

Determination of the absolute configuration of 6β-Hydroxitricyclo[6.2.1.0^{2,7}]undeca-9-ene-3-one by chemical correlation

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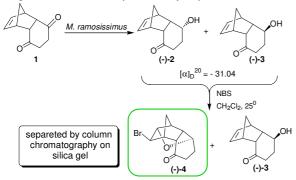
INTRODUCTION

Biotransformation is one of the most efficient methods for production of high optical purity compounds and development of efficient routes for target molecules. Our research group is interested in testing the ability of the microorganisms to perform desymmetrizations of achiral molecules. Our goal is to devise methodologies in order to obtain optically active intermediates for use in biological and, NMR spectroscopy studies and as precursors of chiral compounds or chiral auxiliaries for asymmetric synthesis.^{1,2,3}

In this work, we herein report the determination of the absolute configuration, by chemical correlation, of a polycyclic alcohol obtained from biotransformation tests carried out with the dienedione **1** in liquid culture medium using the fungus *Mucor ramosissimus*.

RESULTS AND DISCUSSION

Biotransformation of diketone **1** gave the ketoalcohol (-)-**2** and their epimer (-)-**3**. The absolute configuration of **2** was previously reported.¹

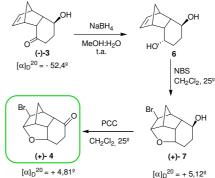


Scheme 1. Synthesis of bromo-ether (-)-4

As attempts to separate **2** and **3** were unsuccessful, and taking advantage of the difference in reactivity of the two epimers, we transformed the alcohol **2** selectively in bromo-ether **(-)-4** (Fig. 1).

The enantiomeric excess of **2** (e.e >99,9%) was determined indirectly from compound **4**, by ¹H NMR experiments using $[(+)-Eu(hfc)]_{3}$

In order to determine the absolute configuration of isomer **3**, we've decided to turn it on the bromo ketone **4** (with already known absolute configuration) through the sequence of reactions shown in Scheme bellow.



Scheme 2. Synthesis of bromo-ether (+)-4

The positive rotation shows that there is an enantiomeric excess of the isomer (+)-**4**. Therefore the absolute configuration of (-)-**3** was determined to be as drawn in Fig. 2.

CONCLUSION

The absolute configuration of alcohol (-)-**3** has been determined by chemical correlation, having the IUPAC systematic name [(1*R*,4*S*,4*aR*,8*S*,8*aS*)-8-hydroxy-4,4*a*,6,7,8,8*a*-hexahydro-1,4-metanonaftalen-5 (1*H*)-one)].

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