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Application of in situ FTIR for the preparation of 17-α-estradiol via Mitsunobu reaction

Flavio S P Cardoso
Libbs Pharmaceuticals, Brazil

An efficient synthesis of 17-α-estradiol 1 is described. Utilization of in situ IR allowed for an online monitoring of the key Mitsunobu reaction and development of a safe and reliable synthesis of 17-α-estradiol 1 in 78% overall yield over three steps. Benzoylation of 17-β-estradiol 2 is conducted at high regioselectivity under phase-transfer catalysis (PTC) conditions, followed by a Mitsunobu reaction to invert the chiral center at C-17 and provide intermediate 5, containing the core structure of 17-α-estradiol 1. Finally, the desired active pharmaceutical ingredient (API) is prepared by saponification of the remaining esters.

Biography

Flavio S P Cardoso obtained a BS degree in Chemistry in 2009 at the State University of Campinas (UNICAMP), Brazil. He performed undergraduate research under the supervision of Prof. Carlos Roque Duarte Correia for a period of nearly three years. His research at UNICAMP focused on the palladium-catalyzed Heck-Matsuda reaction. Next, he started his graduate studies at the University of Florida, USA. Under the guidance of Prof. Aaron Aponick, his PhD studies involved the development of a new class of atropisomers which was ultimately applied in asymmetric catalysis. Upon graduation in 2014, he moved back to Brazil to work at Libbs Pharmaceuticals as a Chemical Development Scientist.

flavio.cardoso@libbs.com.br

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