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Synthesis, Spectroscopic & DFT studies of Novel N-((1H-benzo[d]imidazol-1-yl) methyl)-N-(2-(trifluoromethyl)phenyl)-4,5-dihydrothiazol-2-amine

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Synthesis of N-((1H-benzo[d]imidazol-1-yl)methyl)-N-(2-(trifluoromethyl)phenyl)-4,5-dihydrothiazol-2-amine was done followed by its characterization by various spectral techniques. DFT studies of the compound were performed at B3LYP level to study various structural parameters and thermodynamic variables. The correlation of observed transitions with the electronic transitions had been done via NBO analysis. In addition to it, the HOMO and LUMO energy gaps and identification of sites liable for electrophilic and nucleophilic attack were done by MESP and ESP plots.

Keywords: DFT, Thermodynamic, Spectroscopic properties

1 Introduction

Heterocyclic moieties possessing nitrogen and sulphur nucleus display a myriad of biological activities and possess an important place in the pharmaceutical industry[1-3]. Thiazole, a well known heterocyclic compound, has significant role in the development of newer drugs[4-6]. Among the wide range of pharmacological activities displayed by thiazole, some worth mentioning include antimicrobial, anti allergic, anti hypertensive, anti inflammatory, anti HIV, antioxidant, and antianalgesic [7-28].

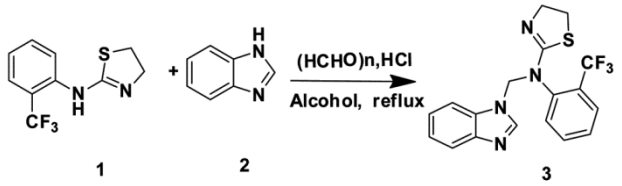
Imidazole nucleus, another therapeutically important moiety, has broad applications as anticancer, antifungal, antiviral, anti tubercular, and antimalarial[29-42] agent. Thus it was thought worth while to synthesize a new hybrid molecule incorporating both thiazole and imidazole moieties with a good activity profile. In this paper, the synthesis of N-((1H-benzo[d]imidazol-1-yl)methyl)-N-(2-(trifluoromethyl)phenyl)-4,5-dihydrothiazol-2-amine (3)along with its characterization by spectral analysis and computational method is described. Experimental and theoretical spectral results for compound **3** have also been compared.

2 Materials and Method

The spectrophotometers used for spectral analysis of molecule are-Bruker 400 MHz for NMR, Perkin-Elmer Fourier transform for IR and Double-Beam spectrophotometer for UV spectroscopy. The solvent used was $CDCl_3$ while tetra methylsilane served the purpose of internal reference.

2.1. Procedure for synthesis of N-((1H-benzo[d]imidazol-1-yl)methyl)-N-(2-(trifluoromethyl)phenyl)-4,5-dihydrothiazol-2-amine(3)

0.014 mole of conc. HCl was added slowly to the solution (ice cold) of 0.01 mole of an amine **2** in 20 ml alcohol. Para form aldehyde was added in small proportions to the reaction mixture while keeping it into the ice for half an hour. 0.01 mole of **1** was added to this and the reaction mixture was refluxed for 2 hrs on water bath. A reddish brown semisolid was obtained as a product after concentrating the reaction mixture (Scheme 1, Fig. 1). Yield-61%, melting point-20-25 ^{0}C, Rf: 0.62(20% $CHCl_3$:CH_3OH), IR (KBr, cm-1): 3018(=C-H stretching), 2850 and 2825 (-CH stretching), 1467(-C=N stretching), 1298(-C-N stretching), 1149 and 1036(-C-F stretching), 773 (-C-S stretching); ^{1}HNMR: δ:3.70-3.67 (t ,2H), 3.84-



Scheme 1 — Synthesis of N-((1H-benzo[d]imidazol-1-yl)methyl)-N-(2-(trifluoromethyl)phenyl)-4,5-dihydrothiazol-2-amine.

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3.81(t,2H) 5.27(s,2H), 7.21-6.96 (m,5H);7.57-6.55 (t, 1H); 8.03-8.02(t, 1H); 7.74-7.72(m,2H)

^{13}CNMR:34.05,61.40,68.76,110.19,116.81,117.39, 119.95,122.54,123.04,124.28,126.06,128.33,131.76,132. 69,141.66, 143.40, 144.00, 160.40; m/z- 377 (M+1)

3 Computational Details

The computational studies of N-((1H-benzo [d] imidazol-1-yl)methyl)-N-(2-(trifluoromethyl) phenyl)-4,5-dihydrothiazol-2-amine were performed at (B3LYP)[43-45] with 6-31G (d,p) as basis set with the Gaussian 09 package[46].

Gauss View 05 program was used to get the graphical presentations of calculated IR and UV spectra. The calculation of **^{1}**H NMR chemical shifts by GIAO method[47]and NBO calculations[48]along with Frontier orbital analysis were also done in $CHCl_3$ by using IEFPCM model. AIM method was employed for studying interactions within the molecule[49].

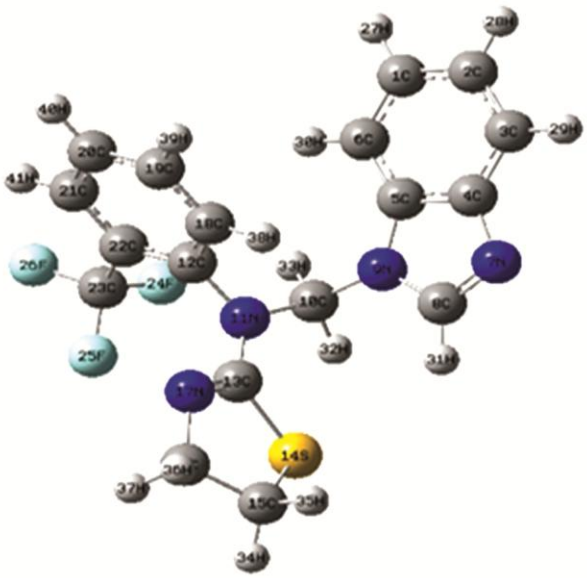

Fig. 1 — Optimized Structure of the title compound.

