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Synthesis of an anti-cancer reagent by using sulfur-based reaction

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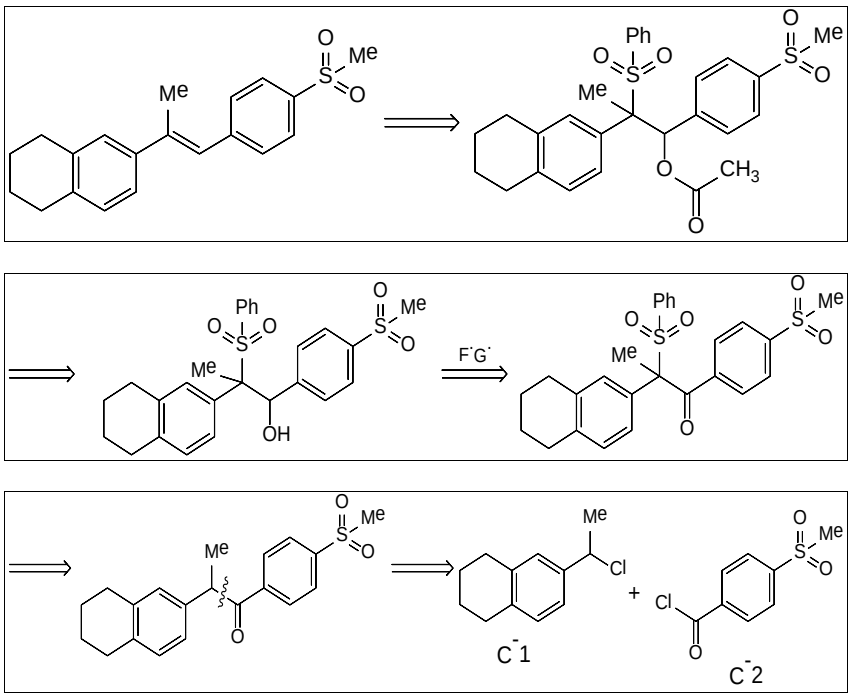
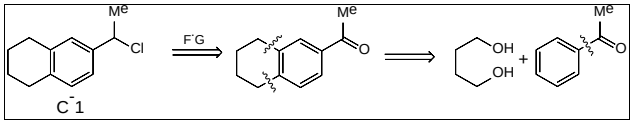
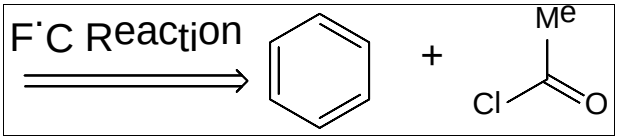
Abstract
In this paper, we have reported the synthesis of an anticancer drug against breast cancer. Constitutionally, it is known as 6-{(*E*)-2-[4-(methylsulfonyl)phenyl]ethenyl}-1,2,3,4 tetrahydronaphthalene During the synthesis, Friedel-Crafts reaction and Grignard reaction were used. The well-known Juliya olefination was used to create the desired stereochemistry of the target molecules, which is required for their ant0-cancer activity. After the completion of synthesis, the vibrational spectroscopy-FTIR has been used to measure the vibrational modes of the target molecules as well as intermediate compounds, which provides information about structure of the drug. From the interpreted spectral data, the structure of the compound was confirmed.

Keywords:

Introduction
Alkenes belong to a chemical functional group that is omnipresent in literally all natural products. Interestingly, since the early times when organic synthesis slowly became a ‘useful’ scientific discipline, many synthetic strategies have focused on the stereoselective synthesis of these structural motives. Especially, methods that allow for the connective stereoselective introduction of the olefin moiety have become very valuable tools for this achievement. Over the past 100 years, many different connective olefination methods[1-4] have been developed, but many of them follow the same retrosynthetic pathway.
The restrosynthetic analysis of the target molecule may be shown as:



