Phenylacetic Acid (3S,6S)-6-Acetoxy-8-methyl-8-aza-bicyclo[3.2.1]oct...

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Phenylacetic Acid (3S,6S)-6-Acetoxy-8-methyl-8-aza-bicyclo[3.2.1]oct-3-yl Ester

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The fact that the configuration of derivatives of acetic acid 8-methyl-8-aza-bicyclo[3.2.1]oct-6-yl ester was considered having significant influence on the muscarinic activity [1] prompted us to synthesize the chiral compounds with the skeleton in order to study the structure-activity relationship.

To a solution of (-)-acetic acid (3*S*,6*S*)-3-hydroxy-8-methyl-8-aza-bicyclo[3.2.1]oct-6-yl ester [2, 3] (0.22 g, 1.1 mmol) in dichloromethane (2 mL) with pyridine (0.1 mL) was added dropwise phenylacetyl chloride (0.23 mL, 1.7 mmol). The mixture was stirred for 24 h at room temperature. The solution was evaporated in vacuo to dryness. The residue was dissolved in water (5 mL) and basified with concentrated aqueous ammonia. The aqueous solution was extracted with chloroform (5×6 mL), and the combined organic layers were dried over anhydrous sodium sulfate, filtered, evaporated in vacuo, to give phenylacetic acid (3*S*,6*S*)-6-acetoxy-8-methyl-8-aza-bicyclo[3.2.1]oct-3-yl ester (0.34 g, 95%) as a pale yellow oil.

$$[a]_D^{20} = +2.0^{\circ} (c 1.05, CHCl_3).$$

IR (KBr): 2947, 2858, 1732, 1604.

¹H NMR (400 MHz, CDCl₃): 1.64-2.15 (m, 6H), 2.03 (s, 3H), 2.44 (s, 3H), 3.08 (s, 1H), 3.21 (m, 1H), 3.61 (s, 2H), 4.95 (m, 1H), 5.21 (dd, J=3.1, 7.6 Hz, 1 H), 7.20-7.36 (m, 5H).

MS: m/z(%) 317 (M⁺,19.58), 182(38.54), 122(53.49), 94(100), 82(9.95), 43(15.63).

Anal. Calc for C₁₈H₂₃NO₄: C 68.14, H 7.26, N 4.42. Found C 67.76, H 7.26, N 4.32.

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References and Notes

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Sample Availability: Available from the authors and from MDPI.

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