4 Results and discussion

4.1 ^{1}H &^{13}C NMR spectra

The experimental and calculated ^{1}H and ^{13}C NMR shift values have been enlisted in Table 1. The correlation graph which is as per the equation, $y = 0.895x + 0.715$, for ^{1}H NMR and $y = 1.021x + 4.219$ for ^{13}C NMR (where 'y' represents experimental value and 'x' manifests calculated shift value in ppm) is shown in Figs. 2(a-b) respectively. The calculated value for protons in aromatic region lies in the range of δ 6.655 to δ8.5784 which matches well with the experimental proton shift at δ 6.96 to δ 8.03. The correlation values (R^2 = 0.912) for ^{1}H NMR and (R^2 = 0.934) for ^{13}C NMR depicted that the experimental and theoretical values are in good accordance with each other. The aromatic proton values in the spectrum at 7.05-7.03 and 8.03-6.96 ppm corresponded to H27, H28, H29, H30, H31, H32, and H33 protons respectively.

Table 1 — Experimental and calculated ^{1}HNMR and ^{13}CNMR chemical shifts of the title compound using DFT/B3LYP 6-31G (d,p).

Carbon atom	Calculated ^{13}CNMR chemical shift (ppm)	Experimental ^{13}CNMR chemical shift (ppm)	Hydrogen atom	Calculated ^{1}HNMR chemical shift (ppm)	Experimental ^{1}HNMR chemical shift (ppm)
1C	121.1	122.54	27H	7.123	7.05
2C	119.878	123.04	28H	7.327	7.05
3C	118.8905	124.28	29H	7.7714	7.03
4C	141.1649	141.66	30H	6.6555	7.03
5C	132.6355	132.69	31H	8.5784	8.03
6C	107.323	119.95	32H	6.6769	6.96
8C	139.7771	143.4	33H	5.4242	6.96
10C	65.4117	68.76	34H	3.4387	3.71
12C	140.9456	144	35H	3.5736	3.71
13C	161.0253	160.4	36H	4.087	3.83
15C	45.9626	34.05	37H	3.8117	3.83
16C	65.3014	61.4	38H	6.7675	6.96
18C	132.5252	110.19	39H	7.347	7.56
19C	130.4564	131.76	40H	7.6085	7.57
20C	126.5229	117.39	41H	7.9288	7.74
21C	126.2921	128.33			
22C	129.3733	116.81			
23C	131.8513	126.06			

4.2 UV-Visible spectrum

The effect of solvent has been considered by employing IEFPCM[50, 51]. The experimental and calculated data for electronic transitions has been depicted in Table 2 (Fig. 3). A HOMO-LUMO transition at 238 nm (f = 0.0638) in chloroform was observed and complied well with experimental data (λ exp. = 270 nm), as shown in Fig. 4.

4.3 Vibrational Assignments

The vibrational analysis of compound showed the presence of 41 atoms which belong to C1 point group possessing 117 normal modes of vibrations. Table 3 contains experimental and scaled[52] calculated wave numbers. Correlation coefficient value (R^2= 0.967) showed a strong correlation between experimental and calculated wave numbers. The correlation graphics has been sketched in Fig. 5 while the FT-IR spectrum (theoretical) is depicted in Fig. 6. The experimental value for vibrational bands of =CH stretching appeared at 3018 cm^{-1} agreed well with the

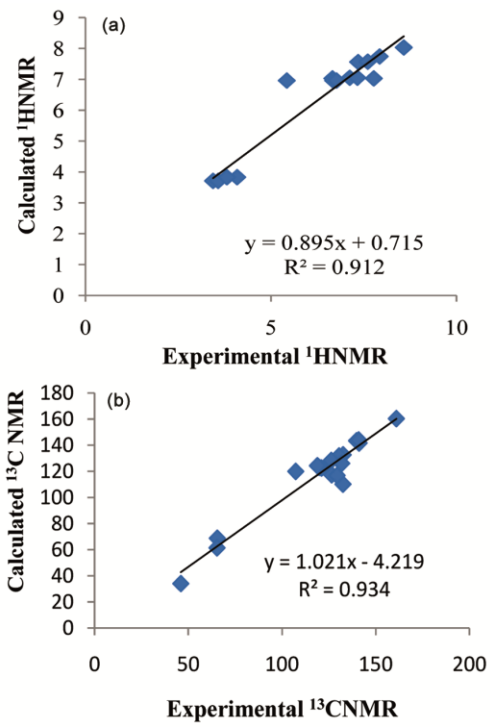

Fig. 2 — Correlation graph between (a) experimental and calculated ^{1}HNMR chemical shifts (b) experimental and calculated ^{13}CNMR chemical shifts using B3LYP 6-31G (d, p).

