Analysis of New Piperidine Substituted Benzothiazole Crystalline Derivatives

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ABSTRACT

Recently, heterocyclic compounds play important role in drug industries. The benzothiazole (BTA) is a bicyclic compound in heterocyclic because of their biological properties. In this paper the synthesis and characterization of benzothiazole were reported. The chemical structures of synthesized compounds were established based on spectral data of 1HNMR, 13CNMR, and IR. The mass of the novel compounds was established with the help of the LCMS test. The formation of the crystal was confirmed by powder XRD and the sharp peaks show the purity and crystalline nature of the samples. The photoluminescence spectra explain the optical property of the compound. The biological studies of synthesized compounds show that compound 5c possesses good antibacterial activity and compound 5d has good antifungal activity.

Keywords: Piperidine derivatives, Benzothiazole, Biological property, Crystallization, Optical activity.

INTRODUCTION

The benzothiazole derivatives possess superior biological and bio-physical properties such as antitumor and metabolic activities1, antimicrobial2-5, imaging agents for β-amyloid6 anti-cancer7, anti-tuberculosis8 anti-viral9, anti-oxidant10 and hence driven the attention of the researchers for further development. Several substituted benzothiazoles have been identified as potent anthelmintic drugs11-14. Aminobenzothiazoles have manifested a large scale of biological activities such as antiparkinsonian, dopa-mine antagonist15-16, schistosomicidal agents17, anticonvulsant activity18, antileishmanial activity19, analgesic agents20, and antiasthmatic drugs21. Moreover, compounds containing condensed pyrimidines have been used as herbicide antidotes22, and diuretics23. The BTA act as an effective catalyst24 and the crystal nature shows fluorophore property25. Based on earlier studies, an attempt is made to prepare benzothiazole derivatives. The prepared samples were characterized for their potential applications.

EXPERIMENTAL

Materials

The chemicals ethyl2-aminobenzo[d] thiazole-6-carboxylate, copper(II)bromide, t-nitrosobutane, piperidine, cesium carbonate,
sodium hydroxide, acetonitrile, dimethylformamide, methanol, hydrochloric acid, ethylacetate, dichloromethane, triethyl amine, sodium sulphate, propene phosphoric acid anhydride, substituted amines were of Sigma-Aldrich. These are used without purification. The dry ethyl acetate, hexane, and ethanol were obtained from Spectrochem for the crystallization process.

**Instruments and methods**

The Perkin-Elmer spectrum 100 series spectrophotometer was used for FTIR studies of the sample. The information about the nature and number of protons was studied from the 1HNMR spectrum. The 1HNMR spectra were studied by using a 400 MHz Varian spectrometer. The information about carbon was obtained from the 13CNMR spectrum of compound which was taken for the samples by subjected to 100MHz Brucker spectrometer with TMS as reference compound.

With the help of Shimadzu mass spectrometer, the mass spectra were obtained. All the reactions were monitored by TLC plates and their spots were visualized by exposing them to a UV lamp, iodine chamber, or KMnO4, and it was performed with silica gel 60-120mesh. The crystal formation and optical properties were ensured by powder XRD and photoluminescence studies respectively. The data were taken by XPERT-PRO-Gonio scan-2 m diffractometer and Cary Eclipse-EL08083851 photo spectrometer. The elemental analysis was done by the Varian instrument (VARIO EL-3 series analyzer).

**Synthesis and characterization**

**Synthesis of Ethyl 2-bromobenz[d]thiazole-6-carboxylate (2)**

In a round bottom flask, 5 g of ethyl2aminobenz[d]thiazole-6-carboxylic acid dissolved in 1 eq of acetonitrile solvent then added 1 eq of copper(II)bromide with t-nitrosobutane. The reaction mixture was mixed thoroughly using a magnetic stirrer up to 16 h maintaining in the room temperature. It was monitored by TLC complies. After that, the ethyl acetate was added with the reaction mixture to dilute it. The 1.5N HCl, water, and brine solution were used to wash the reaction mixture. Now the mixture was dried over sodium sulphate, and concentrated below 50°C. The crude has proceeded to the next step without purification.

