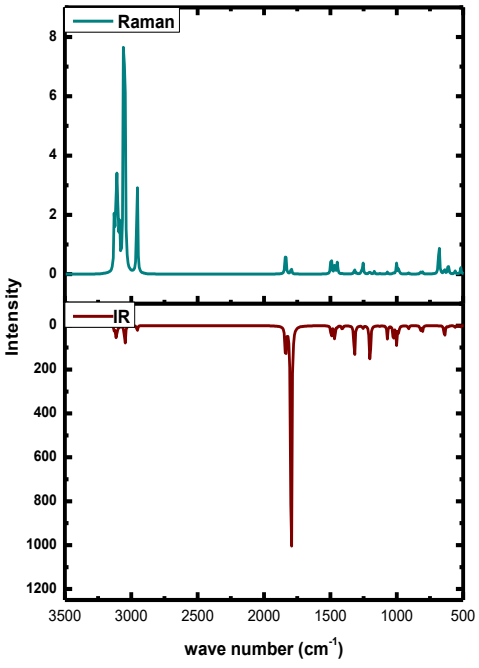

Figure 4: Observed FT-IR & FT-Raman spectra of the 2 -Methylcyclopentane-1,3-dione

Table 1: Optimized Geometrical parameter for 2-Methylcyclopentane-1, 3-dione Computed at B3LPY/6-311++G(d,p)

Bond Length (Å)	B3LYP/ 6-311++G (d,p)	Bond Angle (QUOTE)	B3LYP/ 6-311++G (d,p)	Dihedral Angle (QUOTE)	B3LYP/ 6-311++G (d,p)
C1-C2	1.532	C2-C1-O7	125.1	O7-C1-C2-C3	165.5
C1-O7	1.205	C2-C1-C9	109.3	O7-C1-C2-H5	42.56
C1-C9	1.527	O7-C1-C9	125.5	O7-C1-C2-H15	-72.95
C2-C3	1.540	C1-C2-C3	106.3	C9-C1-C2-C3	-13.55
C2-H5	1.091	C1-C2-H5	108.7	C9-C1-C2-H5	-136.4
C2-H15	1.094	C1-C2-H15	108.2	C9-C1-C2-H15	107.9
C3-C4	1.532	C3-C2-H5	113.7	C2-C1-C9-C4	21.37
C3-H6	1.094	C3-C2-H15	112.8	C2-C1-C9-C10	151.0
C3-H16	1.091	C5-C2-H15	106.6	C2-C1-C9-H14	-87.73
C4-O8	1.205	C2-C3-C4	106.3	O7-C1-C9-C4	-157.6
C4-C9	1.527	C2-C3-H6	112.8	O7-C1-C9-C10	-28.00
C9-C10	1.523	C2-C3-H16	113.7	O7-C1-C9-H14	93.20
C9-H14	1.104	C4-C3-H6	108.2	C1-C2-C3-C4	-0.012
C10-H11	1.092	C4-C3-H16	108.7	C1-C2-C3-H6	118.5
C10-H12	1.090	H6-C3-H16	106.6	C1-C2-C3-H16	-119.7
C10-H13	1.090	C3-C4-O8	125.1	H5-C2-C3-C4	119.7
		C3-C4-H9	109.3	H5-C2-C3-H6	-121.7
		O8-C4-H9	125.5	H5-C2-C3-H16	-0.015
		C1-C9-C4	103.7	H15-C2-C3-H6	-118.5
		C1-C9-C10	116.6	H15-C2-C3-C5	-0.016
		C1-C9-H14	104.4	H15-C2-C3-H16	121.7
		C4-C9-C10	116.6	C2-C3-C4-O8	-165.4
		C4-C9-H14	104.4	C2-C3-C4-C9	13.57
		C10-C9-H14	109.7	H6-C3-C4-O8	72.98
		C9-C10-H11	110.6	H6-C3-C4-H9	-107.9
		C9-C10-H12	110.3	H16-C3-C4-O8	-42.54
		C9-C10-H13	110.3	H16-C3-C4-C9	136.5
		H11-C10-H12	108.0	C3-C4-C9-C1	-21.38
		H11-C10-H13	108.0	C3-C4-C9-C10	-151.0
		H12-C10-H13	109.2	C3-C4-C9-H14	87.72
				O8-C4-C9-C1	157.6
				O8-C4-C9-C10	27.99
				O8-C4-C9-H14	-93.21
				C1-C9-C10-H11	-61.63
				C1-C9-C10-H12	57.92
				C1-C9-C10-H13	178.7
				C4-C9-C10-H11	61.64
				C4-C9-C10-H12	-178.7
				C4-C9-C10-H13	-57.92
				H14-C9-C10-H11	180.0
				H14-C9-C10-H12	-60.43
				H14-C9-C10-H13	60.43

