Experimental spectral characterization, Hirshfeld surface analysis, DFT/TD-DFT calculations and docking studies of (2Z,5Z)-5-(4-nitrobenzylidene)-3-N(2-methoxyphenyl)-2-N'(2-methoxyphenylimino) thiazolidin-4-one

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We reported an experimental and theoretical spectroscopic studies of (2Z,5Z)-5-(4-nitrobenzylidene)-3-N(2-methoxyphenylimino) thiazolidin-4-one (C24H19N3O5S) molecule, using FT-IR, NMR spectroscopy, and density functional theory (DFT) via time-dependent schema (TD-DFT) respectively. The molecular inter-contacts were explored using Hirshfeld surfaces (HS) analysis method. Vibrational frequencies, gauge-independent atomic orbital (GIAO)1H and13C NMR chemical shift values and frontier molecular orbitals (FMOs) have been calculated from the optimized structure of the molecule by DFT/B3LYP functional with 6-31G(d,p) basis set. Our theoretical results show a good agreement with the experimental data. The calculated UV-visible spectrum employing TD-DFT shows electronic transitions at 388 nm and 495 nm. To get insight on the charge interaction happening inside the molecule, HOMO and LUMO were scrutinized and their calculated energy gap was found to be 2.96 eV. The molecular docking was analyzed via interplay study of acetyl cholinesterase, and Butyrylcholinesterase using molecular docking methodology.

1. Introduction

In the last few decades, the design, elaboration and synthesis of new molecules became an active area of research by reason of their widespread applications in several emerging fields such as molecular electronics [1] and nano-biotechnology [2]. In particular, organic molecules and conductive polymers have been already used in many electronic devices such as organic solar cells [3, 4] and single-molecule transistors [5, 6] to name only two. An important class of molecules are the thiazole derivatives. The latter are organic compounds that have five-membered molecular ring structures. They have been emerging as promising materials for several applications in organic electronics and chemical industries including food and pharmaceuticals. As a biologically active agent, thiazole has attracted many research in biology [7, 8, 9, 10]. It has been displayed that the thiazole moiety has antimicrobial activity [11, 12] and the thiazole ring and its compounds are very important pharmacophore [13] and they showed anti-convulsing, anti-inflammatory and anti-tumoractivity [14].

In a recent work, we have determined the structure of the (2Z,5Z)-5-(4-nitrobenzylidene)-3-N(2-methoxyphenylimino) thiazolidin-4-one molecule both experimentally using spectroscopic FT-IR,1H,13C NMR, X-ray single crystal diffraction (XRD) and technically usingB3LYP/6-31G(d,p) [15]. The structure and composition of our molecule are shown in Figure 1. We aim in this paper, to further extend our analysis by studying the vibrational properties and chemical shifts of the C24H19N3O5S molecule, experimentally applying
UV-Visible, NMR spectroscopy and theoretically using Natural Bond Orbital (NBO) and Frontier Molecular Orbitals (FMOs) calculations within the DFT at the B3LYP/6-31G(d, p) level. On the microscopic scale, the later provide a powerful tool to investigate the electronic, magnetic and optical properties of atoms, molecules and condensed phases [16] and their outcomes are proved to fit very well with experiments [17]. It is helpful to conduct a comparison between experimental and theoretical spectra to determine proper assignments and understand the origin of the chemical shift in molecular structure. In order to predict theoretically the UV-Vis spectra of the present molecular system, we have employed a time-dependent (TD-DFT) known to one of the most accurate approaches as regard for computational cost and findings efficiency [18, 19]. For the $^1$H and $^{13}$C chemical shifts, we have used Gauge independent atomic orbital theory (GIAO) [20, 21]. The evaluated HOMO and LUMO energies confirm the existence of charge transfer occurring in the molecule. Throughout the paper, we compared the experimental data with the calculated results.

2. Experimental and theoretical methodologies

FT-IR spectrum was recorded in the 4000–400 cm$^{-1}$ region with a JASCO 4200 FT-IR spectrometer using KBr pellet. $^1$H and $^{13}$C-NMR spectra were recorded at 300 MHz, in CDCl$_3$, on a BRUKER Ac DXP-200 spectrometer. The chemical shifts are reported per million (ppm) down field from internal tetramethylsilane (TMS) (chemical shift in δ values).

Electronic absorption spectrum was measured on a Unicam UV–Vis spectrophotometer in chloroform solvent. Spectrums were recorded at room temperature. All calculations were performed with the Gaussian 03 software package [22] and Gauss-View program [23]. B3LYP method is employed to optimize the molecular structure [24, 25] of the C$_{24}$H$_{19}$N$_3$O$_5$S molecule leading to energy minima in the ground state using the 6-31G(d, p) basis set [26, 27].

3. Results and discussion

3.1. Optimized geometry

The geometrical parameters, namely bond lengths, bond angles, and dihedral angles for C$_{24}$H$_{19}$N$_3$O$_5$S molecule computed by DFT/B3LYP functional with 6-31G(d, p) basis set are listed together with the X-ray diffraction data [15]. The calculated and experimental geometrical parameters of the title compound were found to be close, which indicate that our calculations are good. The small differences can be due to the fact that the calculated values are collected in the gas phase, while experimental data are achieved in the solid state. To make a better comparison of the calculated geometrical parameters, correlation graphs between the calculated and the experimental parameters of bond lengths, bond angles and dihedral angles are plotted and shown in Figure 2. The correlation values R$^2$ obtained by B3LYP functional with 6-31G(d,p) basis set are 0.994, 0.912, and 0.999 for bond lengths, bond angles and dihedral angles, respectively. These graphs confirmed the good agreement between calculated and experimental results.

3.2. Hirshfeld surface analysis

Hirshfeld surface analysis is employed to estimate the distribution of close contact interactions [28]. The structure input file in cif format and the Crystal Explorer have been used to calculate respectively the Hirshfeld surfaces and the related 2D-Fingerprint plots [29]. In the $d_{shape}$ surface, any intermolecular interactions appear as a red spot as shown in Figure 3(a). The presences of π–π stacking interactions are indicated by red and blue triangles on the shape-index surface presented in Figure 3(b). As seen in Figure 3(c), the deep red color indicates hydrogen bonding contacts. For example, a deep red spot indicates the presence of a hydrogen bond, type C–H⋯O (between H7 and O3) and C–H⋯N (between H21 and N3). The 2-D fingerprint plots, which analysis all intermolecular contacts altogether and revealed that the principal intermolecular interactions s is of type H⋯H, H⋯O, H⋯C, H⋯N and C⋯C as shown in Figure 4(a). The two-dimensional fingerprint presentation shows that the majority of contacts are due to H⋯H interaction. This interaction constitute up to 35.8% of the Hirshfeld surface of the (Z,Z)-5-(4-nitrobenzylidene)-3-N(2methoxyphenyl)-2-N’(2-methoxyphenylimino)thiazolidin-4-one molecule. For the present compound, H⋯O contacts that were attributed to C–H⋯O–H bond interactions, appear as two sharp symmetric spikes in the two-dimensional fingerprint map. The existence of these long spikes (displayed in Figure 4(d)) is a proof of strong hydrogen bonds. The intermolecular O⋯H and H⋯O contacts shown in Figure 4 provide a contribution of 22.9% to the HS of the C$_{24}$H$_{19}$N$_3$O$_5$S molecule. In Figure 4(c), the C–H⋯C–H intermolecular interactions comprise 22.9% of the total HS and represent two characteristic wings. The C–C contact includes only 4.3% of the total Hirshfeld surfaces area as shown in Figure 4(e) which is mainly assigned to π–π interaction. The N⋯H/H⋯N interactions comprising 3.7% of Hirshfeld surface area, so appear weekly in the fingerprint plot. Figure 5 shows other contributions that are listed in decreasing order of one percent.

