

SYNTHESIS OF METHYL 4-(4-BROMOPHENYL)-2,7,7-TRIMETHYL-5-OXO-1,4,5,6,7,8-HEXAHYDROQUINOLINE-3-CARBOXYLATE

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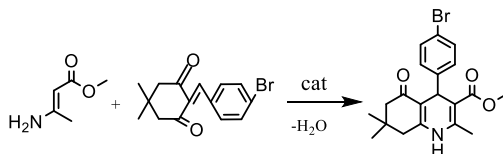
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Most of the widely used organic compounds such as perfumes, cosmetics, pharmaceuticals, vitamins, pesticides, and some nutrients are composed of chiral molecules. The fact that the mentioned substances have special properties is directly related to the chiral nature of the molecules of this type of compounds. One of the main factors that influence substances to have biological, physiological and other properties is the concept of asymmetry, in other words, chirality. For this reason, asymmetric synthesis of physiologically active substances has been of great importance in recent years.

The Hans reaction is the most important reaction for the synthesis of pyridine derivatives. Synthesis of pyridine derivatives always is one of the demand areas in the organic synthesis. Most derivatives of 1,4-dihydropyridine synthesized on the basis of Hans reaction are considered to be highly important compounds in medicine.

From the mechanism of the classic Hans reaction is known that during the reaction of methylene active compound (as an intermediate product)- with aldehyde obtained Knoevenagel adduct but from the reaction with ammonia is obtained enamine. Condensation of this additive and enamel results in the final product acquisition. When using a methylene active compound during the reaction, a symmetric product is obtained. Two different methylene active compounds are used for asymmetric synthesis. The presence of two different methylene active compounds in the environment causes additional intermediate products, which, along with asymmetric products, result in the formation of undesirable symmetric products. This reduces the degree of optical purity and practical output of the product.



Depending on the nature of the chiral organic catalyst during two-component condensation, the degree of optical purity is twice as high as compared to four-component condensation.

The ^1H and ^{13}C NMR spectra of the synthesized substance are as follows.

^1H NMR (400MHz, DMSO- d_6): 0.99 (s, 3H, CH₃), 1.09 (s, 3H, CH₃), 2.19-2.27 (dd, 2H, J = 12.2, J=12.7, CH₂), 2.35-2.43 (dd, 2H, J = 12.9, J=15.2 CH₂), 2.37 (s, 3H, CH₃), 3.68 (s, 3H, OCH₃), 5.04 (s, 1H, CH), 7.37-7.48 (dd, 4H, J=7.3, J=7.7, Ar), 8.75(s,1H,NH).

^{13}C NMR(100MHz, DMSO- d_6): 19.87, 29.76, 31.81, 36.04, 43.06, 52.81, 105.16, 112.24, 126.18, 128.91, 130.92, 145.73, 148.26, 150.34, 168.23, 196.15.