Synthesis of Some New Alkyl Triazolyl Sulphides, Bis-Triazolyl Disulphides, Bis-Triazolyl Ethylene Disulphides and Triazolyl Aryl Dithiocarbamates as Antifungal Agents

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Several new alkyl triazolyl sulphides (1-12), bis-triazolyl disulphides (13-18), bis-triazolyl ethylene disulphides (19-24) and triazolyl aryl dithiocarbamates (25-48) have been prepared. Most of the compounds have been screened for their antifungal activity against two fungi, viz. Aspergillus niger and Helminthosporium oryzae and found to be antifungal. Based on the screening data, possible structure-activity relationship has been discussed.

INTRODUCTION

It is well known that mercapto (—SH) group is an important toxophore especially for pesticidal activity¹. Several heterocyclic sulphides are reported to display antitubercular² and antifungal³ activities. Further, a comparison of biocidal activity of mercapto compounds and their disulphides showed that the latter were relatively more active⁴ than parent mercapto compounds. Similarly, dithiocarbamates possess —N—C=S system, which is an essential structural feature responsible for biocidal activities⁵.6. Keeping these facts in view and in continuation of our ongoing research for new antifungal agents⁵, the title compounds have been prepared.

Alkyl-(3-aryloxymethyl/aryl-4-aryl-1,2,4-triazol-5-yl) sulphides (1-12) were prepared by refluxing a mixture of 3-aryloxymethyl/aryl-4-aryl-5-mercapto-1,2,4-triazoles and alkyl bromide in presence of fused sodium acetate. Oxidation of 3-aryloxymethyl/aryl-4-aryl-5-mercapto-1,2,4-triazoles by bromine afforded bis-(3-aryloxymethyl/aryl-4-aryl-1,2,4-triazol-5-yl)-disulphides (13-18). Bis-triazolyl ethylene disulphides (19-24) were prepared by refluxing a mixture of requisite triazoles, ethylene dibromide and fused sodium acetate. The condensation of aryl isothiocyanate to 3-aryloxymethyl/aryl-4-aryl-5-mercapto-1,2,4-triazoles in pyridine yielded the corresponding triazolyl aryl dithiocarbamates (25-41) (Scheme 1).

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$$R = \frac{1}{N} + \frac{1}{N} +$$

ds were characterised by

Structures of all the compounds were characterised by elemental and spectral data.

SCHEME-1

EXPERIMENTAL

All the melting points were determined in open capillaries and are uncorrected. IR spectra were recorded on Perkin Elmer-710 spectro-photometer in nujol. The completion of reaction and purity of the synthesized compounds were checked by TLC.

Alkyl-(3-aryloxymethyl/aryl-4-aryl-1,2,4-triazol-5-yl) sulphides (1-12)

To a methanolic solution (25 ml) of 3-aryloxymethyl/aryl-4-aryl-5-mercapto-1,2,4-triazole⁷ (0.01 M), fused sodium acetate (2.00 g) and an alkyl bromide (0.01 M) were added. The resulting mixture was gently refluxed for 4 hrs. It was cooled and then poured into water. The solid separating out was filtered, washed and recrystallised from aqueous ethanol to yield 1 54.57%, m.pt. 96°C (Found N, 12.29; S, 9.36. $C_{19}H_{21}N_3OS$ requires N, 12.39; S, 9.44%); v_{max} 1580 (C=N), 1380 (C—CH₃), 1020 and 1240 (=C—O—C) and 760 cm⁻¹ (=C—S—C).

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The compounds thus prepared are given in Table 1 along with their characterisation data.

Bis-(3-aryloxymethyl/aryl-4-aryl-1,2,4-trizol-5-yl) disulphides (13-18)

To an ice-cold methanolic solution (25 ml) of 3-aryloxymethyl/aryl-4-aryl-5-mercapto-1,2,4-triazole⁷ (0.01 m), a cold methanolic solution of bromine (0.005 M) was added dropwise with swirling. It was kept as such for 2 hrs and then evaporated. The residue thus obtained was washed with water, dilute sodium hydroxide, again with water and then recrystallised from aqueousethanol to yield 13 64.52%, m.pt. 48°C (Found: N, 13.43; S, 10.21. $C_{34}H_{32}N_6O_2S_2$ requires N, 13.55; S, 10,32%); v_{max} 1600 (C=N). 1360 (C—CH₃) and 1020 and 1250 cm⁻¹ (=C—O—C).

The compounds thus prepared are given in Table 2 along with their characterisation data.

