Synthesis, Crystal Growth, Crystal Arrangement, Optical, Thermal, NLO and Biological Investigations of Heterocyclic Compounds of N-(1,3-benzothiazol-2-yl)benzamide and N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide

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Abstract — Heterocyclic organic nonlinear optical materials of N-(1,3-benzothiazol-2-yl)benzamide [2-BTBA] and N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide [2-BTFBA] were orchestrated by benzoylation of 2-aminobenzothiazole utilizing subbed benzoyl chloride. The orchestrated mixtures 2-BTBA and 2-BTFBA molecular ion peaks at 253.9 & 272 were affirmed by GC-MS. The grown single crystals of 2-BTBA and 2-BTFBA were developed by slow evaporation method at room temperature with a combination of ethyl acetate & methanol as dissolvable. The X-ray diffraction investigations of equally 2-BTBA & 2-BTFBA crystal have a monoclinic framework with space group $P2_1/n$ individually. The FT-IR spectra of 2-BTBA and 2-BTFBA show absorption peaks at 1670 and 1660 cm^{-1} , indicating the presence of carbonyl functional group vibration modes in the molecules. UV-Vis spectra show a awesome absorbance band at 303 & 300 nm for 2-BTBA and 2-BTFBA molecules, respectively. The number of protons and carbons were predicted using ^1H and ^{13}C NMR spectrum studies. TGA and DTA analyses confirmed the various stages of disintegration of the produced crystals, and they are thermally stable up to 403 K and 333 K for 2-BTBA and 2-BTFBA, respectively. The zone of hindrance method was used to test the antibacterial and antifungal activities of produced single crystals using amphotericin-B and ciprofloxacin as standards. The outcomes prove that the incorporated mixtures display prevalent anti-fungal and antibacterial activity. The non-linear efficiency was affirmed by Kurtz-Perry concentrates strategy for 2-BTBA and 2-BTFBA crystals with the SHG proficiency 2.28 and 2.83 times more prominent than that of potassium dihydrogen phosphate [KDP].

Key words — Crystal growth; XRD; Thermal analysis; Biological activity; Non-linear optical material.

I. INTRODUCTION

In the current scenario, novel optical materials, and their applications, such as organic molecule materials with optical properties that may be modified by an external improvement, need to be affirmed. For quite a while, optical materials used to be latent in organic materials for frequencies transformation or electronic Opto-adjustments [1]. Because there is no p-electron delocalization in inorganic NLO synthon, they exhibit excellent mechanical and thermal stability but have mild optical susceptibilities [2]. Yet, more as of late organic molecular materials have likewise been

utilized for dynamic NLO segments. The upside of organic materials is that they can be enhanced for photo refractivity, holographic memory or electronic Opto-modulations, and different types of NLO applications [3]-[6]. Non-linearity in organic chromophores can be artificially adjusted by changing the arrangement or extent of formed π -frameworks, and by assessing the impacts of different electron-benefactor and acceptor gatherings. The charge transfer between functional groups gives donor-acceptor complexes a high level of polarity [7]-[9]. Organic crystals are frequently shaped by frail Vander Waals and hydrogen bonds prompting a serious level of delocalization [2]. Benzothiazole, a heterocyclic molecule, is being used in research as a starting material for the aggregation of larger, generally bioactive structures. Benzothiazole core is found to have various organic exercises like anti-inflammatory, antimicrobial, antidiabetic, antileishmanial, anticancer, and antiviral [10]-[14].

The existing research effort, synthesis of new heterocyclic molecules N-(1,3-benzothiazol-2-yl)benzamide [2-BTBA] and N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide [2-BTFBA]. 2-BTBA and 2-BTFBA single crystals were developed by a slow solvent evaporation method. The molecular mass of the produced compounds is determined using gas chromatography-mass spectrometry (GC-MS). The primary properties are controlled by the single-crystal X-ray diffraction technique. The quality of 2-BTBA and 2-BTFBA organic single crystals are dictated by a variety of spectroscopic strategies including UV-Vis, FT-IR, ^1H & ^{13}C NMR techniques. Thermal studies were investigated by thermogravimetric (TGA) & differential thermal analysis (DTA). Kurtz powder test conveyed non-linear optical studies and biological properties like antifungal & antibacterial investigations were explored.