3.3. Vibrational assignments

We report in Table 1, both of experimental and computed vibrational frequencies with interrelated vibrational assignments and intensities. Also, we compare the experimental and calculated IR spectra plots in Figure 6. The calculated IR bands were carried out with the DFT with the functional B3LYP in conjunction with the 6-31G(d, p) basis set. Our C$_{24}$H$_{19}$N$_3$O$_5$S molecule consists of (52) atoms having 119 normal modes of vibrations. Also, the calculated vibrational assignments of the normal modes were performed on the basis of the Potential Energy Distribution (PED) and it has been calculated using the Vibrational Energy Distribution Analysis VEDA 4 program [30]. Usually, the calculated vibrational frequencies are higher than the corresponding experimental results. The

Figure 1. (a) Experimental structure and (b) optimized structure using B3LYP/6-31G(d, p) with the atomic numbering for C$_{24}$H$_{19}$N$_3$O$_5$S molecule.
computed wavenumbers values were scaled by scaling factor 0.9608 for DFT [31]. After scaling, the errors are minimized and the calculated vibrations show an excellent compatibility with the experimental values.

### 3.3.1. Benzene ring vibrations

The aromatic C-H stretching modes absorption in poly-substituted benzenes has been reported in the literature to be between 3000 and 3100 cm⁻¹ [32]. Our results are in good accordance with those values. The C–H aromatic stretching mode was observed at 3058 cm⁻¹ experimentally and computed at 3062 cm⁻¹. Our determination of the carbon–carbon stretching vibrations also demonstrates a good agreement between theory and experiments. The carbon–carbon stretching vibrations were observed in the FT-IR spectrum at 1587, 1513, 1504, 1461 cm⁻¹ whereas the corresponding DFT calculated values are found to be 1580, 1571, 1542, 1475 cm⁻¹ respectively. The CCC in plane bending bands are expected in the literature to be between 1000 and 600 cm⁻¹ [33]. In this work, the CCC in plane bending bands were observed at 619 cm⁻¹ in the IR spectrum and calculated at 620 cm⁻¹ using the DFT method. The computed wavenumbers at 1036 cm⁻¹ are identified as CCC out of plane bending vibrations. The wavenumbers of CCC in plane bending vibrations are computed at 672 and 671 with intensities 18.2 and 13.4 respectively.

### 3.3.2. Carbonyl vibrations

The carbonyl group wavenumber (C=O) stretching vibration is expected in the literature to be in the range 1710 cm⁻¹ [34]. In our study, the experimental IR spectrum of carbonyl shows a strong band at 1721 cm⁻¹ and the theoretically calculated value is 1738 cm⁻¹.

### 3.3.3. Methoxy group vibrations

In the FT-IR spectrum, the CH-stretching vibrations in OCH₃ group appeared at 2836 cm⁻¹. However, the DFT calculations lead to values in the range 3033 to 2897 cm⁻¹. The DFT calculated asymmetric stretching vibrations are shifted to the range 3026-2897 cm⁻¹. These values fit well with the results reported in the literature which are in the range 3034-2967 cm⁻¹ and 2917-2904 cm⁻¹ respectively for CH asymmetric and symmetric stretching vibrations [35]. The asymmetric and symmetric O=C=O stretching vibrations of methoxy group attached to an aromatic ring are given in the range 1310–1010 cm⁻¹ [36,37]. In the present work, the symmetric υ₁O-Cₙ vibrations were observed in the medium FTIR band at 1255 cm⁻¹, 1042 cm⁻¹ and calculated at 1258 and 1038 cm⁻¹ by DFT method. The asymmetric υ₂O-Cₙ vibrations were observed in the medium FTIR band at 1490, 1240 cm⁻¹ and calculated at 1258 and 1489, 1482, 1241, 1232 cm⁻¹ by the DFT method.

### 3.3.4. C-S group

In the literature, the C–S stretching vibration was observed between 800 cm⁻¹ and 646 cm⁻¹ for thiazole ring [38]. Our infrared experimental spectrum shows bands at 496 cm⁻¹, 680 cm⁻¹ which is assigned to asymmetric C–S stretching in the thiazole ring. The calculated values are predicted to be 17 cm⁻¹ to 9 cm⁻¹ respectively down than the experimental values.

### 3.3.5. C=N group

In this study, the C–N stretching vibration is observed at 1650 cm⁻¹ in the IR spectrum and it is reported at 1640 cm⁻¹ [39]. The others single C–N bands are cited in the Table 1.

### 3.3.6. NO₂ group

The NO₂ symmetrical stretching vibration is calculated at 1329 cm⁻¹ using the DFT at the B3LYP level. The computed wavenumbers are found to be 834 and 638 cm⁻¹ and they are assigned to N=O–N in plane bending vibrations of the nitro group. It was shown that the aromatic nitro compounds give strong peaks at the range of 1570–1485 cm⁻¹ and 1370–1320 cm⁻¹ due to asymmetric and symmetric stretching vibrations of the NO₂ group, respectively [13, 16].

### 3.4. Electronic properties

#### 3.4.1. Frontier molecular orbital and UV–Vis spectral analysis

The lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO) are very important properties in quantum chemistry. LUMO is not occupied by electrons and produces the capacity to receive an electron. HOMO represents the ability to deliver an electron. The energy difference between them (HOMO and LUMO) is responsible on the chemical reactivity, optical polarizability and chemical hardness–softness of a molecule [40]. It is well known that molecules showing a small frontier orbital gap are easy to polarize and show a high

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![Figure 2](image-url)  
**Figure 2.** Correlation graphics of calculated and experimental bond lengths, bond angles and dihedral angles of C₂₄H₁₉N₃O₅S.
chemical reactivity. They have low kinetic stability and can be seen as soft molecules [41]. In the present research work, we have used the DFT/B3LYP/6-31G (d,p) to calculate the energy values of the HOMO, LUMO, HOMO-1, LUMO+1, HOMO-2 and LUMO+2 (Figure 7). The energy values are given respectively by \(-5.828\) eV, \(-2.858\) eV, \(-6.404\) eV, \(-1.585\) eV, \(-6.434\) eV and \(-0.782\) eV. The value of gap energy excitation from HOMO to LUMO is calculated to be about \(2.969\) eV. It is clear from Figure 7 that the HOMO is located over the benzene related to methoxy group and LUMO, LUMO+1, LUMO+2 are located over the benzene related to the nitro group. Whereas, the HOMO-1 and HOMO-2 are delocalized over the entire molecule.

To compare with the experimental results of the UV-vis spectra, we have employed the TD-DFT method which provides an accurate value for the absorption wavelengths. The latter correlate to vertical electronic transitions computed on the ground state geometry. Calculations of the molecular orbital geometry show that the visible absorption maxima of this molecule correspond to the electron transition between frontier orbital such as translation from HOMO to LUMO. The UV-vis spectrum for our compound is measured in chloroform solvent in the region of 800-200 nm. This spectrum is also obtained using B3LYP level of TD-DFT with 6-31G(d,p) basis. We employed a fully optimized ground-state structure and TD-DFT/B3LYP/6-31G(d,p) calculations to compute the vertical excitation energies, oscillator strength and absorption wavelength. As per the Frank–Condon principle, the maximum absorption peak (\(\lambda_{\text{max}}\)) in a UV spectrum corresponds to vertical excitation. Both of experimental and theoretical UV spectra are plotted in Figure 8.

The DFT calculations based B3LYP/6-31G(d,p) announce that theoretical UV-Vis spectrum shows two absorption peaks at 495 nm and 360 nm with oscillators strengths \(f = 0.0445\) and 0.3692 respectively. Also, we can observe absorption peaks observed in high energy region at 468 nm and 360 nm from the UV-vis absorption spectrum. They are assigned as \(n \rightarrow \pi^*\) and \(\pi \rightarrow \pi^*\) respectively, which are in excellent accord with the DFT calculated maximum values.

