

## Hirshfeld analysis, anticancer efficacy and molecular docking studies for ferrocenecarboxaldehyde oxime and ferrocene-based aldimine

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Ferrocenecarboxaldehyde oxime **1** and ferrocene-based aldimine **2** have been evaluated for their anticancer potentials against MCF-7 and T47D cell lines supported with molecular docking studies. Aldoxime **1** demonstrates an  $IC_{50}$  that is 2.4 to 1.5 times more potent than aldimine **2** against MCF-7 and T47D cancer cell lines, indicating its superior anticancer activity. Molecular docking analyses show that both compounds exhibit strong binding affinities to the EGFR receptor, a well-known cancer receptor. These findings highlight the significant potential of these compounds as effective anticancer agents. In addition, Hirshfeld analysis for molecular packing has been used to inspect the possible contacts which control the molecular packing of both compounds. For aldoxime **1**, the important N...H interactions contribute upto 10.1% while for aldimine **2**, the C...H (25.7%) and O...H (7.0%) contacts are the most significant.

**Keywords:** (*Z*)-Ferrocenecarboxaldehyde aldoxime, (*E*)-Ferrocene-based aldimine, Hirshfeld, Anticancer, Molecular docking