II. EXPERIMENTAL SECTION

A. Materials and Synthesis of 2-BTBA and 2-BTFBA Compounds

Synthetic compounds, for example, 2-aminobenzothiazole, benzoyl chloride, and 2-fluorobenzoylchloride were bought from Sigma-Aldrich (USA). Triethylamine (Et_3N), as well as

solvents like ethyl acetate, acetonitrile, petroleum ether, and methanol, were purchased as AR grade from Spectrochem (India) and used without further cleaning. The adjusted methodology used to the creation of N-(1,3-benzothiazol-2-yl)benzamide [2-BTBA] which is as per the following. 1000 mg, 6.66 mmol of 2-aminobenzothiazole 1 was charged into 15 ml of acetonitrile, and 808 mg, 7.98 mmol triethylamine gradually charged to the response mass. The resulting response combination was chilled to 10°C and 7.33 mmol of benzoyl chloride 2a was added gradually. Dry condition followed each addition. After the addition of benzoyl chloride exothermic noticed, the response temperature raises to 25 °C. The response combination was agitated and refluxed for 1 hr. The reaction development was monitored using thin-layer chromatography (TLC). When the response is finished the combination is permitted to cool 25°C. The mixture was then placed into 25 grams of ice-cold water and stirred for 10 minutes at that point. The separated solid from the mixture was filtered, rinsed with water (2×20 ml), and dried. In ethyl acetate, the crude product was crystallised. Gas chromatographic-mass spectrometry (GC-MS) validated the molecular ion signal at $m/z = 254$ (Fig. 1). Yield: 1.39 g (82%) $R_f = 0.5$ in 80:20 (pet ether: ethyl acetate). The same procedure was followed to syntheses of N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide [2-BTFBA] and molecular ion peak at $m/z = 272$ was established with GC-MS. In Scheme 1, the syntheses of these compounds are shown.

Reaction Scheme

Scheme 1. Synthesis of N-(1,3-benzothiazol-2-yl) benzamides.

Fig. 1 (a-b). GC-MS molecular ion peak spectrum of (a) 2-BTBA (b) 2-BTFBA.

B. Crystal Growth

The orchestrated materials structure has been affirmed by the single crystal of them were developed by a slow evaporation technique by means of ethyl acetate and methanol as a solvent in (1:1) ratio. The single crystals of N-(1,3-benzothiazol-2-yl)benzamide [2-BTBA] and N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide [2-BTFBA] were

developed by slow evaporation technique. A gradual evaporation approach allows the saturated solution of 2-BTBA (3a) and 2-BTFBA (3b) to crystallise at room temperature. The obtained single crystals are optically transparent, pale yellow color (3a) and yellow color (3b) from the mother liquor. The photographs of the developed particular crystals of 2-BTBA (3a) and 2-BTFBA (3b) are shown in Fig. 2. The crystal growth results are showed in supplementary information in Table I.

Fig. 2 (a-b). Grown single crystals image of (a) 2-BTBA (b) 2-BTFBA.