Bis-(3-aryloxymethyl/aryl-4-aryl-1,2,4-triazol-5-yl)-ethylene disulphides (19-24)

A methanolic solution (25 ml) of 3-aryloxymethyl/aryl-4-aryl-5-mer-capto-1,2,4-triazole⁷ (0.01 M), ethylene dibromide (0.005 M) and fused sodium acetate (2.00 g) was refluxed gently for 4 hrs. It was cooled and then poured into water. The solid separating out was filtered, washed and recrystallised from aqueous ethanol to yield 19 66.36%, m.pt. 153°C (Found: N, 12.84; S, 10.00, $C_{36}H_{36}N_6O_2S_2$ requires N, 12.96; S, 9.88%); v_{max} 1580 (C=N), 1400 (S—CH₂), 1380 (C—CH₃) and 1220 and 1240 cm⁻¹ (=C—O—C).

The compounds thus prepared are given in Table 3 along with their characterisation data.

(3-Aryloxymethyl/aryl-4-aryl-1,2,4-triazol-5-yl)-aryl dithiocarbamates (25-48)

A solution of 3-aryloxymethyl/aryl-5-mercapto-1,2,4-triazole⁷ (0.01 M) and an aryl isothiocyanate (0.01 M) in pyridine (10 ml) was refluxed for 6 hrs. It was cooled, poured into water and filtered. The residue thus obtained was washed with ether and recrystallised from aqueous ethanol to yield 25 52.47%, m.pt. 190°C (Found: N, 12.49; S, 14.23. $C_{22}H_{18}N_4OS_2$ requires N, 15.56; S, 14.35%); ν_{max} 3200 (NH), 1540 (C=N), 1360 (C—CH₃), 1040-1240 (=C—O—C) and 1100 cm⁻¹ (C=S).

The compounds thus prepared are given in Table 4 along with their characterisation data.

ANTIFUNGAL SCREENING

Thirty six compounds have been screened for their antifungal activity by agar growth technique⁴ against two fungi, viz. A. niger and H. oryzae.

	YL/ARYL-4-ARYL-1,2,4-TRIAZOL-5-YL) SULPHIDE	
TABLE 1	CHAD ACTEDISATION DATA OF ALKYL-(3-ARYLOXYMETHYL/ARYL-4-ARYL-1,2,4-TRIAZOL-5-YL) SULPHIDE	THE PROPERTY OF THE PROPERTY O
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CHAF	CHARACTERISATION DATA OF ALKYL-(3-ARYLOXYMETHYL/ARYL-4-ARYL-1,2,4-TRIAZOL-5-YL) SULPHIDES	ALKYL-(3	-ARYLOXYMETHYL/A	RYL-4-A	RYL-1,2,	4-TRIAZOL-5-YL) SI	ULPHIDES	
				%	M. Pt.	Melecules formule	% Found/(Calcd)	(Calcd)
Compound No.	~	<u>~</u>	. 2	Yield	့	Moleculai 10111111111	z	S
1	2,3-(CH ₃) ₂ C ₆ H ₃ OCH ₂ -	H	CH,CH,-	54.6	96	C ₁₉ H ₂₁ N ₃ OS	12.29 (12.39)	9.36 (9.44)
7	2,3-(CH ₃) ₂ C ₆ H ₃ OCH ₂ -	H-	CH,CH,CH,-	78.2	<i>L</i> 9	C ₁₀ H ₁₃ N ₅ OS	11.80 (11.90)	9.13 (9.06)
m	2,3-(CH ₁),C ₆ H ₁ OCH ₂ -	H-	CH,CH,CH,CH,-	58.3	47	C ₁₁ H ₂₅ N ₅ OS	11.31 (11.44)	8.62 (8.72)
4	3,4-(CH3)3C6H3OCH2-	H	CH,CH,-	55.2	91	C ₁₉ H ₂₁ N ₃ OS	12.28 (12.39)	9.37 (9.44)
'n	3,4-(CH3)3C6H3OCH2-	Н-	CH,CH,CH,-	75.1	62	C20H23N3OS	11.78 (11.90)	8.95 (9.06)
9	3,4-(CH3),C6H3OCH2-	H-	CH,CH,CH,CH,-	8.09	43	C21H25N3OS	11.33 (11.44)	8.83 (8.72)
7	4-CH ₃ O.C ₆ H ₄ -	H	CH3CH2-	81.0	87	C ₁₇ H ₁₇ N ₃ OS	13.38 (13.50)	10.20 (10.29)
∞	4-CH ₃ O.C ₆ H ₄ -	Н-	CH,CH,CH,-	81.5	127	C ₁₈ H ₁₉ N ₅ OS	12.80 (12.92)	9.93 (9.8 5)
Q	4-CH ₃ O.C ₆ H ₄	Н-	CH,CH,CH,CH,-	9.77	113	C ₁₉ H ₂₁ N ₃ OS	12.25 (12.39)	9.32 (9. 44)
10	4-0H.C ₆ H ₄ -	Ħ	CH ₂ CH ₂ -	81.8	169	C ₁₆ H ₁₅ N ₃ OS	14.02 (14.14)	10.89
11	4-0H.C ₆ H ₄	Ħ	CH,CH,CH,-	79.4	76	C ₁ ,H ₁ ,N ₃ OS	13.38 (13.50)	10.18 (10.29)
12	4-0H.C ₆ H ₄ -	Н-	CH,CH,CH,CH,-	69.2	244	CisH19N3OS	12.81 (12.92)	9.74 (9.85)

