

## <sup>1</sup>H-NMR Studies of 5 and 7-Methyl isomers of 2,4-dichloroquinoline and Synthesis of Dibenzonaphthyridine Isomers

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**ABSTRACT:** The reaction of *m*-toluidine and malonic acid in phosphorous oxychloride resulted in the major formation of 5-methyl isomer (**1a**) and minor formation of 7-methyl isomer (**1b**). Computation study using DFT/B3lyp/6-311++g(d,p) method to calculate the energies of two isomers briefly describe that, the energetically favourable 7-methyl isomer was found to be 6.5937 kcal/mol less energy than the sterically hindered 5-methyl isomer. Overcoming the steric hinderance, the formation of major ratio of 5-methyl isomer when compared to 7-methyl isomer is quite uncertain. Since both the isomers (**1a** and **1b**) could not be separated, the reaction of the both isomers in the construction of angular and linear dibenzonaphthyridines also ended up in the formation of a mixture of positional isomers. All ratio of the products were able to be predicted using <sup>1</sup>H-NMR studies and supported by G.C.Mass spectroscopy.

**Keywords:** 2,4-dichloroquinolines, 5-methyl and 7-methyl isomers, DFT calculations, benzonaphthyridines.

### 1. INTRODUCTION

Cyclic polyaza compounds, such as quinolines, naphthyridines, and phenanthridines, are important structural components of naturally occurring alkaloids and synthetic analogues possessing interesting biological activities [1].

Quinoline core is widely used as central pharmacophore to synthesize compounds of medicinal importance, especially those possessing antimalarial property [2] as well as other biological activities [3-5]. Quinoline derivatives have been examined as inhibitors of tyrosine kinases, proteasome, and topoisomerase, tubulin polymerization, as well as for their function to repair DNA [6]. Natural alkaloids possessing quinoline nucleus also exhibit antitumor activity, e.g., camptothecin [7,8]. Some synthetic anilinoquinoline derivatives proved themselves as antimalarials [9] and were used as potential intermediates to synthesize heterocycles like indoloquinolines [10] and dibenzonaphthyridines [11]. In recent years, the chemistry of naphthyridines and their functional derivatives has attracted interest from synthetic organic chemists

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