TABLE I: CRYSTALLOGRAPHIC DATA OF (A) 2-BTBA (B) 2-BTFBA

Crystal data and Structure refinement	2-BTBA	2-BTFBA
Identification Code	2-BTBA	2-BTFBA
Empirical formula	$C_{14}H_{10}N_2OS$	$C_{14}H_8FN_2OS$
Formula weight	254.30	272.29
Temperature	296(2)K	296(2)K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$
	$a = 5.9479(5)$ Å $\alpha = 90^\circ$	$a = 5.2216(2)$ Å $\alpha = 90^\circ$
Unit cell dimensions	$b = 16.8568(12)$ Å $\beta = 102.343(3)^\circ$ $c = 11.9366(10)$ Å $\gamma = 90^\circ$	$b = 20.2593(9)$ Å $\beta = 90.277(2)^\circ$ $c = 11.3023(5)$ Å $\gamma = 90^\circ$
Volume	$1169.13(16)$ Å ³	$1195.61(9)$ Å ³
Z	4	4
Density (calculated)	1.445 Mg/m ³	1.513 Mg/m ³
Absorption coefficient	0.264 mm ⁻¹	0.275 mm ⁻¹
F(000)	528	560
Crystal size	$0.150 \times 0.150 \times 0.100$ mm ³	$0.150 \times 0.150 \times 0.100$ mm ³
Theta range for data collection	3.494 to 30.507 °	3.514 to 26.995 °
Index ranges	$-8 \leq h \leq 8$, $-24 \leq k \leq 24$, $-17 \leq l \leq 17$	$-6 \leq h \leq 6$, $-25 \leq k \leq 25$, $-14 \leq l \leq 14$
Reflections collected	34145	28778
Independent reflections	3559 [R(int) = 0.0338]	2613 [R(int) = 0.0389]
Completeness to theta = 25.242°	99.5%	99.7%
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6725	0.7461 and 0.6653
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	3559 / 0 / 168	2613 / 0 / 176
Goodness of fit on F ²	1.057	1.149
Final R indices [I > 2 sigma(I)]	$R_1 = 0.0512$, $wR_2 = 0.1273$	$R_1 = 0.0506$, $wR_2 = 0.1127$
R indices (all data)	$R_1 = 0.0683$, $wR_2 = 0.1406$	$R_1 = 0.0592$, $wR_2 = 0.1175$
Extinction coefficient	0.131(10)	n/a
Largest diff. peak and hole	0.296 and 0.363 e Å ⁻³	0.267 and 0.243 e Å ⁻³

C. Instrumentation Details

The single crystals of N-(1,3-benzothiazol-2-yl)benzamide [2-BTBA] and N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide [2-BTFBA] are ready in acceptable characteristics and were exposed to different portrayal examines. The incorporated compounds molecular mass was affirmed by gas chromatography-mass spectrometry at 60 to 300 °C in dormant helium gas environment. The single-crystal X-ray diffraction of produced crystals of 2-BTBA and 2-BTFBA was carried out at room temperature, using a Bruker APEX-II diffractometer with graphite monochromatic MoK α (= 0.7103) radiation and a CCD detector. The functional group vibrational modes of the orchestrated compounds were recorded with a SHIMADZU spectrometer in the wavelength range 400 - 4000 cm⁻¹, as confirmed by FT-IR spectra with KBr pellet method. The ¹H and ¹³C NMR spectra of selected compounds were acquired using DMSO-d₆ as a solvent and a BRUKER 400 MHz NMR spectrometer to track down the number of protons and carbon signals. Using a Lambda-35 spectrometer, the UV-visible absorption spectrums of formed crystals were recorded to determine absorbance signals in the wavelength range 200 nm to 800 nm. On an SDT Q600 V20.9 build 20 instrument with a heating rate of 20°C/min from 0 to 500 °C, TGA and DTA tests were done to assess weight loss and exo-endothermic peaks, and the samples were weighed in an Al₂O₃ crucible. The Second Order Nonlinearity of 2-BTBA and 2-BTFBA single crystals thorough examination was performed by Kurtz - Perry SHG test. These crystals were enlightened using spectrum physics quanta Ray GCR-2(10) Nd: YAG laser with pulse energy of up to 300 mJ and a yield of the first harmonic of 1064 nm. The creation of second harmonic signals by manufactured compounds established the crystals' green radiation emission. The output power of 2-BTBA and 2-BTFBA was estimated and contrasted with the output power of potassium dihydrogen phosphate (KDP) crystal. The biological properties like antifungal & antibacterial examinations were investigated utilizing the standard agar well diffusion strategy.

