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Synthesis and Characterization of Some Fluorinated Heterocycles Like Pyrazolines by Environmentally Benign Process

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Abstract: *Halogenated heterocycles like Pyrazolines shows marked biological activities. 4-fluorobenzaldehyde **1** when treated with substituted hydroxy acetophenones **2** under ultrasonication yields chalcones **3**. These chalcones were subjected with phenyl hydrazine under Ultrasonication gave the compound 5-(4- fluorophenyl)-1,3-diphenyl-4,5-dihydro-1H-pyrazole **4**. On the basis of spectral data, the structures of compounds have been constructed..*

Keywords: Fluorinated heterocycles; pyrazolines, Green method

I. INTRODUCTION

Nowadays Fluorine chemistry has great importance in the drug designing. The most important factors in the drug design is that fluorinated molecule has a higher bioavailability. Fluorine is much more lipophilic than hydrogen, so incorporating fluorine in the molecule makes it more fat soluble, so it percolates into the membrane more readily[1]. Around fifth of all drugs on the market today contain at least one fluorine atom such as Paroxetine, Ezetimibe, Linezolid and Midazolam. Many fluorinated compounds are widely used as antiviral, antimalarial, antipsychotic and antidepressants. Some heterocyclic compounds also act as dyes, pesticides, luminophores and herbicides in nature[2].
Chalcones and their derivatives having an α, β-unsaturated carbonyl system are very versatile substrates for the evaluation of various organic reactions.[3]
The chalcones prepared by the condensation of different substituted aromatic aldehydes and ketones are well known in synthetic chemistry. Synthesized compounds were found to have good antibacterial, analgesic and anti-inflammatory activities.[4] Pyrazolines are widely used as useful synthons in organic synthesis.[5-8] A classical synthesis of 2-Pyrazolines involves the base catalyzed condensation of aryl methyl ketones and aldehydes to give chalcones, which undergoes cyclization with hydrazines yields 2-pyrazolines[9]
Ultrasound is a relatively new way of introducing energy into chemical systems.[10] It has been used to enhance reaction rates[11] in the large number of classical organic reactions. Compared to other processes, ultrasound-assisted organic synthesis produces good yields. It is useful for many organic transformations and has the ability to significantly alter the speeds of chemical reactions.

Present Work:
Substituted hydroxy acetophenones **1** on reaction with 2-fluorobenzaldehyde **2** stirred at room temperature using LiOH / alcohol for 4 hrs. gives respective chalcones **3** which on reaction with Phenyl hydrazine for 6 hrs. which gave pyrazolines 4.

Experimental:
All of the uncorrected melting points were noted in open capillary tubes. The Shimadzu FTIR Spectrophotometer was used to record I.R. spectra in KBr disc. A Bruker Avance II 400 MHz spectrophotometer was used to record 1H NMR spectra using DMSO-d6 as the solvent and TMS as an internal standard (chemical shift in values). A Finnigan mass spectrometer was used to acquire mass spectra. TLC on silica gel G plates was used to verify the compounds' purity.

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Scheme:

Synthesis of Chalcones:
Compound **1** (0.005 mol) & **2** (0.005 mol) were taken in 100 ml RBF with 20 ml ethanol as a solvent. To this reaction 2 gm of LiOH was added & resulting reaction was stirred at room temperature for 4 hrs. Then contents were poured over crushed ice & acidified with conc. HCl, yellow solid thus obtained were separated by filtration & crystallized from ethanol to get compound **3**. Their characterization data is in the table-1

(3a-3e).
Spectral Data
3a- I.R. (KBr, cm-1): 3056 (Ar =C-H), 2925 (C-H), 1655 (–C=O), 1576 (–C=C), 1215 (–C-F),1028 (–C-Br)
NMR (DMSO/ d6): 6.70 -8.12(10 H, m, Ar & =CH protons)

Synthesis of pyrazoline
Compound **3** was taken in 100 ml RBF with 20 ml alcohol. To this reaction mixture 2 ml Phenyl hydrazine was added & the contents were heated under reflux for 3 hrs and to this reaction mixture 2 ml acetic acid was added & heating was continued for further 3 hrs. After cooling contents were poured over crushed ice. Compound 4 was produced by filtering and crystallising the resulting material with alcohol. Spectral data was used to identify the products that were obtained. Table 1 (4a-4e) provides their characterisation data.

Spectral data:
4a I.R. (KBr, cm-1) 3355 (N-H), 2985 (Ar- =CH), 1608 (–C=N), 1576 (–C=C), 1206 (C-F) 1045 (C-Br);
NMR (DMSO/ d6): δ 3.02 (1H, dd, C-H), 3.65 (1H, dd, C-H), 4.78 (1H, dd, C-H), 6.45-7.12 (5H, m, Ar-H), 7.22-7.48 (8H, m, Ar -H for halogenated aromatic rings).

Table 1: Characterization data of synthesized molecules

Compound	R_1	R_2	R_3	R_4	M.P.	Yield
3a	H	H	Br	H	178	67
3b	Cl	H	Cl	H	145	70

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3c	H	CH_3	Cl	H	136	72
3d	H	H	CH_3	H	122	68
3e	H	Cl	H	Cl	165	78
4a	H	H	Br	H	118	65
4b	Cl	H	Cl	H	178	62
4c	H	CH_3	Cl	H	215	58
4d	H	H	CH_3	H	174	56
4e	H	Cl	H	Cl	187	72

II. CONCLUSION

The literature review indicates that pyrazoline derivatives are compounds with biological activity. Numerous fluorinated chemicals are utilised extensively as antidepressants, antiviral, antimalarial, and antipsychotic medications. One relatively recent method of adding energy to chemical processes is ultrasound. It has been applied to many traditional organic processes to increase their rates of reaction. Thus, we used the ultrasonication approach to create fluorinated pyrazoline derivatives.

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