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Synthesis, characterization and biological studies of some novel Schiff bases containing 1, 2,4-triazole ring

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Abstract

In the present study new Schiff base compounds derived from 3,5 di phenyl-4 amino 1,2,4 trizolewith 4 hydroxy benzaldehyde, 4 methoxy benzaldehyde, 2,4 dinito benzaldehyde and 4 nitro benzaldehyde. The synthesized Schiff bases were characterized by IR, 1H NMR, and elemental analysis and crystal studies. The Schiff base ligands have also been testedfor their biologicalactivity.

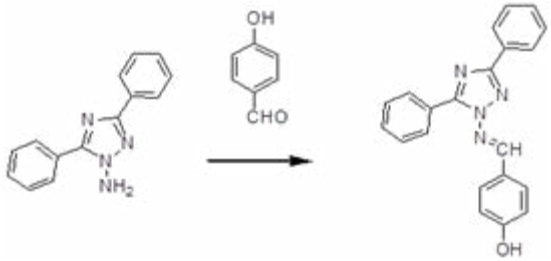
Keywords: Schiff base; characterization;biological activity;anti bacterial ; anti fungal

Keywords: Blue Gold; Urbanization; Industrialization; Biomagnification;

Multicultures; Aerobic; Anaerobic

Introduction

Postprandial Nitrogen containing compounds is very widely distributed in nature and are essential to life; Schiff bases are condensation products of primary amines with carbonyl compounds gaining importance day by day in present scenarioand are found to be a versatile pharmacophore for design and development of various bioactive lead compounds [1]. Schiff bases are the important compound owing to their wide range of biological activities and industrial application.



Schiff Base 1: (E)-4-((3,5-diphenyl-1H-1,2,4-triazol-1-ylimino)methyl) phenol.

1,2,4-triazoles and its derivatives have been reported to possess anti-inflammatory, analgesic, antimicrobial, anticancer, antitumor, antitubercular, anticonvulsant, and antidepressant activity. Therefore, 1,2,4-triazole seems to be an important pharmacophore.

Tautomers of 1,2,4-triazoles

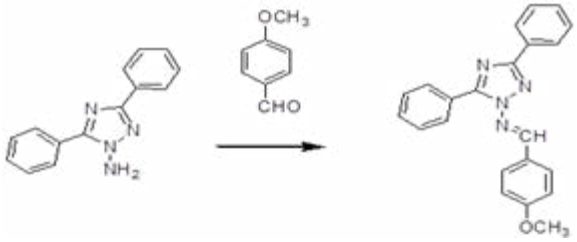
In 1,2,4-triazoles exists in two tautomeric forms. 1H and 4H-1,2,4-triazole isconsideredtobepharmacologicallyimportant nucleus [2].

Patents for synthesis of new triazole Schiff base derivatives and novel applications have been reported. Therefore, the synthesisand characterization of 4-amino-1,2,4-triazole Schiff base derivative is of great importance. In view of these above the biological importance of Schiff bases, we have synthesized some novel Schiff bases evaluated for their characterization and bioactivity.

The present paper describes the synthesis, spectroscopic and molecular structural study ofSchiff base derived from 3,5 diphenyl-4 amino 1,2,4 trizolewith 4 hydroxy benzaldehyde, 4 methoxy benzaldehyde, 2,4 dinito benzaldehyde and 4 nitro benzaldehyde.and to characterize them and study their antibacterial activities [3].

Schiff Base Formation and Mechanism

The reaction between a aldehyde or ketone carbonyl group and an amine gives Schiff bases due to the good electrophilic and nucleophilic characteristic properties of the carbonyl and amine groups, respectively by nucleophilic addition forming a hemiaminal, followed by a dehydration to generate an imines.



Schiff Base 2: (E)-N-(4-methoxybenzylidene)-3,5-diphenyl-1H-1,2,4-triazol-1-amine.

Since the nitrogen of the resulting bond has the basic character (indicated by the lone pair shown explicitly on the nitrogen atom. The reaction can also proceed in an E2 like fashion with the elimination of water occurring at the same time another water deprotonates the nitrogen so it can form a new N=C bond, forming the schiff base or imine.

The synthesis of Schiff base through the water molecule elimination requires an internal equilibrium between the twisted conformation of hemiaminals. The synthesis of hemiaminalincreases with solvent hydrophobicity, whereas a polar solvent shifts the equilibrium towards the Schiff base formation [4].

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Application of the Method

Materials and Method

The purity of the synthesized schiff base compounds was checked by TLC using silica gel plates and spots were developed in iodine chamber, IR spectra were recorded with KBr pellets on Shimadzu FTIR model 8400 spectrophotometer, Elemental analyses were carried out with a CHNS Vario EL III analyzer.The NMR spectra were recorded on a Bruker 300 or 500 MHz spectrometer using solvent as an internal standard. Mass spectra were recorded on VG 7070H mass spectrometer [5].Single crystal X-Ray diffraction data were collected at a Kuma KM4CCD four-circle diffractometer with graphite monochromated Mo Kα radiation (λ = 0.71073 A °) at 100 K using an Oxford Cryosystem adapter.

