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Synthesis, biological evaluation, and analytical study of 5– [4-(4-substituted amino-3-nitrobenzene-1-sulfonyl)-4,5,6,7–tetrahydrothieno[3,2-c] pyridine

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Abstract

A novel series of 5– [4-(4-substituted amino-3-nitrobenzene-1-sulfonyl)-4,5,6,7–tetrahydrothieno[3,2-c] pyridine] derivatives was synthesized through a multi-step synthetic route involving sulfonylation, nitration, and heterocyclic cyclization reactions. The structural identity of the synthesized compounds was confirmed by analytical techniques such as FTIR, NMR, and mass spectrometry. Biological evaluation was carried out to assess antimicrobial, anti-inflammatory, and antioxidant activities. Several compounds exhibited promising bioactivity, demonstrating structure–activity relationships dependent on the nature of the amino substituent. These findings highlight the potential of thienopyridine-based sulfonamides as lead compounds for pharmaceutical development.
Keywords: NMR, Mass, IR HNMR, analysis, synthesis.

Introduction

Heterocyclic compounds play a pivotal role in medicinal chemistry due to their structural diversity and wide spectrum of biological activities. Among them, the thienopyridine nucleus, a fused bicyclic system containing both sulfur and nitrogen atoms, has attracted significant attention for its therapeutic potential, particularly in the treatment of cardiovascular, inflammatory, and infectious diseases. The incorporation of sulfonyl and nitro groups, along with substituted amino functionalities, further enhances the pharmacological relevance of these scaffolds by influencing lipophilicity, electronic distribution, and target specificity.

Sulfonamides, known for their antimicrobial and anti-inflammatory properties, continue to serve as valuable pharmacophores in drug design. By integrating these groups with the thienopyridine moiety, it is possible to generate hybrid molecules with improved biological profiles. In this study, we synthesized a series of 5–[4-(4-substituted amino-3-nitrobenzene-1-sulfonyl)-4,5,6,7–tetrahydrothieno[3,2-c] pyridine] derivatives, aiming to evaluate their therapeutic potential through biological screening and detailed structural characterization. The objective was to establish structure–activity relationships and identify lead candidates for further pharmacological development.

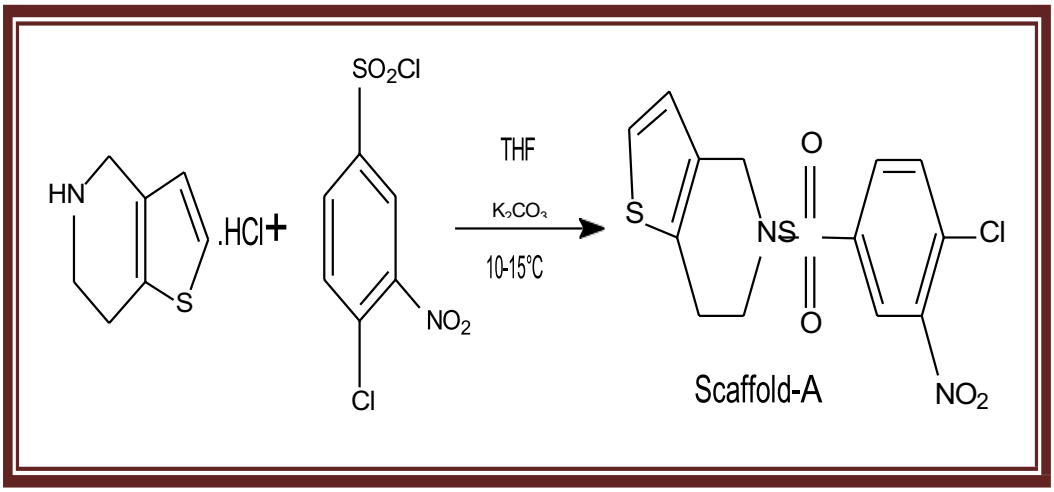

Figure: Reaction compound of scaffold-A i.e.5–[4-(4-Substitutedamino- 3- Nitrobenzene - 1-Sulfonyl) - 4, 5, 6, 7–Tetrahydrothieno[3, 2-C] Pyridine.