TABLE 2
CHARACTERISATION DATA OF BIS-(3-ARYLOXYMETHYL/ARYL-4-ARYL-1,2,4-TRIAZOL-5-YL)-DISULPHIDES

Compd	• R	\mathbb{R}^1	_%_	M·Pt.	1,101000101	% Found/	(Calcd.)
No.	· ·		Yield	°C	formula	N	S
13	2,3-(CH ₃) ₂ C ₆ H ₃ OCH ₂ -	Н-	64.5	48	C34H32N6O2S2	13.43	10.21
						(13.55)	(10.32)
14	3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ -	Н-	62.9	42	C34H32N6O2S2	13,44	10.41
					· · · · · · · · · · · · · · · · · · ·	(13.55)	(10.32)
15	α-C ₁₀ H ₇ OCH ₂ -	Н-	75.3	119	C38H28N6O2S2	12.52	9.73
						(12.65)	(9.64)
16	4-CH ₃ O.C ₆ H ₄ -	Н-	62.1	157	C30H24N6O2S2	14.75	11.23
•						(14.89)	(11.35)
17	4-OH.C ₆ H ₄ -	H-	62.7	215	C28H20N6O2S2	15.56	11.82
						(15.67)	(11.94)
18	4-OH.C ₆ H ₄ -	Cl	56,9	155	C28H18Cl2N6O2S	S ₂ 13.76	10.47
			•		- 20	(13.88)	(10.58)

TABLE 3

CHARACTERISATION DATA OF BIS-(3-ARYLOXYMETHYL/ARYL-4-ARYL-1,2,4-TRIAZOL-5-YL)-ETHYLENE DISULPHIDES

Compd	. R	R¹	% Yield	M.Pt.	11101000101	% Found/(Calcd				
No.			Yield	°C	formula	N	S			
19	2,3-(CH ₃) ₂ C ₆ H ₃ OCH ₂ -	H-	66.4	153	C36H36N6O2S2	12.84	10.00			
						(12.96)	(9.88)			
20	3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ -	H-	64.2	139	C36H36N6O2S2	12.83	9.78			
						(12.96)	(9.88)			
21	α-C ₁₀ H ₇ OCH ₂ -	Н-	67.1	185	C40H32N6O2S2	12.03	9.14			
						(12.14)	(9.25)			
22	4-CH3O.C6H4-	H-	55.7	230	C32H58N6O2S2	14.07	10.69			
						(14.19)	(10.81)			
23	4-OH.C ₆ H ₄ -	Н-	56.0	>360	C30H24N6O2S2	14.77	11.22			
						(14.89)	(11.35)			
24	4-OH.C ₆ H ₄ -	Cl-	67.0	265	C30H22Cl2N6O2S	2 13.15	10.21			
						(13.27)	(10.11)			

