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SYNTHESIS OF A NOVEL HETEROCYCLIC SYSTEM: QUINOXALINO[1,2-*a*]PYRROLO-[2,3-*b*][1,5]BENZOTHIAZEPINE

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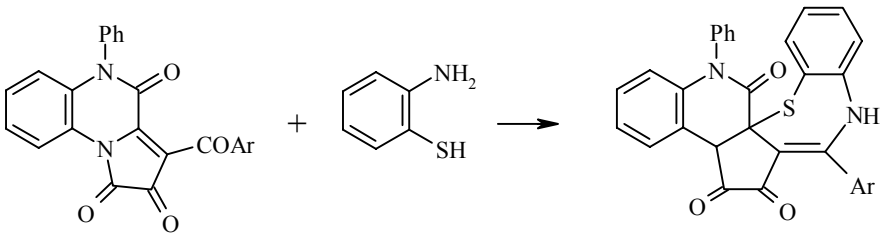
Keywords: *o*-aminothiophenol, 2,3-dihydro-2,3-pyrroledione, pyrrolo[1,2-*a*]quinoxaline-1,2,4-trione, quinoxalino[1,2-*a*]pyrrolo[2,3-*b*][1,5]benzothiazepine.

3-Aroyl-5-unsubstituted and -5-phenyl-1,2,4,5-tetrahydropyrrolo[1,2-*a*]quinoxaline-1,2,4-triones react with *o*-phenylenediamine with successive nucleophilic attack by the amino groups of the reagent with the carbon atoms at the 3a position of the heterocycle and the aroyl carbonyl group and formation of substituted quinoxalino[1,2-*a*]pyrrolo[2,3-*b*][1,5]benzodiazepines [1]. The product of preliminary addition of *o*-aminothiophenol to 5-substituted 3-benzoyl-1,2,4,5-tetrahydropyrrolo[1,2-*a*]quinoxaline-1,2,4-trione could not undergo ring closure under mild conditions [2].

By boiling 3-aroyl-5-phenyl-1,2,4,5-tetrahydropyrrolo[1,2-*a*]quinoxaline-1,2,4-triones **1a,b** with *o*-aminothiophenol in benzene or dioxane for 1 h, we isolated 8-aryl-16-phenyl-7,9,15,16-tetrahydro-6H-quinoxalino[1,2-*a*]pyrrolo[2,3-*b*][1,5]benzothiazepine-6,7,15-triones **2a,b**.



1a,**b** **2a**,**b**

1, **2 a** Ar = *p*-C_6H_4Me, **b** Ar = *p*-C_6H_4OMe

The spectral characteristics of compounds **2a,b** agree well with the proposed structure, and are quite close to those for model aza analogs whose structure has been confirmed by X-ray diffraction data [3].

Compound **2a,b** are probably formed as a result of successive nucleophilic attack by the mercapto and amino groups of *o*-aminothiophenol on the carbon atoms at the 3a position of the heterocycle and the aroyl carbonyl group of compounds **1a,b** and regioselective closure of the thiazepine ring, and the reaction carried out is the first method for constructing the previously inaccessible functionalized condensed heterocyclic system quinoxalino[1,2-*a*]pyrrolo[2,3-*b*][1,5]benzothiazepine.

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16-Phenyl-8-*p*-tolyl-7,9,15,16-tetrahydro-6H-quinoxalino[1,2-*a*]pyrrolo[2,3-*b*][1,5]benzothiazepine-6,7,15-trione (1a). *o*-Aminothiophenol (0.4 mmol) was added to a suspension of compound **1a** (0.4 mmol) in absolute benzene (10 ml), boiled for 1 h, and cooled; the precipitate was filtered out. Yield 0.13 g (64%); mp 284-286°C (with decomposition, from benzene). IR spectrum (vaseline oil), ν, cm^{-1}: 3180 broad (NH), 1737 ($C_{(6)}$=O), 1688 ($C_{(7)}$=O), 1676 ($C_{(15)}$=O). ^{1}H NMR spectrum (400 MHz, DMSO-d_6), δ, ppm: 2.43 (3H, s, CH_3); 6.40 (1H, d, *J* = 7.0 Hz, $C_{(1)}$H); 7.18-7.54 (15H, m, C_6H_5 + $2C_6H_4$ + C_6H_2); 7.93 (1H, d, *J* = 7.0 Hz, $C_{(4)}$H); 10.30 (1H, s, $N_{(9)}$H). Found, %: C 72.12; H 4.13; N 8.22; S 6.20. $C_{31}H_{21}N_3O_3S$. Calculated, %: C 72.22; H 4.11; N 8.15; S 6.22.

8-*p*-Methoxyphenyl-16-phenyl-7,9,15,16-tetrahydro-6H-quinoxalino[1,2-*a*]pyrrolo[2,3-*b*][1,5]-benzothiazepine-6,7,15-trione (1b). Yield 65%; mp 290-292°C (with decomposition, from benzene). IR spectrum (vaseline oil), ν, cm^{-1}: 3210 broad (NH), 1735 ($C_{(6)}$=O), 1689 ($C_{(7)}$=O), 1678 ($C_{(15)}$=O). ^{1}H NMR spectrum (400 MHz, DMSO-d_6), δ, ppm: 3.86 (3H, s, CH_3O); 6.41 (1H, d, *J* = 7.0 Hz, $C_{(1)}$H); 7.05-7.59 (15H, m, C_6H_5 + $2C_6H_4$ + C_6H_2); 7.94 (1H, d, *J* = 7.0 Hz, $C_{(4)}$H); 10.25 (1H, s, $N_{(9)}$H). ^{13}C NMR spectrum (100 MHz, DMSO-d_6), δ, ppm: 55.30 (CH_3); 67.99 ($C_{(14a)}$); 105.78 ($C_{(7a)}$); 113.38-156.70 (Ar); 159.63, 160.85 ($C_{(6)}$=O, $C_{(15)}$=O); 173.85 ($C_{(7)}$=O). Found, %: C 70.12; H 3.99; N 7.88; S 6.12. $C_{31}H_{21}N_3O_4S$. Calculated, %: C 70.04; H 3.98; N 7.90; S 6.03.

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