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Synthesis, Crystal Structure, and Herbicidal Activity of 3-(2-Chloro-6-fluorophenyl)-4-(2-oxooxazolidine-3-carbonyl)-5-methylisoxazole

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ABSTRACT A novel *N*-aroyl diketone derivative, 3-(2-chloro-6-fluorophenyl)-4-(2-oxooxazolidine-3-carbonyl)-5-methylisoxazole ($C_{14}H_{10}ClFN_2O_4$, M_r=324.69), was designed via fragment analysis and coupling strategy that led to highly potent and bio-selective herbicide. The title compound was prepared by a multistep-reaction, including nucleophilic addition and *N*-acylation reaction using 2-chloro-6-fluorobenzaldehyde as the starting materials in 83.4% yield. The product was characterized by infrared, proton nuclear magnetic resonance, Carbon-13 nuclear magnetic resonance, human resource management system, and X-ray diffraction. The title compound crystallized in the monoclinic system, space group $P2_1/n$ with a=10.7119(4) Å, b=17.5875(7) Å, c=11.5151(7) Å, β=100.927(2)°, Z=8, V=2870.0(2) Å^3, $F(000)$=1328, D_c=1.503 Mg/m^3, crystal size: 0.130 × 0.120 ×0.100 mm. The herbicidal activity was tested against the gramineous weed *Echinochloa crus-galli* and broadleaf *Abutilon juncea*.

KEYWORDS 3-(2-Chloro-6-fluorophenyl)-4-(2-oxooxazolidine-3-carbonyl)-5-methylisoxazole, Synthesis, Characterization, Single-crystal structure, Herbicidal activity.

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