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FTIR and UV Spectroscopic Analysis of Sparfloxacin Combined with Theoretical Study Based on DFT Calculations

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Sparfloxacin is analyzed using FTIR and UV-Vis spectrometers; theoretically the structure is geometry optimized using density functional theoretical approach with *B3LYP* **method of calculation. After optimization, the vibrational frequencies are calculated. An acceptable match is observed between the measured and the calculated data. Electron density of the molecule is studied using natural bond orbital method. The energy difference was calculated and found to be 4.314 eV and this represents the difference between the highest occupied molecular orbitals and lowest unoccupied molecular orbitals energies. This value explains the interaction between the charging transfer and the structure that affects the biological behavior. The electrostatic potential map of the molecule shows that the molecular sites having negative potentials are those of oxygen, nitrogen and fluorine atoms and those having positive potentials are those of hydrogen atoms. The UV-VIS analyses of Sparfloxacin was carried out and the results confirmed the charge moving to the molecule.**

Keywords: Quantum molecular physics; density functional theory; Infrared absorption; Orbital energies; Sparfloxacin antibiotic

Introduction

Sparfloxacin (IUPAC name: 5-amino-1-cyclopropyl- 7-[(3R,5S)-3 ,5-dimethylpiperazin-1-yl]- 6,8-difluoro- 4-oxoquinoline- 3-carboxylic acid) is a fluoroquinolone antibiotic indicated for bacterial infections, it derived from nalidixic acid which is commonly used for treating the acute infections of the genitourinary scheme. The mechanism of action of Sparfloxacin is associated with inactivation of the bacterial DNA topoisomerase-II and weak interaction with the Bacterial DNA topoisomerase-IV, which leads to inhibition of the replication process of bacterial cells, leading to their death [1]. Sparfloxacin is one of antibacterial groups used to treat lung diseases, urinary tract infection and dermal allergies. Sparfloxacin is noted for its wide range of activities, strength and excellent pharmacokinetic profiles [2-4]. Sparfloxacin is one of the synthetic drugs which are confirmed and quantified by a multiresidue method which was improved by Lia et al. in 2009[5], they used a liquid chromatography-tandem mass spectrometer in their study. Shah et al. [6] have been developed a simple and accurate process for the spectrometric determination of bulk Sparfloxacin and for the

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pharmaceutical preparations based on quantum-chemical approaches compared to results of simple experimental (shake-flask) technique. Klosinska-Szmurlo et al. [7] identified the bioavailability in silico and in vitro methods of five selected fluoroquinolones. Investigation of the structure the metal complex of sparfloxacin has been conducted by El-Gamel and Zayed [8] Sparfloxacin has been investigated and analyzed after being irradiated in aqueous solution, using LC- UV detectionand LC-MS/MS [9] Attia et al. reported three sensitive, selective and accurate Spectrophotometric and Spectrodensitometric methods for determination of sparafloxacin hydrochloride and besifloxacin hydrochloride in presence of bulk and pharmaceutical formulations of peroxide degradation products [10]. Concurrent short-time reversed phase HPLC method was developed and validated by Gul et al. [11] for the determination of Sparfloxacin, together with meloxicam, diclofenac sodium, flurbiprofen, ibuprofen, mefenemic acid and naproxen in a bulk material, pharmaceutical formulations and human serum. A new rapid and sensitive chemiluminescence method (CL) for determination of Sparfloxacin and other five fluoroquinolones namely, ciprofloxacin, gatifloxacin, levofloxacin, lomefloxacin HCl, and ofloxacin is proposed by Abdel-aal et al. [12]. Jana et al. [13], used FT-IR and UV-Vis spectroscopic techniques to report the effect of the bio-field properties of sparfloxacin. Investigation of mass spectra for sparfloxacin structure obtained using electron ionization (EI) and chemical ionization (CI), procedures have been reported and discussed by Abd El-Kareem et al [14] who toke into consideration the fragmentation process under the two ionization procedures and used the semi-empirical MNDO method. Literature shows that few studies tackle UV spectra and DFT calculations of sparfloxacin have been reported. All spectroscopies analyses by mean of FTIR and UV spectra together with quantum chemical calculations study will aid in Sparfloxacin structure investigation. So, the aim of the work is to study Sparfloxacin molecular structure using its experimental and theoretical vibrational spectra after geometrical optimization using density functional theory DFT with B3LYP method of calculation [15] and 6-311G(d,p) basis set. Hence DFT models are widely used to study the properties of molecular dynamics, including the equilibrium structure and vibrational frequencies [16].

Materials and Methods

Sparfloxacin sample in its pure chemical form was obtained from El-Obour Pharmaceutical Company, Cairo, Egypt. FTIR spectra of the studied Sparfloxacin samples were recorded by Attenuated-Total-reflection Fourier Transform Infrared spectroscopy (A T R -F T I R) using a Shimadzu IRTracer-100 spectrometer. The Geometry of the IR beam includes incidence at angle of 30° enrolls in the range of 4000 - 400 cm^{-1} [17].

Ultraviolet-visible spectrum was performed using a PerkinElmer spectrophotometer (type Lamda-25), registered in the wavelength range of 200-400 nm at ambient atmosphere with air as a reference.

Computational details

The geometric optimization of the studied structure was conducted using density functional theoretical approach of B3LYP as illustrated in a previous study [18]. This method has been used at neutral state using Gaussian 09, Revision C.01 [19]. The optimized molecular geometry with numbering system of sperfloxacin drug is shown in Fig (1).

The ionization potential (I) is determined using the following relation [20-21]:

$$I = -E_{HOMO}\text{, and } A = -E_{LUMO} \qquad (1)$$

Where, A is the electron affinity according to Koopmans' Theory. Electronegativity (χ) of the material together with global chemical rigidity and electronic chemical potential are calculated as follows [22, 23]:

$$\mu = (\partial E / \partial N)\nu(r) = -\chi \qquad (2)$$

$$\eta = 1/2(\partial\mu / \alpha N)(\vec{r}) = 1/2(\partial^2 E / \partial^2 N)\nu(\vec{r}) \qquad (3)$$

Where, E is the energy, N is the number of electrons in external potential of the molecular system under consideration.

From these equations,

$$\chi = (I + A)/2, \eta = (I - A)/2 \text{ , and } \mu = -\chi \quad (4)$$

The electrophilicity index (ω) and the global chemical softness (S) are defined as follows [24, 28]:

$$S = 1/2\eta, and \ \omega = \mu^2 / 2\eta \quad (5)$$

Results and Discussion

Molecular geometry

Sparfloxacin optimization and getting a numbered system was carried out using DFT in B3LYP as shown in Fig.(1). The studied molecule has two C-F bond lengths, eight C-N bond lengths, three C-O bond lengths, sixteen C-C bond lengths, sixteen C-H bond lengths and three N-H bond lengths. Experimental and calculated values are given in Table (1). The calculations showed the C-C bond lengths are ≈ 1.4 (Å) and C-N, C-O bond lengths are ≈ 1.3(Å) and C-F bond lengths are ≈ 1.4(Å) in whole Sparfloxacin molecule. It was observed that the geometrical parameters (bond lengths and angles) estimated by B3LYP level were found to be in excellent agreement with experimental values as shown as in Table (1).

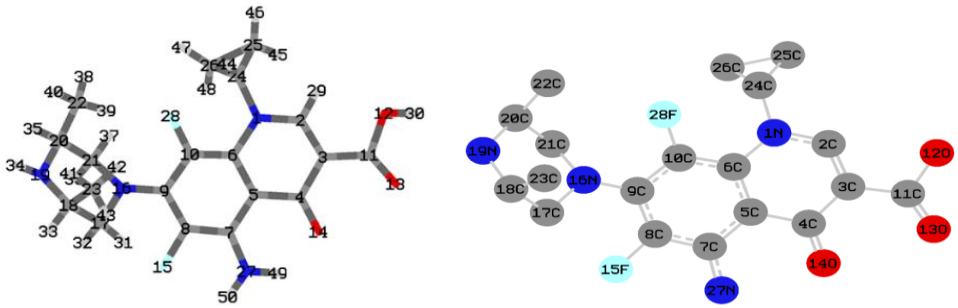
NBO Analysis

Natural Bond Orbital (NBO) is a valuable tool for electron distribution on the molecule [29] The interaction between bonding and antibonding molecular orbitals can be quantitatively described in terms of NBO approach that is expressed by means of second-order interaction energy perturbation E(2). This energy is the estimate of the off-diagonal element of the NBO Fock matrix. The stabilization energy E (2) associated with i (donor) → j (acceptor) delocalization is estimated from the second-order perturbation approach as given below [30]:

$$E(2) = \Delta E_{ij} = q_i \frac{F^2(i, j)}{\varepsilon_j - \varepsilon_i} \quad (6)$$

Where, q_i is the donor orbital occupancy, E_i and E_j are diagonal elements (orbital energies) and $F_{(i,j)}$ is the off-diagonal Fock matrix element.

Table (2) presents the NBO study of the most important hyperconjugative inter actions of Sparfloxacin which were formed because of the overlapping between π(c-c) and π*(c-c) orbitals and the stabilization of the system was attained because of the intra-molecular charge transfer. Such interactions can be detected when the electron density increases in the orbital antibonding system. Some parts of the ring are stabilized because of the high interaction of the p electrons of C-C to anti C-C and C-O bond as shown in Table (2). The donor orbitals πC-C→π*C-C and πC-C→ π*C-O gave more energy than σ C-C $\rightarrow \sigma^*$ C-C. Highly strong interaction has been observed between the lone pair LP N(27) and the σ*C(5)-C(7) with energy (54.88 kcal/ mol). LP O(14) only participates in LPO(14)→σ*C(3)-C(4) interaction with an important value of energy, as shown Table (2). The calculated interaction energies of the BD*(2)C(4)-O(14))→ BD*(2) C(2) - C(3) and BD*(2)C(6)-C(10) →BD*(2) C (5) - C (7) are 192.56 and 329.32 kcal /mol, respectively which indicate a remarkable stabilization in the molecule



(a) (b)

Figure (1: Part a) the optimized geometry of Sparfoxacin; Part b) The structure of Sparfoxacin with atoms numbered according to the text