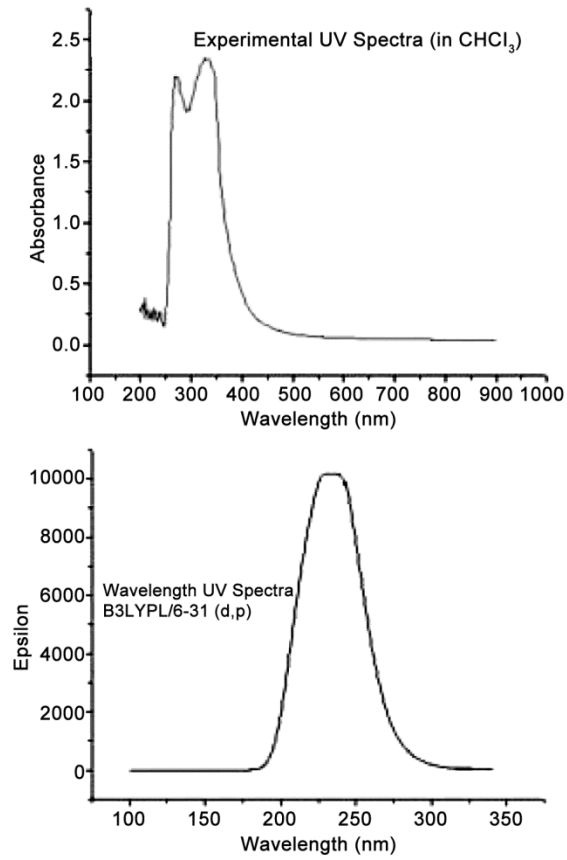

Fig. 3 — Experimental and Theoretical UV spectrum of the title compound.

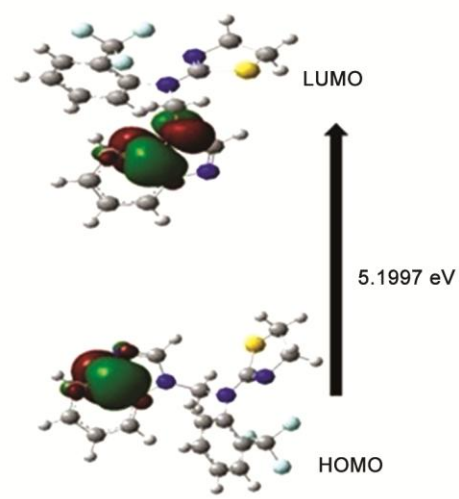

Fig. 4 — HOMO-LUMO molecular orbital of the title compound.

Table 2 — Experimental and theoretical absorption wavelengths λ (nm) and excitation energies E (eV) of title compound using B3LYP functional and 631-G/(d,p) basis set.

S. No.	Major contributing Molecular orbitals	E (eV)	Calculated (λ_{max})	Oscillatory strength (f) B3LYP	Assignment	Observed (λ_{max})
1	H-1→L (33%)	5.1997	238	0.0638	π →π*	270

Table 3 — Experimental FT-IR and calculated vibrational frequencies in cm^{-1} for title compound.

Experimental	Calculated B3LYP	Vibrational assignment
3018	3204	=CH stretching
2850	2940	Symmetric C-H stretching
2825	2452	Symmetric C=N stretching
1467	1548	Symmetric C=N stretching
1298	1340	Symmetric C-N stretching
1149	1132	C-F stretching
1036	1140	C-F stretching
773	780	C-S stretching

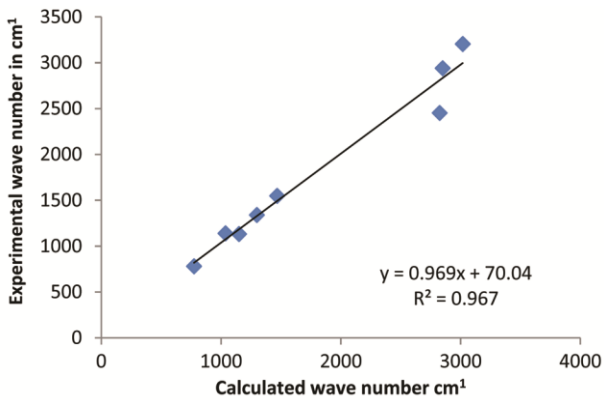

Fig. 5 — Correlation graph between experimental and calculated wave numbers.

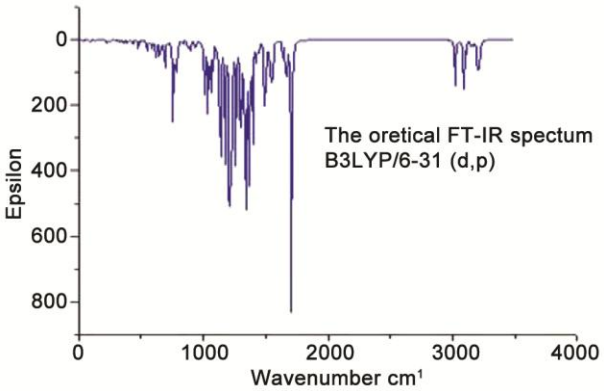

Fig. 6 — Theoretical IR spectrum of the title compound.

calculated value at 3204 cm^{-1}. The experimental and calculated vibrational bands for symmetric C-H stretching appeared at 2850, 2825 cm^{-1}& at 1577, 1548 cm^{-1} respectively. The experimental and calculated C-F stretching appeared at 1149, 1036cm^{-1} & at 1132, 1140 cm^{-1} respectively. The C-S stretching band appeared at 773 & 780 cm^{-1} as observed experimentally and theoretically.

4.4 Molecular electrostatic potential

The MESP (shown in Fig. 7) and ESP maps (shown in Fig. 8) indicated the electron rich and

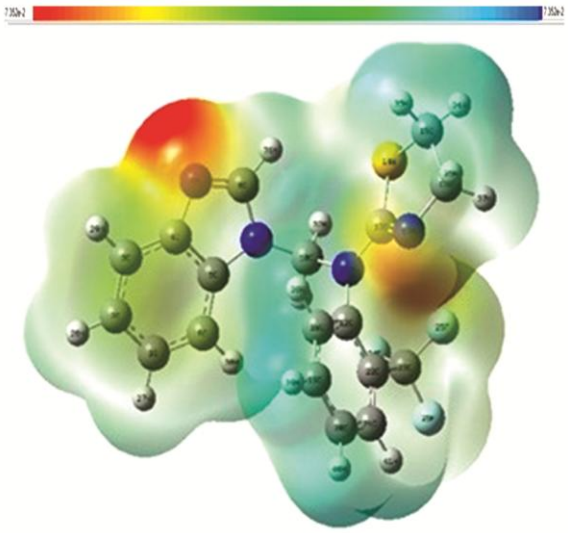

Fig. 7 — 3D plots of the molecular electrostatic potential of the title compound.