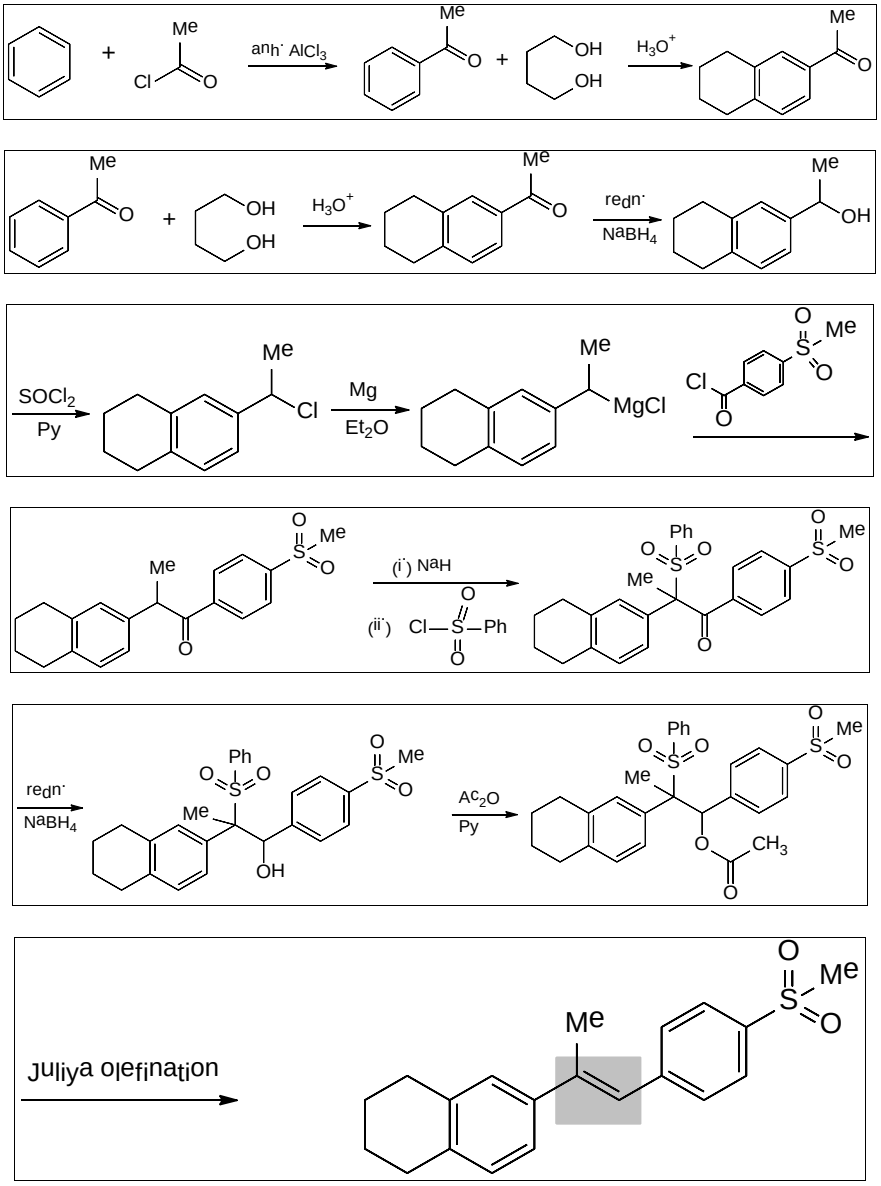




Experimental

All the chemicals benzene, acetyl chloride-methylsulphonylbenzoyl chloride etc. were purchased from the E.Merck and BDH and used as such.

The complete reaction scheme for the synthesis may be shown as:



Mechanism

The Julia olefination reaction mechanism was intensively studied by Silvestre Julia[5] and the study was further extended[6-10] Based on these excellent mechanistical works, the reaction mechanism could be established with respect to the stereochemical outcomes of the reaction. There are following important features of this mechanism.

a) The addition step of metalated sulfone to aldehyde can provide anti-adduct or syn-adduct
b) When stabilized metalated sulfonyl anions are used, the addition step becomes reversible
c) For the elimination step, two borderline mechanisms are generally accepted. In the first, which is the most common, the rearranged intermediate undergoes β-elimination.
d) The most important and most straightforward way to influence the syn/anti-selectivity of the addition step is to choose the right solvent for the transformation. When polar solvents such as THF, DME, or DMF are used, anti-adduct anti is the preferred product of the addition due to solvent stabilization. On the contrary, when nonpolar solvents such as toluene are used, the reaction

proceeds via a closed transition state and syn adduct synis preferred.

e) The addition of the co-solvents to the reaction mixture can also be beneficial when (E)-selectivity is searched. It was observed that the addition of co-solvents such as DMPU or HMPA to the reaction mixtures carried out in the THF or DMF leads to an increase in the (E)-olefin selectivity of the desired product. It is believed that the co-solvent role is in metal cation scavenging with an impact similar to that described in the previous section (Increased reactivity that favors the anti-adduct formation).

Conclusions

Since its first dissemination in 1993 the reaction sequence that is now referred to as the Julia olefination reaction has become very popular late-stage connective method in natural product synthesis, because it combines highly efficient (reaction yield) and selective (predominantly (E)-selective) connective method that proceeds in one-pot protocol and under mild reaction conditions and with broad substrate and functional group tolerance. The past 30 years of reaction development have also identified key mechanistic properties that allow better control of reaction selectivity. Moreover, we have recently introduced a novel modification of the Julia olefination reaction that not only increases the starting material scope since it allows for the use of previously inaccessible carboxylic acid derivatives as substrates but also allows for the selective (E) or (Z)-olefin formation. In addition, this method allows for the first time in the development of the Julia olefination reaction an independent formation of (E) or (Z) olefins starting from the same starting materials by simple reaction work-up protocol alternation.

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