Table (1): Optimized geometrical parameters for Sparfloxacin computed at B3LYP basis set

Bond length	values (Å) B3LYP	Exp. values (Å) *	Bond angle	Value (o) B3LYP	Exp. values (Å) *
N1-C6	1.4172	1.349	A(C2,N1,C24)	118.7482	118.6
N1-C24	1.4666	1.452	A(C6,N1,C24)	122.3717	122.1
C2-C3	1.3701	1.354	A(N1,C2,C3)	120.96	120.9
C3-C4	1.4602	1.462	A(C2,C3,C4)	121.9913	121.2
C3-C11	1.4653	1.440	A(C2,C3,C11)	115.406	114.1
C4-C5	1.4677	1.430	A(C4,C3,C11)	112.53	113.3
C4-O14	1.2672	1.250	A(C3,C4,C5)	124.5542	125.1
C5-N6	1.4278	1.453	A(C3,C4,O14)	119.345	119.3
C5-C7	1.4331	1.429	A(C5,C4,O14)	118.493	117.8
C6-C10	1.3941	1.393	A(C4,C5,C6)	121.885	122.8
C7-C8	1.4004	1.388	A(C4,C5,C7)	122.519	122.9
C7-N27	1.36	1.348	A(C6,C5,C7)	121.7274	121.0
C8-C9	1.396	1.385	A(C1,C6,C5)	115.7499	116.1
C8-F15	1.4162	1.360	A(C1,C6,C10)	120.0233	120.2
C9-C10	1.4125	1.389	A(C5,C6,C10)	119.488	120.5
C9-N16	1.3935	1.391	A(C5,C7,C8)	120.462	119.3
C10-F28	1.4143	1.356	A(C5,C7,N27)	117.950	118.8
C11-O12	1.4076	1.257	A(C8,C7,N27)	122.1544	122.1
C11-O13	1.2302	1.245	A(C7,C8,C9)	120.032	119.0
N16-C17	1.477	1.456	A(C7,C8,F15)	119.8188	120.9
N16-C21	1.4807	1.452	A(C9,C8,F15)	116.1591	116.2
C17-C18	1.539	1.510	A(C8,C9,C10)	123.8131	122.5
C18-N19	1.4743	1.509	A(C8,C9,N16)	121.217	119.9
C18-C23	1.5442	1.512	A(C10,C9,N16)	122.4967	123.0
N19-C20	1.4754	1.496	A(C6,C10,C9)	114.5906	116.9
C20-C21	1.5382	1.515	A(N19,C20,C21)	119.958	118.9
C20-C22	1.5438	1.505	A(N19,C20,C22)	119.4489	116.4
C24-C25	1.5151	1.518	A(C21,C20,C22)	125.3843	124.7
C24-C26	1.5088	1.497	A(N16,C21,C20)	124.1734	122.8
C25-C26	1.5158	1.481			

(*)Experimental values are taken from Ref Acta Cryst. (2000). C56, e115±e116

Table (2) : Natural Bond Orbital of Sparfloxacin neutral molecule

Donor[ia]	Acceptor [j a]	E(2) (kcal/mol) [b]	ΔE a.u.	F(i,j) a.u.
BD(2) C2C3	BD*(2)C4-O14	26.83	0.28	0.079
BD(2)C2C3	BD*(2)C11-O13	27.42	0.27	0.078
BD(2) C5C7	BD*(2)C4-O14	29.15	0.25	0.078
BD(2)C5C7	BD*(2) C6-C10	29.17	0.25	0.077
BD(2)C5C7	BD*(2) C8-C9	16.54	0.25	0.058
BD(2)C6C10	BD*(2)C5-C7	11.09	0.30	0.055
BD(2)C6C10	BD*(2) C8- C9	21.71	0.29	0.075
BD(2)C8C9	BD*(2) C5-C7	23.84	0.29	0.079
BD(2)C8C9	BD*(2) C6 -C10	13.69	0.28	0.058
LP(1)N1	BD*(2)C2-C3	46.83	0.29	0.108
LP(1)N1	BD*(2) C 6 - C10	38.80	0.28	0.094
LP(2) O12	BD*(2) C11 - O13	37.58	0.31	0.100
LP(1)O13	RY*(1) C11	15.05	1.54	0.136
LP(2) O13	BD*(1) C 3 - C11	16.66	0.68	0.098
LP(2) O13	BD*(1) C11 - O 12	37.14	0.51	0.124
LP(1) O14	RY*(1) C4	11.04	1.52	0.116
LP(2) O14	BD*(1) C3 C4	17.96	0.72	0.103
LP(2)O14	BD*(1) C 4 -C5	13.11	0.71	0.087
LP(2)O14	BD*(1) N27 -H 49	9.03	0.71	0.073
LP(3) F15	BD*(2) C8 - C9	12.27	0.40	0.071
LP(1) N16	BD*(2) C8 - C9	28.29	0.25	0.079
LP (1)N19	BD*(1) C18 - C23	9.63	0.60	0.069
LP (1) N19	BD*(1) C20 - C22	9.31	0.60	0.068
LP (1)N27	BD*(2) C5 - C7	54.88	0.25	0.110
LP(3) F 28	BD*(2) C6 - C10	12.36	0.40	0.071
BD*(2)C4O14	BD*(2) C2 - C3	192.56	0.01	0.074
BD*(2) C6 C10	BD*(2) C5 - C7	329.32	0.01	0.077
BD*(2)C11 O13	BD*(2) C2 - C3	101.29	0.02	0.070

[a] see Sparfloxacin numbering system and LP is lone pair.