III. RESULT AND DISCUSSION

A. Single Crystal X-ray Diffraction Study

The arrangement of grown single crystals of N-(1,3-benzothiazol-2-yl)benzamide [2-BTBA] and N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide [2-BTFBA] were affirmed by single crystal XRD investigation. The estimated lattice parameters for 2-BTBA $a = 5.9479(5)$ Å, $b = 16.8568(12)$ Å, $c = 11.9366(10)$ Å and Volume = 1169.13(16) Å³ and 2-BTFBA crystal $a = 5.2216(2)$ Å, $b = 20.2593(9)$ Å, $c = 11.3023(5)$ Å & volume = 1195.61(9) Å³ are in close concurrence with the revealed values. The compounds 2-BTBA & 2-BTFBA expect to be monoclinic structure with P2₁/n space group as displayed in Table 1. It shows the two incorporated crystals have similar lattice parameters. The mixtures 2-BTBA and 2-BTFBA drawing structures were displayed ORTEP (Oak Ride Thermal Ellipsoid Plot) in Fig.3 (a-b). Because it comprises substituted benzene rings that are bridged at perpendicular C-N planes, the compounds are non-planar. The N-C bond distance N(2) – C(7) = 1.366(2) and bond angles N(2) – C(7) – C(6) = 115.75(14) validated the 2-

BTBA molecules N(2) – C(7) bond as revealed by de-protonation on the location. The de-protonation on the position of the N-C bond distance N(1) – C(8) = 1.364(3) and the bond angles N(1) – C(8) – C(9) = 118.9(2) show that the other compound 2-BTFBA molecules N(1) – C(8) bond. De-protonation occurs in compounds because the N-C bond distance is shorter. The compounds have large rotation barriers around the C-N bond, which is also obvious. Normally, the C-N single bond distance is 1.47, but synthesized molecules with shorter bond lengths, ionic pair electrons on the amide nitrogen, and carbonyl oxygen, may produce various isomers of amide derivatives.

Because of the presence of a more electronegative fluoride anion at the ortho position of the amide moiety, the molecule 2-BTFBA has an alternative bond angle and short bond distance of the C-F bond. The delocalization of the π -electron between the benzene ring was confirmed repulsion between the lone pair of electrons with strong electronegativity on F (1). The molecules show a large non-linear optical response in 2-BTBA (3a) and 2-BTFBA (3b) due to the distribution of the electron system in the moiety. It is due to the substituent and resonance effect of and fluoro group in 2-BTFBA (3b) molecules.

Fig. 3 (a-b). Molecular structure of (ORTEP) (a) 2-BTBA (b) 2-BTFBA.

B. FT-IR Spectral Studies

The grown crystals functional groups were studied effectively by FT-IR spectra. Fig. 4 (a-c) & Table II shows the FT-IR spectra of N-(1,3-benzothiazol-2-yl)benzamide [2-BTBA] & N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide [2-BTFBA] crystals and their respective molecular vibration assignments. The observed peaks at 3165 and 3233 cm⁻¹ indicate that N-H stretching vibration of benzamide in 2-BTBA and 2-BTFBA crystals respectively (2-aminobenzothiazole [2-ABT] as beginning material at 3393 cm⁻¹). In contrast to 2-ABT, which has absorption at 1521 cm⁻¹, the aromatic C=C stretching vibration frequency area was seen at 1552 and 1535 cm⁻¹. The stretching frequency of the secondary amide carbonyl (O=C-NH) group peak show up in the range 1670-1620 cm⁻¹. However, an extremely impressive vibration frequency peaks observed at

1670 and 1660 cm^{-1} are because of carbonyl stretching of 2-BTBA and 2-BTFBA compounds, which is clear from the arrangement of carbonyl ($\text{C}=\text{O}$) functional group in synthesized compounds. The observed peaks additionally affirm that the synthesized material has amide ($\text{O}=\text{C}-\text{NH}$) derivatives. The ($\text{C}=\text{O}$) carbonyl stretching vibration of the 2-BTFBA compound has slight variant and it very well might be expected to the $-\text{I}$ effect of the fluorine atom. Mono fluorinated compounds show a prominent band at 1100-1000 cm^{-1} , according to the data. The 2-BTFBA compound shows an absorption region at 1098 cm^{-1} it was affirmed that development of C-F bond. The C-H bending frequencies that have been detected are 748 and 759 cm^{-1} , respectively.

