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Unification and Depiction of a series of 2-Benzylidene N N' Disubstituted Propanediamide Derivatives

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ABSTRACT: Chalcones occupies an important position in the organic synthesis and is used in production of biologically active compounds. An efficient and practical synthesis of chalcones was achieved through condensation of substituted propanediamide derivatives with bezaldehyde in an ethanolic medium using condensing agent. All these compounds were characterized by physical and spectral methods such as melting point, FTIR, H-NMR and mass spectra analysis.

Keywords: Chalcones, Propanediamide derivative, Claisen-schimdt reaction.

I. INTRODUCTION

The chemistry of chalcones has generated intensive scientific studies throughout the world. Especially interest has been focused on the synthesis and biodynamic activities of chalcones. The name “Chalcones” was given by Kostanecki and Tambor [1]. These compounds are also known as benzylidene acetophenone.

Due to the presence of enone functionality in chalcone moiety confers biological activity i.e. anti- cancer, cytotoxic activity, anti-hyperglycemic, anti-inflammatory, antioxidant, antimalerial activity [2-10]. In chalcones, two aromatic rings are linked by an aliphatic three carbon chain. Chalcone bears a very good synthon so that variety of novel heterocycles with good pharmaceutical profile can be designed.

Chalcones are bichromophoric molecules separated by a keto-vinyl chain and constitute an important class of naturally occurring flavonoids exhibiting a wide spectrum of biological activities. The presence of a reactive α, β-unsaturated keto functional group in chalcone is found to be responsible for their broad spectrum activity, which may be altered depending on the type and position of substituents on the aromatic rings.

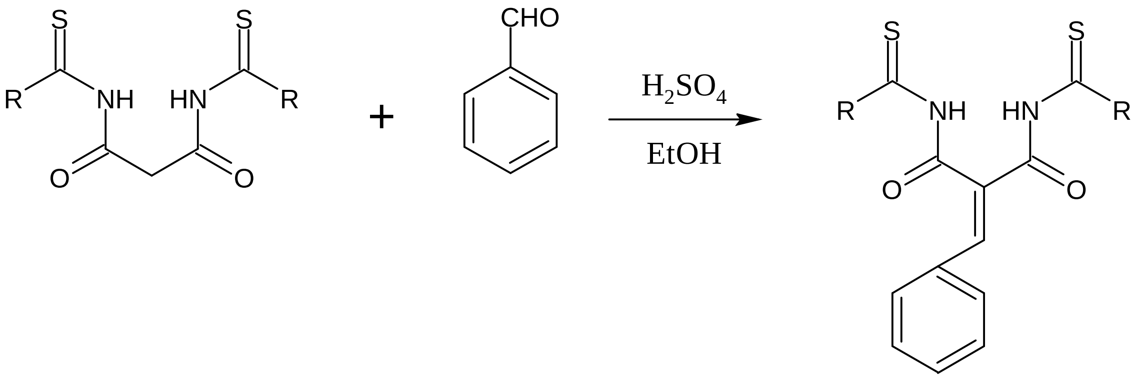
II. MATERIALS AND METHODS

The Identification and characterization of synthesized compounds were carried out by the following procedure to ascertain that all the prepared compounds were of different chemical nature than the respective parent compounds. This involved the determination of the melting point, solubility character’s, and their behaviour in Thin Layer Chromatography (TLC) studies as compared to that of their parent compounds and Nuclear Magnetic Resonance (1H NMR) data, Infra-red spectroscopy. The melting point was determined for the synthesized compounds were taken in open capillary tubes by using Arson digital melting point apparatus which were uncorrected.

General procedure for the synthesis of chalcones (1–5)

Chalcones were synthesized by Claisen‑Schmidt condensation reaction of appropriately substituted malonamide and benzaldehydes.

A mixture of benzaldehyde derivatives (0.01 mol) and substituted propanediamide derivatives (0.01 mol) were condensed in a 250 ml round‑bottomed flask equipped with a magnetic stirrer, for an hour, in presence of concentrate H_2SO_4 as a condensing agent at 150-155 °C . The reaction mixture was cooled and dilute with water. On filtering off, the crude chalcones were dried in air and recrystallized by rectified spirit. The residue was purified on column chromatography (silica gel with 10% ethyl acetate in hexane) to afford pure chalcones. The chemical profile of the compounds is as shown



III. RESULTS AND DISCUSSION

The structures of synthesized compounds were confirmed by IR,1HNMR and mass spectral analysis. The titled compounds were confirmed by IR spectral data showing sharp bands in the range between 1630-1660 cm^{-1} indicated the presence of C=O group. Compounds were also confirmed by 1HNMR spectral analysis.