It was obtained as yellow solid. The yield was 54%. (LCMS: 95% purity). B.pt.139-40°C, IR (KBr, cm⁻¹): νmax 1742(C=O), 1647(C=N), 1324(C-N), 684(C-S), 610(C-Br). 1HNMR (400 MHz, DMSO-d₆, ppm): δ 8.420 (s, 1H, ArH), 7.453-7.482 (d, 2H, J=11.6Hz ArH), 4.302 (m, 2H, -CH₂), 1.289-1.301 (t, 3H, J=4.8Hz -CH₃). 13CNMR (100 MHz, DMSO-d₆, ppm): δ 14.32, 60.50, 121.34, 123.52, 126.40, 128.63, 141.36, 155.77, 165.62. For C₁₀H₈BrNO₂S, Calculated: C-41.97%, H-2.82%, Br-27.92%, N-4.89%, 0-11.19%, S-11.21%. Found: C-42.04%, H-2.90%, Br-27.86%, N-4.92%, 0-11.13%, S-11.15%. LCMS [M+1]+: m/z 287.1.

**Synthesis of Ethyl 2-(piperidin-1-yl)benzo[d]thiazole-6-carboxylate (3)**

The obtained compound (2) was dissolved in DMF and added to the N-alkylation base (CS₂CO₃ 1.5 eq). Now piperidine (1.1 eq) was added and then subjected for thermal treatment to a temperature of 100°C for 3 hours. After complies, it was cooled and purified to get compound (III).

It was obtained as orange solid with 56% yield, (LCMS: 95.7% purity), m.pt.161-162°C, IR (KBr, cm⁻¹): νmax 1740(C=O), 1643(C=N), 1326(C-N), 681(C-S). 1HNMR (400 MHz, DMSO-d₆, ppm): δ 1.536-1.553 (m, 6H, -CH₂), 3.691-3.724, (t, 4H, J=13.2Hz-CH₂) 8.414 (s, 1H, ArH), 7.697-7.721 (d, 2H, J=9.2Hz ArH), 4.292 (m, 2H, -CH₂), 1.292-1.313 (t, 3H, J=8.4Hz -CH₃). 13CNMR (100 MHz, DMSO-d₆, ppm): δ 14.44, 24.21, 25.45, 54.2, 61.02, 116.55, 123.26, 126.57, 130.61, 157.62, 165.87, 168.13. For C₁₅H₁₈N₂O₂S, Calculated: C-62.04%, H-6.25%, N-9.65%, 0-11.02%, S-11.04%. Found: C-61.98%, H-6.27%, N-9.69%, 0-11.05%, S-11.01%. LCMS [M+1]+: m/z 291.3.

**Synthesis of 2-(piperidin-1-yl)benzo[d]thiazole-6-carboxylic acid (4)**

The 2 g measured compound (3) was dissolved in methanol. Now, 2 eq sodium hydroxide solution (NaOH dissolved in water) was added. Now it was stirred for a time duration of 1 h at room temperature. After TLC complies, acidified with 1.5 N HCl. Then it was extracted with ethyl acetate. The organic layer was washed with water, dried, and concentrated. With the help of column chromatography crude was purified and compound eluted with methanol (2.4%) and DCM to get the desired product.
It was obtained as yellow solid of 67% of yield, (LCMS: 95.3% purity), m.pt.169-70°C, IR (KBr, cm⁻¹): νmax 3242(O-H), 1761(C=O), 1645(C=N), 1321(C-N), 684(C-S). ¹H NMR (400 MHz, DMSO-d₆, ppm): δ 1.546-1.5621 (m, 6H, -CH₂), 3.716-3.734 (t, 4H, J=7.2Hz, -CH₂) 8.618, (s, 1H, ArH), 7.882-7.894 (d, 2H, J=7.4Hz ArH), 11.121 (s, 1H, -OH). ¹³CNMR (100 MHz, DMSO-d₆, ppm): δ 24.14, 25.52, 54.36, 116.74, 123.62, 126.88, 130.73, 158.55, 166.72, 168.15. For C₁₃H₁₄N₂O₂S, Calculated: C-59.52%, H-5.38%, N-10.68%, O-12.20%, S-12.22%. Found: C-59.59%, H-5.41%, N-10.72%, O-12.12%, S-12.16%. LCMS [M+1]+: m/z 263.3.