Fig. 4 (a-c). FT – IR Spectra of (a) 2-ABT, (b) 2-BTBA, (c) 2-BTFBA.

TABLE II: ASSESSMENT OF FT – IR SPECTRAL DATA OF(A) 2-BTBA (B) 2-BTFBA

Compound	FT – IR (Wave number (cm^{-1}))				
	N-H	C=N	C-N	C=O	C=C
2-Amino benzothiazole	3393	1626	1281	-	1522
2-BTBA	3165	1595	1273	1670	1553
2-BTFBA	3233	1613	1283	1661	1535

C. ^1H NMR analysis

A popular analytical strategy is to employ nuclear magnetic resonance (NMR) spectral analysis to determine the structure of organic compounds. The proton NMR spectra of N-(1,3-benzothiazol-2-yl)benzamide [2-BTBA] and N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide [2-BTFBA] are shown in Fig. 5 (a-c) with DMSO as the solvent. The NMR spectrum of the reactant molecule 2-aminobenzothiazole (2-ABT) reveals four different peaks, including a singlet at 6.9 ppm, because of the presence of aromatic primary amine. Due to the presence of aromatic protons in the benzene ring in benzothiazole, two doublet peaks and one triplet peak were found at 8.09 ppm (d, 1H, ArH), 8.25 ppm (d, 1H, ArH), and 7.52 ppm (d, 1H, ArH), respectively. The two amide products 2-BTBA (3a) and 2-BTFBA (3b) show no peak at 6.94 ppm, suggesting the nonappearance of a primary N-H proton; but, due to amide coupling, it is moved to a strong resonance at 12.0 to 12.9 ppm. The compound 2-BTBA (3a) shows eight peaks at δ 12.88 ppm (s, 1H, thiazole, amide $-\text{NH}$), δ 8.15 ppm (d, 2H, ArH), δ 8.03 ppm (d, 1H, ArH), δ 7.81 ppm (d, 1H, ArH), δ 7.67 ppm (t, 1H, ArH), δ 7.58 ppm (t, 2H, ArH), δ 7.48 ppm (t, 1H, ArH) and δ 7.35 ppm (t, 1H, ArH). The other Compound 2-BTFBA (3b) has seven distinct proton environments. The peaks appear at δ 12.85 ppm (s, 1H, thiazole, amide, $-\text{NH}$), δ 8.04 ppm (d, 1H, ArH), δ 7.81 ppm (t, 2H, ArH), δ 7.67 ppm (m, 1H, ArH), δ 7.48 ppm (t, 1H, ArH), δ 7.42 ppm (d, 1H, ArH) and δ 7.34 ppm (m, 2H, ArH). The presence of more electronegative fluorine in the benzene ring deshielded the chemical shifts of the aromatic ring protons.

D. ^{13}C NMR Analysis

The ^{13}C NMR spectra of 2-ABT (1), 2-BTBA (3a), and 2-BTFBA are shown in Figs. 6 (a-c) (3b). The compound 2-BTBA shows a carbon signal at 165.7 ppm in the downfield, since the substantially deshielded carbonyl carbon of the benzamide moiety. The eleven peaks at 174.3, 153.2, 134.2, 130.8, 132.1, 128.8, 127.5, 125.3, 124.6, 121.8 and 118.3 ppm in the spectrum of 2-BTBA (3a) corresponds to aromatic carbon of the benzene rings. The compound 2-BTFBA (3b) shows totally thirteen signals. There is a signal at 165.3 ppm in the downfield due to the carbonyl carbon of the benzamide molecule and peaks at 174.5, 159.3, 153.2, 133.7, 131.3, 130.8, 126.0, 125.4, 124.3, 121.8, 118.3 & 115.7 ppm are because of aromatic carbon of the phenyl rings.