TABLE 4

R R³ %idd W.P. formula Molecular of formula % Found/(Ca formula) 2,3-(CH),CaH,OCH;- H- H- 52.5 190 Ca.HaNAOS; 12.49 2,3-(CH),CaH,OCH;- H- Cl- 50.8 197 Ca.HaNAOS; 11.54 2,3-(CH),CaH,OCH;- H- Cl- 50.4 188 Ca.HaNAOS; 11.53 2,3-(CH),CaH,OCH;- Cl- H- 51.0 159 Ca.Ha,CINAOS; 11.53 2,3-(CH),CaH,OCH;- Cl- Cl- Cl- 51.5 159 Ca.Ha,CINAOS; 10.75 2,3-(CH),CaH,OCH;- Cl- Cl- Cl- 50.9 144 Ca.Ha,CINAOS; 10.75 3,4-(CH),CaH,OCH;- H- 54.9 157 Ca.Ha,CINAOS; 11.53 3,4-(CH),CaH,OCH;- H- Cl- 53.3 160 Ca.Ha,CINAOS; 11.53 3,4-(CH),CaH,OCH;- H- Cl- Cl- 53.3 160 Ca.Ha,CINAOS; 11.53 3,4-(CH),CaH,OCH;- Cl- H-	Compd. No. 25 2, 26 2, 27 2. 28 2, 29 2, 30 2,								
R K³ Yièld °C formula N 2,3-(CH),CaH,OCH+- H- H- 52.5 190 Ca.Ha,N.OS1 12.49 2,3-(CH),CaH,OCH+- H- Cl- 50.8 197 Ca.Ha,N.OS2 11.54 2,3-(CH),CaH,OCH+- H- Cl- S0.4 188 Ca.Ha,N.OS2 11.53 2,3-(CH),CaH,OCH+- Cl- H- S1.0 159 Ca.Ha,CIN,OS2 11.53 2,3-(CH),CaH,OCH+- Cl- Cl- Cl- S0.9 144 Ca.Ha,CIN,OS2 10.75 2,3-(CH),CaH,OCH+- Cl- Cl- Cl- S0.9 144 Ca.Ha,CIN,OS2 10.55 3,4-(CH),CaH,OCH+- H- G- S0.9 144 Ca.Ha,CIN,OS2 11.54 3,4-(CH),CaH,OCH+- H- G- S0.9 144 Ca.Ha,CIN,OS2 11.55 3,4-(CH),CaH,OCH+- H- G- S0.9 144 Ca.Ha,CIN,OS2 11.55 3,4-(CH),CaH,OCH+- H- Cl- G- S0.9			i	;	%	M.Pt.	Molecular	% Found/	Calcd.)
2,3-(CH),CAH,OCH,- H- H- 52.5 190 C ₅ ·H ₁ N,OS ₅ 12.49 2,3-(CH),CAH,OCH,- H- Cl- 50.8 197 C ₅ ·H ₁ N,OS ₅ 11.54 2,3-(CH),CaH,OCH,- H- C ₁ H ₂ O- 50.4 188 C ₅ ·H ₁ N,Os ₅ 11.55 2,3-(CH),CaH,OCH,- Cl- H- 51.0 159 C ₁ ·H ₁ OlN _{OS} 11.55 2,3-(CH),CaH,OCH,- Cl- Cl- Cl- 51.5 157 C ₄ ·H ₂ ClN _{OS} 10.75 2,3-(CH),CaH,OCH,- Cl- Cl- Cl- Cl- 54.9 157 C ₄ ·H ₂ ClN _{OS} 10.55 3,4-(CH),CaH,OCH,- H- Cl- 54.9 157 C ₄ ·H ₂ ClN _{OS} 11.54 3,4-(CH),CaH,OCH,- H- Cl- 53.3 160 C ₄ ·H ₃ ·ClN _{OS} 11.53 3,4-(CH),CaH,OCH,- H- Cl- 52.9 140 C ₄ ·H ₃ ·ClN _{OS} 11.54 3,4-(CH),CaH,OCH,- Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-		ĸ	<u>.</u>	R2	Yield	၁့	formula	z	S
2,3-(CH),Ca,H,OCH3- H- Cl- 50.8 197 Ca,H,aCIN,oS3- 11.54 2,3-(CH),Ca,H,OCH3- H- Cl- 50.4 188 Ca,H,aCIN,oS3- 11.53 2,3-(CH),Ca,H,OCH3- Cl- H- C,H3O- 50.9 159 Ca,H,aCIN,OS3- 11.53 2,3-(CH),Ca,H,OCH3- Cl- Cl- Si- 51.9 157 Ca,Ha,aCIN,OS3- 10.75 2,3-(CH3),Ca,H,OCH3- Cl- Cl- Si- 54.9 157 Ca,Ha,aCIN,OS3- 10.85 3,4-(CH3),Ca,H,OCH3- H- Cl- 54.9 157 Ca,Ha,aN,OS3- 11.55 3,4-(CH3),Ca,H,OCH3- H- Cl- 53.3 160 Ca,Ha,N,OS3- 11.55 3,4-(CH3),Ca,Ha,OCH3- H- Cl- 53.9 140 Ca,Ha,N,OS3- 11.53 3,4-(CH3),Ca,Ha,OCH3- Cl- H- 52.9 140 Ca,Ha,N,OS3- 11.53 3,4-(CH3),Ca,Ha,OCH3- Cl- Cl- 64.0 150 Ca,Ha,A,ON-OS3- 11.53 <td< td=""><td></td><td>HOO II O (IIO)</td><td>H.