Table 2: Second order perturbation theory of Fock matrix in NBO basis of 2-Methylcyclopentane-1, 3-dione

Donor	Type of bond	Occupancy	Acceptor	Type of bond	Occupancy	Energy e(2) Kcal/mol	E(j)-e(i)	F(i,j)
O 7	n	0.9998	C 1 - C 2	σ*	0.0344	10.99	0.64	0.107
O 8	n	0.9998	C 3 - C 4	σ*	0.0344	10.99	0.64	0.107
O 7	n	0.9998	C 1 - C 9	σ*	0.0382	10.95	0.65	0.108
O 8	n	0.9998	C 4 - C 9	σ*	0.0382	10.95	0.65	0.108
C 9 - H 14	σ	0.9559	C 1 - O 7	π*	0.0448	3.86	0.52	0.057
C 9 - H 14	σ	0.9596	C 4 - O 8	π*	0.0448	3.86	0.52	0.057
C 2 - H 15	σ	0.9818	C 1 - O 7	π*	0.0448	2.91	0.53	0.05
C 3 - H 6	σ	0.9818	C 4 - O 8	π*	0.0448	2.91	0.53	0.05
C 2 - C 3	σ	0.9905	C 1 - O 7	σ*	0.0063	1.91	1.24	0.061
C 2 - C 3	σ	0.9905	C 4 - O 8	σ*	0.0063	1.91	1.24	0.061
C 10 - H 12	σ	0.9934	C 4 - C 9	σ*	0.0382	1.75	0.87	0.05
C 10 - H 13	σ	0.9934	C 1 - C 9	σ*	0.0382	1.75	0.87	0.05
C 1 - C 9	σ	0.9861	C 4 - O 8	σ*	0.0063	1.71	1.26	0.059
C 4 - C 9	σ	0.9861	C 1 - O 7	σ*	0.0063	1.71	1.26	0.059
C 2 - H 5	σ	0.9861	C 1 - O 7	π*	0.0448	1.56	0.53	0.037
C 3 - H 16	σ	0.9861	C 4 - O 8	π*	0.0448	1.56	0.53	0.037
C 10 - H 11	σ	0.9939	C 9 - H 14	σ*	0.0097	1.53	0.86	0.046
C 9 - H 14	σ	0.9596	C 10 - H 11	σ*	0.0032	1.27	0.91	0.044

Table 3 :Mullikan Charges of 2-Methylcyclopentane-1,3-dione Computed at B3LYP/6-311++G(d,p) basis set.

Atoms	Natural atomic Charge
1 C	0.6021
2 C	-0.4916
3 C	-0.4916
4 C	0.6021
5 H	0.2351
6 H	0.2346
7 O	-0.5411
8 O	-0.5411
9 C	-0.4086
10 C	-0.5724
11 H	0.2085
12 H	0.2186
13 H	0.2186
14 H	0.2567
15 H	0.2346
16 H	0.2351

Table 4: Observed method DFT/B3LYP with 6-311++G(d,p) level calculated vibrational frequencies of 2-Methylcyclopentane-1,3-dione

