ISSN No: 2348-4845
International Journal & Magazine of Engineering, Technology, Management and Research
A Peer Reviewed Open Access International Journal

Synthesis of Heterocyclic Compounds from Alpha- Beta Unsaturated Carbonyl Compounds

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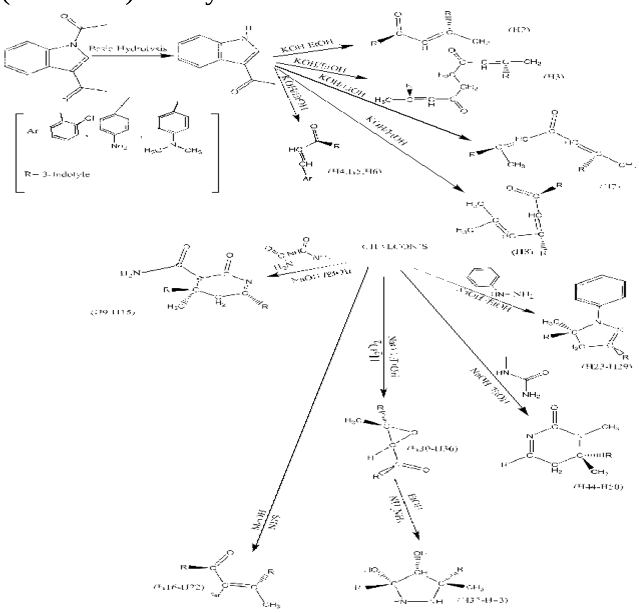
Abstract:

This study include the preparation of 1,3-di acetyleindole from the reaction of indole (with acetic anhydride in presence of acetic acid as acidic media). The compound N-acetyl indole was prepared from the reaction of indole and acetic anhydride and the compunde N-acetophenonindole was prepared from the reaction of α-chloroacetophenone and indole . These three compounds having an alpha acedic hydrogen which could be used in the synthesis of chalcones (H2-H8) using the following carbonyl compounds (4-nitrobenzaldehyde, 2-chlorobenzaldehyde, 4-N, N-dimethylaminobenzaldehyde, 2,5-hexanedione, 3-acetyle indole and acetone) through Aldol condensation to obtain α,β-unsaturated carbonyl compounds . On treatment of 1,3-diacetyl indole with (10%) potassium hydroxide solution , the amid group will be hydrolysis to the amine group in position (1), so the acetyl group in the indole will be the center of the reaction. The prepared chalcons , has been used in the synthesis of many heterocyclic compounds ; when react with biurate give substituted pyrimidinone containing the hexamembered ring (H9-H15). The reaction of chalcone with N-bromosuccinamide gives the monobromo derivatives (H18-H24). The reaction with phenyl hydrazine give the pyrazoline of the pentamembered ring (H25-H31), On the reaction with hydrogen peroxide giving the oxirane (H32-H38).which suffering from the expansion ring through the treatement with hydrazine hydrate gives pyrazolidine diole compounds (H39-H45). The reaction with methylurea gives susbstituted pyrimidinone compounds of hexamembered ring (H46-H52). The synthesis triazole compounds (H53)(which prepared from the reaction of 1,3,4-oxadiazole- 5-thiole with hydrazine hydrate) react (N-acetylindole, 1,3-diaacetylindole) to obtain the imines (H55,H56)respectively. The chalcone (H58) was prepared from the reaction of N-acetophenone indole with 2-chlorobenzaldehyde, this synthesis chalcone was reacted with triazole to obtain the schiff's base (H59). All the synthesized compounds were identified using the available physical and spectroscopic methods [m. p. , color change, (IR, UV and1H- NMR spectra) and some theoretical calculations].

