

Short Note

N-[3-(*N*-*tert*-Butoxycarbonylaminoxy)propyl]-2-[2-(3-butynylcarbonylamino)ethylthio]-1,3-benzothiazole-6-carboxamide

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Abstract

We report the synthesis of a modified benzothiazole sulfide. This compound contains a heterocyclic core, a Boc-protected hydroxylamine, and an appended alkyne. This benzothiazole was accessed through three total steps, including an amidation reaction and two nucleophilic aromatic substitutions. The identity of the title compound was confirmed through ^1H , ^{13}C , ^1H - ^1H COSY, HSQC, and HMBC NMR, in addition to IR, MALDI-MS, HRMS, and HPLC.

Keywords: benzothiazole; alkyne; nucleophilic aromatic substitution

1. Introduction

Benzothiazoles are versatile chemical scaffolds found in a variety of valuable compounds (Figure 1) [1–4]. These heterocycles are easy to access synthetically through various reactions, including condensations between 2-aminothiophenols with aldehydes [5] and carboxylic acid derivatives [6], as well as transition metal-catalyzed approaches [7]. Numerous benzothiazoles are present in therapeutic compounds, including ethoxzolamide [8], which is used to treat glaucoma, flutemetamol [9], which is a diagnostic used for Alzheimer's detection, and tropifexor [10], used to treat liver disease. Medicinally relevant benzothiazoles are often functionalized at various positions, especially the C2 and C6 positions. These heterocycles have also found utility as chemical biology tools. Benzothiazole sulfones with appended alkynes have previously been applied to profile cell lysates for reactive Cys-containing proteins [11]. The sulfone can act as a leaving group for nucleophilic aromatic substitution ($\text{S}_{\text{N}}\text{Ar}$) with free Cys-thiols on proteins [12,13]. The alkyne handle enables reacted benzothiazoles to be isolated from the complex reaction mixture using copper-catalyzed azide–alkyne cycloadditions (CuAAC) [14,15]. A benzothiazole sulfone has also been incorporated into short peptides and used as a cleavable linker [16]. In this context, benzothiazoles containing valuable cargo, such as biotin, can be incorporated onto peptides and cleaved off with thiols through $\text{S}_{\text{N}}\text{Ar}$. Tools such as these are useful for the capture and release of hit peptides during library screening [17–19].

Within this context, our group set out to synthesize a novel benzothiazole, *N*-[3-(*N*-*tert*-Butoxycarbonylaminoxy)propyl]-2-[2-(3-butynylcarbonylamino)ethylthio]-1,3-benzothiazole-6-carboxamide (6, Figure 2). In addition to containing a versatile benzothiazole core, this compound is appended with a protecting hydroxylamine and an alkyne. These traits enable the application of this compound toward two bio-orthogonal transformations. The hydroxylamine can react with aldehydes on small molecules or biomolecules to form oximes [20].



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The alkyne can react with azide-containing compounds in (copper azide–alkyne cycloadditions) CuAAC reactions [14,15]. The benzothiazole sulfide core could be further oxidized to a sulfone, making it reactive toward S_NAr reactions with thiols [12,13,16].

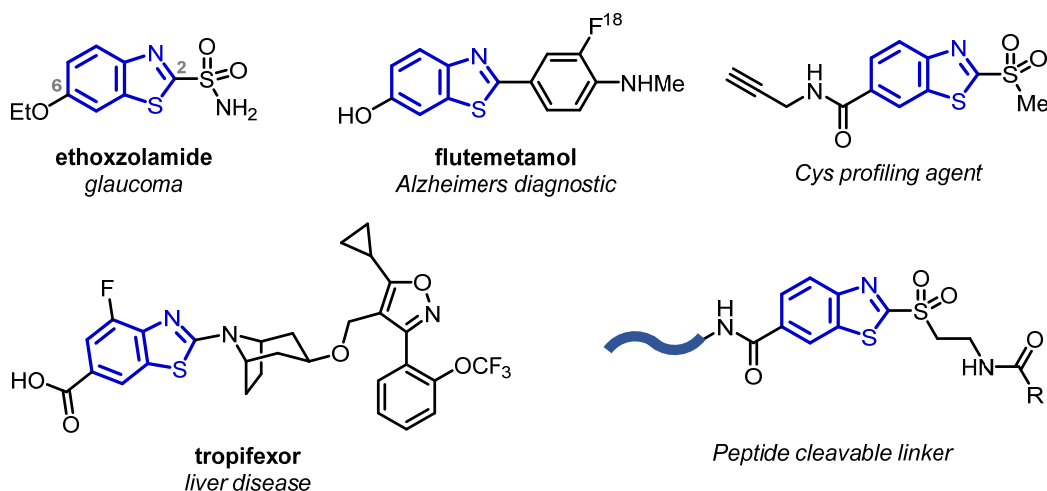


Figure 1. Benzothiazoles are a common motif present in therapeutics and tools for chemical biology.