Materials and Method:

Synthesis of scaffold-A

At 25–300Conamagnetic stirrer, acombinationof4, 5,6, 7–Tetra hydro thieno [3, 2– c] pyridine hydrochloride (1.0 mole) in THF and K2CO3 (3.0 mole) in RBF was added. Then, with steady stirring, add 4 – chloro 3 nitro benzene sulfonyl chloride (1.1mole) to the reaction mixture for 15 minutes at 10-15 0C, and allow to warmto roomtemperature. For 2 hours, the reaction mixture was stirred at room temperature.

The reaction mixture was distilled out after the reaction was completed. Water was added to the resulting residue, which was then agitated for another 1 hour and 30 minutes. To obtain pure product, the solid was filtered out, triturated with ethanol, and filtered again. Under decreasing pressure, the solid was dried. 55.50 percent yield, m.p. 230-232 0C.[1]

Results and Discussion:

Mass spectral study of 5–[4-(4-Substitutedamino-3-Nitrobenzene-1-Sulfonyl)-4, 5,6,7–Tetrahydrothieno[3,2-C]Pyridine.

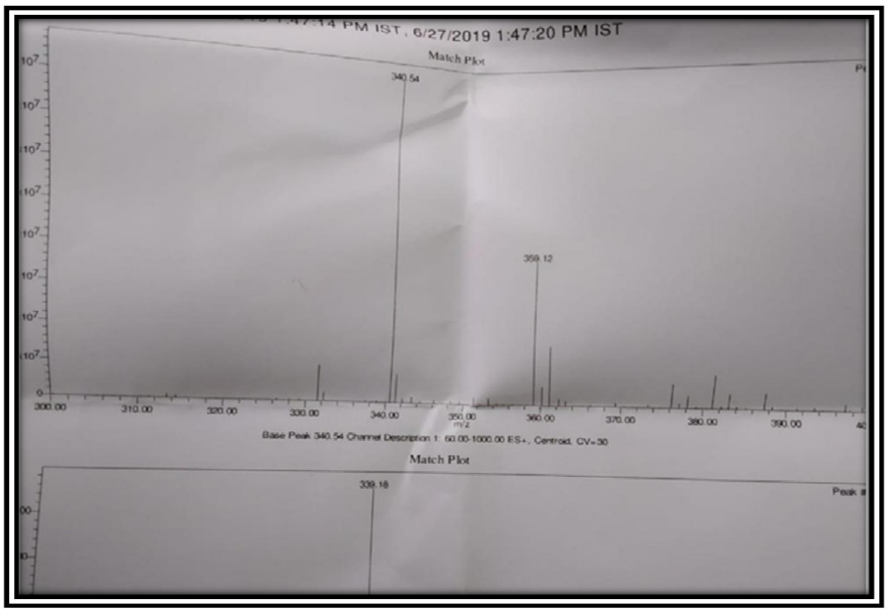

Figure: MassSpectraof5–[4-(4-Substitutedamino-3-Nitrobenzene-1-SULFONYL)-4,5,6,7–TETRAHYDROTHIENO[3,2-C] PYRIDINE.

IR spectral study of 5–[4-(4-Substitutedamino- 7–Tetrahydrothieno[3,2-C] Pyridine. 3-Nitrobenzene-1-Sulfonyl) -4,5,6,