**Preparation of benzothiazole derivatives (5a-e)**

In the solvent dichloromethane (1 mL), one equivalent (100 mg) weighed compound (4) was dissolved. Now the solution was added to simple amine (1 eq), triethylamine (2 eq). The mixture was stirred for 2 hours. Then cooled to zero degrees Celsius. Now, propane phosphoric acid anhydride (T3P) (50% in ethyl acetate) (1.5 eq) was added and again stirred for 12 hours. At the end of the reaction, monitor by TLC, the addition of ice water was done and extracted with dichloromethane. Finally washed in water and brine solution, dried over sodium sulphate, then concentrated. The purification of crude was made by column chromatography (using silica gel) eluent (petroleum ether and 50 – 70% of ethyl acetate) to get desired product (5a-e). All the reaction schemes were shown in Fig. 1. The yield and melting point of these samples are presented in Table 1.

**Table 1: Results of reaction**

| Compound | Simple amine     | Product | Yield % | m.pt °C |
|----------|------------------|---------|---------|---------|
| 5a       | Ailine           |         | 68      | 230 - 31|
| 5b       | t-butyamine      |         | 72      | 233 - 34|
| 5c       | 3,4-difluoro    |         | 63      | 218 - 19|
| 5d       | Morpholine       |         | 70      | 128 - 29|
| 5e       | Cyclo propyl    |         | 76      | 240 - 41|
Synthesis of N-phenyl-2-(piperidin-1-yl)benzo[d]thiazole-6-carboxamide (5a)

The aniline was used to obtain the above compound (5a). The reactions results as white crystalline solid of 68% yield. (LCMS: 96.1% purity), m.pt. 230-31°C, IR (KBr, cm⁻¹): ν max 3230(N-H), 1629(C=O), 1629(C=N), 691(C=S). ¹HNMR (400 MHz, DMSO-d₆, ppm): δ 1.542-1.562 (m, 6H, -CH₂), 3.742-3.761 (t, 4H, J=7.6Hz -CH₂), 7.921-7.942 (d, 1H, J=8.4Hz ArH), 7.635-7.641 (d, 3H, J=2.4Hz ArH), 8.382 (s, 1H, ArH), 9.194 (s, 1H, -NH), 7.293-7.316 (t, 3H, J=9.2Hz ArH). ¹³CNMR (100 MHz, DMSO-d₆, ppm): δ 24.32, 25.26, 54.48, 121.17, 121.73, 123.85, 128.41, 131.07, 137.58, 156.53, 164.36, 167.92. For C₁₉H₁₉N₃O₂S, Calculated: C-67.63%, H-5.68%, N-12.45%, O-4.74%, S-9.50%. Found: C-67.57%, H-5.71%, N-12.41%, O-4.79%, S-9.52%. LCMS [M+1]+: m/z.337.4.

