



**Synthesis, Characterization and Crystal Structure of  
4-Amino-N, N-dibenzyl-2-ethoxy-5-nitrobenzamide**

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**ABSTRACT**

*The amide functionality is a familiar feature in small or complex synthetic or natural molecules and plays a key role for medicinal chemists. And in-depth analysis of the comprehensive medicinal chemistry database revealed that the carboxamide group appears in more than 25% of known drugs. This can be expected, since carboxamides are neutral, are stable and have both hydrogen-bond accepting and donating properties. The newly synthesized 4-amino-N, N-dibenzyl-2-ethoxy-5-nitrobenzamide (3) by hydrolysis of ester (1) to acid (2) with sodium hydroxide in methanol and followed by acid-amine coupling with dibenzylamine to obtain compound 3. The newly synthesized, 4-amino-N, N-dibenzyl-2-ethoxy-5-nitrobenzamide 3 is characterized by LC-MS, IR, <sup>1</sup>H & <sup>13</sup>C NMR studies. The structure is further confirmed by single crystal XRD data. Compound 3 crystallizes in monoclinic centrosymmetric P21/c space group with a = 8.9255(5) Å, b = 17.2482(12) Å, c = 13.5773(8) Å, β = 95.171(6) ° V = 2081.7(2) Å<sup>3</sup> and Z = 4. The dihedral angle between the two phenyl rings which is 6.91°. In the crystal structure of compound 3, there exists a one dimensional chain along crystallographic a axis formed by strong N–H...O hydrogen bonding interaction, it also consists weak C–H...O intramolecular hydrogen bonding interactions.*

**Keywords:** 4-amino-N, N-dibenzyl-2-ethoxy-5-nitrobenzamide, synthesis, characterization, single crystal, N–H...O hydrogen bonds.

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