

Short Note

## 2-(4-Pentyloxyphenyl)benzothiazole

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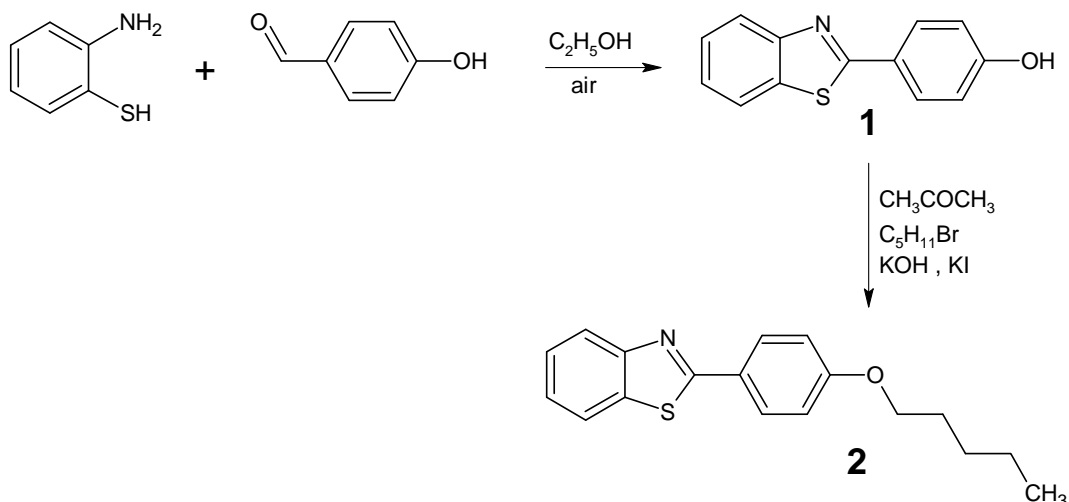
**Abstract:** 2-(4-Pentyloxyphenyl)benzothiazole was synthesized and its IR, <sup>1</sup>H NMR and MS spectroscopic data are presented.

**Keywords:** 2-(4-pentyloxyphenyl)benzothiazole; heterocyclic fused-ring; ether chain

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There has been considerable interest in heterocyclic molecules due to their diversified molecular design and remarkable optical [1–3], liquid crystalline [4] and electronic properties [5]. In view of the importance of these compounds, chemists are prompted to generate the derivatives by introducing different substituents into the existing skeleton of the molecule [6–8].

**Preparation of Benzothiazole 1:** This intermediate compound was first reported by Bogert and Corbitt in year 1926 [9]. 2-Aminothiophenol (5.01 g, 40 mmol) and 4-hydroxybenzaldehyde (4.88 g, 40 mmol) in absolute ethanol (40 mL) was heated under reflux for 6 hours. The reaction mixture was subsequently cooled to room temperature, then distilled water (60 mL) was added slowly until the mixture turned cloudy. It was kept overnight at 20 °C and the solid formed was filtered and washed with cold ethanol:water (1:1.5) and dichloromethane.



**Preparation of Benzothiazole 2:** In analogy to a recently published procedure [10], benzothiazole **1** (4.55 g, 20 mmol) in acetone (40 mL), was added to a solution of potassium hydroxide (1.12 g, 20 mmol) in distilled water (5 mL). This was followed by addition of a small amount of potassium iodide into the mixture. The reaction mixture was heated under reflux for an hour upon stirring. 1-Bromopentane (3.78 g, 25 mmol) was then added to the flask and reflux was continued for 20 hours. The solid obtained was repeatedly recrystallized from absolute ethanol whereupon the pure compound was isolated as a white solid (3.04 g, 51%).

Melting Point: 72.3 °C.

EI-MS  $m/z$  (rel. int.%): 297(37) [ $M^+$ ], 227(100), 198(11), 108(7), 43(8).

IR (KBr,  $cm^{-1}$ ): 2955, 2870 (C-H aliphatic); 1606 (C=N); 1266, 1020 (C-O ether).

$^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta/ppm$  0.95 (t,  $J = 7.1$  Hz, 3H,  $CH_3$ -), 1.37-1.50 (m, 4H,  $CH_3$ -( $CH_2$ )<sub>2</sub>- $CH_2$ - $CH_2$ -O-), 1.82 (q,  $J = 7.4$  Hz, 2H, - $CH_2$ - $CH_2$ -O-), 4.02 (t,  $J = 6.6$  Hz, 2H, - $CH_2$ -O-), 6.98 (d,  $J = 6.8$  Hz, 2H, Ar-H), 7.35 (t,  $J = 8.3$  Hz, 1H, Ar-H), 7.46 (t,  $J = 8.3$  Hz, 1H, Ar-H), 7.86 (d,  $J = 7.8$  Hz, 1H, Ar-H), 8.01 (m, 3H, Ar-H).

Elemental analysis: Calculated for  $C_{18}H_{19}NOS$ : C, 72.69%, H, 6.44%, N, 4.71%; Found: C, 72.60%, H, 6.53%, N, 4.77%.

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## References and Notes

1. Chen, X.L.; Jenekhe, A. *Macromolecules* **1996**, *29*, 6189–6192.
2. Chou, S.S.P.; Sun, D.J.; Lin, H.C.; Yang, P.K. *Chem. Commun.* **1996**, 1045–1046.
3. Raimundo, J.M.; Blanchard, P.; Ledoux-Rax, I.; Hierle, R.; Michaux, L.; Roncali, J. *Chem. Commun.* **2000**, 1597–1598.
4. Lee, C.H.; Yamamoto, T. *Mol. Cryst. Liq. Cryst.* **2001**, *363*, 77–84.
5. Maruyama, T.; Suganuma, H.; Yamamoto, T. *Synthetic Metals* **1995**, *74*, 183–185.
6. Prajapati, A. K.; Bonde, N. L. *J. Chem. Sci.* **2006**, *118*, 203.
7. Ha, S.T.; Koh, T.M.; Yeap, G.Y.; Lin, H.C.; Boey, P.L.; Yip, F.W.; Ong, S.T.; Ong, L.K. *Mol. Cryst. Liq. Cryst.* **2009**, *506*, 56.
8. Ha, S.T.; Koh, T.M.; Yeap, G.Y.; Lin, H.C.; Beh, J.K.; Win, Y.F.; Boey, P.L. *Chin. Chem. Lett.* **2009**, *20*, 1081.
9. Bogert, M.T.; Corbitt, H.B. *J. Am. Chem. Soc.* **1926**, *48*, 783.
10. Ha, S.T.; Ong, L.K.; Wong, J.P.W.; Win, Y.F.; Koh, T.M. *Molbank* **2009**, *1*, M598.

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