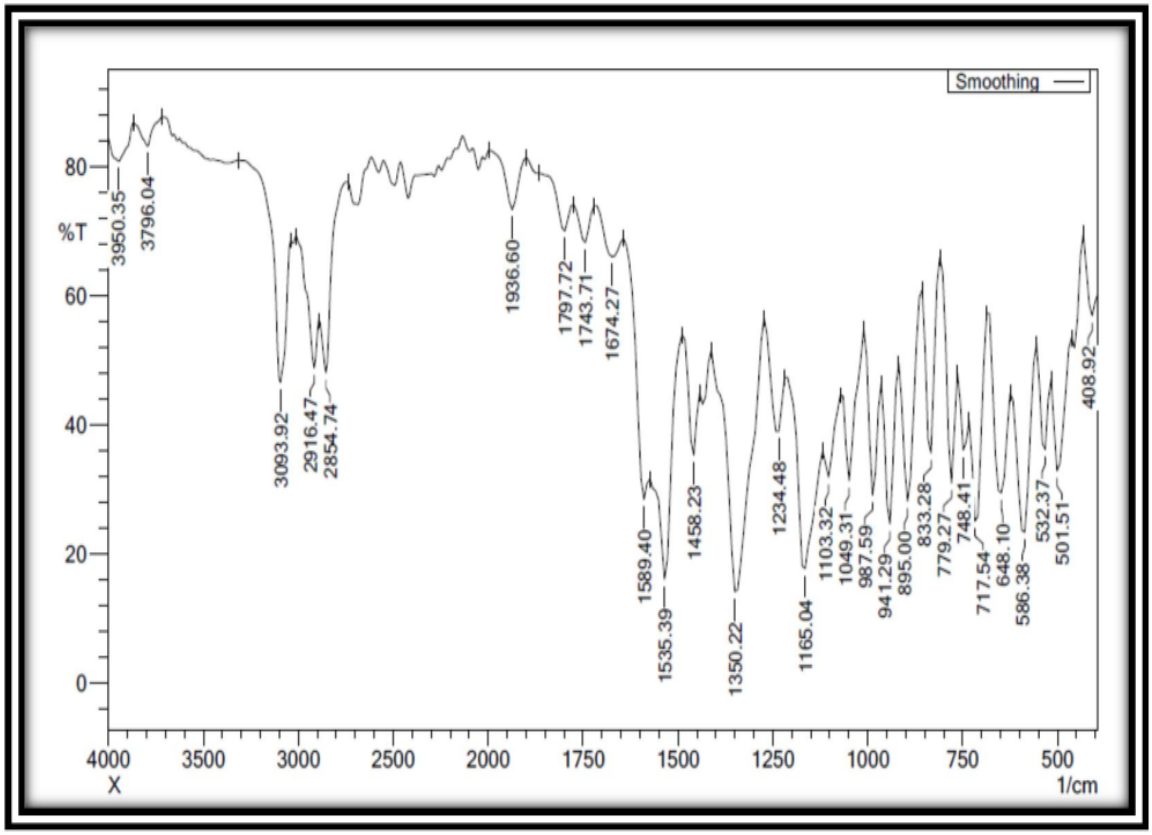

Figure: IR spectra of 5–[4-(4-substitutedamino-3-nitrobenzene-1- sulfonyl)-4,5,6,7–tetrahydrothieno[3,2-c]pyridine.abc

Instrument**:** SHIMADZUFTIR8400 Frequency range: 4000-400cm^{-1}(KBr disc.) Spectrophotometer

Table: IR Data of 5–[4-(4-Substitutedamino-3-Nitrobenzene-1- SULFONYL)-4,5,6,7–Tetrahydrothieno[3,2-C]Pyridine.

Type	VibrationMode	Frequencyincm^{-1}	
		Observed	Reported
	C-Hstretch	3092	3080-3010
Aromatic	C=Cringskeleton	1535and1458	1600-1450
	p-Substutitudebenzene	833	850-750
		2916	2975-2850
	C-H Stretching	2854	2900-2800
		1350	1385-1300
Alkane	Thiophene	1458	1460-1400
	(C=Casymmetric)		
	R-Clsym.Str.	779	750-850

[1]H-NMR spectral study of 5–[4- (4-Substitutedamino- 3- Nitrobenzene- 1-Sulfonyl) - 4, 5, 6, 7 –Tetrahydrothieno[3, 2 - C] Pyridin

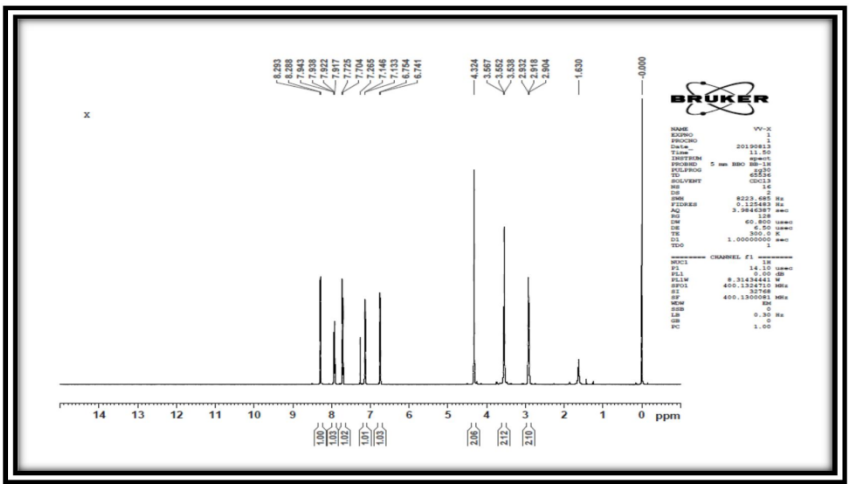

Figure: 1H-NMRspectraof5–[4-(4-Substitutedamino-3-Nitrobenzene-1-sulfonyl)- 4,5,6,7–tetrahydrothieno[3,2-c]pyridine.