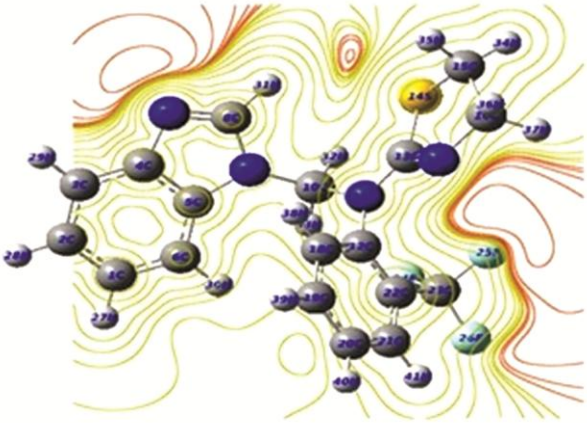

Fig. 8 — Electrostatic potential contour surface of the title compound.

electron deficient centres[53-55]. The tendency to accept electrons for a specific site follows the order as red < yellow< green < light blue < blue[56-60]. As per the MESP map, it is observed that the most preferred region for electrophilic and nucleophilic attack are around C10, C15 & C16 (MESP value=-7.352 a.u.) and N7 (MESP value=+7.352 a.u.) respectively. Magnitude of positive charge on H34 atom and negative charge over oxygen atom affirms the presence of the C-H…O hydrogen bonding in the molecule **3**.

4.5 Natural bond orbital analysis

Natural bond orbital (NBO) analysis[61] has been used time and again to explore the charge transfer within the molecular systems. The NBO analysis has been in Table 4.

Table 4 — Second order perturbation theory analysis of Fock matrix in NBO basis of the title compound.

Donar	Type	ED/e	Acceptor	Type	ED/e*	(E2)[a]	(Ej-Ei)[b]	(Fij)[c]
BD(1)C1-C6	n	1.972	BD*(1)C5-N9	σ*	0.033	7.06	1.14	0.08
BD(2)C1-C6	σ	1.728	BD*(2)C2-C3	σ*	0.307	17.22	0.29	0.064
BD(2)C1-C6	σ	1.728	BD*(2)C4-C5	σ*	0.474	19.53	0.28	0.07
BD(1)C2-C3	n	1.978	BD*(1)C4-N7	σ*	0.02	5.25	1.06	0.035
BD(2)C2-C3	σ	1.715	BD*(2)C1-C6	σ*	0.0334	20.24	0.28	0.068
BD(2)C2-C3	σ	1.715	BD*(2)C4-C5	σ*	0.474	18.34	0.27	0.066
BD(1)C4-C5	σ	1.967	BD*(1)N9-C10	σ*	0.054	5.6	1	0.067
BD(2)C4-C5	σ	1.596	BD*(2)C1-C6	σ*	0.334	18.85	0.28	0.066
BD(2)C4-C5	σ	1.596	BD*(2)N7-C8	σ*	0.307	14.5	0.29	0.067
BD(2)C4-C5	σ	1.596	BD*(2)N7-C8	σ*	0.306	14.5	0.26	0.056
BD(1)C4-N7	n	1.976	BD*(1)C8-H31	σ*	0.022	5.59	1.23	0.074
BD(1)N7-C8	n	1.985	BD*(1)C3-C4	π*	0.023	5.71	1.42	0.081
BD(1)C8-C9	n	1.985	BD*(1)C5-C6	π*	0.021	5.02	1.37	0.074
BD(2)C12-C18	π	1.656	BD*(2)C19-C20	π*	0.311	19.47	0.29	0.067
BD(2)C12-C18	π	1.656	BD*(2)C21-C22	π*	0.357	20.72	0.28	0.069
BD(2)C19-C20	π	1.646	BD*(2)C12-C18	π*	0.326	20.7	0.28	0.068
BD(2)C19-C20	π	1.646	BD*(2)C12-C18	π*	0.326	22.25	0.28	0.07
BD(2)C21-C22	π	1.67	BD*(2)C12-C18	π*	0.326	20.73	0.29	0.069
BD(2)C21-C22	π	1.67	BD*(2)C19-C20	π*	0.311	18.26	0.29	0.065
LP(1)N9	n	1.602	BD*(2)C4-C5	σ*	0.474	32.66	0.3	0.089
LP(1)N11	n	1.746	BD*(1)C12-C18	π*	0.026	6.56	0.83	0.07
LP(1)N11	n	1.746	BD*(1)C12-C22	σ*	0.034	5.85	0.81	0.065
LP(1)N17	n	1.86	BD*(1)C15-C16	σ*	0.03	5.28	0.69	0.55

[a]E(2) means energy of hyperconjugative interactions (stabilization energy in Kcal/mol)
[b] Energy difference between donor and acceptor i and j NBO orbitals in a.u.
[c] F(ij) is the Fock matrix elements between i and j NBO orbitals in a.u.

Table 5 — Dipole Moment μ, Polarizability α_{tot} ($\times 10^{-24}$esu) and first order static hyperpolarizability β_{tot} (10^{-30}) data of the title compound.

