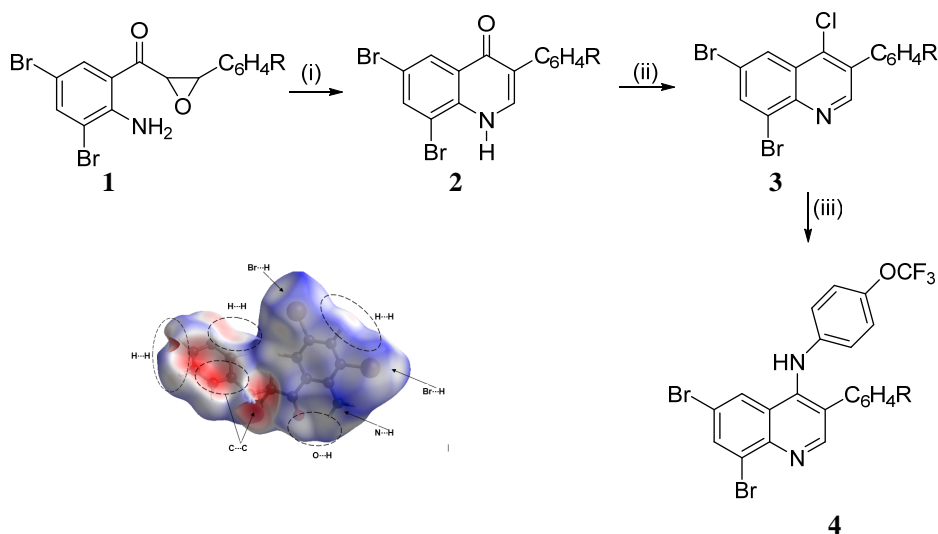


# POTENTIALLY TAUTOMERIC 3-ARYLQUINOLIN-4(1H)-ONES VERSUS 3-ARYLQUINOLIN-4-OLS: SPECTROSCOPIC, DFT AND X-RAY ANALYSES

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Continued interest in the synthesis of primary 4-aminoquinoline derivatives stems from their importance as antimalarial, anti-inflammatory, antibacterial, and antihypertensive agents [1] as well as immunostimulants and non-nucleoside HIV-1 inhibitors [2]. Although there are several methods described in the literature for the synthesis of primary 4-amino-2-arylquinolines [3], corresponding data for the synthesis of the 3-substituted 4-aminoquinoline derivatives is considerably less well documented. Consequently, we decided to employ the epoxides **1** as substrates for the synthesis 3-arylquinolin-4(1*H*)-ones **2**. Since no qualitative structural analysis of these potentially tautomeric compounds **2** has been performed before, we decided to investigate the geometry of the dominant form of these tautomers in solution and solid state using spectroscopic and X-ray diffraction techniques complemented with density functional theory (DFT) methods. The heterocyclic ring of compounds **2** was aromatized, and the intermediate 3-aryl-4-chloroquinolines **3** transformed into the primary 4-amino-3-arylquinolines **4** via nucleophilic displacement leading to  $Csp^2$ -heteroatom (N) bond formation.



[1] *Tetrahedron Lett.* **2001**, 42, 2553–2555.

[2] *Synthetic Commun.* **2009**, 39, 4249–4263

[3] *Chem. Med. Chem.* **2008**, 3, 1077–1082.