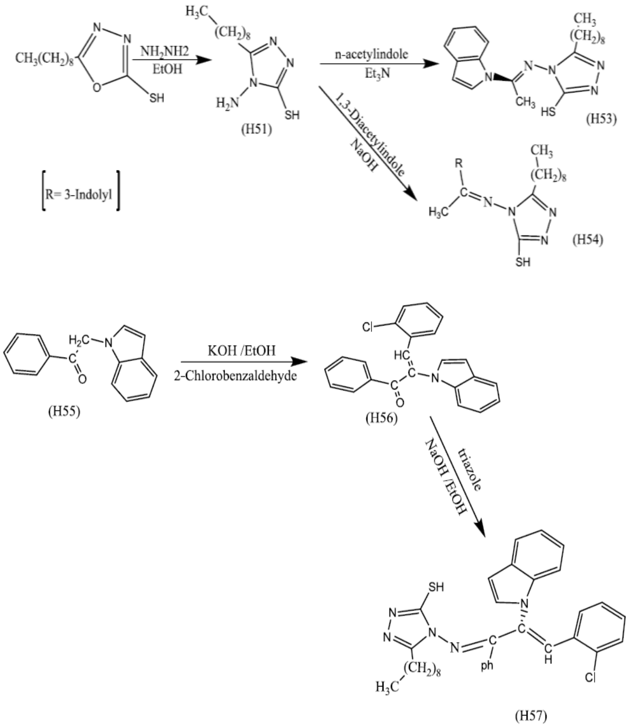
Introduction

α, β-Unsaturated ketones are convenient and easilyavailable starting materials or intermediates for the synthe-sis of a wide variety of heterocyclic compounds. The α,β-enone unit is favourable for dipolar cycloaddition reac-tions with various reagents affording heterocyclic com-pounds of different ring sizes with one or more heteroatoms. Their reactions with dinucleophiles provide impor-tant and useful heterocyclic ring systems as well. Amongthe α,β-unsaturated ketones, chalcones and their analogueshave a prominent place as starting materials for the synthe-sis of, first of all, nitrogen-containing heterocyclic com-pounds. Such reactions have been reviewed in severalaccounts [1-5].

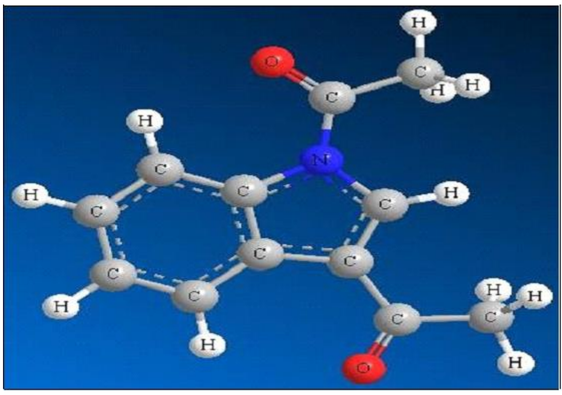
Utilization of the related exocyclic α, β- unsaturate dketones for such purposes made possible the synthesis ofvarious polycyclic ring systems. Probably the most impor-tant types of these polycyclic compounds are their fusedheterocyclic and spiroheterocyclic representatives.Although such compounds have been known for decades,their syntheses have hitherto been scarcely reviewed [6,7].For this reason, the major aim of our present review articleis to compile the most important types of heterocycliccompounds synthesized by the reactions of selected groupsof exocyclic α,β-unsaturated ketones, represented by2-arylidene-1-indanones (1), -1-tetralones (2), -1-benzo-suberones (3), 3-arylidenechromanones (4), -1-thiochro-manones (5), -flavanones (6) and -1-thioflavanones (7).2. Synthesis of Exocyclic α,β-Unsaturated Ketones 1-7Several representatives of the above-mentioned exo-cyclic α,β-unsaturated ketones 1 - 7 have been well knowncompounds for a long time. 2-Arylidene-1-indanones (1), -1-tetralones (2) and -1-benzosuberones (3) were synthe-sized by base- [8-20] and acid-catalyzed [21-26] condensa-tion of 1-indanone, 1-tetralone and 1-benzosuberone witharomatic aldehydes (Scheme 1). 3-Arylidenechromanones



