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Structure and Reactivity StudyofMannich base, N-[(1-yrrolidinobenzyl)]semicarbazide

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Abstract: The synthesis of various substituted N-[(1-pyrrolidinobenzyl) semicarbazide] (**PBSC**) have been synthesized and characterized by IR and 1H-NMR spectral analysis. The antimicrobial activity of the various substituted N-[**(**1-pyrrolidinobenzyl)]semicarbazide compounds has been extensively studied on microorganisms such as *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli* and *Pseudomonas aeruginosa* by well- diffusion method using DMSO as solvent. The values of zone of inhibition were found out at 37^0C for a period of 24 h. It has been found that all the inhibitory action gets enhanced with the introduction of electron- withdrawing groups in the phenyl ring.
Key words: Mannich base, N-[(1-pyrrolidinobenzyl)]semicarbazide, antibacterial activity, Hammet effect.

Introduction

Coordination compounds occur widely in nature and they comprise a largebody of current inorganic research. The availability of the latest physical techniquesand the development of ligand field and molecular orbital theories tend to be a majorreason for the flourishment of research activities in the field of coordinationchemistry.Synthetic organic chemistry is one of the most developing, expanding and successful branches of science. During the last fifteen years, synthetic organic chemistry has seen enormous growth, not only in terms of development of new methodologies for construction of carbon-carbon and carbon-hetero atom bonds but also in terms of development of new strategies, reagents, catalysts, transformations and technologies. From the survey of existing literature[1-7]it appears that Mannich bases have played a vital role in the development of synthetic organic chemistry. It is well known from the literature that the compounds containing amide moiety as a functional group have been found to possess donor properties and exhibit a wide range of biological activities[8-13]. Literature study also reveals that a broad spectrum of biological activity is reported to be associated with a number of heterocyclic compounds. Keeping the above facts in mind and as part of continuing efforts on Mannich bases, in the present paper the synthesis and characterization of various substituted N- [**(**1-pyrrolidinobenzyl)]semicarbazide compounds and studied the antimicrobial activity to find out the substituent effect on PBSC.

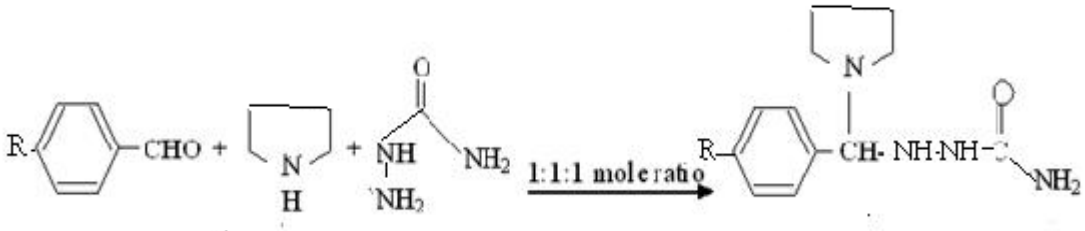
Experimental

Melting points were determined in an open capillary tube with a Buchi melting point apparatus and are uncorrected. Elemental analyses were carried out using Perkin-Elmer 240C CHN-analyzer.

Synthesis of Mannich base, PBSC:

The Mannich base, was synthesised by the condensation of an ethanolicsolution of benzaldehyde, pyrrolidine and semicarbazide were taken in 1:1:1 mole ratio. Semicarbazide hydrochloride (1.1 g, 10 mmol) in 10 ml of ethanol was neutralized with ammonia. To this solution benzaldehyde (1 mL, 10 mmol) and pyrrolidine (1 mL, 10 mmol) were added dropwise with constant stirring under the same condition. After 5 min the colourless solid obtained was filtered and recrystallized from ethanol. Yield: 68%; m.p: 191^{0}C.

In the same manner, various substituted Mannich bases have been synthesized in reasonable yields.



R=H, CH3, OCH3, Cl, CN

Table 1.Analytical data of the Mannich bases

Compoundwith mol.formula	**Found(calculated)**			**m.p.**	**Yield(%)**
	C%	**H%**	**N%**		
H-PBSC $C_{12}H_{18}N_4O$	60.84 (61.84)	7.91 (8.02)	20.68 (22.38)	184^{0}C	70
4-CH_3-PBSC $C_{13}H_{20}N_4$	61.80 (62.12)	7.26 (8.19)	18.86 (20.37)	192^{0}C	72
4-OCH_3-PBSC $C_{13}H_{20}N_4O$	57.82 (60.43)	7.25 (7.61)	19.62 (19.12)	186^{0}C	74
4-Cl-PBSC $C_{12}H_{17}N_4ClO$	55.75 (56.31)	5.66 (5.83)	18.62 (18.88)	184^{0}C	73
4-CN-PBSC $C_{13}H_{18}N_5$	60.12 (60.53)	7.24 (7.12)	22.18 (24.64)	198^{0}C	76

Antibacterial study:

The ligand and its complexes were tested for antibacterial activity. Mueller- Hinton agar was used for testing the susceptibility of microorganisms by well diffusion method[14-17] using DMSO as solvent, at a concentration of 0.01 M against Gram positive (*Staphylococcus aureus, Bacillus subtilis)* and Gram negative *(Escherichia coli, Pseudomonas auroginosa)* bacteria. The zone of inhibition against the growth of microorganisms was determined at the end of an incubation period of 24 h at 370 C (**Table 2**).

Table2.AntibacterialactivityoftheMannichbases

Compound	InhibitionZone(mm)			
	S.aureus	***E.coli***	***P.auroginosa***	***B.subtilis***
H-PBSC	15	18	20	17
4-CH_3-PBSC	14	17	19	16
4-OCH_3-PBSC	13	16	15	15
4-Cl-PBSC	16	19	21	19
4-CN-PBSC	18	22	23	20
Ampicillin (standard)	9	11	10	12

The order of activity of PBSC compounds towards *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli* and *Pseudomonas auroginosa* is: CN>Cl>H>CH3>OCH3. It has been found that the inhibitory action gets enhanced with the introduction of electron-withdrawing cyano and chloro groups in the phenyl ring. The compounds, however, with electron-releasing methyl and methoxy groups are lesser active compared to unsubstituted phenyl ring. It appears that there is a linear relationship between logarithm of zone of inhibition and Hammet substituent constant. The substituent constant **(**σ) for H, CH3, OCH3, Cl and CN is 0, -0.17, -0.27, 0.23 and 0.66. According to Hammet, substituents that enhance activity relative to unsubstituted benzene ring will have positive σ values (σ>0).

Conclusion

In this research paper, we have successfully and effectively synthesizedvarious substituted N-[(1-pyrrolidinobenzyl)semicarbazide] and antimicrobial activity of the various compounds has been extensively studied on microorganisms. It has been found that all the inhibitory action gets enhanced with the introduction of electron- withdrawing groups in the phenyl ring.

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