

Analytical, theoretical, and evaluation of biological activities of a new azo dye derived from the drugs procaine and kojic acid

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ABSTRACT A new azo dye, (2-(diethylamino)ethyl (*E*)-4-((3-hydroxy-6-(hydroxymethyl)-4-oxo-4*H*-pyran-2-yl)diazenyl) benzoate), was synthesized by diazotization of procaine followed by coupling with kojic acid in alkaline condition. The results showed a stable ionization approach since it works well in liquids with varying pH levels. The theoretical study on azo dye includes atomic close-contact calculations, (-N=N-) group and its related atoms, and analysis utilizing internal coordinate mechanics. The chemical azo dye showed a potential antibacterial activity against *Staphylococcus aureus*, *Aspergillus niger* and *Candida albicans*, and negative against *Escherichia coli*.

KEY WORDS Azo dye, Internal coordinate mechanics, Conformational analysis, Sensitizer.

How to cite this article: Abdullmaged, H.A., Al-Waeli, J.H. and Mirdan, G.A. Analytical, theoretical and evaluation of biological activities of a new azo dye derived from the drugs procaine and kojic acid, *Indian J. Heterocycl. Chem.*, **2025**, 35, 861-867. <https://doi.org/10.59467/IJHC.2025.35.861>