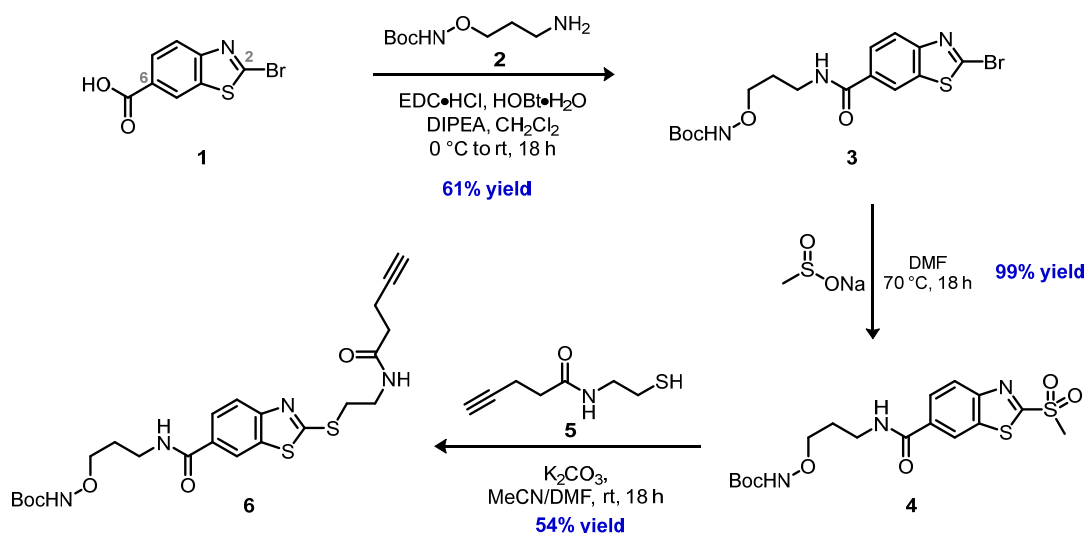


Figure 2. Synthesis of benzothiazole 6.

2. Results and Discussion

In this work, we report a three-step synthesis of benzothiazole **6** (Figure 2). This synthesis commenced from commercially available benzothiazole **1**, which contains a bromide and a carboxylic acid at the C2 and C6 positions respectively. Compound **1** was coupled to amine **2**, which contains an appended Boc-protected hydroxylamine, using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) and 1-hydroxybenzotriazole (HOBt)-based amidation conditions, yielding **3** in 61% crude yield [16]. Bromo-benzothiazole **3** was next transformed to sulfone **4** in a nucleophilic aromatic substitution reaction (S_NAr). Treatment of compound **3** with sodium methyl sulfinate at 70 °C produced sulfone **4** in 99% yield [11].

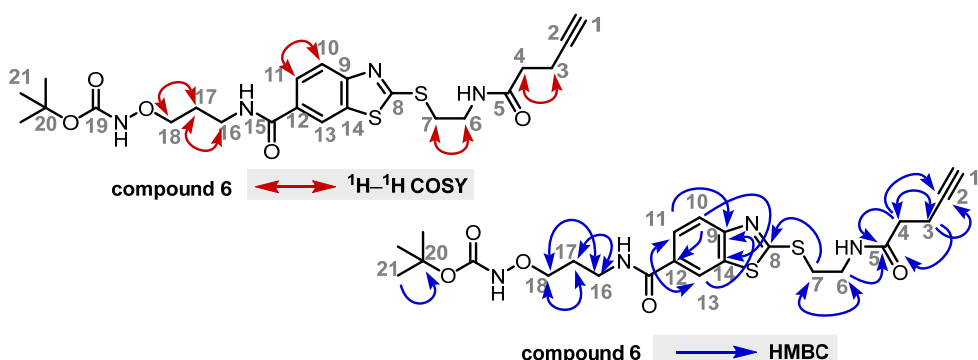
Benzothiazole sulfones like **4** are known to function as strong electrophiles for S_NAr with thiols. The sulfone motif presumably serves as the leaving group for S_NAr , being displaced as a sulfinate. S_NAr was utilized to incorporate an alkyne attached to a thiol onto the benzothiazole core. Thiol **5** has previously been synthesized and can be accessed