### 3.4.2. Global reactivity descriptors

Global chemical reactivity descriptors (GCRD) parameters are a good indication to highlight the relationship between chemical reactivity and strength of structure. GCRD parameters can be obtained using the following equations:

\[
\eta = \frac{1}{2} (E_{\text{LUMO}} - E_{\text{HOMO}}); \quad \mu = \frac{1}{2} (E_{\text{LUMO}} + E_{\text{HOMO}}); \quad S = \frac{1}{2} \eta; \\
\chi = \frac{1}{2} (E_{\text{LUMO}} + E_{\text{HOMO}}); \quad \omega = \frac{\mu^2}{2\eta}; \quad E_A = -E_{\text{LUMO}} \quad \text{and} \quad I_p = -E_{\text{HOMO}}
\]

where \(\eta\) is the global hardness, \(\mu\) is the chemical potential, \(S\) is the global softness, \(\chi\) is the electronegativity, \(\omega\) is the electrophilicity index.

According to the Table 2, the chemical hardness value (\(\eta\)) was calculated at 1.485 eV using functional B3LYP in conjunction with the 6-31G(d,p) basis set, indicating that charge transfer occurs within the molecule. The electrophilic conduct of the molecule is confirmed by the global electrophilic index (\(\omega\)) which has a value of 17.732 eV. On the additional hand, the chemical stability of the titer molecule is expressed by the chemical potential value (\(\mu\)) which is \(-7.257\) eV.

### 3.4.3. Optical band gap

The gap energy between HOMO and LUMO can be measured experimentally by spectroscopic methods and conductivity [42]. The UV-visible spectrum can be used as a simple and straight forward technique to accurately estimate the gap energy for \(\pi\)-conjugated materials.
From UV-visible spectrum, the optical gap can be estimated according to equation (1).

$$E_g (eV) = \frac{h \cdot v}{\lambda_{Eg}} \approx \frac{1240}{\lambda_{Eg} (nm)}$$

The optical gap, $E_g$, is expressed in eV and $\lambda_{Eg}$ is the absorption band expressed in nm obtained from the intersection of the two lines as shown in Figure 9 [43].

From the experimental UV-visible spectrum, the wavelength is $\lambda_{Eg} = 423$ nm, so the optical gap value is equal to 2.931 eV, this value is close to the band gap value calculated by DFT, 2.969 eV. This work has shown that UV-Vis analysis in the CHCl₃ solution can be used as an easy and direct technique to accurately estimate the band gap energy of conjugated $\pi$ organic compounds, which is a crucial property to evaluate the optical and conductive properties of a material. The experimental value approach and calculated by the functional B3LYP and the bases 6-31G(d, p) confirms the correct choice of models of calculations.

### 3.4.4. $^1$H and $^{13}$C NMR spectra

The use of $^1$H and $^{13}$C NMR spectroscopy is one of the important tools in characterizing molecules. The $^1$H and $^{13}$C NMR spectra of the C₂₄H₁₉N₃O₅S molecules are performed by Bruker Ac DPX-200 (300 MHz) spectrometer in CDCl₃ as solvent. The experimental results are compared to the GIAO (gauge-independent atomic orbital) $^1$H and $^{13}$C chemical shift values. The latter were computed from B3LYP functional and 6-31G(d, p) basis set. The geometry of C₂₄H₁₉N₃O₅S together with that of tetramethylsilane (TMS) were fully optimized. For comparing the theoretical $^1$H NMR chemical shifts of our compound with the experimental data, the $^1$H and $^{13}$C NMR chemical shifts were converted to the TMS scale by subtracting the calculated absolute chemical shielding of TMS with values of 31.75 ppm ($^1$H) and 192.82 ppm ($^{13}$C) for B3LYP/6-31G (d, p). Experimental results together with the theoretical one are gathered in Table 3.

The formation of the C₂₄H₁₉N₃O₅S was clearly proved by the appearance of singlet two peaks of OCH₃ at 3.72 ppm and 3.82 ppm. Note that the chemical shift of the protons of the methoxy group (O–CH₃) is deblinded, following the delocalization of the free doublet of oxygen generated by the group imino (C= N). The corresponding theoretical values of the mentioned peaks are observed at 3.46–3.90 ppm and 3.62–3.97 ppm, respectively. In the $^1$H NMR spectrum, the aromatic proton signals appear as a multiplet at 6.79–8.18 ppm regions whereas the calculated values are observed at 6.63–8.44 ppm. The peak of methine proton exo-cyclic appeared at 7.73 ppm experimentally and observed at 7.64 ppm from computations. Signals exhibited at 8.42 and 8.44 ppm might be attributed to H6, H2 protons respectively close to the nitro group. While the $^{13}$C NMR spectra of the title compound showed the presence of carbonyl carbon atoms at 165.69 ppm. This value is observed at 160.50 ppm theoretically. Carbons of methoxy groups (C23 and C24) are calculated at 53.88 ppm and 53.55 ppm respectively, these values are observed at 55.98 ppm and 55.90 ppm experimentally. As reported by these results, the calculated chemical shifts are in good compliance with...
| Mode no. | Experimental wavenumbers (cm$^{-1}$) | Theoretical wavenumbers (cm$^{-1}$) (B3LYP/6-31G(d,p)) | Assignments with PED (≥10 %) |
|---------|-----------------------------------|-------------------------------------------------|----------------------------------|
|         | Unscaled                          | Scaled                                          | $I_{nm}$                          |
| 118     | 3248                              | 3120                                           | 1.4                              |
| 117     | 3247                              | 3120                                           | 0.8                              |
| 116     | 3229                              | 3102                                           | 8.5                              |
| 115     | 3227                              | 3100                                           | 4.6                              |
| 114     | 3225                              | 3098                                           | 14.2                             |
| 113     | 3219                              | 3093                                           | 12.0                             |
| 112     | 3210                              | 3085                                           | 16.4                             |
| 111     | 3205                              | 3080                                           | 14.8                             |
| 110     | 3200                              | 3074                                           | 4.5                              |
| 109     | 3198                              | 3072                                           | 16.4                             |
| 108     | 3190                              | 3065                                           | 4.2                              |
| 107     | 3058                              | 3062                                           | 0.2                              |
| 106     | 3169                              | 3045                                           | 0.9                              |
| 105     | 3033                              | 3033                                           | 15.8                             |
| 104     | 3150                              | 3026                                           | 19.4                             |
| 103     | 2994                              | 2969                                           | 29.6                             |
| 102     | 2942                              | 2975                                           | 38.0                             |
| 101     | 3024                              | 2906                                           | 54.4                             |
| 100     | 3016                              | 2897                                           | 71.4                             |
| 99      | 1721                              | 1738                                           | 87.7                             |
| 98      | 1650                              | 1677                                           | 872.0                            |
| 97      | 1606                              | 1604                                           | 122.3                            |
| 96      | 1660                              | 1595                                           | 49.7                             |
| 95      | 1659                              | 1594                                           | 35.3                             |
| 94      | 1587                              | 1580                                           | 22.1                             |
| 93      | 1644                              | 1579                                           | 83.8                             |
| 92      | 1643                              | 1579                                           | 51.2                             |
| 91      | 1513                              | 1571                                           | 6.3                              |
| 90      | 1504                              | 1542                                           | 120.0                            |
| 89      | 1490                              | 1489                                           | 109.1                            |
| 88      | 1542                              | 1482                                           | 70.6                             |
| 87      | 1461                              | 1475                                           | 14.7                             |
| 86      | 1518                              | 1459                                           | 51.2                             |
| 85      | 1517                              | 1458                                           | 44.0                             |
| 84      | 1506                              | 1447                                           | 12.3                             |
| 83      | 1505                              | 1446                                           | 4.8                              |
| 82      | 1505                              | 1446                                           | 4.8                              |
| 81      | 1499                              | 1440                                           | 2.7                              |
| 80      | 1481                              | 1423                                           | 18.9                             |
| 79      | 1410                              | 1421                                           | 27.4                             |
| 78      | 1376                              | 1396                                           | 13.1                             |
| 77      | 1395                              | 1340                                           | 58.8                             |
| 76      | 1336                              | 1333                                           | 208.2                            |
| 75      | 1384                              | 1329                                           | 982.9                            |
| 74      | 1358                              | 1305                                           | 42.4                             |
| 73      | 1357                              | 1303                                           | 22.6                             |
| 72      | 1356                              | 1303                                           | 45.8                             |
| 71      | 1290                              | 1277                                           | 23.7                             |
| 70      | 1280                              | 1270                                           | 69.2                             |
| 69      | 1318                              | 1266                                           | 80.7                             |
| 68      | 1255                              | 1258                                           | 123.8                            |
| 67      | 1240                              | 1241                                           | 154.7                            |
| 66      | 1283                              | 1232                                           | 63.1                             |
| 65      | 1252                              | 1203                                           | 45.52                            |
| 64      | 1184                              | 1170                                           | 8.4                              |
| 63      | 1172                              | 1167                                           | 23.5                             |