Experimental wavenumber (cm $^{-1}$)	Calculated wavenumber (cm^{-1})	PED %	
FT-IR	***FT-RAMAN***		
3080	3080	3079	ν CH 50
		3066	ν CH 55 + ν CH 22
		3058	ν CH 38 +ν CH 12
		3042	ν CH 41
	3019	3010	ν CH 12 + ν CH 38
		3001	ν CH 41 + ν CH 45 + ν CH 28
		3001	ν CH 41 + ν CH 45 + ν CH 28
2948		2911	ν CH 99
		1809	ν CH 45 + ν OC 45
1717	1712	1768	ν CH 46 +ν OC 46
		1474	β HCH 38 + β HCH 40 + τ HCCC 16
1461	1452	1469	β HCH 18 + τ HCCC 11 + τ HCCC 12
1435		1444	β HCH46 + β HCH 45
1414		1425	β HCH 41 + β HCH 41
1336	1244	1388	β HCH 25 + β HCH 45
		1298	νCC 13 + β HCC 12 + τ HCCC 21
		1282	ν CC 11 + 12 + τ HCCC 13 + τ HCCC 12
1258		1247	β HCC 11 + τ HCCC 10 + τ HCCC 12
1227	1231	1235	β HCC 23 + HCC 16 + τ HCCC 11 + τ HCCC 15 + 13
		1191	β HCC 22 + τ HCCC 16 + τ HCCC 13
1182		1182	ν CC 10 + β HCC11 +τ HCCC τ HCCC 10
1129		1151	β HCC 15 + τ CCCC 10
	1109	1111	β HCC 15 + τ HCCC 11 + τ HCCC 10
	1035	1054	ν CC 15+ β OCC 10+ τ HCCC 15
		1009	ν CC 27 + 14 + τ HCCC 20
995	993	985	β CCC 26 + β CCC 23
		969	ν CC 13 + β HCC 10 + τ HCCC 16
895		897	β HCC 11
		808	τ HCCC 11 + γ OCCC 15 + γ CCCC 10
761		792	ν CC 27
670		670	ν CC 13
		630	ν CC 10 + β CCC 30
		602	β CCC 20 + τ HCCC 12
533		552	ν CC 10 + β OCC 29
		510	ν CC 10 + β CCC 10 + γ CCCC 12
		468	γ OCCC 26
	370	385	β OCC 24 + β CCC 22
		245	γ OCCC 14 + CCCC 53
	232	228	β CCC 73
	144	154	τ HCCC 28
	68	60	τ CCCC 30
		24	τ HCCC 19

Table 5: Theoretical electronic absorption spectra of 2 Methylcyclopentane-1,3-dione (absorption wavelength λ (nm)), excitation energies E (ev) and oscillator strengths (f) using TD-DFT/B3LYP/6-311++G(d,p) method

Theo-retical	Experi-mental	E	f	Oscillator strengths
360.7	355	3.437	0.0000	HOMO(A)->LUMO(A) (42%)
327.4		3.786	0.0000	H-1(A)->LUMO(A) (23%)
318.7		3.889	0.0019	HOMO(A)->LUMO(A) (46%)

Table 6: Details of the ligand-protein interaction of 2-Methylcyclopentane-1,3-dione

Protein (PDB ID)	Binding energy	RMS	bond	Bonded Residues	Bond Distance
3HMC	-5.27	28.53	2	MET 129 TRY 130	1.8 2.0

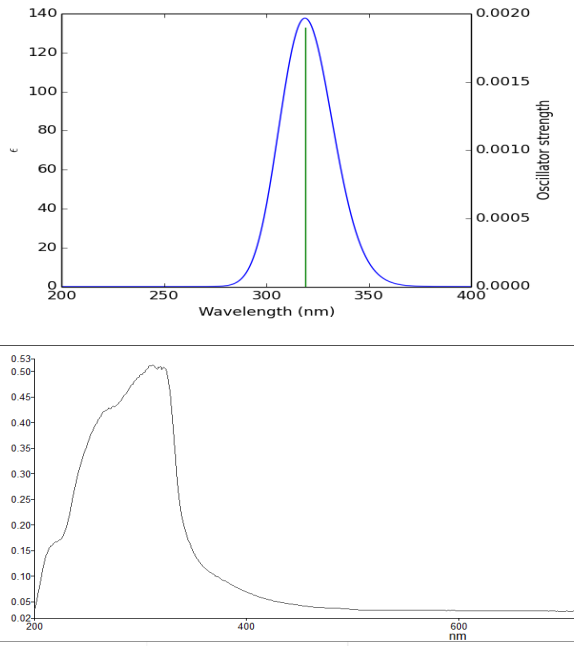

Figure 5: Experimental and Theoretical and UV-Vis Spectra of using 2-Methylcyclopentane-1,3-dione