Synthesis of N-(tert-butyl)-2-(piperidin-1-yl)benzo[d]thiazole-6-carboxamide (5b)

The t-butyl amine was added that reacts to give the compound 5(b). It was obtained as a white crystalline solid with a 72% yield. (LCMS: 95.3% purity), m.pt. 233-34°C, IR (KBr, cm⁻¹): ν max 3333(N-H), 1625(C=O), 1625(C=N), 1321(C-N), 694(C-S). ¹HNMR (400 MHz, DMSO-d₆, ppm): δ 1.548-1.591 (m, 6H, -CH₂), 3.695-3.702 (t, 4H, J=2.8Hz -CH₂), 7.878-7.895 (d, 1H, J=6.8Hz ArH), 7.672-7.685 (d, 1H, J=5.2Hz ArH), 8.402 (s, 1H, ArH), 1.402 (s, 9H, -CH₃). ¹³CNMR (100 MHz, DMSO-d₆, ppm): δ 24.58, 25.32, 29.15, 54.62, 59.57, 121.17, 121.67, 123.96, 130.85, 156.42, 168.12. For C₁₇H₂₃N₃OS, Calculated: C-64.32%, H-7.30%, N-13.24%, O-5.04%, S-10.10%. Found: C-64.38%, H-7.26%, N-13.21%, O-5.01%, S-10.14%. LCMS [M+1]+: m/z.317.4.

Synthesis of N-(3,4-difluorophenyl)-2-(piperidin-1-yl)benzo[d]thiazole-6-carboxamide (5c)

The compound 5(c) was obtained by the addition of 3,4-difluoro aniline. It was obtained as a white crystalline solid with a 63% yield, (LCMS: 95.6% purity), m.pt. 218-19°C, IR (KBr, cm⁻¹): ν max 3267(N-H), 1623(C=O), 1623(C=N), 1290(C-F), 1148(C-S). ¹HNMR (400 MHz, DMSO-d₆, ppm): δ 1.358-1.556 (m, 6H, -CH₂), 3.707-3.719 (t, 4H, J=4.8Hz -CH₂), 7.796-7.812 (d, 1H, J=6.4Hz ArH), 7.578-7.601 (d, 3H, J=9.2Hz ArH), 8.412 (s, 1H, ArH), 9.562 (s, 1H, -NH), 7.742 (s, 1H, ArH). ¹³CNMR (100 MHz, DMSO-d₆, ppm): δ 1.536-1.569 (m, 6H, -CH₂), 3.695-3.702 (t, 4H, J=6.8Hz -CH₂), 7.878-7.895 (d, 1H, J=6.8Hz ArH), 7.672-7.685 (d, 1H, J=5.2Hz ArH), 8.402 (s, 1H, ArH), 2.765 (m, 1H, -CH), 0.612-0.850 (m, 4H, -CH₂). For C₁₉H₁₇F₂N₃OS, Calculated: C-61.11%, H-4.59%, F-10.18%, N-11.25%, O-4.28%, S-8.59%. Found: C-61.02%, H-4.52%, F-10.24%, N-11.30%, O-4.31%, S-8.61%. LCMS [M+1]+: m/z.473.4.

Synthesis of morpholine(2-(piperidin-1-yl)benzo[d]thiazol-6-yl)-methanone (5d)

The addition of morpholine yields compound 5(d). It was obtained as pale yellow crystalline solid, with a 70% yield. (LCMS: 93% purity), m.pt. 128-29°C, IR (KBr, cm⁻¹): ν max 3332(N-H), 1625(C=O), 1625(C=N), 1320(C-N), 682(C-S). ¹HNMR (400 MHz, DMSO-d₆, ppm): δ 1.526-1.549 (m, 6H, -CH₂), 3.720-3.738 (t, 4H, J=7.2Hz -CH₂), 7.901-7.925 (d, 1H, J=9.6Hz ArH), 7.645-7.681 (d, 1H, J=14.4Hz ArH), 8.421 (s, 1H, ArH), 3.591-3.615 (t, 8H, -CH₂). ¹³CNMR (100 MHz, DMSO-d₆, ppm): δ 24.29, 25.63, 36.47, 46.33, 54.37, 66.18, 121.22, 121.67, 123.96, 131.10, 156.45, 168.17, 168.81. For C₁₇H₂₁N₃O₂S, Calculated: C-61.61%, H-6.39%, N-12.68%, O-9.65%, S-9.67%. Found: C-61.68%, H-6.35%, N-12.64%, O-9.69%, S-9.64%. LCMS [M+1]+: m/z.331.4.