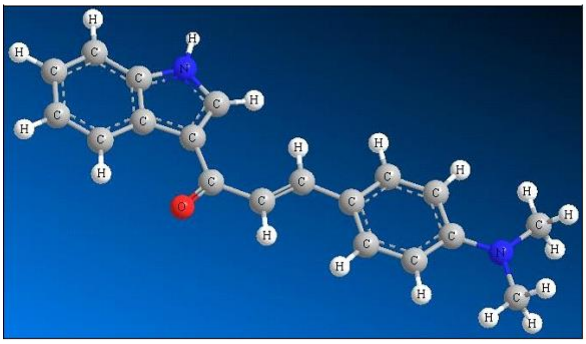
Scheme 1



Scheme 2



Total Energy: 10.3313Kcal / mol
Form compound H1



Total Energy: 23.5553 Kcal / mol Form compound H6

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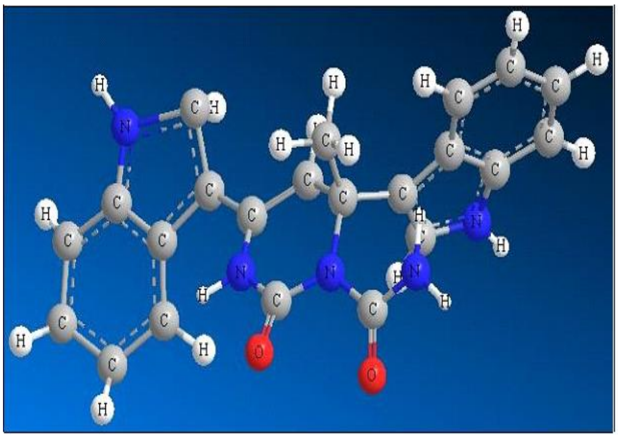
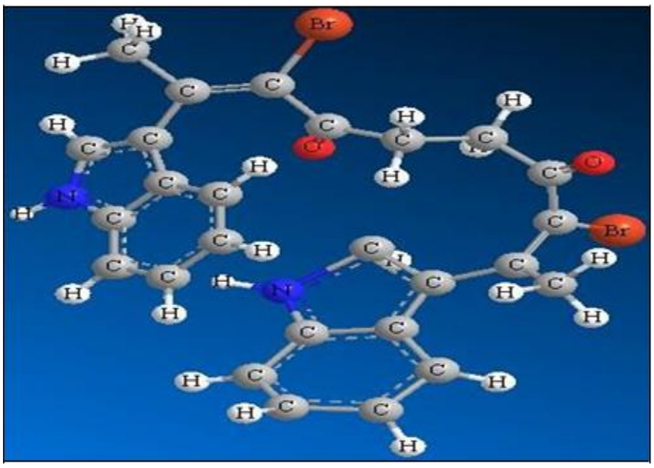
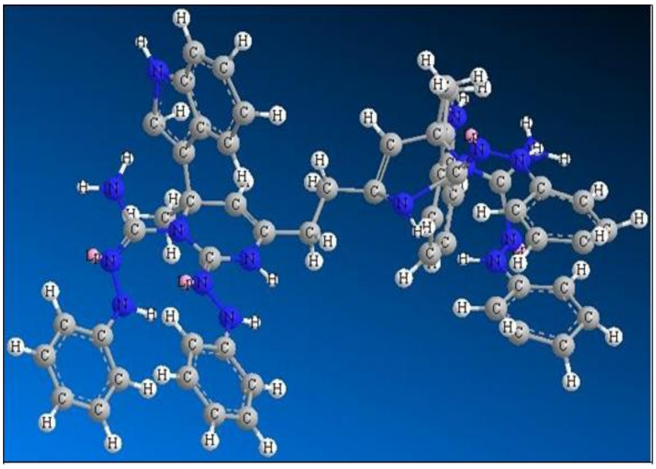


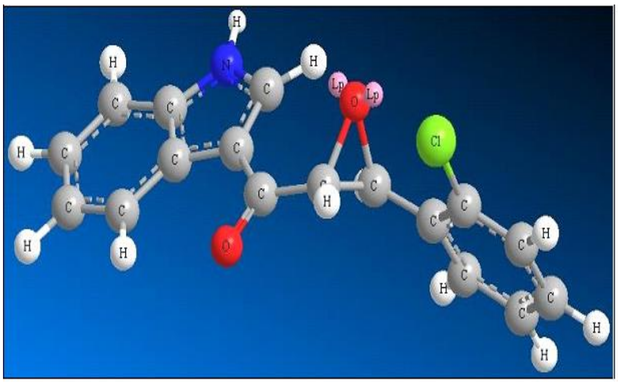
Total Energy: 0.4658Kcal / mol
Form compound H6



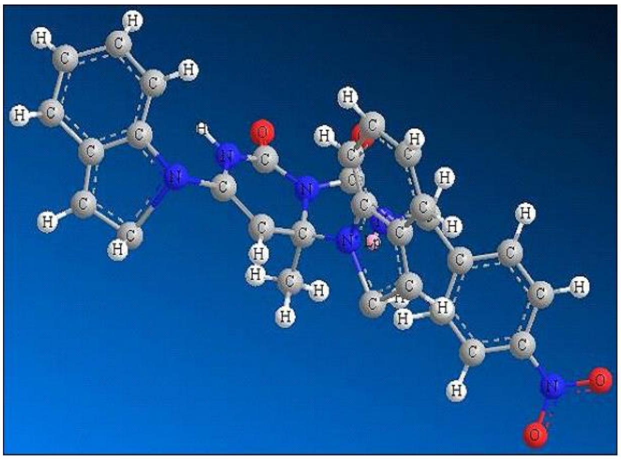
Total Energy: 7.2708Kcal / mol
Form compound H17