[b] E(2) second energy order

It could be noted that the carbon atom has positive and negative charge and hydrogen atomic charges is found to be totally positive and arranged in an the order from 0.19087 to 0.47904 due to charge transfer from H to carbon atom. Additionally, the three oxygen atoms are negative and arranged in an the order -0.54461 to -0.73027, the magnitudes of the atomic charge of the three Nitrogen atoms have negative values and arranged in the order -0.38511 to -0.74591and the magnitudes of the atomic charge of the two fluorine atoms are negative (-0.37197 , -0.37629) indicating that a Sparfloxacin molecule has a highly electronegative atoms O, N and F atoms as presented in Table (3). The authors of the present study suggest that N1 and O14 in Sparfloxacin qinolone ring have a lone pair electrons ionization processes which may take place at these atoms. The histogram of NBO atomic charges for Sparfloxacin at DFT/B3LYP/6-311G level is shown in Figure (2).

The Highest_Occupied_Molecular_Orbital (HOMO) and the Lowest Unoccupied_Molecular Orbital (LUMO) are very important parameters for studying molecule kinetic stability OMO is

responsible for donating an electron and LUMO is responsible for accepting this electron. The HOMO-LUMO energy values were calculated by B3LYP method using 6-311 G (d, p) basis sets for evaluating the behavior of the compound under study. Figure (2) shows HOMO and LUMO of Sparfloxacin red color represent ing the positive area and green color representing negative HOMO which is basically consisted of O(12)O(14), O(18) and N(1) of bicyclic ring, N(16) of piperazyinyl ring. N(27) attached to the two methyl groups. LUMO is distributed inside molecule except the methyl groups bounded to N(27). The energy gap ΔE is equal to the absolute value of the (HOMO - LUMO) energy difference, hence it is an important value which serves as an index of stability. A large HOMO-LUMO gap, involves the lower reactivity of high molecular stability in chemical reactions [31, 32]. Figure (3) shows the energy distribution for the molecular orbits HOMOLUMO with the related energy gap. The energy gap value of HOMO-LUMO ΔE was found to be 4.086 eV, which explains biological activity properties. The relative high values of ΔE, HOMO, LUMO show high chemical stability and low reactivity of the structure. Other energies and physical properties have been calculated and reported in Table (4) which helps to understand the molecular structure and reactivity.

Table (3): NBO and Mulliken atomic charges of Sparfloxacin drug calculated at DFT/B3LYP/6-311G level of theory

Atom	NBO [ac]	Mulliken [ac]	Atom	NBO [ac]	Mulliken [ac]	Atom	NBO [ac]	Mullikenac
N1	-0.38511	-0.782212	H40	0.19087	0.157470	H46	0.21264	0.200562
C2	0.12926	0.227414	H41	0.19484	0.163328	H47	0.21209	0.198361
C3	-0.26880	-0.262686	H42	0.20036	0.189747	H48	0.21360	0.202252
C4	0.46048	0.444639	O12	-0.73027	-0.615042	H49	0.43307	0.382845
C5	-0.16888	-0.225364	O13	-0.54461	-0.328071	H50	0.39067	0.342179
C6	0.14302	0.477575	O14	-0.61545	-0.431057	H43	0.19531	0.166800
C7	0.17704	0.422334	F15	-0.37629	-0.347725	C23	-0.59877	-0.496579
C8	0.31550	0.170910	N16	-0.47895	-0.649429	C24	-0.02587	-0.000126
C9	0.10980	0.324875	C17	-0.18257	-0.136223	C25	-0.39523	-0.387134
C10	0.31335	0.220402	C18	-0.00173	-0.052605	C26	-0.37978	-0.330371
C11	0.75746	0.468526	N19	-0.69848	-0.573318	N27	-0.74591	-0.911112
H34	0.35490	0.283192	C20	-0.00168	-0.046082	F28	-0.37197	-0.341801
H35	0.19259	0.175982	C21	-0.18074	-0.178286	H29	0.24168	0.246166
H36	0.18450	0.186254	C22	-0.59544	-0.484849	H30	0.47904	0.386661
H37	0.21149	0.198478	H43	0.19531	0.166800	H31	0.21154	0.192832
H38	0.19416	0.161405	N44	0.22054	0.219535	H32	0.19112	0.187865
H39	0.20526	0.193741	H45	0.21548	0.207893	H33	0.19486	0.179847