Dipole moment	B3LYP 6-31G (d,p)	Hyperpolarizability	B3LYP6-31G (d,p)
μ_x	1.511	β_{xxx}	0.395501
μ_y	-1.4388	β_{xxy}	0.798569
μ_z	1.3088	β_{xyy}	0.75098
μ	2.463	β_{yyy}	-0.04315
Polarizability			
α_{xx}	36.60095	β_{xxz}	-0.06566
α_{xy}	3.690254	β_{xyz}	0.129544
α_{yy}	37.46941	β_{yyz}	0.419359
α_{xz}	-2.60948	β_{xzz}	-0.25118
α_{yz}	-0.90724	β_{yzz}	0.159932
α_{zz}	24.03611	β_{zzz}	0.040234
(α)	32.70216	βtotal (esu)	**1.3396**

The NBO analysis[62] disclosed that significant delocalization can be affirmed within the system as evident from the charge transfer from π (C_{19}-C_{20}) to π* (C_{12}-C_{18}) and from N_9 to σ* (C_4-C_5) with stabilization energy values of 22.25 and 32.66 kcal mol^{-1}. Apart from these transisitions other π→π * and n→π* intra molecular transistions are also seen with stabilisation energy values ranging between 5-20 kcal mol^{-1} thus showing delocalisation of electrons within the system.

4.6 Non -linear optical analysis

NLO analysis, has always allured the interest of researchers due to its application[63,64] in signal processing, modulation, optical logic and other such fields. The presence of conjugation in organic systems can be attributed to polarization leading to a high value of NLO coefficient.

The corresponding NLO analysis is presented in Table 5. The calculated dipole moment[65], polarizability α_{tot} and first hyper polarizability for the

title compound are 2.463 D, 32.70216×10^{-24} esu and 1.3396×10^{-30} esu respectively for B3LYP level.

4.7 Thermodynamical analysis

Thermodynamic data (heat capacity and entropy) tabulated in the supplementary Table 6(a-b) for the title compound 3, while the correlation graphics is shown in Fig. 9. The results indicated that the values of thermodynamic parameters increase with rise in temperature which is attributed to the progression in vibrational intensities with temperature.

4.8 Reactivity descriptors

4.8.1 Global Reactivity Descriptors

Global reactivity descriptors are used to establish the structure-stability relationship. These descriptors are listed in Table 7. In this regard, Koopman's theorem can be very well employed for ascertaining reactivity in chemical environment and selectivity of a particular electronic site[66-70]. The value of chemical potential is a clear indicator of stability of 3.

Table 6(a) — Calculated thermodynamic parameters of title compound.

Parameters	B3LYP/6-31 G(d,p)
Zero-point vibrational energy (Kcal/mol)	193.7399
Rotational temperatures (K)	0.01196
	0.00814
	0.00600
Rotational constants (GHZ)	
X	0.24921
Y	0.16958
Z	0.12508
Total Energy Etotal (Kcal/mol)	207.252
Translational	0.889
Rotational	0.889
Vibrational	205.475

Table 6(b) — Thermodynamic functions at different temperatures at the B3LYP/6-31-G(d,p) level.

Temperature(T) (K)	Heat Capacity(CV) (Cal/mol K) B3LYP	Entropy(S)(Cal/Mol K) B3LYP
100	33.589	100.32
200	57.158	132.077
298.15	83.08	160.50
300	83.568	161.028
400	108.479	189.131
500	129.366	216.106

4.8.2. Local reactivity descriptors

Local reactivity descriptors[71,72] are used for the analysis of reactivity orientation of specific sites within the molecule (Table 8). The relatively enhanced values of reactivity descriptors observed at C10,C15 and C16 are indicator of sites of nucleophilic activity while the increased values of these descriptors at N7 suggest it to be a site of electrophilic activity.

4.9 AIM approach

Molecular graph of **3** is sketched in Fig. 10. The intense, average and weak H-bonds can be

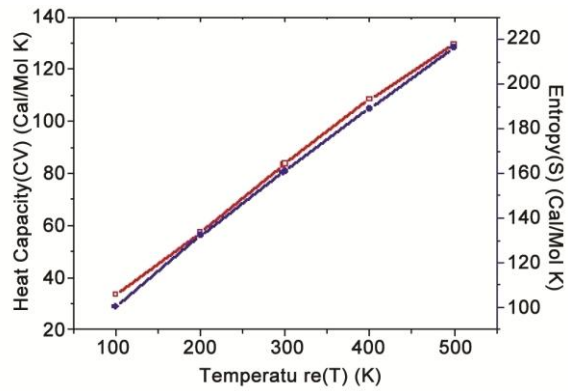

Fig. 9 — Correlation graphs of heat capacity and entropy calculated at various temperatures using B3LYP.

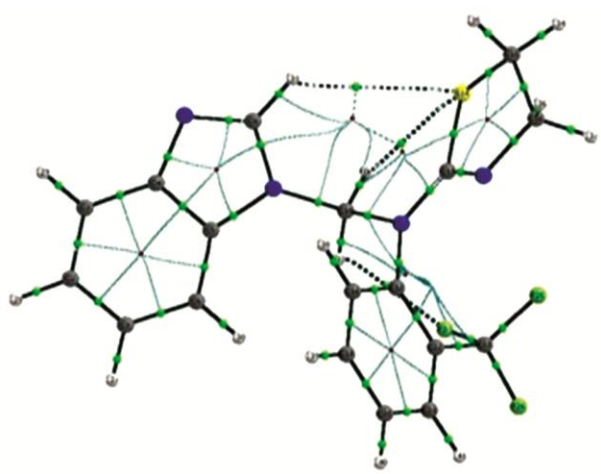

Fig. 10 — Molecular graph of the title compound using AIM program at B3LYP/6- 31G (d,p) level ring critical points (small blue sphere), bond paths (red lines).

