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Cyclisierungsversuche von substituierten Bis(brommethyl)benzolen mit methylenaktiven Verbindungen

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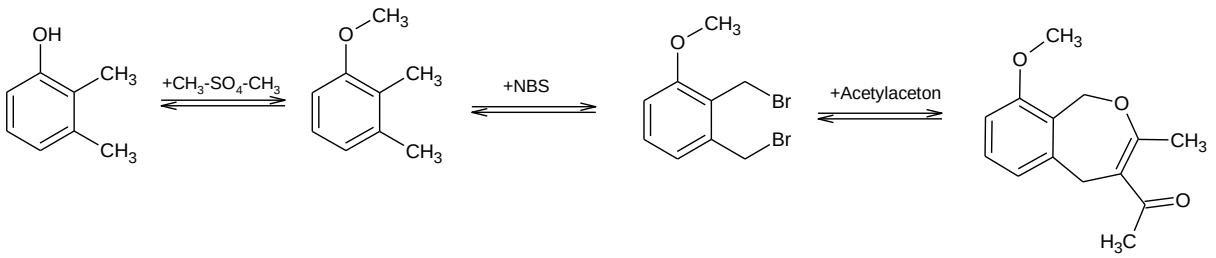
Firstly, the 2,3-dimethylphenol reacts via a Williamson-ether-synthesis, a S_N2-mechanism, to methylate the hydroxyl-group. To generate an appropriate reactant for the cyclization both of the methylgroups get brominated via the Wohl-Ziegler-reaction with the regionally selective reagent N-bromosuccinimide. Afterwards, the phase-transfer catalyst reaction happens, which generates either a benzoxepin- as well as an indane-derivative and some side-products. Within the substituent on the benzene-ring the reaction can be controlled in both directions. Especially the electron density at the methylene groups is highly important and is related to the mesomeric effect of the methoxy group. With the chosen +M-substituent (methoxy group) the reaction should be ending up with the benzoxepin as the main product. The most challenging step of the synthesis was the purification, because during the process, a lot of the benzoxepine deteriorated. An optimization of this task is still needed.



Fazit

Das gewünschte 4-Acetyl-9-methoxy-3-methyl-1,5-dihydro-2-benzoxepin ließ sich charakterisieren, jedoch nicht rein kristallisieren. Nachfolgend das 1H-Spektrum, bei dem der Peak bei 5.42 die Synthese des 1,5-Dihydro-2-benzoxepins belegt, hier allerdings verunreinigt mit dem Indanderivat: