



## Synthesis, Characterization and Crystal Structure Analysis of 2-(1-(4-butylphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-4-chlorophenol

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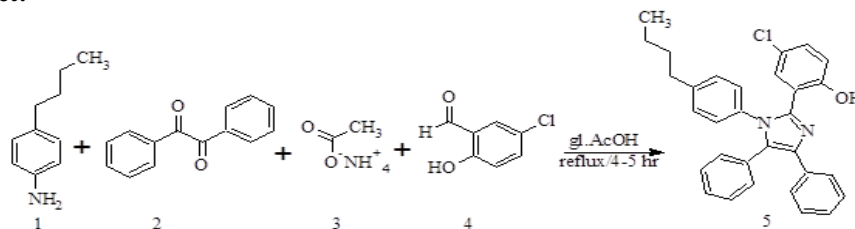
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### ABSTRACT

High efficiency process for the synthesis of 2-(1-(4-ethylphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-4-chlorophenol (5) through a four-component condensation reaction of 4-butylaniline (1), Benzyl (2), Ammonium Acetate (3) and 4-chloro-salicylaldehyde (4) in a acetic acid media with 2-3 drops of con  $H_2SO_4$  has been reported. The compound obtained was characterized spectroscopically by IR,  $^1H$ -NMR,  $^{13}C$  NMR, SEM and EDAX techniques and finally the structure of 2-(1-(4-ethylphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-4-chlorophenol (5) was established by X-ray diffraction studies. The compound crystallizes in the triclinic *p-1* space group with cell parameters  $a = 10.253(15) \text{ \AA}$ ,  $b = 11.107(16) \text{ \AA}$ ,  $c = 12.481(19) \text{ \AA}$ ,  $\alpha = 99.560(16)^\circ$ ,  $\beta = 130.254(8)^\circ$ ,  $\gamma = 93.785(3)^\circ$  and  $Z = 2$ . The imidazole ring in the structure is planar. The structure exhibits intramolecular hydrogen bonds of the type  $O-H \dots N$  and  $C-H \dots N$  hydrogen bonds which contribute for the stability of the compound. Further, the Hirshfeld surface analysis reveals the nature of intermolecular contacts; the fingerprint plot provides the information about the percentage contribution from the intermolecular contacts to the surface.

### Graphical Abstract:



Synthesis of 2-(1-(4-butylphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-4-chlorophenol

**Keywords:** Antiaging, Imidazole,  $O-H \dots N$  and  $C-H \dots N$  hydrogen bonds, Hirshfeld surface.