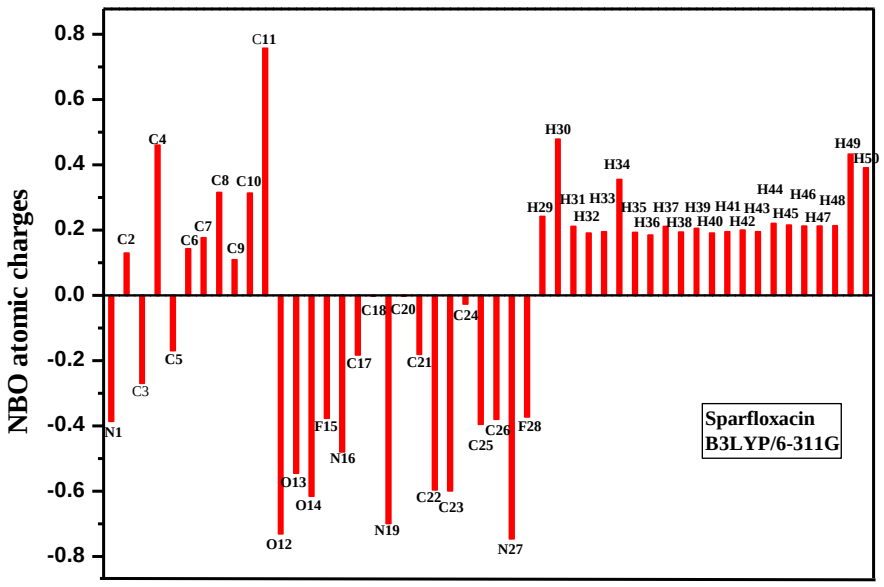


Figure (2): NBO atomic charges Sparfloxacin drug calculated at DFT/B3LYP/6-311G level of theory

Table (4): Energies and some physical properties of Sparfloxacin calculated at B3LYP/6-311G(d,p) level

Molecular parameters	B3LYP/6-311G(d,p)
Total energy (HT)	-1381.5592
Dipole moment (Deby)	7.1431
E_{Homo}(eV)	-5.721
E_{Lumo}(eV)	-1.635
ΔE_{gap}(eV)	-4.086
Ionization potential_IP (eV)	5.721
Electron affinity_EA (eV)	1.635
Hardness(η) (eV)	2.043
Softness(S) (eV)-1	0.4895
Electronegativity(χ)	3.678
Chemical potential, (μ)	-3.678

Electrophilicity, (ω)[33]	3.311

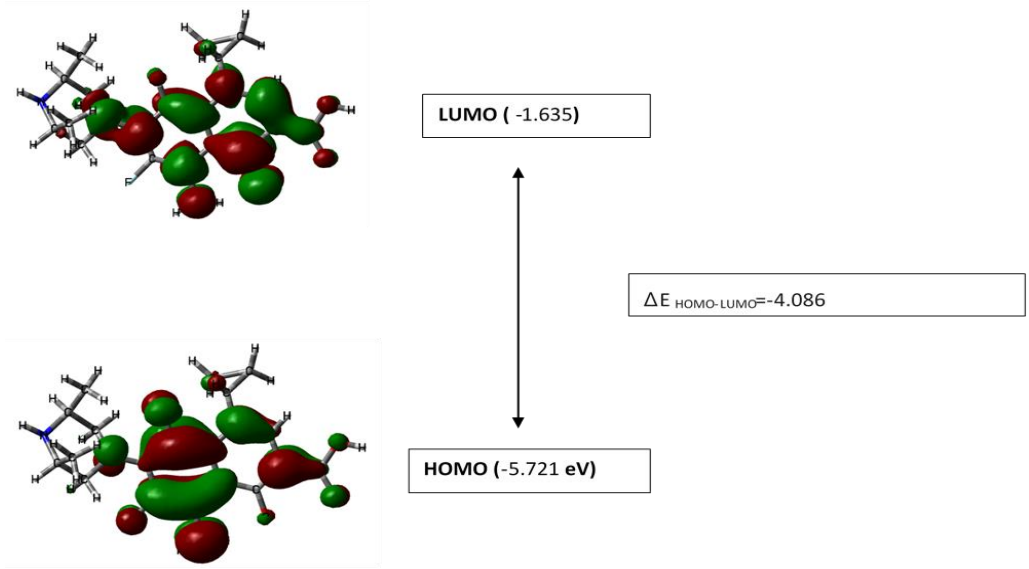


Figure (3): HOMO and LUMO, energy gap of Sparfloxacin

Molecular Electrostatic Potential (MEP)

MEP together with electron density are very important to indicate the sites for electrophilic and nucleophilic reactions [34]and to identify reactive sites of electrophilic or nucleophilic properties of Sparfloxacin. Red color surface means negative and accept proton while blue is positive and do not accept proton Figure (4) shows the total electron density surface mapped with molecular electrostatic potential MEP plot in solid and mesh view. From the MEP, it is blurred that the negative area covers the C4=O14group of qinolone ring and C11=O13 group carboxyl group attached to the qinolone ring of the title compound, another negative region were localized at O12 group carboxyl group, N27 at qinolone ring and N16, N19 of piperazinyl group attached with quinolone ring and the positive region is over the hydrogen of the aromatic qinolone ring and over the hydrogen of piperazinyl ring. The electrostatic potential value is largely responsible for bindings between the substrate and its receptor sites since the receptor and the corresponding ligands recognized

recognize each other at their molecular surface [35].