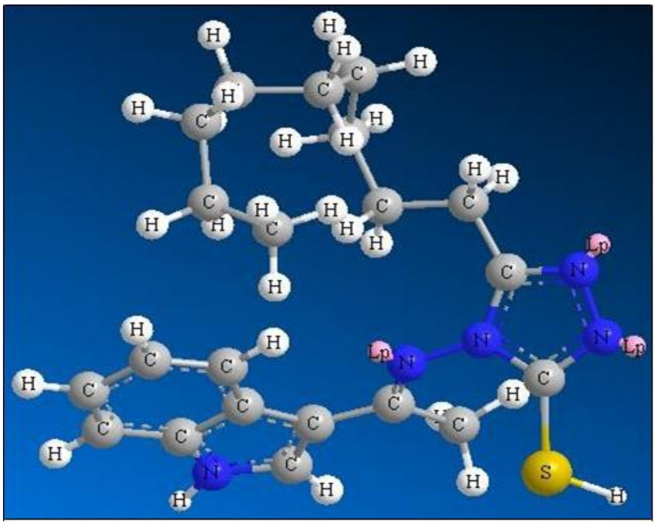
Total Energy: -30.1769Kcal / mol
Form compound H9



Total Energy: 107.9837Kcal / mol
Form compound H35



Total Energy: -9.7397Kcal / mol
Form compound H17



Total Energy: 33.3833 Kcal / mol
Form compound H56

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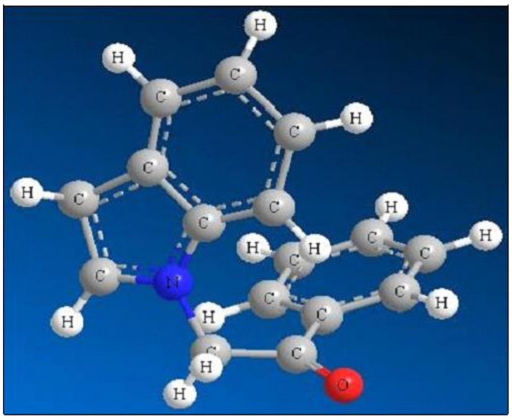
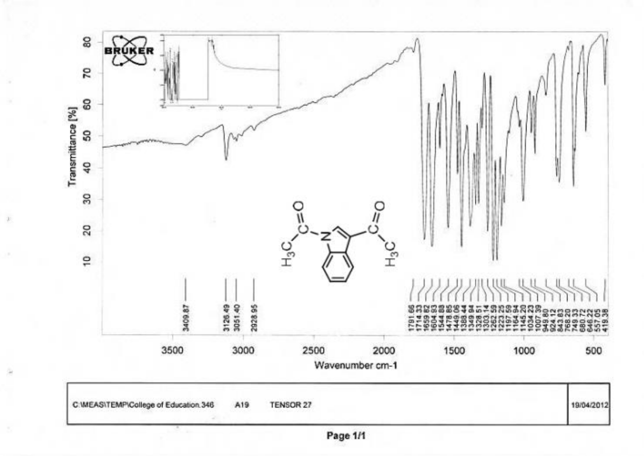
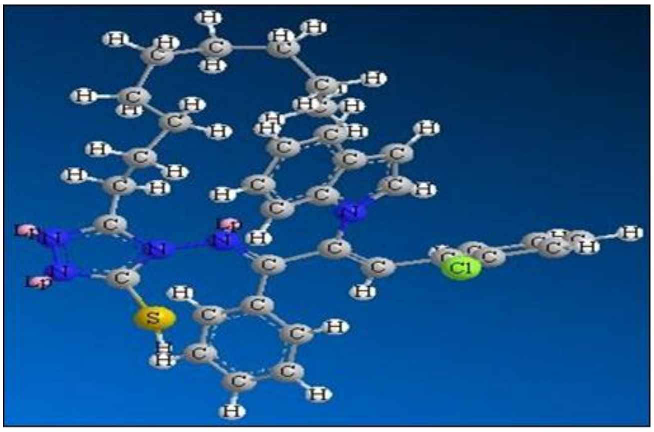


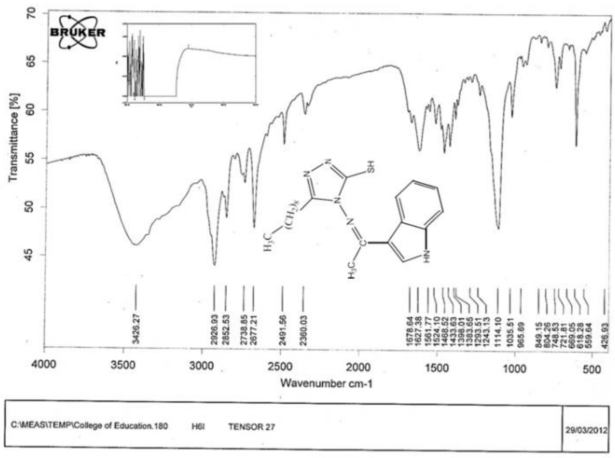
Total Energy: 8.6623Kcal / mol
Form compound H57



