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SYNTHESIS AND THEORETICAL STUDY OF 4-ACETYL-5-(2-NAPHTYL)-2,3-DIHYDRO-2,3-FURANDIONE WITH SOME NITROGENOUS NUCLEOPHILES

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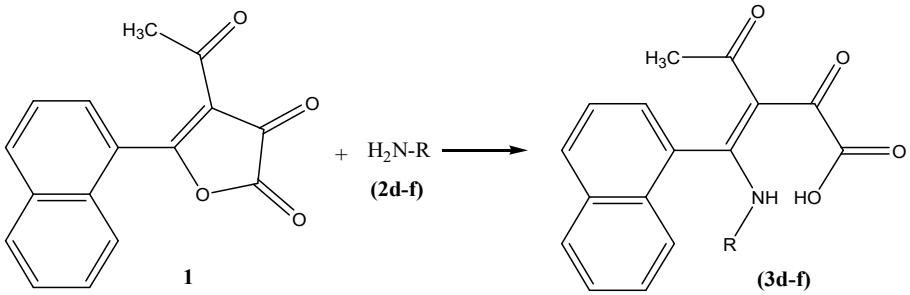
Abstract: The 2,4-dioxopentanoic acid derivatives **(3d-f)** were obtained from the reaction of 4-acetyl-5-(1-naphthyl)furan-2,3-dione **(1)** with various nitrogenous nucleophiles **(2d-f)**. The structures of these newly synthesized compounds **(3d-f)** were determined from the FT-IR, ^{1}H and ^{13}C NMR spectroscopic data and elemental analyses. Theoretical Study of derivatives of (3*Z*)-3-{2-naphthyl[2-(4-nitrophenyl)hydrazino]methylene}-2,4-dioxopentanoic acid **(3d-f)** were carried out by using DFT/B3LYP method with basis set of the 6-311G(d,p) in order to find molecular properties by Gaussian 03 program [1](see **Schemes 1**and **2**). According to E_{HOMO} and softness values; electronic give trends for investigated molecules can be written as: **3f**>**3d**>**3e**.The E_{HOMO} and E_{HOMO} energy gap of a measure of stability. Additionally, according to E_{HOMO} and E_{HOMO} energy gap; stability give trends for investigated molecules can be written as: **3e**>**3d**>**3f**.

Keywords: *Furan-2,3-dione; Nitrogenous Nucleophiles; 2,4-dioxopentanoic Acid; Quantum Chemical Calculations.*



Scheme 1. Short representation of the synthesized molecules **(3d-f).**

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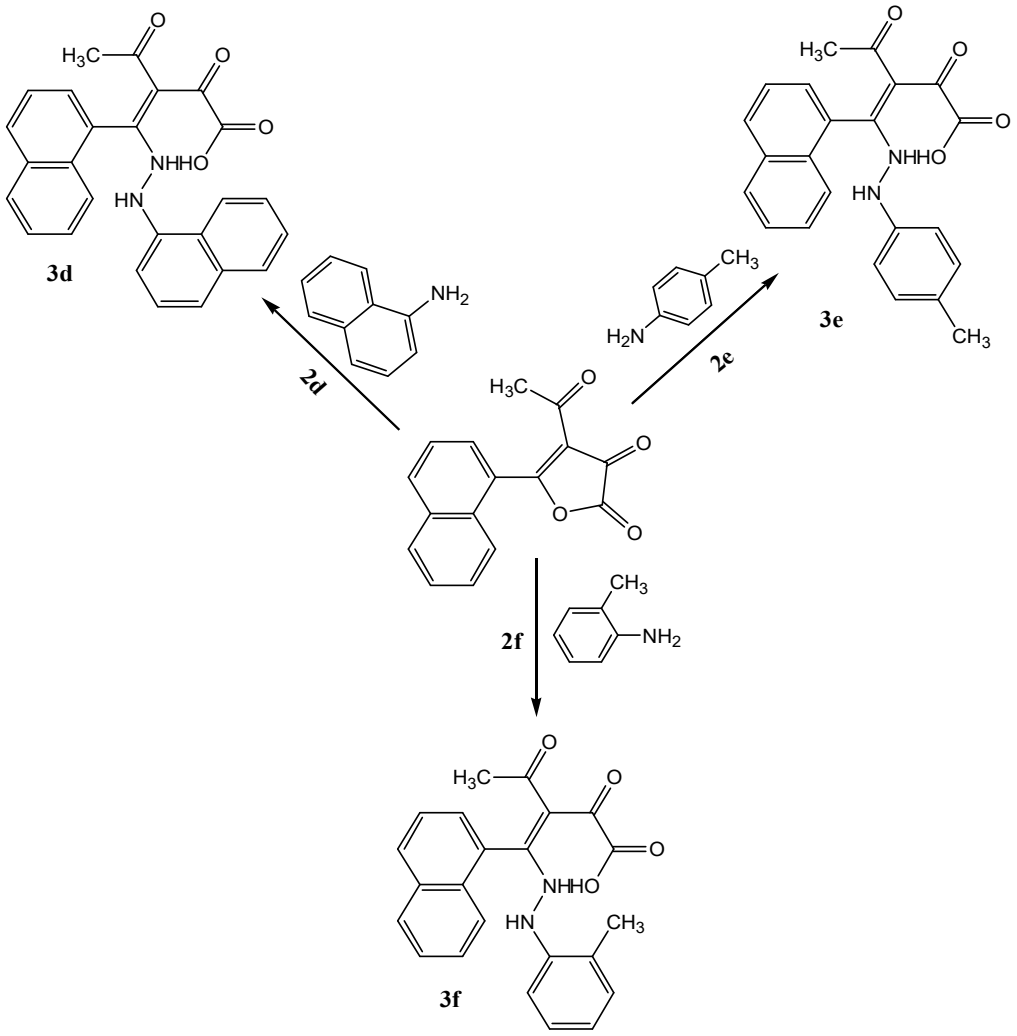

Scheme 2. Synthesis of molecules **(3d-f).**

Reference

[1] M.J. Frisch, *et. al.*, Gaussian 03 W, Gaussian Inc., Wallingford, CT, 2004.