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2-Bromo-3-ethylthiazolium Tetrafluoroborate (BET)

Györgyi Kovács [1*], Zoltán Kele [1], Péter Forgó [2] and Lajos Kovács [1]

1. Department of Medicinal Chemistry, University of Szeged, Dóm tér 8, H-6720 Szeged, Hungary.
Phone: +36 62 54 51 45, Fax: +36 62 54 59 71, *E-mail: gyorgyi@ovrisc.mdche.u-szeged.hu
2. Department of Organic Chemistry , University of Szeged, Dóm tér 8, H-6720 Szeged, Hungary

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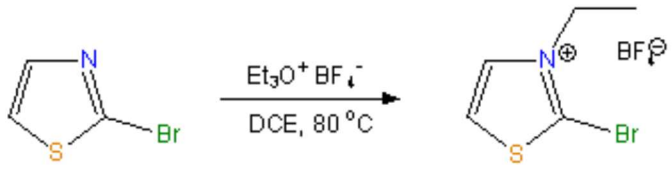

Recent progress in peptide synthesis resulted in the elaboration of novel coupling agents. One successful approach involves the application of thiazolium salts, *e.g.* 2-bromo-3-ethyl-4-methylthiazolium tetrafluoroborate (BEMT) [1-3]. This compound can be prepared from 2-bromo-3-ethyl-4-methylthiazole [1, 2]. We have found that a simpler analogue, 2-bromo-3-ethylthiazolium tetrafluoroborate (BET), can be prepared in convenient steps from the commercially available 2-aminothiazole using the procedure by Dondoni *et al*. [4] to obtain 2-bromothiazole which, in turn, was readily transformed into the title compound. In our experience BET is a highly efficient coupling reagent in the synthesis of peptide nucleic acid (PNA) oligomers in solution phase.
To a stirred solution of 2-bromothiazole [4] (1.78 mL, 20.0 mmol) in 1,2-dichloroethane (DCE, 20 mL) the solution of triethyloxonium tetrafluoroborate (11.4 g, 60.0 mmol) in DCE(60 mL) was added over 45 min. at 80 °C. When the reaction was complete (16 h) according to TLC (n-buthanol : acetic acid : water = 4:1:1) the solution was concentrated *in vacuo*. After the residue was precipitated from diethyl ether it was recrystallized from *abs*. acetonitrile/ethyl acetate to afford white plates. Yield: 4.48 g (80 %).

Mp: 137.9-139.2 °C.

^{1}H NMR (DMSO-d$_6$, 500 MHz, d, ppm): 1.47 (t, J = 7.0 Hz, 3H, CH_2CH_3); 4.52 (q, J = 7.0 Hz, 2H, CH_2CH_3); 8.35 (d, J = 4.1 Hz, 1H, aryl); 8.56 (d, J = 4.1 Hz, 1H, aryl).

^{13}C NMR (DMSO-d$_6$, 125 MHz, d, ppm): 14.19 (CH_2CH_3); 50.61 (CH_2CH_3); 127.45 (C-5); 137.73 (C-4); 146.50 (C-2).

ESI-MS (m/z, %): 191.8 (100, $[C_5H_7{}^{79}BrNS]^+$); 193.8 (97, $[C_5H_7{}^{81}BrNS]^+$).

Anal. cald. for $C_5H_7BBrF_4NS$ (279.891): C, 21.45; H, 2.52; Br, 28.55; F, 27.15; N, 5.00; S, 11.46; found C, 21.47; H, 2.51; Br, 28.52; F, 27.20; N, 5.01; S, 11.44.

References

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Sample availability: sample available from the authors and MDPI.