Fig.5 (a-c). ^1H NMR Spectral data of (a) 2-ABT (b) 2-BTBA (c) 2-BTFBA.

Fig.6 (a-c). ^{13}C NMR Spectral data of (a) 2-ABT (b) 2-BTBA (c) 2-BTFBA.

E. UV-Visible Spectral Analysis

The UV-Visible spectrums of a grown single crystal are displayed in Fig. 7. 2-ABT (1), 2-BTBA (3a), and 2-BTFBA (3b) had experimental cutoff wavelengths of 262, 303, and 300 nm, respectively. The $n-\pi^*$ and $\pi-\pi^*$ transitions from aromatic ($\text{C}=\text{C}$) bonds and carbonyl group ($\text{C}=\text{O}$) in the compounds cause a huge difference in cutoff wavelengths between reactant and product molecules. When an electron donor group or an electron withdrawing group is present in a molecule, it improves polarization, causing higher absorbance. In the N-benzoylated benzothiazole molecule, the absorption band found in the visible range is assigned. In the visible area, the formed crystals have a good absorption property. It clearly shows that the crystals can be used for NLO purposes. The optical band gap energy (E_g) calculated in Fig. 8 (a-c) are 4.40, 3.83 & 3.86 eV for 2-ABT (1), 2-BTBA (3a) & 2-BTFBA (3b) single crystals correspondingly. In comparison to 2-BTFBA (3b) crystals, the 2-BTBA (3a) crystal has a lower band gap, according to the above research.

Fig.7.UV- Vis – NIR absorption Spectra of (a) 2-ABT (b) 2-BTBA (c) 2-BTFBA.

Fig. 8 (a-c).Optical band gap energy plots of (a) 2-ABT (b) 2-BTBA (c) 2-BTFBA.

F. Thermal Analysis

Fig 9 (a-c) shows the thermo gravimetric analysis (TGA) and differential thermal analysis (DTA) curves of 2- ABT (1), 2-BTBA (3a), and 2-BTFBA (3b) respectively. Perkin Elmer Diamond TG/DTA instrument used to find the thermal analysis of grown crystal in the range of 25°C to 600 °C at a

heating rate $20^{\circ}\text{C min}^{-1}$ in the inert nitrogen environment. The weight loss (from TGA) and melting point (from DTA) of generated single crystals were calculated. We can see that there is a single stage consecutive mass loss (99.46%, 99.65%, and 96%) commencing at roughly 110°C , 130°C , and 60°C , respectively, from the TGA curves of 2-ABT (1), 2-BTBA (3a), and 2-BTFBA (3b). There is no water crystallisation in 2-ABT (1) and 2-BTBA (3a) because the decomposition temperatures are higher than 100°C . The TGA curve of 2-BTFBA (3b) shows water crystallization as the decomposition starts 60°C itself and it shows that the three stages of weight loss. Small weight loss occurs in the first phase at temperatures ranging from 60 to 180°C , with a total weight loss of 5.093 percent. This mass loss indicates that water has been removed from the crystallisation process. The second stage is from 180 to 400°C , with an 88.24 percent mass loss, while the third stage is from 400 to 490°C , with a 2.218 percent mass loss. 2-ABT (1), 2-BTBA (3a), and 2-BTFBA (3b) had substantial endothermic peaks at 135.55°C , 193.97°C , and 159.40°C , respectively, on the DTA curve. At 325.30°C , Compound 2-BTFBA (3b) exhibits an exothermic peak, while the other two samples exhibit endothermic peaks. DTA analysis confirmed the absence of physically absorbed solvent or water crystallisation. In all of the 2-ABT (1), 2-BTBA (3a), and 2-BTFBA (3b) compounds, the TGA-DTA analysis reveals no phase transition before decay. These crystals have also been found to be thermally stable up to 110°C and 130°C , respectively. Because of its high thermal stability, the 2-BTFBA (3b) crystal is a superior candidate for NLO applications.