***2-Benzylidene N*-{[(3-chloro -2-hydroxy phenyl) (phenyl)methyl] carbamo thioyl-*N*'-{[(2-hydroxyphenyl)(phenyl)methyl]carbamothioyl}propanediamide**

IR (KBr, cm^{-1}): 1647 (C=O)ketone, 1610 (CH=CH) ethylene , 1600(CH=CH) aromatic, 3225-3371 (-NH_2), 3100(-CH) alkenes, 3076(-CH) aromatic; 1H NMR (CDCl3) ;1H-NMR (δ, CDCl3): 4.69 (2H, s, CH2), 7.08-8.21, 8.27 (1H, s, NH); MS: m/z: 707.

***2-Benzylidene N*-{[(5-amino -2-hydroxyphenyl)(phenyl) methyl]carbamoyl-*N*'-{[(2-hydroxyphenyl) (phenyl) methyl]carbamothioyl} propanediamide**

IR (KBr, cm-1): 1732 (C=O) amide, 1680 (C=O)ketone, 1670 (N=CH) imine, 1614(CH=CH) ethene, 1519(CH=CH) aromatic, 3192(-CH) alkene, 3421(-NH). 1H NMR ($CDCl_3$) d: 8.05 (s, H, OH), 8.0 (s, H, NH_2), 7.7-7.9(m, 2H, NH),; MS: m/z: 659.

***2-Benzylidene N*-{[(2,5-di hydroxyphenyl) (phenyl) methyl] carbamothioyl-*N*'-{[(3-chloro-2-hydroxy phenyl) (phenyl)methyl] carbamo thioyl}propanediamide**

IR (KBr, cm^{-1}) : 1680 (C=O)ketone, 1654 (N=CH) imine, 1600(CH=CH) ethene,1595(CH=CH) aromatic, 2995(-CH) aliphatic; 1H-NMR (δ, $CDCl_3$): 1.17 (3H, CH_2CH_3), 2.26 (3H, s, Me), 2.53 (2H, CH_2CH_3), 4.79 (2H, s, CH_2), 7.10 -8.11 (m), 8.30 (1H, s, NH); MS: m/z: 702.

***2-Benzylidene N*-{[(2-hydroxy-4-methyl phenyl) (phenyl)methyl] carbamoyl-*N*'-{[(3-chloro-2-hydroxy phenyl)(phenyl) methyl] carbamothioyl}propane diamide**

IR (KBr, cm^{-1}): 1683 (C=O)ketone, 1650 (N=CH) imine, 1626(CH=CH) ethene,1595(CH=CH) aromatic, 2966(-CH) aliphatic, 3080(-CH) aromatic, 3120(-CH) alkene, 3394(-OH). 1H NMR ($CDCl_3$, δppm): 3.85 (3H, CH_3),), 4.70 (2H, s, CH_2) 2.20 (1H, d, -CO-CH=), 6.90 – 7.60 (18H, Ar-H) 8.80(1H,CH=N) ,11.20(1H,O-H) . MS: m/z: 705.

Table 1: Analytical Data of the Synthesized Compounds.

Compound	Molecular weight	Molecular formula	MP (°C)	Yield	Element Anal. Calculation			
					C	H	N	S
1	$C_{38}H_{31}ClN_4O_4S_2$	707.26014	81°C	23.10%	64.53%	4.42%	7.92%	9.07%
2	$C_{38}H_{33}N_5O_5S$	671.76412	69°C	23.33%	67.94%	4.95%	10.43%	4.77%
3	$C_{39}H_{33}ClN_4O_4S_2$	721.28672	109°C	34.3%	64.94%	4.32%	7.75%	8.87%
4	$C_{39}H_{33}ClN_4O_5S$	705.22112	98°C	30.1%	66.42%	4.72%	7.94%	4.55%
5	$C_{38}H_{33}N_5O_6S$	687.76352	91°C	37.5%	66.36%	4.84%	10.18%	4.66%

2-Benzylidene _N_-{[(5-amino-2-hydroxy phenyl)(phenyl)methyl] carbamoyl-_N'_-{[(2,5-dihydroxyphenyl) (phenyl)methyl]carbamothioyl }propanediamide

IR (KBr, cm^{-1}) : 1683 (C=O)ketone , 1650 (N=CH) imine, 1626(CH=CH) ethene,1595(CH=CH) aromatic, 2966(-CH) aliphatic, 3080(-CH) aromatic, 3120(-CH) alkene, 3394(-OH) ; 1HNMR:- 2.30(s, 3H, CH_3),7.37(1H,H_2), 7.46(1H,),7.62 (1H,CH=N) 13.40(s, 1H, OH). 3.20 (1H, d, -CO-CH=),; MS: m/z: 690.

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