

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

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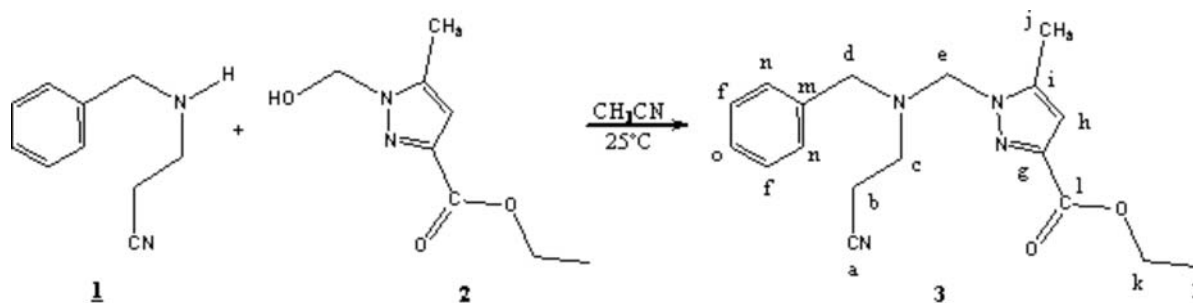
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Received: 19 July 2006 / Accepted: 31 July 2006 / Published: 1 September 2006

**Keywords:** pyrazole; propionitrile and tridentate ligand.

The products of aza-type *Michael* addition, *i.e.*,  $\beta$ -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,  $\beta$ -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 ethyl ester **2** [4] (1.15g, 6.25 mmol) in 20 ml of acetonitrile was stirred at room temperature for four days, then the mixture was dried with Na<sub>2</sub>SO<sub>4</sub> and filtered. The solvent was evaporated under reduced pressure. The product **3** obtained with an 81% yield as yellow oil.

<sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  = 7.34 (CH<sub>arom</sub>, 5H, s); 6.55 (CH<sub>pyr</sub>, 1H, s); 4.94 (pyr-CH<sub>2</sub>-N, 2H, s); 4.33-4.4 (OCH<sub>2</sub>, 2H, q, J = 8Hz); 3.750 (C<sub>6</sub>H<sub>5</sub>-CH<sub>2</sub>, 2H, s); 3.00-3.1 (CH<sub>2</sub>-CH<sub>2</sub>-CN, 2H, t, J = 7.33Hz); 2.34-2.38 (N-CH<sub>2</sub>, 2H, t, J = 8Hz); 2.18 (CH<sub>3</sub>, 3H, s) and 1.39-1.34 (CH<sub>3</sub>, 3H, t, J = 8Hz).

<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 75 MHz):  $\delta$  = 162.94 (l); 143.26 (i); 141.432 (g); 137.51 (m); 129.16; 129.06 (n); 128.83 (f); 128.23 (o); 119.00 (a); 109.19 (h); 67.70 (e); 61.26 (k); 56.76 (d); 48.34 (c); 17.44 (b); 14.77 (p); 11.55 (j).

EI-MS (70 eV, m/z): 173; 171; 154 (51.4); 119; 91 (60.6).

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