

# Flavours and Fragrances: Chemistry, Bioprocessing and Sustainability



Short Note

## (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 4-Aminobutyrate Hydrochloride

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**Abstract:** The title ester (1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl 4-aminobutyrate hydrochloride was obtained in 96% yield via Steglich esterification. The structure of the target compound was established by FTIR, HR-MS, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR spectral analysis, and single crystal X-ray diffraction study. Single crystals of the title ester suitable for X-ray investigation were obtained by slow evaporation of the methanolic solution at room temperature. The purity of compound was assessed using HPLC coupled to mass spectrometry.

**Keywords:** terpene; *l*-menthol; ester; X-ray diffraction

### 1. Introduction

Since the identification, cloning, and characterization of the transient receptor potential (TRP) ion channels, special attention has been focused on terpenes and their derivatives as against/antagonist of aforementioned pharmacological targets. Cyclic terpene alcohol menthol is one of TRP modulators possessing antinociceptive and local anesthetic effects [1,2]. Among four pairs of optical isomers (–)-menthol—also known as *l*-menthol with (1*R*,2*S*,5*R*) configuration—occurs most widely in the nature and has the greatest cooling activity [3,4]. Besides binding to TRP channels, *l*-menthol was found to act as positive allosteric modulators of  $\gamma$ -aminobutyric acid (GABA)<sub>A</sub> receptors [5].

Based on the foregoing, the combination of *l*-menthol residues with GABA into one molecule is reasonable to enhance the effect of each component. Thus, the current note is devoted to the detailed description and determination of ester structure based on menthol and GABA—(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl 4-aminobutyrate hydrochloride.

### 2. Results and Discussion

(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 4-aminobutyrate hydrochloride was synthesized via Steglich esterification with *N,N'*-dicyclohexylcarbodiimide (DCC) and 4-dimethylaminopyridine (DMAP) as a catalyst in dichloromethane, as shown in Scheme 1. Synthesized ester was isolated in 96% yield as white solid soluble in methanol and dimethyl sulfoxide and fully characterized by <sup>1</sup>H-NMR, FTIR-spectroscopy and FAB-ESI-mass spectrometry. Additionally, the HPLC analysis was carried out to determine the purity of the title compound. For this purpose, reversed-phase HPLC method with

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