(continued on next page)
| Mode no. | Experimental wavenumbers (cm⁻¹) | Theoretical wavenumbers (cm⁻¹) (B3LYP/6-31G(d,p)) | Assignments with PED (≥ 10 %) |
|---------|-------------------------------|---------------------------------|--------------------------------|
| 62      | 1160                          | 1214, 1166                      | δ HCC (133) + δ HCCC (13) + δ HCCC (44) |
| 61      |                               | 1194, 1147                      | ν δHCC37 (10)                  |
| 60      |                               | 1192, 1145                      | δ HCC (ring2) (80)            |
| 59      |                               | 1190, 1143                      | ν CCCCring3 (10) + ν HCCC (ring2) (60) |
| 58      |                               | 1182, 1136                      | ν HCCC (31)                   |
| 57      |                               | 1179, 1133                      | δ HCCCring3 (25) + δ HCCC (methoxy) (27) |
| 56      |                               | 1178, 1132                      | δ HCC (ring2) (25) + δ HCCC (methoxy) (73) |
| 55      |                               | 1146, 1100                      | δ HCC (ring1) (45)            |
| 54      |                               | 1140, 1095                      | ν HCCC (ring3) (10)           |
| 53      | 1051                          | 1131, 1087                      | ν HCCC (ring1) (56) + δ HCC (ring3) (11) + γ HCC (ring1) (12) |
| 52      | 1042                          | 1080, 1038                      | ν HCCC (methoxy) (38) + ν HCCC (ring3) (13) |
| 51      |                               | 1078, 1036                      | ν HCCCring2 (47) + ν HCCC (ring2) (11) + γ HCCC (ring2) (10) |
| 50      | 1022                          | 1064, 1023                      | ν HCCC (ring2) (59)           |
| 49      |                               | 1064, 1022                      | ν HCCCring2 (66)              |
| 48      |                               | 1059, 1017                      | ν HCCC (ring3) (20) + δ HCCC (ring3) (10) |
| 47      |                               | 1029, 988                       | δ HCCC (ring1) (14) + δ HCCC (ring1) (77) |
| 46      |                               | 993, 954                        | τ HCCC (ring3) (79)           |
| 45      |                               | 981, 943                        | τ HCCC (ring3) (59) + τ HCCC (ring3) (11) |
| 44      | 935                            | 979, 941                        | τ HCCC (ring2) (70) + τ HCCC (ring2) (10) |
| 43      | 929                            | 966, 928                        | τ HCCCring3 (65) + τ HCCC (ring3) (27) |
| 42      | 913                            | 943, 906                        | τ HCCCring2 (10) + τ HCCC (ring2) (76) |
| 41      |                               | 941, 904                        | τ HCCC (ring3) (73)           |
| 40      |                               | 927, 891                        | τ HCCC (ring3) (87)           |
| 39      | 871                            | 909, 874                        | τ HCCC (ring3) (14)           |
| 38      | 850                            | 874, 839                        | τ HCCC (ring3) (12)           |
| 37      |                               | 868, 834                        | ν HCCC (ring1) (24) + ν HCCC (ring1) (33) |
| 36      |                               | 863, 829                        | τ HCCC (ring1) (72)           |
| 35      | 826                            | 860, 826                        | τ HCCC (ring3) (57)           |
| 34      | 817                            | 855, 822                        | τ HCCC (ring1) (71)           |
| 33      |                               | 838, 805                        | ν δHCCC (ring3) (20)          |
| 32      |                               | 838, 805                        | τ HCCC (ring1) (88)           |
| 31      | 770                            | 805, 774                        | ν δHCCC (ring2) (10)          |
| 30      |                               | 787, 756                        | δ HCCC (ring1) (14)           |
| 29      | 749                            | 777, 746                        | τ HCCC (ring3) (17)           |
| 28      |                               | 763, 733                        | τ HCCC (ring3) (19)           |
| 27      |                               | 763, 733                        | τ HCCC (ring3) (59) + τ HCCC (ring2) (40) + γ OCCC (ring2) (12) |
| 26      | 731                            | 762, 732                        | τ HCCC (ring3) (72)           |
| 25      |                               | 740, 711                        | τ HCCC (ring3) (12) + τ HCCC (ring3) (51) |
| 24      |                               | 734, 705                        | τ HCCC (ring3) (66)           |
| 23      | 689                            | 723, 695                        | τ HCCC (ring3) (16) + τ HCCC (ring2) (12) |
| 22      |                               | 700, 672                        | δ HCCC (ring1) (10) + τ HCCC (ring3) (41) |
| 21      | 680                            | 698, 671                        | ν as CH (thioamide) (12) + δ HCCC (ring1) (21) + τ HCCC (ring3) (18) |
| 20      | 650                            | 664, 638                        | ν δHCCC (ring3) (13) + δ HCCC (ring2) (11) + δ HCCC (ring2) (12) |
| 19      | 619                            | 646, 620                        | δ HCCC (ring3) (14) + ν HCCC (ring3) (21) |
| 18      | 631                            | 651, 626                        | δ HCCC (ring3) (27) + δ HCCC (ring3) (12) |
| 17      | 595                            | 614, 589                        | δ HCCC (ring3) (25) + τ HCCC (ring2) (13) |
| 16      |                               | 609, 585                        | ν δHCCC (ring3) (13)          |
| 15      |                               | 600, 577                        | τ HCCC (ring3) (20)           |
| 14      | 559                            | 575, 553                        | δ HCCC (ring3) (10) + δ HCCC (ring3) (20) + δ HCCC (methoxy) (17) |
| 13      |                               | 571, 549                        | δ HCCC (ring3) (10) + τ HCCC (ring2) (10) |
| 12      |                               | 565, 543                        | δ HCCC (ring3) (19)           |
| 11      | 530                            | 559, 537                        | τ HCCC (ring3) (14) + τ HCCC (ring3) (23) + δ HCCC (ring3) (18) |
| 10      | 516                            | 557, 516                        | τ HCCC (ring3) (11) + τ HCCC (ring3) (11) + τ HCCC (ring2) (10) |
| 9       | 533                            | 512, 509                        | ν OCCC (10) + τ HCCC (ring2) (10) |
| 8       | 530                            | 509, 498                        | ν OCCC (20) + τ HCCC (ring2) (10) |
| 7       | 498                            | 498, 498                        | ν δHCCC (28)                 |
| 6       | 496                            | 499, 479                        | ν HCCC (ring3) (22) + δ HCCC (methoxy) (15) |
| 5       | 469                            | 481, 462                        | τ HCCC (13) + ν HCCC (ring3) (13) + γ N2CC6C12 (10) |

(continued on next page)
the experimental data. Furthermore, the small shifts might be due to the molecular environmental change.

