

3-Bromomethyl-1,5-diphenyl-1*H*-pyrazolo[4,3-*e*][1,2,4]triazine and 3-Dibromomethyl-1,5-diphenyl-1*H*-pyrazolo[4,3-*e*][1,2,4]triazine

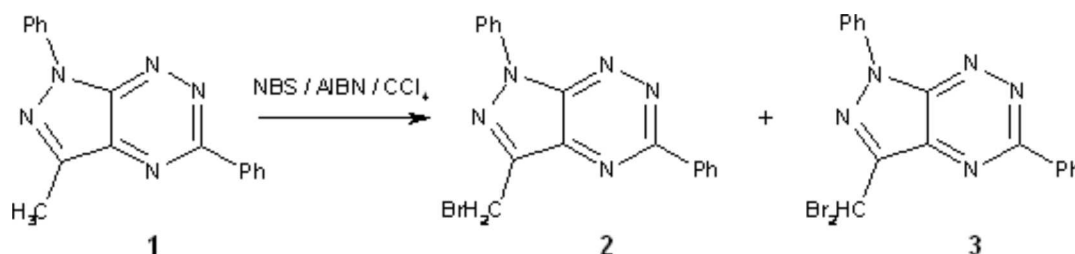
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As part of our research programme we have synthesized the title compounds as valuable intermediates for the preparation of acyclonucleosides-biologically active molecules. The starting material **1** was obtained according to the reported procedure [1] and title compounds were obtained using N-Bromosuccinimide (NBS) as brominating agent.



To a solution of **1** (72 mg, 0.25 mmol) in CCl₄ (10 ml) NBS (178 mg, 1 mmol) and Azobis(isobutyronitrile) (AIBN) (17 mg, 0.1 mmol) were added. The mixture was refluxed for 4.5 h. The solvent was evaporated *in vacuo* and the residue was purified by column silica gel chromatography (silica gel 230-400 mesh, CHCl₃/n-hexane mixture 1:1) to give 99 mg (0.27 mmol, 54%) of **2** and 63 mg (0.14 mmol, 28%) of **3**.

3-Bromomethyl-1,5-Diphenyl-1*H*-Pyrazolo[4,3-*e*][1,2,4]Triazine (**2**)

Melting Point: 185-187°C

¹H-NMR (200 MHz, CDCl₃): δ= 8.67-8.72 (m, 2H); 8.41-8.46 (m, 2H); 7.55-7.65 (m, 5H); 7.42-7.46 (m, 1H); 5.02 (s, 2H).

IR (KBr, cm⁻¹): 3032; 1595; 1500; 1421; 1213; 1109; 1080; 753; 689.

MS- EI (*m/z*, %): 365 (6) [M⁺]; 339 (32); 337 (32); 286 (14); 259 (29); 258 (100); 218 (20); 155 (51); 115 (17); 77 (18).

HR-MS (EI, 70eV) Calculated for C₁₇H₁₂⁷⁹BrN₅: 365.02761. Found: 365.02685.

3-Dibromomethyl-1,5-Diphenyl-1*H*-Pyrazolo[4,3-*e*][1,2,4]Triazine (**3**)

Melting Point: 200-202°C

¹H-NMR (200 MHz, CDCl₃): δ= 8.70-8.75 (m, 2H); 8.41-8.46 (m, 2H); 7.57-7.66 (m, 5H); 7.44-7.48 (m,

1H); 7.18 (s, 1H).

IR (KBr, cm^{-1}): 2922; 1593; 1500, 1420; 1108; 775; 690.

MS- EI (m/z , %): 445 (10) [M^+]; 419 (29); 417 (58); 415 (29); 366 (23); 364 (22); 339 (32); 338 (100); 337 (32); 336 (98); 258 (37); 235 (38); 233 (40); 218 (14); 155 (10); 77 (30).

HR-MS- EI: Calculated for $\text{C}_{17}\text{H}_{12}^{79}\text{Br}^{81}\text{BrN}_5$: 444.93607. Found: 444.93751.

References:

1. Rykowski, A.; Mojzych, M.; Karczmarzyk, Z. *Heterocycles*, **2000**, 53, 2175.

Sample Availability: Available from MDPI.

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