Vibrational assignments

The Sparfloxacin molecule consists of 50 atoms and has144 symmetrical normal modes. Experimental and calculated FTIR and normal mode descriptions are presented in Table (5) (Table S1 supplementary file) and are shown in Fig.(5).

Experimental FT-IR spectrum of Sparfloxacin is shown in Figure (5), which shows the vibrational peaks at 3093.64-3461.80 cm^{-1} related to O-H and N-H stretching. The vibrational peaks appeared at 2845.29-2962.12 cm^{-1} for C-H (CH3) stretching. Furthermore, the vibrational peaks were observed at 1716.12 cm^{-1} and 1640.78 cm^{-1} due to C=O (COO-) and C=O (pyridone) stretching, respectively. The IR peaks appeared at 1585.33, and 1532.51cm^{-1} related to C=C (benzene ring) stretching and N-H bending, respectively. C-H bending and C=O (COO-) stretching peaks appeared at 1439.40 and 1333.73 cm^{-1} respectively C-N (aryl) stretching and C-F stretching peaks were observed at 1183.98-1293.13 cm^{-1} and 1149 .91 cm^{-1}, respectively. Moreover, the IR peaks appeared at 1084.76, 1027.95, and 670.92 cm^{-1} were assigned to C-O (COO-) stretching C-N (alkyl) stretching, and =C-H bending respectively. The FT-IR experimental data of Sparfloxacin was in well agreement with the calculated DFT and supported by the literature data [13].

UV-vis studies and electronic properties

UV data of Sparfloxacin have been carried out using TD-DFT calculations on Sparfloxacin at two states (gas phase and ethanol) and reported in Table (6). The theoretical and experimental UV-visible spectra are visualized in Figure (6 a &b). As can be seen from Table (6), the calculated absorption maxima values for the title compound were found to be 368.46, 353.01 and 330.74 nm. This band is recorded experimentally as a shoulderat 294 nm. The wavelength calculated at 368.46 nm (f = 0.0432) primarily produced molecular orbital HOMO excitations to LUMO.

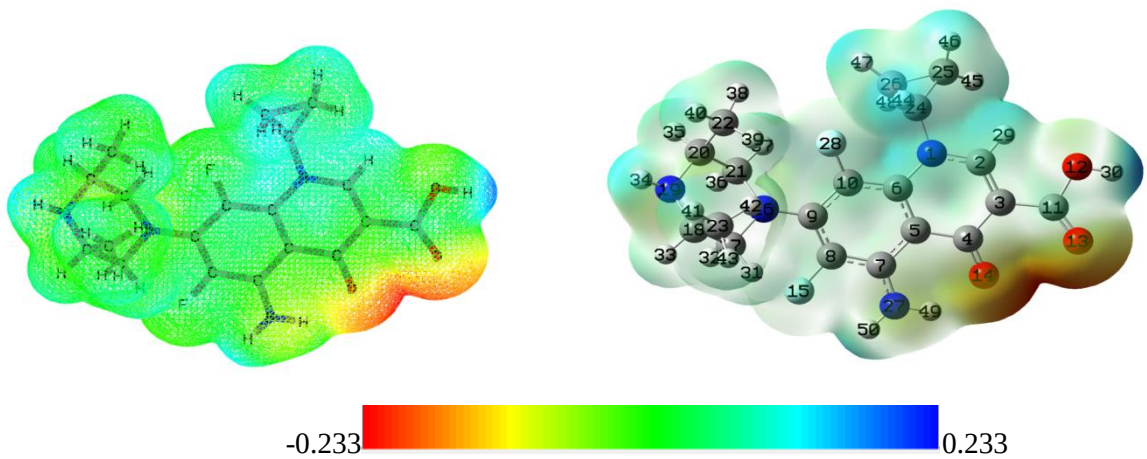


Figure (4): MEP mapped plot in (solid and mesh view) for Sparfloxacin calculated by B3LYP method