Fig.9 (a-c). TGA-DTA Curves of(a) 2-ABT (b) 2-BTBA (c) 2-BTFBA.

G. Non-linear Optical Studies

The second harmonic generation (SHG) proficiency estimated from the Kurtz –Perry powder test of the developed crystals 2-BTBA (**3a**) and 2-BTFBA (**3b**) contrasted and assessed with potassium dihydrogen phosphate (KDP). A micro capillary tube was utilized to tightly pack the powdered samples and position them in the path of the optical source, a Q- Switched Nd: YAG laser. A standard laser beam with an energy of 1.2 mJ per pulse, a wavelength of 1064 nm, a pulse width of 10 ns, and a frequency of 10 Hz was used to fall naturally on the samples. The light (Green) released by the samples is detected by an oscilloscope assembly, which uses a photo multiplier tube as a detector. The output of the second harmonic signal ($\lambda = 532$ nm) for 2-BTBA (**3a**) and 2-BTFBA (**3b**) molecules was 91 mV and 113 mV, respectively. For a similar frequency range, the reference material KDP yields 40 mV. The SHG conversion efficiency of these three crystals is found to be 2.28 and 2.83 times greater than that of reference sample and they are listed in Table 3. The laser damage threshold studies show that 1.28 and 1.68 (GWcm⁻²) for 2-BTBA (**3a**) and 2-BTFBA (**3b**) compounds, respectively. The reference material KDP shows 0.2 (GWcm⁻²) of the same damage threshold regions. The Nonlinear Optical property confirms by all the synthesized material was emitted green light. The SHG test also demonstrates the fact that the 2- BTFBA crystal has higher SHG efficiency and laser damage threshold.

TABLE III: EVALUATION OF NLO PROPERTY AND LASER DAMAGE THRESHOLD OF (A) 2-BTBA (B) 2-BTFBA.

Sample code	Output energy (mV)	Input energy (mJ/pulse)	Damage Thersold (GWcm ⁻²)
KDP	40	1.2	0.2
2-BTBA	91	1.2	1.28
2-BTFBA	113	1.2	1.68

H. Biological Applications

Because of the amino group in the second position of the benzothiazole ring, the benzothiazole and its analogues had moderate to high activity against gramme +ve and gramme –ve bacteria. The antimicrobial activity of 2-amino benzothiazole and its derivatives 2-BTBA (**3a**) and 2-BTFBA (**3b**) was investigated and tested in vitro against e. faecalis, pseudomonas aeruginosa, staphylococcus aureus, and aspergillus niger, aspergillus flavus, and Candida albicans as antibacterial and antifungal organisms, respectively.

Ciprofloxacin was utilized as a typical for antibacterial agent. The antibacterial test used Ciprofloxacin as a control, whereas the antifungal test used Amphotericin B as a control. The antibacterial activity was tracked using the conventional Agar well diffusion approach. With the suspension of each bacterial cell, the Brain Heart Infusion (BHI) broth technique was used. The immunised plates are incubated for 12-24 hours at 37°C. Using vernier callipers, the presence of a zone of restraint assessed in measurement (mm) during this time period corroborated the activity. When compared to control, the range of the zone is the proportion of antibacterial and antifungal effects induced by the concentrates. For the test, the orchestrated compounds were dissolved in Dimethyl sulfoxide (DMSO).