Synthesis of N-cyclopropyl-2-(piperidin-1-yl)benzo[d]thiazole-6-carboxamide (5e)

The reaction of cyclopropyl amine and the compound (5) results the compound 5(e) in the form of white crystalline solid. Its yield percentage is 76% (LCMS: 95.4% purity), m.pt. 240-41°C, IR (KBr, cm⁻¹): ν max 3267(N-H), 1623(C=O), 1623(C=N), 1290(C-F), 1148(C-S). ¹HNMR (400 MHz, DMSO-d₆, ppm): δ 1.536-1.569 (m, 6H, -CH₂), 3.695-3.702 (t, 4H, J=6.8Hz -CH₂), 7.901-7.925 (d, 1H, J=9.6Hz ArH), 7.645-7.681 (d, 1H, J=14.4Hz ArH), 8.421 (s, 1H, ArH), 2.765 (m, 1H, -CH), 0.612-0.850 (m, 4H, -CH₂). ¹³CNMR (100 MHz, DMSO-d₆, ppm): δ 1.536-1.569 (m, 6H, -CH₂), 3.695-3.702 (t, 4H, J=6.8Hz -CH₂), 7.901-7.925 (d, 1H, J=9.6Hz ArH), 7.645-7.681 (d, 1H, J=14.4Hz ArH), 8.421 (s, 1H, ArH), 3.591-3.615 (t, 8H, -CH₂). For C₁₆H₁₉N₃OS, Calculated: C-63.76%, H-6.35%, N-13.94%, O-5.31%, S-10.64%. Found: C-63.68%, H-6.35%, N-13.94%, O-5.31%, S-10.64%. LCMS [M+1]+: m/z.473.4.
RESULT AND DISCUSSION

The functional groups present in all the compounds were identified by FTIR spectra of these compounds. The compound 5c shows an additional peak due to C-F functional group at 1240 cm\(^{-1}\). The result of FTIR confirms the formation of the synthesized compounds. In \(^1\)HNMR, all the compounds display the almost same chemical shift values. However, in compound 5d singlet due to N-H is disappeared. It is because of the presence of two R-groups instead of one R-group and one H-atom which were present in all other groups. Similarly, when comparing the \(^1\)HNMR spectrum of the compounds 5a and 5c, it is observed that the doublet at \(\delta (7.635-7.641 \text{ ppm})\) is changed as a singlet at \(\delta (7.742 \text{ ppm})\). It is due to the substitution of fluorine that replaces hydrogen at C-3 in aniline. The same result was also obtained in \(^{13}\)CNMR the chemical shift value changes from 128.41 to 145.26 ppm. The structure of these compounds was confirmed from the \(^{13}\)CNMR and \(^1\)HNMR. From the Table 1, it is observed that the melting point of the synthesized compounds is almost the same except for compound 5d. The compound 5d shows a lower melting point value. The addition of heterocyclic compound (Morpholine) weakens the bond and hence reduces the melting point. The results of LCMS analysis establish the formation of the products. The percentage of the elements present in the products was obtained from elemental analysis. These values agree with theoretically calculated values. Hence the formation of the products is also confirmed from this analysis.

Antibacterial and antifungal activity

Antibacterial activity

In earlier days, simple and easy method of screening the antibacterial activity of a sample by the agar well diffusion method was used (Perez et al., 1990, Perez et al., 1999, Bagamboula et al., 2004 and Erdemoglu et al., 2003). In Brain Heart Infusion (BHI) (Difco, Detroit, MI) broth the microorganism was suspended. It was diluted to roughly 106 colony-forming units (cfu) per mL. On the surface of BHI agar and Sabouraud Dextrose Agar (SDA) (Difco, Detroit, MI), these diluted microorganisms were spread as “flood-inoculated”. Then it was dried. The SDA was used for \(C.\) albicans and \(C.\) tropicalis. The wells of 5 mm size were cut from the agar using a sterile cork-borer. Now 25 μL of the sample solutions were poured in these wells. The plates were kept in an incubation chamber for 18 h at 35°C. The measurement of zone of inhibition gives the antimicrobial activity of the samples. Ciprofloxacin (10 μg/mL) was the standard drug for antibacterial activities. The tests were carried out in duplicates. The diameter of inhibition zone was measured and interpreted.

