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LETTERS TO THE EDITOR

NEW SYNTHESIS OF BENZO[*b*]FURAN-, BENZO[*b*]THIOPHENE- AND BENZO[*b*]-SELENOPHENE-3-ACETIC ACIDS

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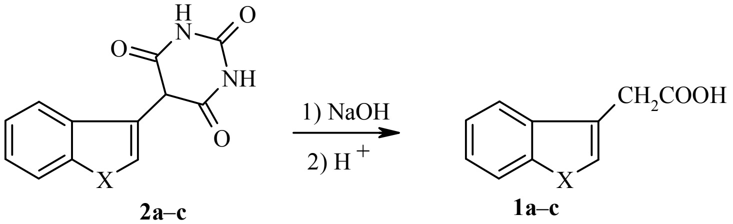
Heterylacetic acids hold interest as compounds with potential biological activity and reagents for fine organic synthesis. Benzo[*b*]furan-3-acetic acid (**1a**) and benzo[*b*]thiophene-3-acetic acid (**1b**) are plant growth stimulants. Benzo[*b*]-3-selenophene-3-acetic acid (**1c**) was recently found to have stronger auxin-like activity than indolyl-3-acetic acid [1, 2]. While there are well-developed methods for the synthesis of acids **1a** and **1b**, benzo[*b*]selenophene-3-acetic acid has not been readily available. The only method for the preparation of acid **1c** was described by Laitem and Critiaens [3].



1, **2** **a** X = O, **b** X = S, **c** X = Se

We propose a new synthesis for benzo[*b*]furan- (**1a**), benzo[*b*]thiophene- (**1b**), and benzo[*b*]selenophene-3-acetic acids (**1c**), involving the alkaline hydrolysis of the corresponding 5-(3-heteryl)hexahydropyrimidine-2,4,6-triones (**2a-c**) obtained by the condensation of benzo[*b*]furan-3[2H]-one, benzo[*b*]thiophene-3[2H]-one, and benzo[*b*]selenophene-3[2H]-one with barbituric acid according to previous procedures [4, 5]. ^{1}H NMR spectroscopy showed that compounds **2a-c** in DMSO-d$_6$ solution contain about 65% of the keto form, as indicated by the 5-H signals at 5.37-5.50 ppm.

5-(3-Benzo[*b*]furyl)hexahydropyrimidine-2,4,6-trione (2a) was obtained in 92% yield; mp 229-230°C (acetic acid). ^{1}H NMR spectrum (200 MHz), δ, ppm, (*J*, Hz): 5.40 (1H, s, 5-H); 7.29 (1H, t, *J* = 7.2, 6-H); 7.38 (1H, t, *J* = 7.7, 5-H arom); 7.49 (1H, d, *J* = 7.2, 7-H); 7.65 (1H, d, *J* = 7.7, 4-H); 7.95 (1H, s, 2-H); 10.90 (2H, br. s, NH); 11.56 (1H, br. s, OH enol). Found, %: C 59.31; H 3.48; N 11.40. $C_{12}H_8N_2O_4$. Calculated, %: C 59.02; H 3.30; N 11.47.

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5-(3-Benzo[*b*]thienyl)hexahydropyrimidine-2,4,6-trione (2b) was obtained in 91% yield; mp 260°C (acetic acid). ^{1}H NMR spectrum, δ, ppm: 5.50 (1H, s, 5-H); 7.30-8.00 (5H, m, H arom); 10.90 (2H, br. s, NH); 11.51 (1H, br. s, OH enol). Found, %: C 55.61; H 3.24; N 10.60, S 12.40. $C_{12}H_8N_2O_3S$. Calculated, %: C 55.38; H 3.10; N 10.76; S 12.32.

5-(Benzo[*b*]selenophene-3-yl)hexahydropyrimidine-2,4,6-trione (2c) was obtained in 91% yield; mp 157-158°C (acetic acid). ^{1}H NMR spectrum, δ, ppm: 5.37 (1H, s, 5-H); 7.20-7.56 (3H, 5-, 6-, 7-H arom); 7.90 (1H, s, 2-H); 8.00 (1H, m, 4-H); 10.83 (2H, br. s, NH); 11.45 (1H, br. s, OH enol). Found, %: C 46.75; H 2.35; N 9.35; Se 25.54. $C_{12}H_8N_2O_3Se$. Calculated, %: C 46.92; H 2.63; N 9.12; Se 25.71.

Benzo[*b*]furan-3-acetic Acid (1a) was obtained in 68% yield; mp 89°C (heptane) (mp 89°C [6]). Found, %: C 68.36; H 4.42. $C_{10}H_8O_3$. Calculated, %: C 68.18; H 4.58.

Benzo[*b*]thiophene-3-acetic Acid (b) was obtained in 66% yield; mp 108-109°C (heptane) (mp 108-109°C [7]). Found, %: C 62.23; H 4.27; S 16.53. $C_{10}H_8O_2S$. Calculated, %: C 62.48; H 4.19; S 16.68.

Benzo[*b*]selenophene-3-acetic Acid (1c) was obtained in 58% yield; mp 149-150°C (cyclohexane) (mp 150°C [3]). ^{1}H NMR spectrum (DMSO-d_6), δ, ppm, (*J*, Hz): 3.73 (2H, s, CH_2); 7.28 (1H, t, $J = 7.3$, 6-H); 7.38 (1H, t, $J = 7.7$, 5-H); 7.72 (1H, d, $J = 7.7$, 4-H); 7.90 (1H, s, 2-H); 7.94 (1H, d, $J = 7.3$, 7-H); 12.18 (1H, br. s, CO_2H). Found, %: C 50.41; H 3.11; Se 33.28. $C_{10}H_8O_2Se$. Calculated, %: C 50.23; H 3.37; Se 33.02.

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