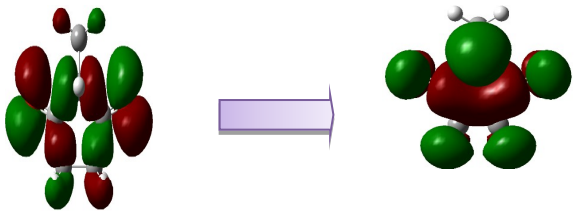

Figure 6: Frontier molecular orbitals of 2-Methylcyclopentane-1,3-dione

Table 7: Homo, Lumo, Kubo gap, global electronegativity, global hardness and softness, global electrophilicity index of 2-Methylcyclopentane-1, 3-dione

Parameters	Gas
EHOMO (ev)	0.0574
ELUMO (ev)	0.0628
ΔEHOMO-LUMO gap (ev)	-0.0054
Elecronegativity (χ)	-0.0601
Global hardness (η)	0.0027
Global softness (S)	0.0108
Chemical Potential (μ)	0.6688

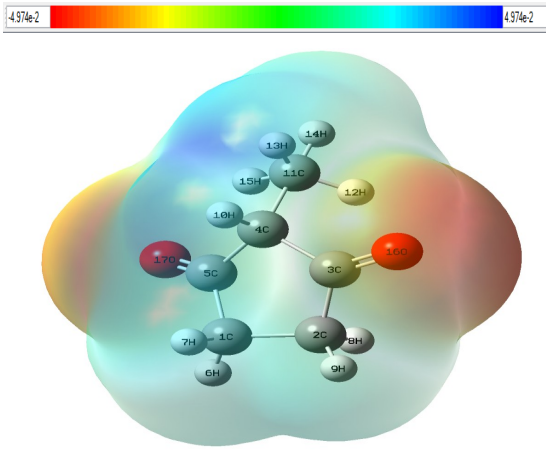

Figure 7: Molecular electrostatic potential

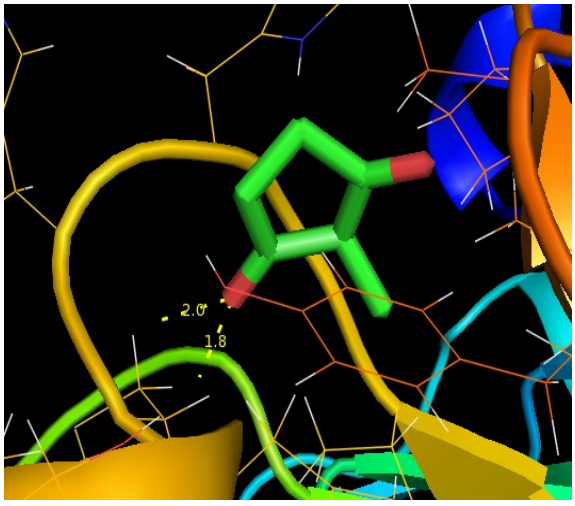

Figure 8: Molecular binding pose

IV. CONCLUSION

An attempt has been made in the present work for the proper frequency assignments for the compound 2-Methylcyclopentane-1,3-dione from the FT-IR and FT-Raman spectra. The structural conformational, geometrical analysis vibrational NBO, HOMO-LUMO,UV-vis Mullikan atomic charge. The FT-IR and FT-Raman spectra of the present moleculespectra provides evidence for the charge transfer interaction between the donor and acceptor groups through the π system and enhances bioactivity of the title molecule. Using the comparison we analyses the different type's vibration. In present study, MEP surface mapped that there are significant difference in electron density in different regions of the molecule. HOMO-LUMO values denoted good stability having this compound. Role of net charge on catalytic domain and influence of cell wall binding domain on bactericidal activity, specificity, and host range of phage lysine.

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