### 3.4.5. Natural bond orbital analysis

NBO analysis provides useful information about intra-and intermolecular bonding. Also, it gives details dealing with interactions in connection with bonds, and can be seen as a convenient tool for exploring charge transfer within molecular systems. The NBO calculations were performed using NBO program [44] as implemented in the Gaussian03 software package. Again, we employed DFT/B3LYP/6-31G(d,p) approach to draw a picture about the intra-molecular hybridization and delocalization of electron density within the molecule. The π-electron delocalization is maximum around π(C1-C6), π(C2-C3) and π(C4-C5) distributed to π* anti-bonding of π*(C2-C3), π*(C4-C5) and π*(C1-C6) with a stabilization energy of about 17.29–23.93 kcal mol⁻¹ as shown in Table 4. The analysis for the title compound shows strong intra-molecular hyper-conjugated interactions π(C11-C12) shows strong stabilization energies of 21.96 kcal mol⁻¹ and 16.17 kcal mol⁻¹ with π*(C16-C15) and π*(C14-C13) respectively and π(C16-C15) shows comparable stabilization energy of 17.05 kcal mol⁻¹ and 22.38 kcal mol⁻¹ with π*(C11-C12) and π*(C14-C13) respectively. This reveals that (C16-C15) prefers to be acceptor than to be a donor with (C11-C12). Conversely π(C14-C13) involves interaction with π*(C11-C12) and π*(C16-C15) with stabilization energy of 23.23 kcal mol⁻¹ and 17.31 kcal mol⁻¹ indeed it gives the explanation that (C11-C12) prefers to be an acceptor with (C14-C13). The important intra-molecular hyper-conjugated interactions are: (N3-C10) from (S1) of n2(S1) → π*(C16-C15) (26) + π*(C16-C15) (19).

### Table 1 (continued)

| Mode no. | Experimental wavenumbers (cm⁻¹) | Theoretical wavenumbers (cm⁻¹) (B3LYP/6-31G(d,p)) | Assignments with PED (≥10 %) |
|----------|---------------------------------|-------------------------------------------------|------------------------------|
|          | Unscaled                        | Scaled                                          | Iₚ  |                         |
| 4        | 448                             | 460                                             | 442 | 0.6                      | τCCCC(ring3) (50) |
| 3        | 433                             | 447                                             | 429 | 1.2                      | τCCCC(ring1) (54) |
| 2        | 408                             | 419                                             | 402 | 0.5                      | τHCCC (ring1) (11) + τCCCC(ring1) (62) |
| 1        | 417                             | 417                                             | 400 | 18.4                     | θ adv13C (29) + θ adv13C (19) |

ν: Stretching; s: symmetric; as: asymmetric; δ: in plane bending; γ: out of plane bending; τ: twisting; ρ: rocking. Scaled frequencies are in units of cm⁻¹, Iₚ infrared intensities are in units of km mol⁻¹.

Figure 6. Comparison between experimental and calculated FT-IR spectra of using B3LYP/6-31G(d, p) approach.

Figure 8. UV-visible theoretical spectrum and experimental in chloroform solvent.

Figure 7. Molecular orbital surfaces and energy levels for the HOMO, LUMO, HOMO-1, LUMO+1, HOMO-2 and LUMO+2 of the C₂₅H₁₉N₃O₅S molecule computed at B3LYP/6-31G(d, p) level.
(N3-C10),(C9-N2) from (O3) of n2 (O3)→π* (C9-N2),(C16-C15) from (O4) of n2 (O4)→π* (C16-C15) and (C22-C21) from (O5) of n2 (O5)→π* (C22-C21) with electron densities 1.76144, 1.84216, 1.83710, 1.83777 e and stabilization energies 21.91, 29.32, 31.93, 30.98 kcal mol⁻¹. The energy value of the interactions π* (C16-C15) →π* (C14-C13) is 281.71 kcal mol⁻¹, indicating that these interactions produce a great stabilization in the molecule. The delocalization of electrons due to n3 (O2) →π* (O1-N1), n1 (N2)→π* (C9-O3) and n1 (N2)→π* (N3-C10) having the highest intra-molecular charge transfer interaction (ICT) energies (E(2)) of 163.38, 54.70 and 44.18 kcal mol⁻¹ respectively.

In Table 5, σ (C1-C6) orbital with 1.97633 electrons has 51.03% C1 character in a sp¹.65 hybrid and has 48.97% C6 character in a sp¹.98 hybrid. The sp¹.65 hybrid on C has 62.29% p character and sp¹.98 hybrid on C have 66.46% p character C24H19N3O5S molecule. The σ (C2-C3) orbital with 1.97569 electrons has 50.19% C2 character in a sp¹.80 hybrid and has 49.81% C3 character in a sp¹.84 hybrid. The sp¹.80 hybrid on C has 64.31% p-character and the sp¹.83 hybrid on C has 64.58% p-character in a sp¹.65 hybrid.

3.4.6. Molecular electrostatic potential (MEP)

The distribution of charges (either positive or negative) in molecules/crystal can be understood from calculation of the molecular electrostatic potential (MEP) [45]. The electrostatic potential is important in the study of intermolecular interactions of molecular systems and it can be obtained from the experimental X-ray diffraction data and the ab-initio theoretical calculations [46, 47]. To study the reactive sites of our molecule, the molecular electrostatic potential was computed from the optimized geometry using B3LYP/6-31G(d,p) functional and its surface map is shown in Figure 10.

As can be seen in Figure 10, the different values of the electrostatic potential of our molecule are represented by different colors in the ranges -0.05072 and +0.05072. The electrostatic potential map and the ab-initio theoretical calculations [46, 47]. To study the reactive sites of our molecule, the molecular electrostatic potential was computed from the optimized geometry using B3LYP/6-31G(d,p) functional and its surface map is shown in Figure 10.

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Table 2. Calculated quantum chemical reactivity descriptors for C24H19N3O5S molecule.

| Parameters          | B3LYP/6-31G(d,p) |
|---------------------|-----------------|
| E_LUMO (eV)         | 5.828           |
| E_HOMO (eV)         | -2.858          |
| E_LUMO-E_HOMO (eV)  | 2.970           |
| IP (eV)             | 5.828           |
| EA (eV)             | 2.858           |
| γ (eV)              | 7.257           |
| μ                   | -7.257          |
| η (eV)              | 1.485           |
| S                   | 0.743           |
| ω                   | 17.732          |

Figure 9. Schematic representation of experimental UV-Vis spectrum and the band gap energy estimation.

4. Molecular docking methodology

Molecular docking has now become an increasingly significant tool for drug discovery and docking small molecular systems into binding site of DNA, enzymes and proteins. Presently Chemical Computing Inc., MOE: 2017 software was used to import, optimize and dock the molecular structure of C24H19N3O5S into binding pockets of two acetylcholinesterase and butyrylcholinesterase enzymes. Molecular structures of PB were imported and optimized using MM force field and entered into MOE database by selecting entries. The optimized X-ray crystallographic structure of Acetylcholinesterase (PDB ID: 2X8B), XRD resolution of 2.95 Å and Butyrylcholinesterase (PDB ID: 1XLW), XRD resolution of 2.1 Å was obtained from PDB [48, 49] and imported to MOE visualization to arrange for molecular docking simulation. Docking preparation includes removal of water molecules from XRD structure and protonation of both enzymes to lowest energy state using the MOPAC 7.0 and amber force field. All water molecules were removed macromolecular system. Before docking simulations. After pre-preparation of 2X8B and 1XLW and C24H19N3O5S molecule, XRD structure of 2X8B and 1XLW was allowed to dock with the optimized molecule of C24H19N3O5S molecules under default parameters with RMS gradient of 0.01 kcal mol. Several conformations of docked poses were obtained based on minimum free energy values. The docked conformation fitting into pockets of binding pockets of acetylcholinesterase and butyrylcholinesterase having minimum energy and maximum stability was selected as a final docking pose [50, 51].

