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Synthesis and characterization of C-5 substituted barbituric acid derivatives for the evaluation of anticancer activity against breast cancer cell michigan cancer foundation-7

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ABSTRACT Two series of hybrids bridged between the C-5 position of barbituric acid and ortho/para-substituted aromatic amines through azo/imine linkages were synthesized. Azo group-linked compounds were synthesized through azo-coupling reaction of diazotized salt of amine and barbituric acid. Imine-linked compounds were synthesized by the reaction of barbituric acid with trimethyl orthoacetate, followed by amines. The structures of all the compounds were confirmed by spectral techniques. Absorption, Distribution, Metabolism, Excretion, and Toxicity profiling of the compounds by Swiss ADME indicated favorable pharmacokinetic properties for the active derivatives. Docking studies with mechanistic target of rapamycin using Autodock showed that quinoline/naphthyl–barbituric acid hybrids to possess activity comparable to doxorubicin. Among the synthesized compounds, naphthyl and quinoline hybrids with promising docking scores displayed strong antiproliferative effects in 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assays, with IC_{50} values of 150–200 μM. Structure–activity relationship analysis revealed that electron-withdrawing or bulky aromatic substituents at the C-5 position markedly enhance cytotoxicity.

KEY WORDS ADME analysis, Anticancer activity, Barbituric acid derivatives, 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assay.

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