</td><td>H.</td><td>52.5</td><td>190</td><td>C24H22N4OS2</td><td>12.49</td><td>14.23</td></td<>		HOO II O (IIO)	H.	H.	52.5	190	C24H22N4OS2	12.49	14.23
2,3-(CH),CaH,OCH3- H- Cl- 50.8 197 CaH3,CIN,OS3, 11.54 2,3-(CH),CaH,OCH3- H- CaH5O- 50.4 188 CaH3,CIN,OS3, 11.53 2,3-(CH),CaH,OCH3- Cl- H- 51.0 159 CaH3,CIN,OS3, 11.53 2,3-(CH),CaH,OCH3- Cl- Cl- Cl- 51.5 157 CaH3,CIN,OS3, 10.75 2,3-(CH),CaH,OCH3- Cl- Cl- Cl- 54.9 144 CaH3,CIN,OS3, 10.55 3,4-(CH),CaH,OCH3- H- H- 54.9 157 CaH3,CIN,OS3, 11.55 3,4-(CH),CaH,OCH3- H- Cl- 54.9 157 CaH3,INAOS3, 11.55 3,4-(CH),CaH,OCH3- H- Cl- 53.3 160 CaH3,INAOS3, 11.55 3,4-(CH),CaH,OCH3- H- Cl- 52.9 140 CaH3,INAOS3, 11.53 3,4-(CH),CaH,OCH3- Cl- Cl- 64.0 150 CaH3,INAOS3, 11.54 3,4-(CH),CH3,CH3,OCH3- Cl-		3-(CH3)2C6H3OCH2-	4	4)		(12.56)	(14.35)
2.3-(CH) ₁ C ₄ H ₃ OCH ₃ - H- C ₁ H ₅ O- 50.4 188 C ₂ dH ₃ M ₃ OS ₃ 11.32 2.3-(CH) ₁ C ₄ H ₃ OCH ₃ - Cl- H- 51.0 159 C ₃ dH ₃ CIN ₄ OS ₃ 11.55 2,3-(CH) ₁ C ₄ H ₃ OCH ₃ - Cl- Cl- Cl- Cl- 51.5 157 C ₃ dH ₃ CIN ₄ OS ₃ 10.75 2,3-(CH) ₁ C ₄ H ₃ OCH ₃ - Cl- Cl- Cl- Cl- 50.9 144 C ₃ dH ₃ CIN ₄ OS ₃ 10.55 3,4-(CH) ₁ C ₄ H ₃ OCH ₃ - H- H- 54.9 157 C ₃ dH ₃ CIN ₄ OS ₃ 10.55 3,4-(CH) ₁ C ₄ H ₃ OCH ₃ - H- Cl- 53.3 160 C ₄ dH ₃ CIN ₄ OS ₃ 11.55 3,4-(CH) ₁ C ₄ H ₃ OCH ₃ - H- Cl- 52.9 140 C ₄ dH ₃ CIN ₄ OS ₃ 11.55 3,4-(CH) ₁ C ₄ H ₃ OCH ₃ - Cl- Cl- 64.0 150 C ₄ H ₃ CIN ₄ OS ₃ 11.53 3,4-(CH) ₁ C ₄ H ₃ OCH ₃ - Cl- Cl- G ₄ H ₂ CIN ₄ OS ₃ 10.74 3,4-(CH) ₁ C ₄ H ₃ OCH ₃ - Cl- Cl- G ₄ H ₂ CIN ₄ OS ₃ 10.74 3,4-(CH) ₁ C ₄ H ₃ OCH ₃ - Cl- Cl-			1	-	50.8	197	C24H21CIN4OS2	11.54	13.21
2.3-(CH ₁) ₁ C ₄ H ₁ OCH ₁ - H- C ₁ H ₅ O- 50.4 188 C ₃ H ₃ N ₄ O ₅ S ₃ 11.32 2,3-(CH ₁) ₁ C ₄ H ₃ OCH ₁ - Cl- H- 51.0 159 C ₄ H ₃ CIN ₄ OS ₃ 11.55 2,3-(CH ₁) ₁ C ₄ H ₃ OCH ₁ - Cl- Cl- Cl- 51.5 157 C ₄ H ₃ CIN ₄ OS ₃ 10.75 2,3-(CH ₁) ₁ C ₄ H ₃ OCH ₁ - Cl- Cl- Cl- 50.9 144 C ₄ H ₃ CIN ₄ OS ₃ 10.85 3,4-(CH ₃) ₁ C ₄ H ₃ OCH ₁ - H- H- 54.9 157 C ₄ H ₃ IN ₄ OS ₃ 12.48 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₁ - H- Cl- 53.3 160 C ₄ H ₃ IN ₄ OS ₃ 11.55 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₁ - H- Cl- 53.3 160 C ₄ H ₃ IN ₄ ON ₂ S ₃ 11.55 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₁ - Cl- H- 52.9 140 C ₄ H ₃ IN ₄ ON ₂ S ₃ 11.54 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - Cl- Cl-		,3-(СПз)2С6ПзОСП2-	:	5				(11.65)	(13.32)
