In recent years, there has been increased attention towards the synthesis of isoxazole derivatives, since they possess a broad spectrum of biological activities. Isoxazoles are one of the key oxygen and nitrogen containing five-membered ring heterocycles that possess significant roles in the medicinal chemistry. Considerable attention has been focused on isoxazoline derivatives due to their interesting biological activities. The synthesis of novel isoxazoline derivatives remains the main focus due to their diverse pharmacological activities. Owing to their versatile chemotherapeutic importance, a significant amount of research effort has been focused on preparing new derivatives of isoxazole compounds. Isoxazole derivatives are a promising structural moiety for drug designing, which are reported to possess antibacterial, anticonvulsant, antipsychotic, anti-inflammatory, antitumor, analgesic, insecticidal, antioxidant, antidepressant and antimicrobial activities. In addition, isoxazoline derivatives have played a crucial role as intermediates in the organic synthesis of a number of hetero-cyclic pharmacologically active compounds. Encouraged by the diverse biological activities of isoxazole compounds, it was decided to prepare a new compound, 5-(3-dimethylene-p-tolylsulfonyl)-propyl-3-(4-flurophenyl)-isoxazole.

The intermediate 4-fluro-benzaldoxime was prepared from X-ray diffraction studies. The title compound crystallizes in the triclinic crystal class in the space group $P\overline{1}$ with cell parameters $a = 5.9350(6)$ Å, $b = 10.1850(14)$ Å, $c = 14.8270(2)$ Å, $\alpha = 104.938(4)^\circ$, $\beta = 97.960(8)^\circ$, $\gamma = 90.933(6)^\circ$ and $Z = 2$. The isoxazole ring is planar. The molecular structure exhibits intermolecular hydrogen bonds of the type C–H $\cdots$ O. The final residual factor is $R_1 = 0.0433$.

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4-fluorobenzaldehyde with hydroxylamine hydrochloride in the presence of sodium acetate in methanol at 60°C for 5 - 6 h. After completion of the reaction, the solvent was evaporated under a vacuum; 40 ml of distilled water was added and cooled to 5 - 8°C for 1 h and filtered at the same temperature to obtain a white solid.

After a solution of 4-fluorobenzaldoxime (1 equivalent) in ethanol was taken in a round-bottomed flask, 2 - 5 equivalents of CAT and 2 equivalents of dipolarophiles 3 were added. The reaction mixture was stirred for 8 to 10 h at room temperature, and the solvent was evaporated under a vacuum; 40 ml of distilled water was added and cooled to 5 - 8°C for 1 h and filtered at the same temperature to obtain a white solid.

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