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ISSN: 2278-1862

Journal of Applicable Chemistry

2019, 8 (1): 293-301

(International Peer Reviewed Journal)

Crystal Structure Study, Hirshfeld Surface Analysis and *in vitro* Antibacterial Activity of *p*-tolyl 4-fluorobenzoate

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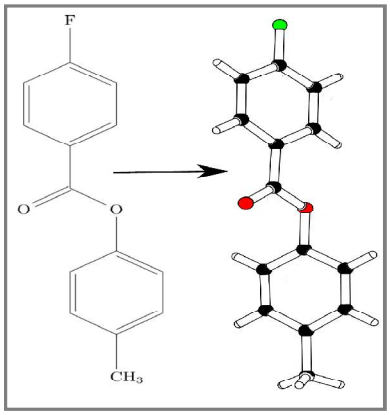
Accepted on 30th November, 2018

ABSTRACT

The title compound $C_{14}H_{11}FO_2$ crystallizes in orthorhombic crystal system with space group $P2_12_12_1$. The compound exhibits inter-molecular interaction of the types C–H…O, and C–H…π; intra-molecular interaction of the type and C–H…O. The inter-contacts are also studied using Hirshfeld surface analysis. The compound was screened for anti-bacterial activity which revealed medium to low activity against certain bacteria.

Graphical Abstract



Highlights

- This manuscript discusses the procedure to synthesis *p*- tolyl 4- fluorobenzoate.
- Elemental analysis, ^{1}H NMR, FT-IR spectral analysis was studied.
- The X-ray crystal structure study reveals that the compound crystallizes in orthorhombic crystal system with space group $P2_12_12_1$.
- The compound exhibits inter-molecular interaction of the types C–H…O, and C–H…π; intra-molecular interaction of the type and C–H…O.

- The inter-contacts are also studied using Hirshfeld surface analysis.
- The compound was screened for anti-bacterial activity which revealed medium to low activity against certain bacteria.

Keywords: *Bacillus subtilis, Staphylococcus aureus, Proteus vulgaris, Escherichia coli,* fingerprint plots, Streptomycin, Resazurin assay, phenyl benzoate, Hirshfeld surface analysis.