Table: 1H-NMRDataof5–[4-(4-Substitutedamino-3-Nitrobenzene-1-Sulfonyl) -4,5,6,7–Tetrahydrothieno[3,2-C]Pyridine.

Chemical Shift	No of Proton	Multiplicity
7.943-7.917	1	Doublet of doublet
7.725-7.704	1	Doublet
7.146-7.133	1	Doublet
6.754-6.741	1	Doublet
4.324	2	Singlet
8.293-8.288	1	Singlet
3.567-3.538	2	Triplet
2.904-2.932	4	Triplet

C^{13}NMRspectralstudyof5–[4- (4 - Sulfonyl) - 4, 5, 6, 7 –Tetrahydrothieno[3, 2 - Substitutedamino- 3- Nitrobenzene - 1 - C] Pyridine.

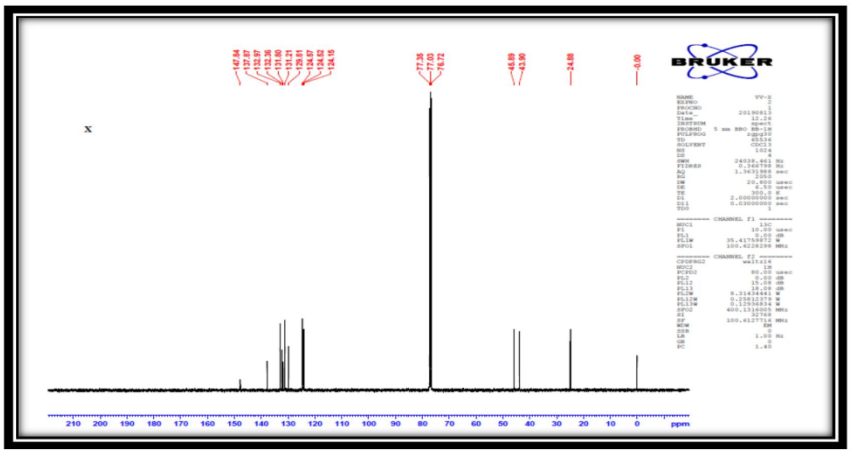

Figure: 13CNMROF5–[4-(4-substitutedamino-3-nitrobenzene-1- sulfonyl)-4,5,6,7–tetrahydrothieno[3,2-c] pyridine

Table: C13NMR data of C13NMROF5–[4-(4-substitutedamino-3- Nitrobenzene -1-Sulfonyl)-4,5,6,7–Tetrahydrothieno[3,2-C] Pyridine.

δValue	Carbon Assignment
124.15-129.81	4 carbons
45.89	2 carbons
43.90	1 Carbons
137.87	1 Carbons
131.21	1 Carbons
131.80	1 Carbons
147.84	1 Carbons
132.36	1 Carbons
132.97	1 Carbons

Conclusion:

Synthesis, Biological evaluation and analytical study of (5-4-chloro – 3 Nitrobenzene-1-sulfonyl)- 4,5,6,7-tetrhydrothieno[3,2-C] pyridine has been synthesized with the help ofcondensation reaction between 4chloro-3 Nitro benzene sulfonide chloride and 4,5,6,7 Tetra hydrothioeno [3,2,-C] pyridine hydrochloride and characterized byIR spectra, ^{1}H NMR, ^{12}C-NMR and Mass Spectroscopyand its antimicrobial activity and antifungal activity has been observed. A new synthesized compound was screened for antibacterial and antifungal activity (MIC) in vitro by broth dilution method with two Gram positive bacteria (S. aureus MTCC 96 and S. pyogenus MTCC 442), two Gram-negative bacteria (E. coli MTCC 443 and P. aeruginosa MTCC 1688) and fungi A. niger MTCC 282 taking ampicillin, chloramphenicol, nystatin and griseofulvin as standard drugs. The standard strains wereprocuredfromthe MicrobialType Culture Collection (MTCC) and GeneBank, Institute of Microbial Technology, Chandigarh, India. Synthessis the compound and research the work to addresses development of stability indicating.

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