4.1. DNA-binding studies by molecular docking

Molecular docking is widely a probed computational method to determine covalent and non-covalent interactions between small molecules and macromolecules i.e.; enzymes, proteins and DNA. It is most suitable and reliable methods for structure-based and ligand-based drug designing [51]. Computational screening of biological and biochemical molecules before experimental synthesis can be facile and cost effect way [45, 50, 51].

Present section involves C24H19N3O5S molecule probe into interaction study of acetylcholinesterase (PDB ID: 2X8B), and Butyrylcholinesterase (PDB ID: 1XLW) using molecular docking methodology. The lowest energy docked pose of the C24H19N3O5S molecule is presented in Figure 12. Ligplot (right side of Figure 12A/C) are demonstrating interaction profiles revealed that blue blurred regions indicate direct exposure of C24H19N3O5S molecule to the residues of acetylcholinesterase and Butyrylcholinesterase. Dotted lines in the shape of curves...
### Table 3. Comparison of the experimental and calculated NMR values.

| ATOMS   | EXP (δ ppm) B3LYP/6-31G(d,p) | ATOMS   | EXP (δ ppm) B3LYP/6-31G(d,p) |
|---------|------------------------------|---------|------------------------------|
| H2      | 8.18                         | 8.44    | C1                           | 147.46                         |
| H3      | 7.54                         | 7.68    | C2                           | 121.85                         |
| H5      | 7.54                         | 7.46    | C3                           | 126.07                         |
| H6      | 8.18                         | 8.42    | C4                           | 140.12                         |
| H7      | 7.73                         | 7.64    | C5                           | 130.38                         |
| H12     | 7.52                         | 7.38    | C6                           | 121.21                         |
| H13     | 7.38                         | 7.11    | C7                           | 126.93                         |
| H14     | 7.52                         | 7.47    | C8                           | 131.12                         |
| H15     | 6.90                         | 6.78    | C9                           | 165.69                         |
| H18     | 7.01                         | 6.82    | C10                          | 150.09                         |
| H19     | 7.10                         | 6.93    | C11                          | 124.17                         |
| H20     | 7.33                         | 7.14    | C12                          | 129.85                         |
| H21     | 6.79                         | 6.63    | C13                          | 120.98                         |
| H23A    | 3.82                         | 3.87    | C14                          | 127.44                         |
| H23B    | 3.82                         | 3.64    | C15                          | 112.59                         |
| H23C    | 3.72                         | 3.62    | C16                          | 155.02                         |
| H24A    | 3.72                         | 3.90    | C17                          | 137.33                         |
| H24B    | 3.72                         | 3.60    | C18                          | 120.99                         |
| H24C    | 3.72                         | 3.46    | C19                          | 120.97                         |
| C20     | 123.15                       |        | C20                          | 121.35                         |
| C21     | 112.24                       |        | C21                          | 106.80                         |
| C22     | 150.65                       |        | C22                          | 147.15                         |
| C23     | 55.98                        |        | C23                          | 53.88                          |
| C24     | 55.90                        |        | C24                          | 53.55                          |

### Table 4. Natural bond analysis of the C_{24}H_{19}N_{3}O_{5}S molecule.

| Donor (i) | ED/e | Acceptor (j) | ED/e | E(2) (kcal/mol) | E(j)-E(i) (a.u.) | F(i,j) (a.u.) |
|-----------|------|--------------|------|-----------------|------------------|---------------|
| π (C1–C6) | 1.63134 | π* (C2–C3) | 0.27849 | 20.15 | 0.29 | 0.070 |
| π (C1–C6) | 1.63134 | π* (C4–C5) | 0.37850 | 18.51 | 0.29 | 0.065 |
| π (C2–C3) | 1.66209 | π* (C1–C6) | 0.38966 | 19.46 | 0.28 | 0.066 |
| π (C2–C3) | 1.66209 | π* (C4–C5) | 0.37850 | 20.25 | 0.28 | 0.068 |
| π (C4–C5) | 1.58603 | π* (C1–C6) | 0.38966 | 23.93 | 0.27 | 0.072 |
| π (C4–C5) | 1.58603 | π* (C2–C3) | 0.27849 | 17.29 | 0.28 | 0.064 |
| π (C11–C12) | 1.70924 | π* (C16–C15) | 0.38405 | 21.96 | 0.28 | 0.072 |
| π (C11–C12) | 1.70924 | π* (C14–C13) | 0.33235 | 16.17 | 0.29 | 0.062 |
| π (C16–C15) | 1.65449 | π* (C11–C12) | 0.35331 | 17.05 | 0.29 | 0.063 |
| π (C16–C15) | 1.65449 | π* (C14–C13) | 0.33235 | 22.38 | 0.29 | 0.073 |
| π (C14–C13) | 1.67663 | π* (C11–C12) | 0.35331 | 23.23 | 0.28 | 0.073 |
| π (C14–C13) | 1.67663 | π* (C16–C15) | 0.38405 | 17.31 | 0.27 | 0.062 |
| π (C17–C18) | 1.69087 | π* (C22–C21) | 0.38608 | 19.64 | 0.28 | 0.068 |
| π (C17–C18) | 1.69087 | π* (C19–C20) | 0.34132 | 18.09 | 0.29 | 0.066 |
| π (C22–C21) | 1.68124 | π* (C17–C18) | 0.37690 | 17.25 | 0.29 | 0.064 |
| π (C22–C21) | 1.68124 | π* (C19–C20) | 0.34132 | 20.50 | 0.30 | 0.070 |
| π (C19–C20) | 1.69328 | π* (C17–C18) | 0.37690 | 20.74 | 0.28 | 0.069 |
| π (C19–C20) | 1.69328 | π* (C22–C21) | 0.38608 | 17.97 | 0.27 | 0.06 |
| π (C4–C5) | 1.58603 | π* (C7–C8) | 0.21467 | 18.46 | 0.28 | 0.067 |
| π (C7–C8) | 1.84225 | π* (C4–C5) | 0.37850 | 11.77 | 0.31 | 0.057 |
| π (C7–C8) | 1.84225 | π* (C9–O3) | 0.28608 | 18.33 | 0.30 | 0.068 |
| π (C7–H7) | 1.96338 | σ* (C8–S1) | 0.03789 | 10.14 | 0.71 | 0.076 |
| σ (O1–N1) | 1.98523 | n3 (O2) | 1.44613 | 12.20 | 0.18 | 0.078 |
| π (C1–C6) | 1.63134 | π* (O1–N1) | 0.63210 | 28.36 | 0.15 | 0.062 |
| n2(O2) | 1.89839 | σ* (C1–N1) | 0.10337 | 12.51 | 0.57 | 0.076 |
| n2 (O2) | 1.89839 | σ* (O1–N1) | 0.05676 | 19.23 | 0.71 | 0.105 |
| n3(O2) | 1.44613 | π* (O1–N1) | 0.63210 | 163.38 | 0.14 | 0.139 |