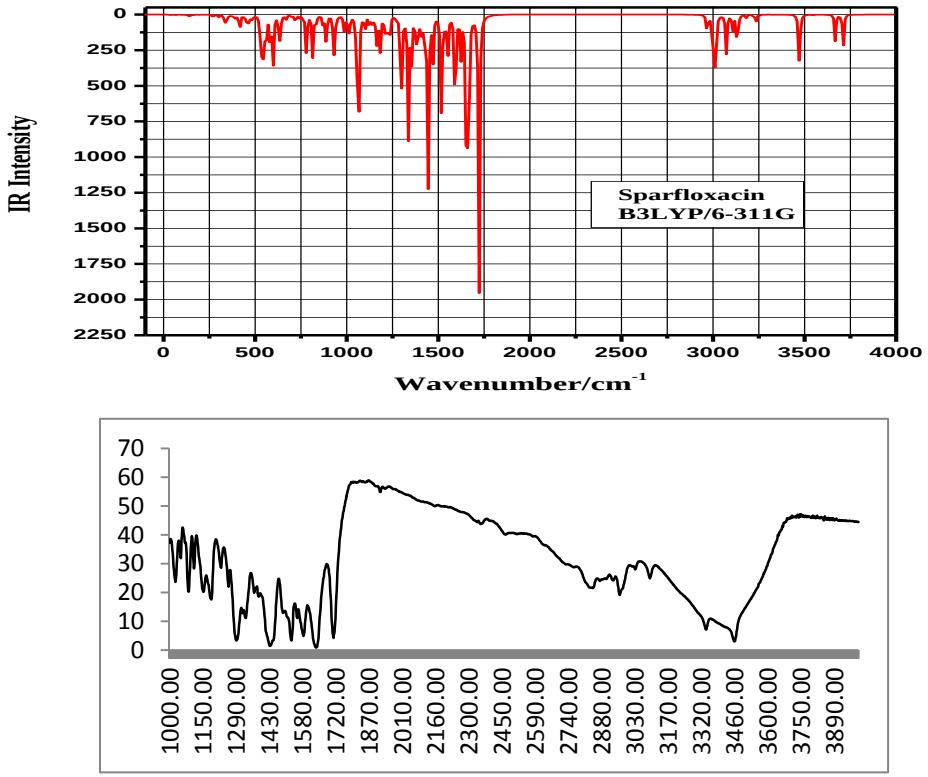


Figure (5): Calculated and experimental FTIR spectra of Sparfloxacin compound

Table (5): Experimental and calculated FTIR spectra of Sparfloxacin

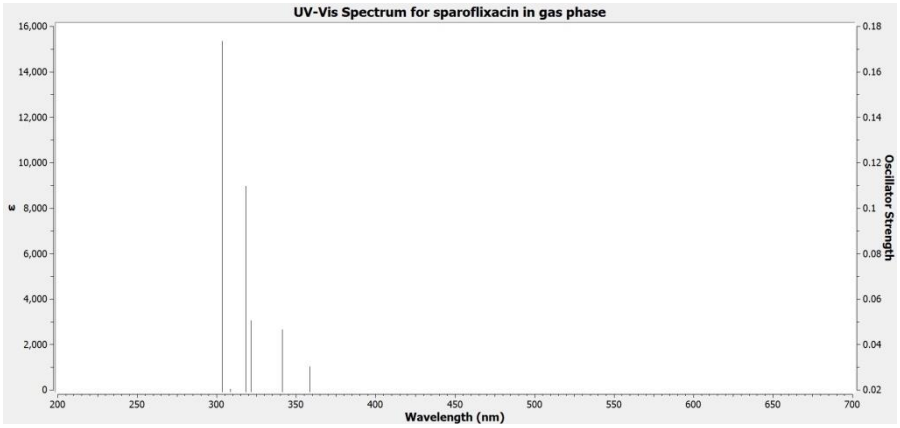
	Observed fundamentals (cm^{-1})	Calculated frequencies νi (cm^{-1}) B3LYP/6-311 G(d,p)		
number		Scal. Frequency	UnScal. Frequency	IR Intensity
1	401	400.81388	414.9212	38.1746
2	424	424.25986	439.1924	2.8214
3	436	435.85476	451.1954	18.2919
4	449	448.92512	464.7258	17.0394
5	459	459.35609	475.5239	4.7524
6	467	467.68861	484.1497	11.0851
7	507	507.33866	525.1953	30.3541
8	519	519.70365	537.9955	109.2297
9	528	528.40519	547.0033	78.9699
10	540	540.02308	559.0301	61.9497
11	563	563.33865	583.1663	75.7629
12	577	577.39047	597.7127	95.3488

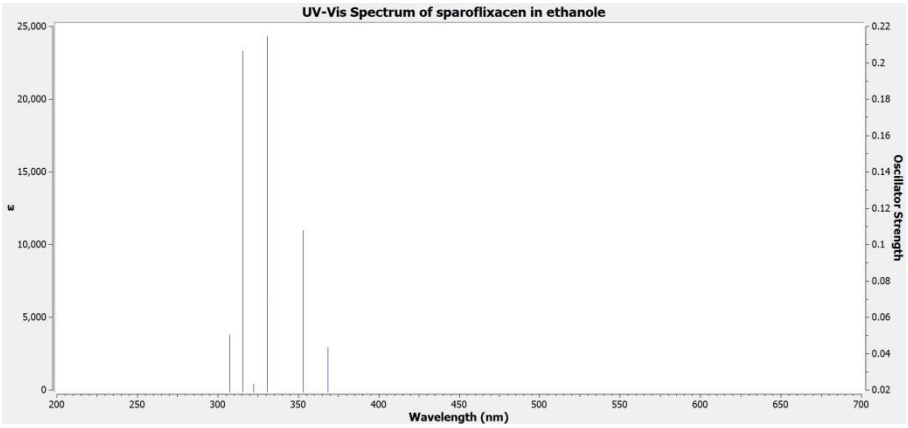
13	579	578.82498	599.1977	0.9245
14	609	608.51566	629.9334	45.2100
15		612.15111	633.6968	19.2710
16	617	616.59703	638.2992	21.2538
17		645.38296	668.0983	10.5173
18		676.27409	700.0767	4.4375
19	694	694.426	718.8675	19.2448
20		718.40937	743.6950	6.3458
21	737	737.04573	762.9873	9.1156
22		752.74371	779.2378	82.1705
23		760.81513	787.5933	6.3225
24		783.84708	811.4359	15.0677
25		786.41123	814.0903	74.5999
26	795	794.89764	822.8754	2.9149
27		803.06806	831.3334	13.0933
28		808.81122	837.2787	3.7330
29	841	841.38339	870.9973	28.2241
30	858	858.06998	888.2712	68.5820
31		892.31159	923.7180	15.5702
32	901	900.69077	932.3921	85.6219
33		908.91809	940.9090	4.8283
34		954.21045	987.7955	14.5372
35	960	959.55137	993.3244	1.0261
36		966.93277	1000.9656	13.6853
37	980	980.06651	1014.5616	46.4282
38	1010.00	1014.56565	1050.2750	27.2882
39	1030.00	1026.27521	1062.3967	352.0324
40	1060.00	1061.84729	1099.2208	29.6988
41		1063.08667	1100.5038	4.4099
42	1080.00	1081.92618	1120.0064	4.6446
43		1083.80003	1121.9462	13.3013
44	1090.00	1092.48205	1130.9338	6.2400
45	1100.00	1102.49087	1141.2949	24.5487
46		1120.12279	1159.5474	21.3721
47	1120.00	1124.21013	1163.7786	0.9440
48	1130.00	1127.36122	1167.0406	61.9158