Table 7 — Calculated ε_{LUMO}, ε_{HOMO}, energy band gap $\varepsilon_{HOMO}-\varepsilon_{LUMO}$, ionization potential (IP), electron affinity (EA), electronegativity (χ), global hardness (η), chemical potential (μ), global electrophilicityindex (ω), global softness (S) and additional electronic charge (ΔNmax) in eV for the title compound, using DFT/B3LYP/6-31G(d,p).

ϵ_H	ϵ_L	ϵ_H-ϵ_L	I	A	X	η	μ	ω	S	ΔN_{Max}
-7.0095	-0.03673	-6.97282	7.0097	0.03673	3.52314	3.4864	-3.5231	1.7801	1.7432	1.01053

Table 8 — Fukui functions (fk^+,fk^-), Local softness (sk^+sk^-) in eV, Local electrophilicity indices (wk^+,wk^-) in eV for specific atomic sites of the title compound.

Atoms	q_N	q_N+1	q_N-1	f_k+	f_k-	sk^+	sk^-	w_k^-	w_k^+
1 C	0.005583	0.059766	-0.04753	0.054183	0.053108	0.013649	0.013378	0.157889	0.154757
2 C	-0.02422	0.055447	-0.11048	0.079669	0.08626	0.020069	0.021729	0.232155	0.251362
3 C	0.066555	0.051623	0.023143	-0.01493	0.043412	-0.00376	0.010935	-0.04351	0.126503
4 C	0.181424	0.327256	0.162139	0.145832	0.019285	0.036735	0.004858	0.424954	0.056196
5 C	0.062145	0.093621	0.066016	0.031476	-0.00387	0.007929	-0.00098	0.091721	-0.01128
6 C	-0.02914	-0.05066	-0.08578	-0.02152	0.056638	-0.00542	0.014267	-0.0627	0.165043
7 N	-0.57965	-0.68738	-0.58829	-0.10773	0.008643	-0.02714	0.002177	-0.31392	0.025186
8 C	0.437848	0.611499	0.373951	0.173651	0.063897	0.043743	0.016096	0.506019	0.186196
9 C	0.040277	-0.05155	0.033344	-0.09183	0.006933	-0.02313	0.001746	-0.26759	0.020203
10 C	0.227316	0.326354	0.167412	0.099038	0.059904	0.024948	0.01509	0.288597	0.17456
11 C	0.184922	0.18098	0.186966	-0.00394	-0.00204	-0.00099	-0.00051	-0.01149	-0.00596
12 C	0.100987	0.043082	0.108188	-0.05791	-0.0072	-0.01459	-0.00181	-0.16874	-0.02098
13 C	-0.03672	0.022189	-0.08586	0.058908	0.049138	0.014839	0.012378	0.171658	0.143188
14 C	-0.00126	0.04985	-0.05098	0.051105	0.04972	0.012873	0.012524	0.14892	0.144884
15 C	-0.01577	0.021029	-0.05944	0.036801	0.043669	0.00927	0.011	0.107238	0.127251
16 C	-0.0089	0.043396	-0.01913	0.052299	0.010229	0.013174	0.002577	0.152399	0.029807
17 O	-0.10937	-0.46971	-0.14579	-0.36035	0.036423	-0.09077	0.009175	-1.05005	0.106137
18 O	-0.23856	-0.20467	-0.29299	0.033888	0.054433	0.008536	0.013712	0.09875	0.158618
19 C	0.103464	0.166891	0.082497	0.063427	0.020967	0.015977	0.005282	0.184826	0.061098
20 C	0.078419	0.096224	0.070549	0.017805	0.00787	0.004485	0.001982	0.051884	0.022933
21 N	-0.42095	-0.33046	-0.42001	0.090499	-0.00094	0.022797	-0.00024	0.263714	-0.00275
22 C	-0.1239	-0.14966	-0.12968	-0.02576	0.005783	-0.00649	0.001457	-0.07506	0.016852
23 C	0.004138	0.071025	-0.05311	0.066887	0.057247	0.016849	0.014421	0.194909	0.166818
24 C	0.002448	0.05635	-0.05469	0.053902	0.057134	0.013578	0.014392	0.15707	0.166488
25 C	-0.01469	0.032205	-0.06627	0.046894	0.051583	0.011813	0.012994	0.136649	0.150313
26 C	-0.18143	0.05325	-0.21222	0.234677	0.030792	0.059115	0.007757	0.683849	0.089728
27 C	0.152208	0.21862	0.163994	0.066412	-0.01179	0.016729	-0.00297	0.193525	-0.03434
28 C	-0.00241	0.054398	-0.02665	0.056805	0.024247	0.014309	0.006108	0.16553	0.070656
29 C	-0.01009	0.044521	-0.0401	0.054612	0.03001	0.013757	0.00756	0.159139	0.087449
30 C	0.003856	0.05844	-0.02402	0.054584	0.027876	0.01375	0.007022	0.159058	0.081231
31 C	0.173736	0.214022	0.17231	0.040286	0.001426	0.010148	0.000359	0.117393	0.004155
32 Cl	-0.02828	-0.00796	-0.0975	0.020314	0.06922	0.005117	0.017437	0.059195	0.201707

Table 9 — Topological parameters for intramolecular interactions in compound electron density (ρ_{BCP}), Laplacian of electron density ($\nabla^2\rho_{BCP}$), electron kinetic energy density (G_{BCP}), electron potential energy density (V_{BCP}), total electron energy density (H_{BCP}), Hydrogen bond energy (E_{HB}) at bond critical point (BCP).