Experimental

4-hydroxybenzaldehyde in ethanol (20 mmol) are mixed with 20 mmol of 3,5-diphenyl-1H-1,2,4-triazol-1-amine , and the mixture is refluxed for 8-10 hours under constant stirring. After completion of the reaction the solution was poured into crushed ice. The separated product was filtered, washed with ice cold water, and recrystallized with a 1:1 solution of DMF & methanol [6].

Experimental

4-methoxy benzaldehyde in ethanol (20 mmol) are mixed with 20 mmol of 3,5-diphenyl-1H-1,2,4-triazol-1-amine , and the mixture is refluxed for 10-12 hours under constant stirring. After completion of the reaction the solution was poured into crushed ice. The separated product was filtered, washed with ice cold water, and recrystallized with a 1:1 solution of ethyl acetate& methanol [7].

Experimental

2,4 dinitro benzaldehyde in ethanol (20 mmol) are mixed with 20 mmol of 3,5-diphenyl-1H-1,2,4-triazol-1-amine and the mixture is refluxed for 6-8 hours under constant stirring. After completion of the reaction the solution was poured into crushed ice. The separated product was filtered, washed with ice cold water, and recrystallized with a 1:1 solution of DMF & methanol.

Experimental

4-nitro benzaldehyde in ethanol (20 mmol) are mixed with 20mmol of 3,5-diphenyl-1H-1,2,4-triazol-1-amine , and the mixture is refluxed for 8hours under constant stirring [8]. After completion of the reaction the solution was poured into crushed ice. The separated product was filtered, washed with ice cold water, and recrystallized with a 1:1 solution of hexane & methanol.

Biological Activity

Antibacterial

The biological studiesof the synthesized schiffbasecompounds were tested against the bacteria Bacillus subtilis. Paper discs of Whatman filter paper no. 1 were cut and sterilized in an autoclave [9]. The paper discs were saturated with 10 µl of the compounds dissolved in dimethyl and was placed aseptically in the Petri dishes containing Nutrient agar media inoculated with the above mentioned two bacteria separately. The petridishes were incubated at 350C and the inhibition zones were recorded after 24 h of incubation.

Antifungal

The Schiff base complexes were screened for their antifungal activity against fungi viz. candida. Filter paper discs of 5 mm in size, prepared by using Whatman filter paper no. 1 (sterilized in an autoclave) was saturated with 10 µl of the compounds dissolved in DMSO solution. The fungal culture plates were inoculated and incubated at 25± 20C for 48 h. The plates were then observed and the diameters of the inhibition zones (in mm) were measured and tabulated [10].

Result and Discussion

To The synthesized Schiff base compounds were characterized with spectral.Quantum-chemical calculationsindicated also that modification of 4-amino-1,2,4-triazole in 3,5 position with almost all small substituents with different electronic effect results in a favorable stabilization of hemiaminal.

The 1H-NMR spectral data of stable hemiaminals obtained from 4-amino-3,5-diphenyl-1,2,4-triazole with 2,4 dinito benzaldehyde and 4 nitro benzaldehydeshowed that they are stretched conformers.

Schiff bases shows IR absorption peak at 1615-1530 cm-1 (C=N stretching). All the compounds show NMR signalsat their respective positions. 1H NMR(CDCL3) δ 8.1 (S, 1H, N=CH), 7.0to 9.5 (m, Ar-H).

Single crystal X-ray diffraction studies of hemiaminals obtained from 4-amino-3,5-diphenyl 2-yl-1,2,4- triazolerevealed the formation of centro symmetric dimers linked by strong O-H….N1Tr hydrogen bonds.

Crystal structurereveals that two aromatic rings, phenyl and triazole are linked through a N3-N4-C7-C1 fragment, central part of molecule. The N3-N4-C7-C1 torsion angle is determined by the type of molecules – either stretched or twisted.

The synthesized Schiff base [SB-3] (E)-N-(2,4-dinitrobenzylidene)-3,5-diphenyl-1H-1,2,4-triazol-1-amineis found to be more active against Bacillus subtilis withstandard antibacterial drug amoxicillin and against fungi viz. candida with standard antifungaldrug fluconazole.In accordance with the data obtained from antimicrobial activity, the synthesized Schiff bases of have shown good activity against the tested microbes.

Conclusion

In this review, the biological activities of Schiff base have been summarized. Thus the synthesized Schiff basescan be further explored for development of potent medicinal agents. The research study report suggest that the successful synthesized Schiff bases were characterized through elemental analysis, IR, 1H NMR, Crystal structure , Mass spectral data and anti bacterial studies.

Hence, further study of a synthesized Schiff base compound (E)-N-(2,4-dinitrobenzylidene)-3,5-diphenyl-1H-1,2,4-triazol-1-amine in antimicrobial andmay become fruitful.

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Competing Interests

All authors declare no competing interests.

Author Contributions

All authors planned the study. MH screened control patients and performed mixed meal testing. KA and PW did PET/CT readings. MH, KA, and PW did the analysis and wrote the first draft of the manuscript. All authors critically proved data, edited and approved the manuscript.

Data Availability

All data is available from the corresponding author on request.

Ethics approval

The study was approved by the local ethics committee (Ethikkommission Nordwest-und Zentralschweiz, Basel, Switzerland, EKBB 163/12).

Consent to participate

Informed consent was obtained from all individual participants included in the study.

Consent to publish

All authors approved the manuscript for submission.

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