Correction factor for B3LYP/6-311G is 0.966 [https://cccbdb.nist.gov/vibscalejust.asp]

Table (6): theoritical maximum absorption wavelengths (λ_{max}), excitation energies (ΔE) and oscillator strengths (f) of Sparfloxacin by TD-DFT/B3LYP/6-311g method

Sparfloxacin		Gas phase	In ethanol
Excited State 1	λMax (nm)	358.54	368.46
	ΔE(eV)	3.4580	3.3650
	f(a.u.)	0.0302	0.0432
Excited State 2	λMax (nm)	341.23	353.01
	ΔE(eV)	3.6335	3.5122
	f(a.u.)	0.0466	0.1079
Excited State 3	λMax (nm)	321.42	330.74
	ΔE(eV)	3.8573	3.7487
	f(a.u.)	0.0506	0.2148





Figure(6a):Theoretical UV spectra in gas phase and ethanol

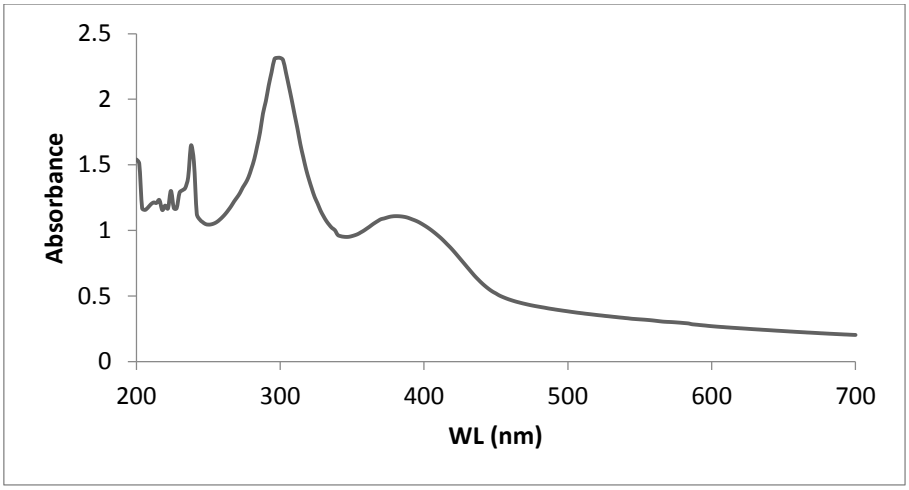


Figure (6 b): Experimental UV spectra

Conclusions

A complete vibrational dynamical and molecular structure analysis of Sparfloxacin has been performed, based on the quantum chemical approach by DFT (B3LYP) calculations. The spectral characterization studies such as FTIR for Sparfloxacin have been carried out. A good agreement was found between the experimental and the calculated normal vibration modes. The assignment of fundamentals was established by the qualitative concurrence between the calculated and the observed band intensities and is assumed to be correct. The NBO results show that the most negative atomic charges are localized at O12, O14 and N27of the qunoline ring and N16 of the piperazyinyl ring. HOMO - LUMO energy gap was reported to be -4.086 eV. This value explains the possible charge transfer interaction with the molecule, which affects structure reactivity of the compound. The relatively high value of $\Delta E_{HOMO-LUMO}$ indicates that the title compound presents a high chemical stability and it has a low reactivity. Molecular Electrostatic Potential map shows that the negative potential sites are on oxygen, nitrogen and fluorine atoms and that the positive potential sites are around the hydrogen atoms. The theoretical UV-vis spectral analysis has also provided insight into the excitation energy and oscillator strength and predicted mainly the $\pi \rightarrow \pi^*$ type electronic transitions which are of intra-molecular charge transfer type. The present quantum chemical study may lead to the understanding of the properties and activity of Sparfloxacin and may also help in extending its use for more medical applications.

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