Interactions	ρ_{BCP}	$\nabla^2\rho_{BCP}$	G_{BCP}	V_{BCP}	H_{BCP}	$E_{HB(Elipticity)}$
C8-H31⋯S14	0.005956	0.017975	0.003451	-0.002409	0.000087	0.017150
C10-H32⋯S14	0.013745	0.055005	0.011449	-0.009147	-0.000872	0.921598
C10-H33⋯F24	0.010307	-0.334598	0.009827	-0.008290	-0.00125	0.260783

ρ_{BCP}, $\nabla^2\rho_{BCP}$, G_{BCP}, V_{BCP}, H_{BCP} in a.u. and E_{HB} in (kcal/mol)

denoted by $\nabla^2\rho$(BCP) < 0 and *H*BCP < 0, $\nabla^2\rho$ (BCP) > 0 and *H*BCP < 0 and $\nabla^2\rho$(BCP) > 0 and *H*BCP > 0 respectively[73].

Geometrical and topological parameters along with ellipticity (ε) values, are given in Table 9. According to AIM computations, the overall energy of interactions within the molecule comes out to be -0.0903 kcal/mol. Along with this, delocalization was further confirmed by the decreased ellipticity data.

5 Conclusion

The present work comprises of synthesis and respective characterization NovelN-((1H-benzo[d] imidazol-1-yl)methyl)-N-(2-(trifluoromethyl) phenyl)-4,5-dihydrothiazol-2amine(3) by spectral and computational methods. The experimental and theoretical results were found in good compliance with each other. The biological activity of the molecule could be anticipated by HOMO-LUMO values. As per the results obtained from NLO

analysis, the molecule turns out to be a potent NLO material. Ellipticity and hydrogen bonding interatctions, as investigated by the AIM, depicted π-character of bonds in the aromatic ring and weak hydrogen bonds.

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Conflict of interests

The authors declare no conflict of interests.

References

1 Fei X P, Hui Z Z, Ping H X, Yi Z Z, Liang Z R & Chin J, *Chem Soc*, 51 (2004) 315.
2 Ibis C, Tuyun A F, Gunes Z O, Bahar H, Stasevyc M V, Musyanovych R Y, Porokhnyavets O K & Novikov V, *Eur J Med Chem*, 46 (2011) 5861.
3 Jain A K, Vaidya A, Ravichandran V, Kashaw S K & Agrawal R K, *Bioorg Med Chem*, 20 (2012) 3378.
4 Rollas S & Kucukguzel S G, *Molecule*, 12 (2007) 1910.
5 El-Sayed R & Chin, *J Chem*, 28 (2010) 594.
6 Mor S, Mohil R, Kumar D & Ahuja M, *Med Chem Res*, 21 (2011) 3541.
7 Rollas S, Gulerman N & Edeniz H, *Farmaco*, 57 (2002) 17.
8 Capilla J, Serena C, Javier Pastor F, Ortoneda T & Guarro J, *Antimicrob Agents Chemother*, 47 (2003) 3976.
9 Loncle C, Brunel J M, Vidal N, Dhebomez M & Letourneux Y, *Eur J Med Chem*, 39 (2004) 1067.
10 Abdel-Aal M T, El-Sayed W A & El-Ashry E H, *Arch Pharm Chem Life Sci*, 339 (2006) 656.
11 Savini L, Chiasserini L, Travagli V, Pellerano C, Novellino E, Consentino S & Pisano M B, *Eur J Med Chem*, 39 (2004) 113.
12 Bijew A, *Lett Drug Des Discov*, 3 (2006) 506.
13 Goksen U S, Gokhan-Kelekci N, Goktas O, Koysal Y, Kilic E, Isik S, Aktay G & Ozalp M, *Bioorg Med Chem*, 15 (2007) 5738.
14 Imramovsky A, Polanc S, Vinsova J, Kocevar M, Jampilek J, Reckova Z & Kaustova J, *Bioorg Med Chem*, 15 (2007) 2551.
15 Jani Y L, *Bioorg Med Chem*, 15 (2007) 2479.
16 Walcourt A, Loyevsky M, Lovejoy D B, Gordeuk V R & Richardson D R, *Int J Biochem Cell Biol*, 36 (2004) 401.
17 Dimmock J R, Vashishth S C & Stables J P, *Eur J Med Chem*, 35 (2000) 241.
18 Silva G A, Costa L M M, Brito F C F, Miranda A L P, Barreiro E J & Fraga C A M, *Bioorg Med Chem*, 12 (2004) 3149.
19 Vijesh A M, Isloor A M, Prabhu V, Ahmad S & Malladi S, *Eur J Med Chem*, 45 (2010) 5460.
20 Hargrave K D, Hess F K & Oliver J T, *J Med Chem*, 26 (1983) 1158.
21 Steinbaugh B A, Batley B L, Painchaud C A, Rapundalo S T, Michniewicz B M & Olson S S C, *J Med Chem*, 35 (1992) 2562.
22 Rostom S A F, El-Ashmawhy M I, El-Razik H A A, Badr M H & Ashour H M A, *Bioorg Med Chem*, 17 (2009) 882.
23 Tsuji K & Ishikawa H, *Bioorg Med Chem Lett*, 4 (1994) 1601.
24 Bell F W, Cantrell A S, Hogberg M, Jaskunas S R, Johansson N G, Jordon C L, Kinnick M D, Lind P, Morin J M, Norren R, Oberg B, Palkowitz J A, Parrush C A, Pranc P, Sahlberg C, Ternansky R J, Vasileff P T, Vrang L, West S L, Zhang H & Zhou X, *J Med Chem*, 38 (1995) 492.
25 Devasagayam T P A, S De S, Adhikari S, Jain J K & Menon V P, *Chem Bio Interact*, 173 (2008) 215.
26 Shiradkar M, Suresh K G V, Dasari V, Tatikonda S, Akula K C & Shah R, *Eur J Med Chem*, 42 (2007) 807.
27 Harnett J J, *Bioorg Med Chem Lett*, 14 (2004) 157.
28 Shih M H & Ying Ke F, *Bioorg Med Chem*, 12 (2004) 4633.
29 Katritzky A R, *Comprehens Heterocycl Chem*, 5 (1984) 469.
30 Grimmett M & Imidazole R, Benzimidazole Synthesis, Academic Press, (1997).
31 Brown E G, Ring Nitrogen and Key Biomolecules, Kluwer Academic Press, (1998).
32 Pozharskii A F, Heterocycles in Life and Society, John Wiley & Sons, (1997).
33 Gilchrist TL, Heterocyclic Chemistry, The Bath Press, (1985).
34 Congiu C M, Cocco & Onnis V, *Bio Med Chem Lett*, 18 (2008) 989.
35 Venkatesan A M, Agarwal A, Abe T, Ushirogochi H O, Santos D, Li Z, Francisco G, Lin Y I, Peterson P J, Yang Y, Weiss W J, Shales D M & Mansour T S, *Bioorg Med Chem*, 16 (2008) 1890.
36 Nakamura T, Kakinuma H, Umemiya H, Amada H, Miyata N, Taniguchi K, Bando K & Sato M, *Bioorg Med Chem Lett*, 14 (2004) 333.
37 Su H M & Kim D H, *Bioorg Med Chem Lett*, 11 (2001) 1425.
38 Roman G, Riley J G, Vlahakis J Z, Kinobe R T, Brien J F, Nakatsu K & Szarek W A, *Bio Med Chem*, 15 (2007) 3225.
39 Bbizhayev M A, *Life Sci*, 78 (2006) 2343.
40 Nantermet P G, Barrow J C, Lindsley S R, Young M, Mao S, Carroll S, Bailey C, Bosserman M, Colussi D, McMasters D R, Vacca J P & Selnick H G, *Bioorg Med Chem Lett*, 14 (2004) 2141.
41 Adams J L, Boehm J C, Gallagher T F, Kassis S, Webb E F, Hall R, Sorenson M, Garigipati R, Don E, Griswold & John C, *Med Chem Lett*, 11 (2001) 2867.
42 Bhandari K, Srinivas N, Keshava G B S & Shukla P K, *Eur J Med Chem*, in press, 43.
43 Becke A D, *J Chem Phys*, 98 (1993) 1372.
44 Becke A D, *Phys Res A*, 38 (1988) 3098.
45 Lee C, Yang W & Parr R G, *Phys Rev B*, 37 (1988) 785.
46 Schlegel H B, *Comput J Chem*, 3 (1982) 214.
47 Wolinski K, Hinton J F & Pulay P, *J Am Chem Soc*, 112 (1990) 8251.
48 Glendening E D, NBO 5.0, Theoretical Chemistry Institute, University of Wisconsin, *Madison*, (2001).
49 Bader R F W & Cheeseman J R, *AIMPAC*, (2000).
50 Cossi M & Barone V, *J Chem Phys*, 115 (2001) 4708.
51 Adamo C & Barone V, *Chem Phys Lett*, 330 (2000) 152.
52 Hiroshi Y & Akito E, *Chem Phys Lett*, 325 (2000) 477.

