Synthesis and Characterization of 5-Substituted Derivatives of 2, 4-Dithio-3-phenyl-6-chalcone-1,3,5-Triazines

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A B S T R A C T
Present research work involves, Synthesis of novel series of (2E)-1-[4-(2,4-dithio-3-phenyl-5-substituted-1,3,5-triazino-6-yl)aminophenyl]-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Ia-e) by the isomerisation of series of (2E)-1-[4-(2-phenylimino-4-substitutedimino)amino-1,3,5-dithiazino-6-y]aminophenyl]-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Ia-e) under the presence of sodium bicarbonate in aqueous ethanol. All the synthesized compounds were justified on the axis of chemical tests, elemental study and spectral characterization.

Keywords: Isomerisation, sodium bicarbonate, ethanol and spectral Characterization

1. Introduction
Heterocyclic plays a crucial role in the in the activities of the drugs or natural products. Nitrogen and sulphur are the important class of the hetero atoms in the formation of heterocycles. Many times nitrogen and sulphur in the same heterocycles reflects variety of applications. 1,3,5-Triazine is one of the enormously biologically potent heterocycle among the encyclopedia of heterocycles. Marvelous activities of the 1,3,5-Triazine are to the basic structure. The heterocycles containing s-triazines in the nucleus had successfully tested against various microorganisms and it...
was found that they possess potential therapeutic value for several diseases. So these compounds possess their own importance in medical faculty, pharmaceutical, industrial and agricultural field. Different substituent’s at different positions displayed variety of applications. Day by day bacteria becoming resistant to the existing drugs; Hence need of todays era is to design and synthesize new heterocycles based drugs.

Considering all the significances of the s-triazine and its different derivatives, it was planned to synthesize novel series of (2E)-1-[4-(2,4-dithio-3-phenyl-5-substituted-1,3,5-triazino-6-yl)aminophenyl]-3-(3,4-dimethoxy phenyl) prop-2-en-1-one (Ia-e) by the isomerisation of series of (2E)-1-[4-(2-phenyl-imino-4-substitute dimino) amino-1,3,5-dithiazino-6-yl) aminophenyl]-3-(3,4-dimethoxy phenyl) prop-2-en-1-one (Ia-e) on refluxing with 10% aqueous sodium bicarbonate in ethanol on water bath for half hours. The method used in the present synthesis is simple, cheaper and less time consumable.

2. Experimental

**Materials:** The entire chemicals used in the present research were MERCKS Chemicals (India Made). Starting compounds (Ia-e) were synthesized by literature method.

**Method**

Method adopted for the synthesis of all the compounds in the present investigation was conventional refluxing under water bath to attain constant temperature. Melting points of all the synthesized compounds estimated using paraffin oil and uncorrected. The carbon, hydrogen and nitrogen analysis was carried out on Carlo-Ebra-1106 analyzer and Colman-N-analyzer-29 respectively. IR spectra were recorded on SCIMADZU FTIR spectrometer in the range 4000-400 cm⁻¹ in KBr pellets. PMR spectra were recorded on BRUKER AVANCE II 400 NMR spectrometer with TMS as an internal standard using CDCl₃ and DMSO-d₆ as a solvent.

**General Procedure**

(2E)-1-[4-(2-phenylimino-4-substitutedimino) amino-1,3,5-dithiazino-6-yl) amino phenyl]-3-(3,4-dimethoxy phenyl) prop-2-en-1-one (Ia-e) was isomerized by 10% aqueous sodium bicarbonate solution ethanol medium. During heating reactants dissolved into the solvent. After completion of the reaction, excess solvent distilled out. Yellow crystals were obtained, which on recrystalized from glacial acetic acid to obtain (2E)-1-[4-(2,4-dithio-3-phenyl-5-substituted-1,3,5-triazino6-yl) amino phenyl]-3-(3,4-dimethoxy phenyl) prop-2-en-1-one (Ia-e).

Similarly, (2E)-1-[4-(2-phenylimino-4-(prop-2-en-1-yl) imino-1,3,5-dithiazino-6yl)aminophenyl]-3-(3,4-dimethoxy phenyl) prop-2-en-1-one (Ia), (2E)-1-[4-(2-phenylimino-4-ethylimino)-1,3,5-dithiazino-6yl) amino phenyl]-3-(3,4-dimethoxyphenyl) prop-2-en-1-one (Ib), (2E)-1-[4-(2-phenylimino-4-(2-methyl prop-2-yl)imino)-1,3,5-dithia-zino-6yl) amino phenyl]-3-(3,4-dimethoxy phenyl) prop-2-en-1-one (Ic), (2E)-1-[4-(2-phenylimino-4-phenylimino)-1,3,5-dithiazino-6yl]aminophenyl]-3-(3,4-dimethoxy phenyl) prop-2-en-1-one (Id), (2E)-1-[4-(2-

3. Results and Discussion

Elemental and IR Spectra and PMR spectral analysis of all the synthesized compound is given below, (2E)-1-[4-(2,4-dithio-3-phenyl-5-(prop-2-en-1-yl)-1,3,5-triazino-6-yl) amino phenyl]-3-(3,4-dimethoxy phenyl) prop-2-en-1-one (Ia)

Cream yellow solid, C₃₅H₂₅N₄O₃S₃, Yield-72%, M.P.- 173°C Composition-found(calculated) C 63.74 (63.49), H 4.61 (4.76), N 10.58 (10.58) and S 11.16 (12.11); FTIR (KBr) v cm⁻¹: 3069.64 (Ar=C-H stretching), 3349.69 (N-H stretching), 1687.26 (C=O stretching), 1139.82 (C=S stretching), 1032.06 (C=O-C stretching) and 1212.66 (C-N stretching); ¹H NMR (400 MHz CDCl₃, 6 ppm) singlet of 6H of –OCH₃ at δ 3.40 ppm, singlet of 2H of –CH=CH₂ at δ 3.63-3.77 ppm, multiplet of 12H of Ph at δ 6.69-8.11 ppm, singlet of 1H of –NH at δ 9.82 ppm and pentate of 1H of –NH and of 2H of allyl at δ 82.1, 1.31 and 2.10 respectively; Mol. Wt.: 529.

(2E)-1-[4-(2,4-dithio-3-phenyl-5-ethyl-1,3,5-triazin06-yl) aminophenyl]-3-(3,4-dimethoxy phenyl)prop-2-en-1-one (Iib): Dark yellow solid, C₃₇H₃₅N₄O₃S₂, Yield-80%, M.P.-
5. References


4. Conclusion

All the synthesized compound were analyzed, found and confirmed by their elemental study, IR spectra and PMR spectra. Similar method and procedure can be adopted for the synthesis of variety of derivatives of 1, 3, 5-triazines.

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