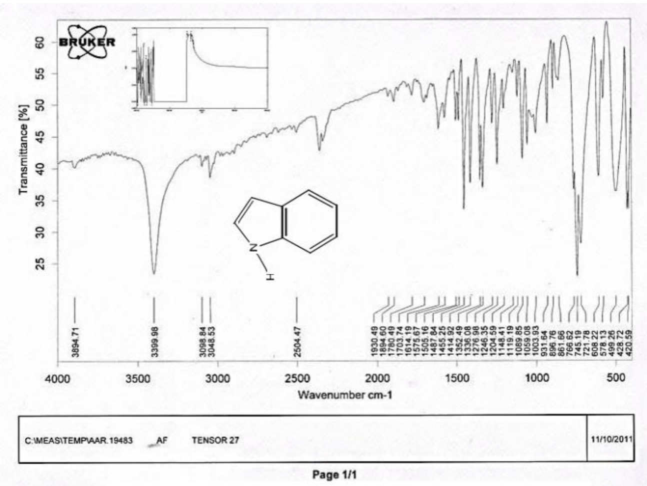
IR & UV of Compound 1,3-Di acetyl indol



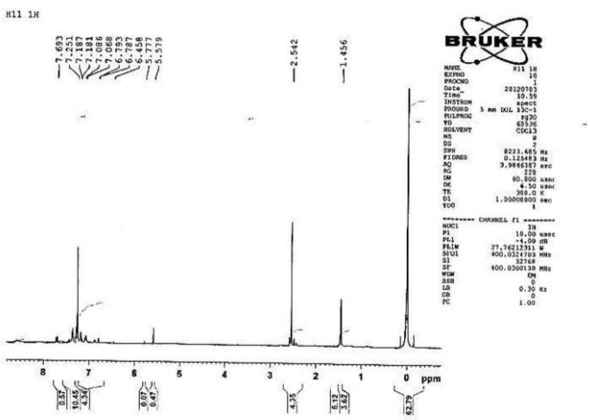
Total Energy: 42.0151Kcal / mol
Form compound H59



IR & UV of Compound H54



IR & UV of Compound H1 Indol



NMR of Compound H2

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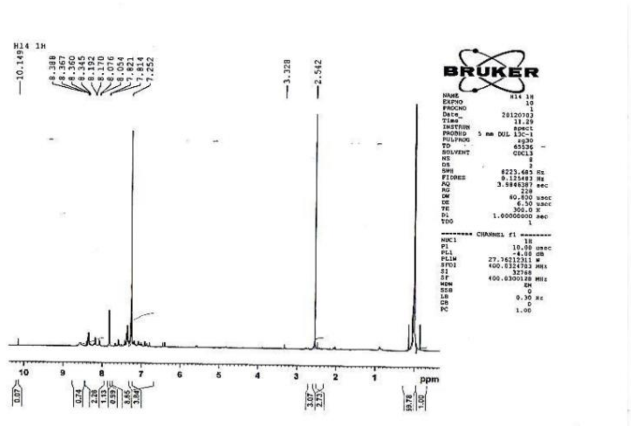
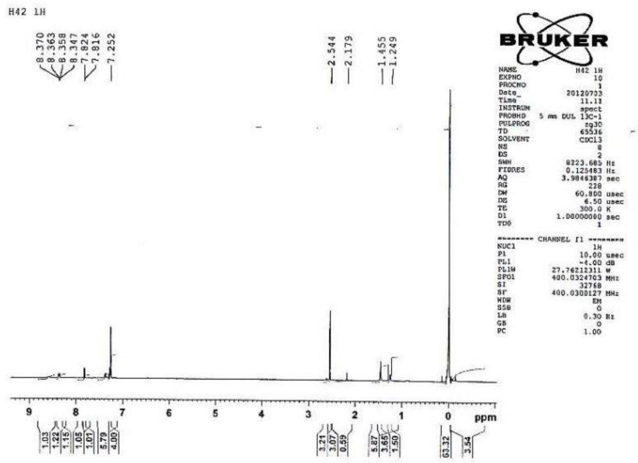


NMR of Compound H5



NMR of Compound H37

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