1-[[Benzyl-(2-cyano-ethyl)-amino]-methyl]-5-methyl-1H-pyrazole-3-carboxylic acid methyl ester

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The products of aza-type Michael addition, i.e., β-amino carbonyl compounds and their derivatives, are often used as peptide analogs or precursors of optically active amino acids, amino alcohols, diamines, and lactams [1]. Moreover, β-amino carbonyl functionalities are ubiquitous motifs in natural products such as alkaloids and polyketides [2]. Herein, we report the synthesis of new product using aza-type Michael reactions under mild conditions.

A mixture of 3-(benzylamino)propionitrile 1 [3] (1g; 6.25mmol) and 1-Hydroxymethyl-5-methyl-1H-pyrazole-3-carboxylic acid methyl ester 2 [4] (1.062g; 6.25 mmol) in 20 ml of acetonitrile was stirred at room temperature for four days, then the mixture was dried with Na2SO4 and filtered. The solvent was evaporated under reduced pressure. The product 3 has been obtained with a 99% yield as yellow oil.

1H-NMR (300 MHz, CDCl3): δ = 7.31 (CH arom, 5H, s); 6.56 (CH pyr, 1H, s); 4.94 (OCH 3, 3H, s); 3.89 (N-CH 2-N, 2H, s); 3.75 (C6H5-CH 2, 2H, s); 3.01-3.06 (CH2-CH 2-CN, 2H, t, J = 7.33 Hz); 2.33-2.37 (N-CH 2, t, J = 7 Hz) and 2.18 (CH 3, 3H, s).

13C-NMR (CDCl3, 75 MHz): δ = 163.32 (l); 142.91 (i); 141.56 (g); 137.46 (m); 129.154 (n); 129.03; 129.08 (f); 128.26 (o); 118.97 (a); 109.30 (h); 67.82 (e); 56.79 (d); 52.37 (k); 48.36 (c); 17.46 (b); 11.55 (j).

EI-MS (70 eV, m/z): 173 (16); 171; 119 (22); 91 (100).

References:

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