The Minimal Inhibitory Concentration (MIC) and Minimal Bactericidal Concentration (MBC) was measured by the broth dilution method (Van der Berghe and Vlietinck, 1991). About 1.0 to 0.25 mg/mL diluted plant extract was used. Test bacteria culture with concentration of 105 CFU/mL was used. After 24 h of incubation at 37°C the MIC values were taken as the lowest plant extracts concentration which restricts visible bacterial growth and MBC was the lowest concentration that completely inhibited bacterial growth. In this method the reference was Ciprofloxacin. The experimental procedure was done thrice.

The antibacterial activity of all the synthesized compounds was tested \textit{In vitro} against pathogenic \textit{Enterococcus faecalis}, \textit{Staphylococcus aureus}, \textit{Escherichia coli}, and \textit{Salmonella typhi}. The results are presented in Table 2.

Table 2: Antibacterial activity of the compounds

| Microorganisms          | Control | 5a  | 5b  | 5c  | 5d  | 5e  | Ciprofloxacin |
|-------------------------|---------|-----|-----|-----|-----|-----|--------------|
| Zone of inhibition in mm|          |     |     |     |     |     |              |
| \textit{Enterococcus faecalis} | 10.5±0.55 | 11.24±0.67 | 18.45±0.44 | 07.44±0.56 | 11.54±0.67 | 35.56±0.55 |
| \textit{Staphylococcus aureus} | 08.42±0.10 | 07.12±0.10 | 10.56±0.66 | 12.34±0.30 | 07.55±0.10 | 40.54±0.48 |
| \textit{Escherichia coli}  | 07.55±0.00 | 08.15±0.00 | 11.87±0.54 | 13.44±0.45 | 08.45±0.00 | 38.54±0.60 |
| \textit{Salmonella typhi}  | 06.67±0.22 | 09.21±0.00 | 08.22±0.00 | 08.57±0.00 | 09.45±0.00 | 35.76±0.10 |
Antifungal activity

As reported earlier by Alves and Cury, 1992, the samples were examined for antifungal activity by dilution in agar technique. A 100 mg plant extracts were dissolved in 1 mL of dimethyl sulfoxide (DMSO) and then undergone two fold dilution in Yeast Nitrogen Base Phosphate (YNBP) agar (Merck, Germany) to get a concentration range of 31.25-1000 µL/mL. The YNBP agar plates having only DMSO diluted in the same way, that didn’t influence the fungal growth, were used as controls. These fungal strains were suspended in sterile physiological Tris buffer (pH 7.4, 0.05M), homogenized, and adjusted to an OD (530nm) of 0.05 (equivalent to 1 X 106 CFU/mL). This suspension was used as the inoculum for the test in the agar plates. Using an automatic micropipette, the fungal suspensions (3 µL) were inoculated. These plates (diameter: 25 cm) were kept for incubation at 37°C for 48 hours. The minimal inhibitory concentration (MIC) is defined as the minimum concentration of the plant extracts required to inhibit completely the visible growth of the fungus. Ketoconazole was used as a reference and appropriate controls with no plant extracts were used. Each experiment was carried out for three times.