53 Prabavathi N & Senthil N, *Spectrochim Acta Part A*, 129 (2014) 572.
54 Prasad M V S, Chaitanya K, Udaya Sri N & Veeraiah V, *J Mol Struct*, 1047 (2013) 216.
55 Fatma S, Bishnoi A & Verma A K, *J Mol Struct*, 1095 (2015) 112.
56 Glossman-Mitnik D, *Proc Comput Sci*, 18 (2013) 816.
57 Singh R N, Kumar A, Tiwari R K & Rawat P, *Spectrochim Acta Part A*, 113 (2013) 378.
58 Zaater S, Bouchoucha A, Djebbar S & Brahimi M, *J Mol Struct*, 1123 (2016) 344.
59 Saha S K, Hens A, Murmu N C & Banerjee P, *J Mol Liquids*, 215 (2016) 486.
60 Parr R G & Yang W, Density Functional Theory of Atoms and Molecules, Oxford University Press, 47 (1993) 101.
61 Glendening E D, Reed A E, Carpenter J E & Weinhold F, NBO Version 3.1, TCI University of Wisconsin, *Madison*, (1998).
62 Reed A E, Curtis L A & Weinhold F, *Chem Rev*, 88 (1988) 899.
63 Andraud C, Brotin T, Garcia C, Pelle F, Goldner P, Bigot B & Collet A, *J Am Chem Soc*, 116 (1994) 2094.
64 Nakano M, Fujita H, Takahata M & Yamaguchi K, *J Am Chem Soc*, 124 (2002) 9648.
65 Geskin V M, Lambert C & Bredas J L, *J Am Chem Soc*, 125 (2003) 15651.
66 Prabavathi N & Senthil N, *Spectrochim Acta Part A*, 129 (2014) 572.
67 Soliman S M, Hagar M, Ibid F, Sayed E & Ashry H E, *Spectrochim Acta Part A*, 145 (2015) 270.
68 Sethi A & Prakash R, *J Mol Struct*, 1083 (2015) 72.
69 Parr R G, Szentpaly L & Liu S, *J Am Chem Soc*, 121 (1999) 1922.
70 Arivazhagan M & Senthil K J, *Spectrochim Acta Part A*, 137 (2015) 490.
71 Chattaraj K & Giri S, *J Phys Chem*, 111 (2007) 11116.
72 Rozas I, Alkorta I & Elguero J, *J Am Chem Soc*, 122 (2000) 11154.
73 Matta L F & Boyd R J, An Introduction of the Quantum theory of Atom in Molecule, Wiley- VCH Verlag GMBH, (2007).