2,3-(CH),1,C,H,OCH,- Cl- H- 51.0 159 C ₁ ,H ₁ ,CIN,OS ₁ 11.55 2,3-(CH),1,C,H,OCH,- Cl- Cl- Cl- 51.5 157 C ₂ ,H ₂ ,CIN,OS ₂ 10.75 2,3-(CH),1,C,H,OCH,- Cl- C ₂ H,O- 50.9 144 C ₂ ,H ₂ ,CIN,OS ₂ 10.55 3,4-(CH),1,C,H,OCH,- H- H- H- 54.9 157 C ₂ ,H ₂ ,CIN,OS ₂ 11.56 3,4-(CH),1,C,H,OCH,- H- C ₁ H,O- 53.3 160 C ₂ ,H ₂ ,IN,OS ₂ 11.55 3,4-(CH),1,C,H,OCH,- H- C ₂ H,O- 54.1 145 C ₂ H ₂ IN,ONOS ₂ 11.54 3,4-(CH),1,C,H,OCH,- Cl- Cl- 52.9 140 C ₂ H ₂ IN,ONOS ₂ 11.54 3,4-(CH),1,C,H,OCH,- Cl- Cl- 64.0 150 C ₂ H ₂ IN,CIN,OS ₂ 11.54 3,4-(CH),1,C,H,OCH,- Cl- Cl- G ₂ H ₂ O 52.9 140 C ₂ H ₂ IN,CIN,OS ₂ 11.54 3,4-(CH),1,C,H,OCH,- Cl- Cl- G ₂ H ₂ O 52.9 140 C ₂ H ₂ IN,CIN,OS ₂ 10.74 3,4-(CH),1,C,H,OCH,- Cl		HOOH O (HO) 6	Ħ	C.H.O.	50.4	188	C26H26N4O2S2	11.32	13.17
2,3-(CHJ),C,H,OCH,- Cl- H- 51.0 159 C ₁ H ₂ ICIN ₁ OS ₂ 11.55 2,3-(CH ₂),C,H,OCH ₂ - Cl- Cl- Cl- 51.5 157 C ₄ H ₂ ICIN ₁ OS ₂ 10.75 2,3-(CH ₃),C,H,1OCH ₂ - Cl- C ₂ H ₂ O- 50.9 144 C ₄ H ₂ ICIN ₁ OS ₃ 10.68 3,4-(CH ₃),C,H,1OCH ₂ - H- H- S4.9 157 C ₄ H ₂ ICIN ₁ OS ₃ 11.55 3,4-(CH ₃),C,H,1OCH ₂ - H- C ₁ H ₂ O- 54.1 145 C ₄ H ₂ ICIN ₁ OS ₃ 11.55 3,4-(CH ₃),C,H,1OCH ₂ - Cl- H- 52.9 140 C ₄ H ₂ ICIN ₁ OS ₃ 11.43 3,4-(CH ₃),C,H,1OCH ₂ - Cl- Cl- G ₂ H ₃ O- 52.9 140 C ₄ H ₂ ICIN ₁ OS ₃ 10.74 3,4-(CH ₃),C,H,1OCH ₂ - Cl- Cl- G ₂ H ₃ O- 52.9 150 C ₄ H ₂ ICIN ₁ OS ₃ 10.76 3,4-(CH ₃),C,H ₃ OCH ₂ - Cl- Cl- G ₂ H ₃ O- 52.4 130 C ₄ H ₂ ICIN ₁ OS ₃ 10.76 3,4-(CH ₃),C,H ₃ OCH ₂ - Cl- Cl- G ₄ H ₃ O- 52.4 130 C ₄ H ₃ ICIN ₁ OS ₃ <		.5-(CH3)2C6H3OCH2-	1	01110	• • •)		(11.43)	(13.06)
2,3-(CH3)ACM1-CATA CI- CI- CI- 51.5 157 C ₂ AH ₂ OCINAOS ₂ 10.75 2,3-(CH3)ACM1-CATA CI- CI- CI- CI- CH5O- 50.9 144 C ₂ AH ₂ CINAOS ₂ 10.55 2,3-(CH3)ACM1-CATA H- H- H- 54.9 157 C ₂ AH ₂ INAOS ₂ 12.48 3,4-(CH3)ACM1-CH3-CM1-CM3-CM4-CM4-CM3-CM4-CM3-CM4-CM4-CM3-CM4-CM3-CM4-CM3-CM4-CM3-CM4-CM4-CM4-CM4-CM4-CM4-CM4-CM4-CM4-CM4			5	H	51.0	159	C24H21CIN4OS2	11.55	13.22
2,3-(CH ₃) ₂ C ₆ H ₃ OCH ₁ - Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl		,5.(С113)1С6113	5	1				(11.65)	(13.32)