(continued on next page)
Table 4

| Donor (i) | ED/e | Acceptor (j) | ED/e | E(2) (kcal/mol) | E(j)-E(i) (a.u.) | F(j) (a.u.) |
|-----------|------|--------------|------|----------------|----------------|------------|
| n2 (O1)  | 1.89839 | σ* (Cl-N1) | 0.10337 | 12.52 | 0.57 | 0.076 |
| n2 (O1)  | 1.89839 | σ* (O2-N1) | 0.05677 | 19.24 | 0.71 | 0.105 |
| n2 (S1)  | 1.76144 | π* (C7-C8) | 0.21647 | 21.91 | 0.28 | 0.070 |
| n2 (S1)  | 1.76144 | π* (N3-C10) | 0.27332 | 21.91 | 0.28 | 0.070 |
| n2 (O3)  | 1.84216 | σ* (C8-C9) | 0.08180 | 21.74 | 0.65 | 0.108 |
| n2 (O3)  | 1.84216 | σ* (C9-N2) | 0.09450 | 29.32 | 0.67 | 0.127 |
| n2 (O4)  | 1.83710 | π* (C16-C15) | 0.38405 | 31.93 | 0.34 | 0.099 |
| n1 (N3)  | 1.80732 | σ* (S1-C10) | 0.11228 | 25.75 | 0.47 | 0.100 |
| n1 (N3)  | 1.80732 | π* (C17-C18) | 0.37690 | 12.77 | 0.37 | 0.064 |
| n2 (O5)  | 1.83777 | π* (C22-C21) | 0.38608 | 30.98 | 0.34 | 0.097 |
| n1 (N2)  | 1.63308 | π* (C9-O3) | 0.28608 | 54.70 | 0.27 | 0.112 |
| n1 (N2)  | 1.63308 | π* (N3-C10) | 0.27332 | 44.18 | 0.28 | 0.103 |
| π* (C16-C15) | 0.38405 | π* (C14-C13) | 0.33235 | 281.71 | 0.01 | 0.080 |
| π* (O1-N1) | 0.63210 | π* (C1-C6) | 0.38966 | 16.75 | 0.14 | 0.060 |
| π* (C9-O3) | 0.28608 | π* (C7-C8) | 0.21467 | 134.78 | 0.01 | 0.071 |
| π* (N3-C10) | 0.27332 | π* (C17-C18) | 0.02535 | 15.97 | 0.02 | 0.029 |

Table 5. NBO results showing formation of Lewis and non-Lewis orbital for the title compound.

| Bond (AB) | ED/energy (a.u.) | EDA (%) | EDB (%) | NBO | S (%) | p (%) | d (%) |
|-----------|------------------|---------|---------|------|-------|-------|-------|
| σ (Cl–C6) | 1.97633 | 51.03 | 48.97 | 0.7143 (sp1.65) C+ 0.6998 (sp1.86) C | 37.68 | 62.29 | 0.03 |
| π (Cl–C6) | 1.63134 | 54.53 | 45.47 | 0.7385 (sp1.86) C+ 0.6743 (sp1.66) C | 37.68 | 62.29 | 0.03 |
| π*(Cl–C6) | 0.02229 | 48.97 | 51.03 | 0.6998 (sp1.86) C+ 0.7143 (sp1.66) C | 37.68 | 62.29 | 0.03 |
| π+(Cl–C6) | 0.38966 | 45.47 | 54.53 | 0.6743 (sp1.66) C+ 0.7385 (sp1.86) C | 37.68 | 62.29 | 0.03 |
| σ (C2–C3) | 1.97569 | 50.19 | 49.81 | 0.7085 (sp1.86) C+ 0.7057 (sp1.86) C | 35.65 | 64.31 | 0.04 |
| π (C2–C3) | 1.66269 | 48.65 | 51.35 | 0.6975 (sp1.86) C+ 0.7166 (sp1.86) C | 35.65 | 64.31 | 0.04 |
| σ*(C2–C3) | 0.04149 | 49.81 | 50.19 | 0.7057 (sp1.86) C+ 0.7085 (sp1.86) C | 35.65 | 64.31 | 0.04 |
| π*(C2–C3) | 0.27849 | 51.35 | 48.65 | 0.7166 (sp1.86) C+ 0.6975 (sp1.86) C | 37.68 | 62.29 | 0.03 |
| σ (C4–C5) | 1.97565 | 51.22 | 48.78 | 0.7156 (sp1.86) C+ 0.6985 (sp1.86) C | 33.13 | 66.83 | 0.04 |
| π (C4–C5) | 1.58603 | 49.92 | 50.08 | 0.7065 (sp1.86) C+ 0.7077 (sp1.86) C | 33.13 | 66.83 | 0.04 |
| σ*(C4–C5) | 0.02090 | 48.78 | 51.22 | 0.6985 (sp1.86) C+ 0.7156 (sp1.86) C | 33.13 | 66.83 | 0.04 |
| π*(C4–C5) | 0.37850 | 50.08 | 49.92 | 0.7077 (sp1.86) C+ 0.7065 (sp1.86) C | 33.13 | 66.83 | 0.04 |
| σ (C7–C8) | 1.84225 | 46.31 | 53.69 | 0.6805 (sp1.86) C+ 0.7327 (sp1.86) C | 33.50 | 66.50 | 0.04 |
| π*(C7–C8) | 0.21467 | 53.69 | 46.31 | 0.7327 (sp1.86) C+ 0.6805 (sp1.86) C | 33.50 | 66.50 | 0.04 |
| π*(C9-O3) | 0.28608 | 68.81 | 31.19 | 0.8295 (sp1.86) C+ 0.5585 (sp1.86) O | 33.50 | 66.50 | 0.04 |
| σ (C7–H7) | 1.96338 | 63.53 | 36.47 | 0.7971 (sp1.86) C+ 0.7358 (sp1.86) H | 26.60 | 73.30 | 0.10 |
| π*(C8–S1) | 0.03789 | 45.86 | 54.14 | 0.6772 (sp1.86) C+ 0.7358 (sp1.86) S | 26.60 | 73.30 | 0.10 |
| σ (O1-N1) | 1.98523 | 60.13 | 39.87 | 0.7754 (sp1.86) O+ 0.6314 (sp1.86) N | 26.60 | 73.30 | 0.10 |
| π*(C1–N1) | 0.10337 | 62.18 | 37.82 | 0.7885 (sp1.86) C+ 0.6150 (sp1.86) N | 26.60 | 73.30 | 0.10 |
| π*(O2–N1) | 0.05677 | 48.62 | 51.38 | 0.6973 (sp1.86) C+ 0.7168 (sp1.86) N | 26.60 | 73.30 | 0.10 |

(continued on next page)
reveal solvent contact with the C24H19N3O5S molecule. Probing into ligplot interaction shows hydrogen bonding between H-atom of aromatic ring of C24H19N3O5S molecule with O-atom of LeusineLeu(519) of acetylcholinesterase (Figure 12B). We can deduce that Leu (380), Phe (535), Ala (377) and Phe (531) developed hydrophobic interactions with C24H19N3O5S molecule. On the other hand, Butyrylcholinesterase furnished only Vander Waal’s interactions with C24H19N3O5S molecule as indicated in ligplot of Butyrylcholinesterase (Figure 12D). Due to more considerable interactions acetylcholinesterase showed higher binding constant and greater spontaneity of reaction (more negative free energy values).

For the comprehensive understanding of macroscopic interaction, a number of electronic and steric descriptors have been calculated on the basis of molecular docking data (Table 6). Energies of frontier molecular orbitals i.e.; E_HOMO and E_LUMO are measure of electron donating and accepting character of a compound [50]. The compounds are considered to be strong electron as they are donating to who has more significant value of E_HOMO, and those compounds which have a low value of E_LUMO, have grander tendency to accept electrons. Therefore, in the present study C24H19N3O5S molecule acts as electron donors while associating with Butylcholinesterase due immenser E_HOMO as compared to its interaction with Actylcholinesterase due to smaller E_HOMO. This shows that when C24H19N3O5S molecule networks with acetylcholinesterase, it withdraws electrons from enzyme residues thus developing strong interactions and high binding strength leading to greater value of binding constant (Table 7). Steric descriptor calculated from simulation results were molar refractivity (MR), heat of formation (Hf) and hydrophobic surface volume (Vsurf). MR, which is a measure of the polarizability of the molecule and is directly related with the binding strength, was found to be higher for acetylcholinesterase furnishing the huger binding strength.