through various synthetic methods [21–23]. Benzothiazole sulfone **4** and thiol **5** were coupled together in the presence of potassium carbonate to yield title compound **6** in 54% yield [16]. The reactions of **3** to **4** and **4** to **6** were performed in solvent mixtures of DMF and other organic cosolvents. Lithium chloride washes were utilized to remove residual DMF. The total yield of the three-step synthesis of benzothiazole **6** was 33%.

Benzothiazole **6** was characterized by 2D NMR, including ^1H NMR, ^{13}C NMR, ^1H – ^1H COSY, HSQC, and HMBC experiments (Figures S8–S12). The observed ^1H and ^{13}C shifts are summarized and assigned to specific atoms on benzothiazole **6** in Table 1. Key COSY and HMBC correlations were also displayed. Of note, aromatic protons on C10, C11, and C13 were assigned based on their coupling constants, which correlate with observed *ortho* (8.6 Hz), *meta* (1.8 Hz), and *para* (0.6 Hz) J-values on benzene derivatives [24]. H-atoms with similar chemical shifts on C6 and C7, as well as C3 and C4, were differentiated based on their HMBC correlations to nearby atoms. The C8 carbon, which was assigned due to its HMBC cross-peak with C7–H, exhibits a significant downfield shift that matches the literature precedent [25].

Additional characterization of benzothiazole **6** was performed using IR, MALDI-MS, HRMS, and HPLC. Mass spectrometry of compound **6** revealed an $[\text{M} + \text{H}]^+$ mass of 507.1734, which was in good accordance with the expected mass of 507.1730 (Figures S14 and S15). HPLC analysis with UV–Vis detection of heterocycle **6** showed one main peak exhibiting strong absorbance at 293 nm, a characteristic trait of benzothiazoles (Figure S16) [26].

Table 1. NMR data and ^1H – ^1H COSY and HMBC correlations for benzothiazole **6**.



Position	δ_{H} (J = Hz)	δ_{C}	Position	δ_{H} (J = Hz)	δ_{C}
1	2.26 (2.6)	70.4	11	7.94 (8.6, 1.8)	126.7
2	—	83.4	12/14	—	131.9/136.6
3	2.48–2.41	15.6	13	8.38 (1.8, 0.6)	121.9
4	2.41–2.34	36.0	15	—	169.2
5	—	174.3	16	3.59–3.51	38.5
6	3.64	40.0	17	1.92 (6.3)	28.7
7	3.59–3.51	33.6	18	3.92 (5.9)	75.6
8	—	171.7	19	—	159.5
9	—	156.3	20	—	82.3
10	7.86 (8.6, 0.6)	121.9	21	1.48	28.6

3. Materials and Methods

Room temperature is defined as 21–25 °C. All reagents and solvents were purchased from commercial sources and used as received, unless otherwise noted.

^1H NMR spectra were recorded on 400 MHz or 500 MHz Bruker spectrometers (Billerica, MA, USA) at ambient temperature. Samples were prepared in chloroform-*d* (CDCl_3),

DMSO- d_6 , or mixtures of CD_3CN/D_2O . ^1H NMR data are reported as chemical shifts with multiplicity, coupling constants (J) in Hz, and integrations. Proton chemical shifts are reported in ppm (δ) and referenced to residual solvent ($CHCl_3$, δ 7.26 ppm; CD_3OD , δ 3.31 ppm) [27]. Multiplicity is reported as follows: singlet (s), broad singlet (bs), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), pentet (p), multiplet (m), and overlapping multiplets (overlapping m). ^{13}C NMR spectra were recorded on 500 (126) MHz Bruker spectrometers (Billerica, MA, USA) with complete proton decoupling at ambient temperature. Carbon chemical shifts are reported in ppm (δ) and referenced to solvent ($CDCl_3$, δ 77.2; CD_3OD , δ 49 ppm) [27].