2,3-(CH),C ₆ H,OCH ₂ - Cl- C ₂ H ₅ O- S ₁ O ₂ H,C ₁ H ₁ CCH ₂ - Cl- C ₂ H ₅ O- S ₂ O ₃ H ₂ CH ₁ CCH ₂ - Cl- C ₂ H ₅ O- S ₃ O ₃ H ₄ CH ₁ CH ₂ CH ₂ CCH ₂ - Cl- S ₃ O ₄ C(H),C ₆ H ₂ CCH ₂ - H- Cl- S ₃ O ₄ C(H),C ₆ H ₂ CCH ₂ - H- Cl- S ₃ O ₄ C(H),C ₆ H ₂ CCH ₂ - H- Cl- S ₂ O ₄ H ₂ CH ₂ CH ₃ CCH ₂ - H- S ₂ O ₄ H ₂ CH ₃ CCH ₃ - Cl- H- S ₂ O ₄ H ₂ CH ₃ CCH ₃ - Cl- H- S ₂ O ₄ H ₂ CCH ₃ CH ₃ CCH ₃ - Cl- H- S ₂ O ₄ H ₂ CCH ₃ CH ₃ CCH ₃ - Cl- H- S ₂ O ₄ H ₃ CCH ₃ - Cl- H- S ₂ O ₄ H ₃ CCH ₃ CH ₃ CCH ₃ - Cl- H- S ₂ O ₄ H ₃ CCH ₃ CH ₃ CCH ₃ - Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl		2 CU. C. H.OCH	7	C	51.5	157	C24H20Cl2N4OS2	10.75	12.50
2,3-(CH3),CeH3OCH2- CI- C2,H5O- 50.9 144 C2,4H2,CIN,O3S 10.55 3,4-(CH3),CeH3OCH2- H- H- H- 54.9 157 C2,4H2,IN,OSS 12.48 3,4-(CH3),CeH3OCH2- H- C1- 53.3 160 C2,4H2,ICIN,OSS 11.55 3,4-(CH3),CeH3OCH2- H- C1-B5O- 54.1 145 C3,H2,ICIN,OS2 11.65) 3,4-(CH3),CeH3OCH2- C1- H- 52.9 140 C2,4H2,ICIN,OS2 11.54 3,4-(CH3),CeH3OCH2- C1- C1- 64.0 150 C2,4H2,ICIN,OS2 10.74 3,4-(CH3),CeH3OCH2- C1- C1- 64.0 150 C2,4H2,ICIN,OS2 10.74 3,4-(CH3),CeH3OCH2- C1- C1- C3- 130 C3,4H2,ICIN,OS2 10.74 3,4-(CH3),CeH3OCH2- C1- C1- C3- 130 C3,4H2,ICIN,OS2 10.74 3,4-(CH3),CeH3OCH2- C1- C3- C3- 130 C3,4H2,ICIN,OS2 10.74		,5-(C113)26113	5	·			•	(10.87)	(12.43)
3,4(CH ₃)C ₆ H ₃ OCH ₂ - H-		3-(CH3)-CH3OCH3-	5	C,H,O-	50.9	144	C26H25CIN4O2S2	10.55	12.07
3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - H- H- Cl- 53.3 H- Cl- 53.3 H- Cl- 53.3 H- Cl- 53.3 H- Cl- 54.1 H- Cl- 53.3 H- Cl- 11.55 (11.65) 11.55 (11.65) 3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - Cl- H- 52.9 H- 52.9 H- 52.9 H- 52.9 H- 52.9 H- 64.0 C ₄ H ₂ ICIN ₄ OS ₂ 11.54 (11.65) 11.54 (11.65) 3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl		7110 06110 7(611) - 6	;					(10.68)	(12.20)
3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - Cl- Cl- Cl- Cl- 64.0 15.56 (11.65) (11.65) 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - Cl- Cl- Cl- Cl- Cl- Cl- Cl- C		4-(CH ₁),C ₂ H ₂ OCH ₂ -	H-	H-	54.9	157	C24H22N4OS2	12.48	14.46
3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - H- Cl- 53.3 160 C ₂ H ₂ ICIN ₄ OS ₂ 11.55 (11.65) 3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - Cl- H- 52.9 140 C ₂ H ₃ ICIN ₄ OS ₂ 11.33 (11.43) 3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - Cl- Cl- 64.0 150 C ₂ H ₃ ICIN ₄ OS ₂ 10.74 (10.87) 3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - Cl- C ₃ H ₅ O- Cl- C ₃ H ₃ O- C ₃ H ₃ CIN ₄ OS ₂ 10.74 (10.87)		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,						(12.56)	(14.35)