### Table 5 (continued)

| Bond (AB) | ED/energy (a.u.) | EDA (%) | EDB (%) | NBO | S (%) | p (%) | d (%) |
|-----------|-----------------|---------|---------|-----|-------|-------|-------|
| π* (N3-C10) | 0.27332 | 39.94 | 60.06 | 0.6320 (sp^2.99) | N-0.775 (sp^2.99) | C | 0.38 | 99.38 | 0.24 |
| σ* (C8-C9) | 0.08180 | 47.58 | 52.42 | 0.6898 (sp^1.17) | C-0.7240 (sp^4.83) | C | 31.53 | 68.42 | 0.05 |
| σ* (C9-N2) | 0.09450 | 64.11 | 35.89 | 0.8007 (sp^1.36) | O-0.5991 (sp^2.46) | N | 30.62 | 69.25 | 0.12 |
| π* (C16-C15) | 0.38405 | 54.24 | 45.76 | 0.7365 (sp^1.80) | C-0.6764 (sp^4.60) | C | 15.06 | 84.25 | 0.59 |
| σ* (S1-C10) | 0.11228 | 52.48 | 47.52 | 0.7244 (sp^4.89) | S-0.6894 (sp^4.69) | C | 28.68 | 71.22 | 0.10 |
| π* (C17-C18) | 0.37690 | 48.88 | 51.12 | 0.6991 (sp^1.99) | C-0.7150 (sp^1.79) | C | 0.03 | 99.93 | 0.04 |
| π* (C22-C21) | 0.38608 | 52.95 | 47.05 | 0.7277 (sp^1.89) | C-0.6859 (sp^1.89) | C | 0.00 | 99.95 | 0.04 |
| π* (C5-O3) | 0.01086 | 64.88 | 35.12 | 0.8055 (sp^1.89) | C-0.5926 (sp^1.89) | C | 33.87 | 66.03 | 0.09 |
| π* (C14-C13) | 0.53235 | 52.05 | 47.95 | 0.7214 (sp^1.80) | C-0.6925 (sp^1.80) | C | 41.81 | 57.84 | 0.35 |

n(O2) (sp^2.99) 0.00 99.99 0.00
n(O2) (sp^2.99) 0.00 99.99 0.00
n(O1) (sp^2.99) 0.00 99.99 0.00
n(O1) (sp^2.99) 0.00 99.99 0.00
n(S1) (sp^2.99) 0.00 99.99 0.00
n(O3) (sp^2.99) 0.00 99.99 0.00
n(O4) (sp^2.99) 0.00 99.99 0.00
n(N3) (sp^2.99) 0.00 99.99 0.00
n(O3) (sp^2.99) 0.00 99.99 0.00
n(O4) (sp^2.99) 0.00 99.99 0.00

Figure 10. Molecular electrostatic potential (MEP) map calculated with B3LYP/6-31G(d, p) functional.

Figure 11. Orientation of the molecular dipole moment of the C24H19N3O5S molecule; the origin is at the center of mass of the molecule.
Table 6. Binding constants and free energy values of C24H19N3O5S molecule for the Acetylcholinesterase and Butylcholinesterase calculated from molecular docking data.

| Complex code | Molecular docking | \( K_b \) /M\(^{-1} \) | (-ΔG) KJmol\(^{-1} \) |
|--------------|-------------------|-----------------|-------------------|
| Acet –2      |                   | 1.70 \times 10^4 | -24.14            |
| Buty –2      |                   | 1.06 \times 10^3 | -17.25            |

Table 7. Data set of electronic descriptors calculated from molecular docking data.

| Complexes | \( E_{HOMO} \) (kcal/mol) | \( E_{LUMO} \) (kcal/mol) | \( E_{ele} \) (kcal/mol) | \( E_{vander} \) (kcal/mol) | \( E_{IP} \) (kcal/mol) | \( E_{Total} \) (kcal/mol) |
|-----------|------------------|-----------------|-----------------|------------------|-----------------|-------------------|
| Acet-2    | -9.18822         | -1.7942         | -1034645.0      | 12.6166945       | 9.1882          | -122140.09       |
| Buty-2    | -8.92967         | -1.537209       | -1043527.7      | 15.312981        | -8.929670       | -121562.9        |

Table 8. Data set of steric descriptors calculated from Molecular docking data.

| Complexes | \( H_s \) (kcal/mol) | \( M_R \) | Slog P | \( V_{surf} \) | Dipole |
|-----------|---------------------|---------|-------|---------------|--------|
| Acet-2    | 16.12               | 12.1500 | 5.0136 | 458.18        | 4.3368 |
| Buty-2    | 16.86               | 11.5960 | 5.426  | 447.78        | 8.3612 |
of Acetylcholinesterase with C$_{24}$H$_{19}$N$_3$O$_5$S molecule, Table 8, stable and strong complexes have smaller positive value of heat of formation (H$_f$). In this work, Acetylcholinesterase has smaller positive value of heat of formation (H$_f$) with stronger complex formation and high binding constant as compared to Butyrylcholinesterase (Table 8). It was also observed that the value of hydrophobic surface volume (V$_{surf}$) is comparatively bigger for Acetylcholinesterase than Butyrylcholinesterase due to the greater hydrophobic surface contact of the compound PB with Acetylcholinesterase. Higher hydrophobic surface area is attributed to the huger overlapping of C$_{24}$H$_{19}$N$_3$O$_5$S molecule with a greater number of enzyme residues.

5. Conclusion

The molecular system (2Z,5Z)-5-(4-nitrobenzylidene)-3-N(2-methoxyphenyl)-2-N’(2-methoxyphenylimino) thiazolidin-4-one, has been synthesized and characterized by FT-IR, UV (1H, 13C) NMR spectroscopy and single crystal X-ray diffraction techniques. We investigated the optimized molecular structure and related harmonic vibrational frequencies, UV-visible, 1H and 13C NMR chemical shifts using density functional theory with the hybrid functional B3LYP in combination with 6-31G(d, p) basis set. DFT calculations and comparison of proton and carbon NMR chemical shifts have been a supplementary tool for confirming the correctness of the structure. The comprehensive vibrational analysis of the molecule has shown an excellent concordance with secured experimental data. However, differences observed between the experimental and computed values are associated to the assumption of considering the simulated compound as a single molecule in the gas phase, whereas the experimental values were recorded in the solid phase by exploring the presence of intermolecular interactions. Furthermore, the UV-Vis spectrum was obtained in chloroform solution. The stability of the molecule arising from hyper-conjugated interaction and charge delocalization was explored with NBO tool. Also, we have reported HOMO and LUMO energies and energy band gap with the hybrid B3LYP method. The slight difference in energy band gap between HOMO and LUMO has shown that synthesized molecule carries high charge mobility with small excitation energy. These results made C$_{24}$H$_{19}$N$_3$O$_5$S molecule potentially easy to polarize. Molecular electrostatic potential indicates clearly that the oxygen and nitrogen atoms are the most reactive sites in the electrophilic attack, while the preferred sites for the nucleophilic attack are on the phenyl and methyl groups. We completed the present investigations with molecular docking in order to understand the covalent and non-covalent interactions between the present C$_{24}$H$_{19}$N$_3$O$_5$S molecule and enzymes: Acetyl cholinesterase and Butyrylcholinesterase. We hope that the synthesis, crystallographic and spectroscopic characterization and DFT studies of (2Z,5Z)-5-(4-nitrobenzylidene)-3-N(2-methoxyphenyl)-2-N’(2-methoxyphenylimino) thiazolidin-4-one will be useful in designing new devices for organic electronics based biological materials.

Declarations

Author contribution statement

Ahmed Djafri, Fouzia Perveen, Rachida Rahmani, Souraya Goumiri-Said: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Nadia Benhalima, Nawel Khellouli, Rachida Rahmani, Ayada Djafri, Abdelkader Chouihi, Mohammed Benali Kanoun: Conceived and designed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

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Data availability statement

Data will be made available on request.

Declaration of interests statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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