Automatic normal-phase column chromatography was carried out with a Biotage Selekt flash purification system using a silica column with an appropriate gradient of EtOAc/Hexanes. Infrared spectra were obtained using a Nicolet ATR/FT-IR spectrometer (Thermo Fisher Scientific Inc., Waltham, MA, USA), and ν_{max} (cm^{-1}) were partially recorded in accordance with convention.

Low-resolution mass spectrometry (MS) was acquired on a Shimadzu AXIMA MALDI-TOF (Columbia, MD, USA). High-resolution mass spectra (HRMS) were analyzed with a Q Exactive HF-X (ThermoFisher, Bremen, Germany) mass spectrometer. High-performance liquid chromatography (HPLC) was acquired on a Shimadzu Prep-Scale HPLC with PDA detection and a Kromasil 100–5-C18 column. The general method for HPLC analysis is as follows: Kromasil 100-5-C18 column; LC conditions: 1% MeCN (0.08% TFA; B) 99% H_2O (0.1% TFA, A) from 0 to 1 min, linear ramp from 5% to 95% B from 1 to 55 min, 95% B from 55 to 59 min, linear ramp from 95% to 1% B from 59 to 60 min; and 0.5 mL/min flow rate.

3.1. *N*-[3-(*N*-*tert*-Butoxycarbonylaminoxy)propyl]-2-bromo-1,3-benzothiazole-6-carboxamide (**3**)

Following a procedure adapted from the literature [16], a 100 mL RB flask was charged with 2-bromo-benzothiazole-6-carboxylic acid (0.71 g, 2.9 mmol, 1.1 eq), *tert*-butyl-3-aminopropoxycarbamate (0.50 g, 2.6 mmol, 1.0 eq), EDC·HCl (0.61 g, 3.2 mmol, 1.2 eq), and HOBt· H_2O (0.48 g, 3.2 mmol, 1.2 eq). The mixture was cooled to 0 °C and dissolved in CH_2Cl_2 (12 mL). The reaction was allowed to warm to rt and stirred overnight for 18 h. After completion, the crude material was transferred to a separatory funnel and washed with satd $NaHCO_3$ (1 $\times$ 25 mL), 10% citric acid (1 $\times$ 25 mL), and satd brine (1 $\times$ 25 mL). The organics were dried over Na_2SO_4 , filtered, and concentrated to yield 0.76 g of **3** as a colourless oil, 61% crude yield, which was used without further purification. ^1H NMR (500 MHz, $CDCl_3$) δ 8.51–8.47 (m, 1H), 8.33 (bs, 1H), 8.14–8.05 (m, 1H), 8.04–7.94 (m, 1H), 7.44 (bs, 1H), 4.04 (t, J = 5.3 Hz, 2H), 3.75 (q, J = 5.7 Hz, 2H), 1.92 (p, J = 5.5 Hz, 2H), 1.53 (s, 9H). R_f (1:2 Hex/EtOAc) 0.66.

3.2. *N*-[3-(*N*-*tert*-Butoxycarbonylaminoxy)propyl]-2-mesyl-1,3-benzothiazole-6-carboxamide (**4**)

Following a procedure adapted from the literature [11], compound **3** (0.75 g, 1.7 mmol, 1.0 eq) was added to a 50 mL RB flask, followed by DMF (7.0 mL) and sodium methanesulfinate (0.27 g, 2.6 mmol, 1.5 eq). The solution was heated to 70 °C and stirred overnight for 18 h. Upon completion of the reaction, the solution was cooled and diluted with 50 mL EtOAc. The organics were extracted with 5% LiCl (3 $\times$ 50 mL), dried over Na_2SO_4 , filtered, and concentrated to yield 0.74 g of **4** as a beige solid, 99% yield. ^1H NMR (500 MHz, $CDCl_3$) δ 8.69 (d, J = 1.7 Hz, 1H), 8.57 (s, 1H), 8.25 (dd, J = 8.7, 1.5 Hz, 1H), 8.19 (d, J = 8.7 Hz, 1H), 7.71 (s, 1H), 4.04 (t, J = 5.4 Hz, 2H), 3.74 (q, J = 5.8 Hz, 2H), 3.44 (s, 3H), 1.91 (p, J = 5.6 Hz, 2H), 1.52 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.3, 165.9, 157.9, 153.9, 136.5, 134.6, 127.3, 124.9, 122.1, 82.6, 75.8, 42.4, 37.9, 28.3, 26.8. IR (cm^{-1} , neat), 3304, 2928, 1711, 1636, 1538, 1476, 1393, 1367, 1319, 1272, 1251, 1146, 1110, 1025, 955, 912, 837, 757, 730. R_f (1:2 Hex/EtOAc) 0.35.