The antibacterial outcomes are displayed in Fig. 10 and recorded in Table IV for 2-amino benzothiazole (**1**) and synthesized (**3a-b**) compounds alongside the examination of principles. The analyzed outcomes show 2-amino benzothiazole (**1**) was more active and other all synthesized intensifies 2-BTBA (**3a**) and 2-BTFBA (**3b**) are respectably dynamic to idle with standard. The antifungal activity data shown in Fig. 11 and Table V show that 2-amino benzothiazole (**1**) has unmatched activity, while the other two compounds, 2-BTBA (**3a**) and 2-BTFBA (**3b**), were moderately active when compared to standards. This is due to the benzoyl and 2-fluorobenzoyl groups protecting the active 2-amino primary group in the benzothiazole ring.

Fig.10 (a-c) Antibacterial activity of synthesized compounds with (a) Enterococcus faecalis (b) Pseudomonas aeruginosa, (c) Staphylococcus aureus and Ciprofloxacin as a standard.

Fig. 11 (a-c). Antifungal activity of synthesized compounds with (a) Aspergillus niger, (b) Aspergillus flavus (c) Canida albicans and Amphotericin B as a standard.

TABLE IV: COMPARISON OF ANTIBACTERIAL ACTIVITY OF SYNTHESIZED COMPOUNDS WITH ENTEROCOCCUS FAECALIS PSEUDOMONAS AERUGINOSA, STAPHYLOCOCCUS AUREUS AND CIPROFLOXACIN AS A STANDARD

S.No	Microorganisms	Control	2-ABT	2-BTBA	2-BTFBA	Cipro floxacin
Zone of inhibition in mm						
1.	<i>Enterococcus faecalis</i>	-	10	-	5	13
2.	<i>Pseudomonas aeruginosa</i>	-	-	-	-	25
3.	<i>Staphylococcus aureus</i>	-	15	7	10	30

TABLE V: COMPARISON OF ANTIFUNGAL ACTIVITY OF SYNTHESIZED COMPOUNDS WITH ASPERGILLUS NIGER, ASPERGILLUS FLAVUS, CANDIDA ALBICANS AND AMPHOTERICIN B AS A STANDARD

S.No	Microorganisms	Control	2-ABT	2-BTBA	2-BTFBA	Amphotericin-B
Zone of inhibition in mm						
1.	<i>Aspergillus niger</i>	-	20	5	8	12
2.	<i>Aspergillus flavus</i>	-	20	5	6	13
3.	<i>Candida albicans</i>	-	20	10	7	12

IV. CONCLUSION

We have introduced 2-aminobenzothiazole benzamide subsidiaries (3a-b) in the current study by benzylation of 2-aminobenzothiazole in its basic state. Great worth single crystals of N-(1,3-benzothiazol-2-yl)benzamide [2-BTBA] and N-(1,3-benzothiazol-2-yl)-2-fluorobenzamide [2-BTFBA] Compounds were produced at room temperature using a slow evaporation process. The crystals 2-BTBA and 2-BTFBA crystallise as monoclinic crystal systems with the P_{21}/n space group. The functional groups and environments of proton and carbon locations contained in the 2-BTBA and 2-BTFBA single crystals were identified using FT-IR and NMR spectrum studies. The thermal stability of these crystals is up to 403 K, among the 2-BTFBA crystal having the best thermal strength. All 2-BTBA (3a) and 2-BTFBA (3b) single crystals exhibit frequency doubling. Their laser damage threshold and NLO efficiency show that 2-BTFBA (3b) is the best contender for all NLO applications. When tested for gramme +ve and gramme -ve bacterial cultures, 2-ABT and derivatives of 2-BTBA and 2-BTFBA show good to moderate antibacterial and antifungal activity against a variety of bacterium strains. It was observed that a good activity for (2-ABT, 2-BTBA) against all the tested bacterial strains compared with 2-BTFBA (3b) shows inactivity to moderate activity.

SUPPORTING INFORMATION

The Cambridge Crystallographic Data Centre has deposited crystallographic data for the structure described in this research. 2-BTBA (3a) and 2-BTFBA (3b) crystal copies of the data can be obtained in (CCDC 2002996) and (CCDC 2002997). UK [email: deposit@ccdc.cam.ac.uk].

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