The antifungal activity of all the synthesized compounds was tested in vitro against pathogenic Aspergillus niger, Aspergillus flavus, Candida albicans, and Penicillium sps. The results are given in Table 3.

| Microorganisms         | Control | 5a       | 5b       | 5c       | 5d       | 5e       | Ketoconazole |
|------------------------|---------|----------|----------|----------|----------|----------|--------------|
| Aspergillus niger      | -       | 07.32±0.10| 08.13±0.00| 10.55±0.20| 10.67±0.10| 08.34±0.00| 12.54±0.50   |
| Aspergillus flavus     | -       | 06.35±0.00| 06.64±0.10| 08.22±0.01| 09.56±0.30| 07.10±0.10| 09.30±0.30   |
| Candida albicans       | -       | 08.34±0.10| 11.24±0.20| 07.35±0.00| 10.45±0.00| 12.15±0.20| 12.44±0.40   |
| Penicillium sps        | -       | 07.10±0.00| 07.15±0.10| 7.50±0.00 | 08.25±0.02| 07.40±0.10| 15.34±0.10   |

Powder XRD studies

The powder XRD pattern is shown in Fig. 4. From the graph, it is observed that the peaks are sharp and intense. This shows that the sample is pure and crystalline in nature.

The crystalline size is calculated from the Debye-scherrer formula:

\[ D = \frac{0.9 \times \lambda}{\beta \cos \theta} \]

where:
- \( \lambda \rightarrow \) wavelength 1.546 Å
- \( \beta \rightarrow \) Full width half (0.1476 deg = 0.002576 rad)
- \( \theta \rightarrow \) Angle of diffraction (16.1967/2 = 8.0935 deg = 0.14134 rad)
- \( D = 0.9 \times 0.154/0.002576 \times \cos (0.14134) \)
- \( D = 54.3652 \) nm.

Table 3: Antifungal activity of the compounds

Fig. 2. Antibacterial activity

Fig. A. 3. Antifungal activity

Fig. 4. Powder X-ray diffraction pattern of N-phenyl-2-(piperidin-1-yl)benzo[d]thiazole-6-carboxamide(5a)
Fig. 5. Powder X-ray diffraction pattern of compounds 5b to 5e

Table 4: Crystalline size of the compounds

| S. No | Compound name | Size (nm) |
|-------|---------------|-----------|
| 1     | 5a            | 54.3652   |
| 2     | 5b            | 54.4454   |
| 3     | 5c            | 54.2976   |
| 4     | 5d            | 54.4046   |
| 5     | 5e            | 54.6069   |

The crystalline size of the samples are calculated and presented in Table 2.

Photoluminescence

The photoluminescence (PL) spectrum examines material for its wide applications in the field of medical, biochemical, and chemical research. In PL spectroscopy, generally, a beam of light excites the electrons in the molecule of given materials and causes them to emit light in a longer wavelength than the observed radiation. The figures Fig. 9 to Fig. 13 show the PL spectra of the samples. These spectra give the absorption wavelength at 362 to 381nm which means the emission of blue radiation. The absorption peak is due to the band-to-band electronic transition in a material. The result predicts the use of the materials as a color filter.
CONCLUSION

The synthesis of derivatives of benzothiazole (5a-e) was carried out. The functional groups present in the samples were studied from the FTIR spectra and thus it confirms the synthesis of the compounds. The proton and carbon positions of these were obtained through ¹H NMR and ¹³C NMR spectra respectively. The LCMS study indicates the good yield of all the compounds. The synthesized compounds exhibited antibacterial and antifungal activities. From the antibacterial test the compounds 5c, 5d, 5e, and 5e are show the highest activity of Enterococcus faecalis, Staphylococcus aureus, Escherichia coli, and Salmonella typhi, respectively. In the antifungal activity test the compounds 5c & 5d, 5d, 5b & 5e, and 5d show the higher activity of Aspergillus niger, Aspergillus flavus, Candida albicans, and Penicillium sps, respectively. The crystalline nature of the samples was confirmed by the powder X-ray diffraction studies. These samples show good optical nature as studied from the PL study. Hence the synthesized compounds can be used as color filters and in pharmaceutical applications.

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Conflict of interest

The authors declare no conflict of interest.

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