3.3. *N*-[3-(*N*-tert-Butoxycarbonylaminoxy)propyl]-2-[2-(3-butynylcarbonylamino)ethylthio]-1,3-benzothiazole-6-carboxamide (**6**)

Following a procedure adapted from the literature [16], to a 25 mL RB flask was added benzothiazole **4** (0.50 g, 1.2 mmol, 1.0 eq), thiol **5** (0.52 g, 3.3 mmol, 2.0 eq), K₂CO₃ (0.24 g, 1.7 mmol, 1.5 eq), CH₃CN (5 mL), and DMF (1 mL). The reaction was stirred at rt for 18 h overnight. After completion, the CH₃CN was removed under vacuum and EtOAc (25 mL) was added. The organics were extracted with a 1:1 solution of 10% citric acid and 5% LiCl (1 × 50 mL). The aqueous later was re-extracted with EtOAc (50 mL). The combined organics were extracted with a 1:1 solution of satd NaHCO₃ and 5% LiCl (1 × 75 mL), and satd brine (1 × 75 mL). The resulting solution was dried over Na₂SO₄, filtered, and concentrated. The crude material was purified by automatic normal phase chromatography, eluting with a gradient of 25–100% EtOAc/Hex to yield 0.32 g of pure **8** in 54% yield as a white solid. **¹H NMR** (400 MHz, CD₃OD) δ 8.38 (dd, *J* = 1.8, 0.6 Hz, 1H), 7.94 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.86 (dd, *J* = 8.6, 0.6 Hz, 1H), 3.92 (t, *J* = 5.9 Hz, 2H), 3.64 (t, *J* = 6.0 Hz, 2H), 3.59–3.51 (overlapping m, 4H), 2.48–2.41 (m, 2H), 2.41–2.34 (m, 2H), 2.26 (t, *J* = 2.6 Hz, 1H), 1.92 (p, *J* = 6.3 Hz, 2H), 1.48 (s, 9H). **¹³C NMR** (126 MHz, CD₃OD) δ 172.9, 170.3, 167.8, 158.1, 154.9, 135.2, 130.5, 125.3, 120.5, 120.5, 82.0, 80.8, 74.2, 69.0, 38.6, 37.1, 34.6, 32.2, 27.3, 27.2, 14.2. **IR** (cm^{−1}, neat) 3310, 3209, 2934, 2880, 2397, 1711, 1634, 1548, 1438, 1347, 1317, 1251, 1120, 998, 764. **MALDI MS** *m/z*: [M + Na]⁺ calculated for C₂₃H₃₀N₄O₅S₂Na 529.2, found 529.3. **HRMS**: (HESI-Q Exactive HF-X) *m/z*: [M + H]⁺ calcd for C₂₃H₃₁N₄O₅S₂ 507.1730, found 507.1734. **HPLC** (General Method) 37.9 min, UV absorbance at 293 nm. **R_f**(1:2 Hex/EtOAc) 0.48.

4. Conclusions

In this work, we have reported a three-step synthesis of a novel benzothiazole sulfide derivative (**6**). Compound **6** was constructed using an amidation reaction, as well as two sequential S_NAr reactions, with a total yield of 33%. This hydroxylamine- and alkyne-appended heterocycle was characterized using ¹H-, ¹³C-, ¹H–¹H COSY, HSQC, and HMBC NMR, in addition to IR, MALDI-MS, and HPLC. Various 2D NMR correlations on compound **6** have also been assigned.

Supplementary Materials: The following supporting information can be downloaded online, Figure S1. ¹H NMR of benzothiazole **3**. Figures S2–S7. Data for benzothiazole **4**. Figures S8–S16. Data for benzothiazole **6**.

Author Contributions: Conceptualization, C.R.S.; methodology, C.R.S.; data curation, C.R.S., G.G.M. and N.N.V.; writing—original draft preparation, C.R.S.; writing—review and editing, C.R.S., G.G.M. and N.N.V. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The data presented in this study are available in the article and Supplementary Materials.

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Conflicts of Interest: The authors declare no conflicts of interest.

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