3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - Cl- H- 52.9 140 C ₄ H ₃ C ₁ N ₄ OS ₂ 11.54 (11.65) 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - Cl- Cl- Cl- 64.0 150 C ₄ H ₃ C ₁ N ₄ OS ₂ 10.74 (10.87) 3,4-(CH ₃) ₂ C ₄ H ₃ OCH ₂ - Cl- C ₃ H ₅ O- C ₄ H ₃ OCH ₂ - Cl- C ₄ H ₅ O- 52.4 130 C ₄ H ₃ C ₁ N ₄ OS ₂ 10.56 (10.68)		4-(CH ₂),C ₂ H ₂ OCH ₂ -	H	C-C	53.3	160	C24H21CIN4OS2	11.55	13.22
3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - H- C ₂ H ₅ O- 54.1 145 C ₃ c ₄ H ₃ c _N O ₂ S ₃ 11.33 (11.43) 3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - C - C - C - C - C - C - C - C - C - C		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	ŀ					(11.65)	(13.32)
3,4-(CH ₃),C ₆ H ₃ OCH ₂ - Cl- H- 52.9 140 C ₂ ,H ₃ ,CIN ₄ OS ₂ 11.54 (11.65) 3,4-(CH ₃),C ₆ H ₃ OCH ₂ - Cl- Cl- 64.0 150 C ₂ ,H ₂ ,CI ₂ N ₄ OS ₂ 10.74 (10.87) 3,4-(CH ₃),C ₆ H ₃ OCH ₂ - Cl- C ₃ H ₅ O- 52.4 130 C ₄ ,H ₃ ,CIN ₄ O ₂ S ₂ 10.56 (10.68)		4-(CH:), C.H;OCH;-	H	C2H5O-	54.1	145	C26H26N4O2S2	11.33	13.14
3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₃ - Cl- H- 52.9 140 C ₃ H ₃ ICIN ₄ OS ₂ 11.54 (11.65) 3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₃ - Cl- Cl- 64.0 150 C ₃ H ₃ CI ₃ N ₄ OS ₂ 10.74 (10.87) 3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - Cl- C ₃ H ₅ O- 52.4 130 C ₃ cH ₃ 5CIN ₄ O ₅ S ₂ 10.56 (10.68)		,+-(•					(11.43)	(13.06)
3,4-(CH ₃),C ₆ H ₃ OCH ₂ - Cl- Cl- 64.0 150 C ₄ H ₃ oCl ₂ N ₄ OS ₂ 10.74 (10.87) (10.87) (10.87) (10.88) (10.68)		4-(CH:), C.H:OCH:-	O 1	H-	52.9	140	C24H21CIN4OS2	11.54	13.21
3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - Cl- Cl- 64.0 150 C ₂ AH ₂ oCl ₂ N ₄ OS ₂ 10.74 (10.87) 3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - Cl- C ₃ H ₅ O- 52.4 130 C ₃ cH ₃ sClN ₄ O ₅ S ₂ 10.56 (10.68)		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	}					(11.65)	(33.32)
3,4-(CH ₃) ₂ C ₆ H ₃ OCH ₂ - C - C ₃ H ₅ O- 52.4 130 C ₃ 6H ₃ 5ClN ₄ O ₅ S ₂ 10.56 (10.68)		A_(CH ₁),C ₂ H ₂ OCH ₂ -	5	C-	64.0	150	C24H20Cl2N,OS2	10.74	12.31
3,4-(CH ₃),C ₆ H ₃ OCH ₂ - Cl- C ₂ H ₃ O- 52.4 130 C ₃ cH ₃ sClN ₄ O ₃ S ₂ 10.56 (10.68)		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,						(10.87)	(12.43)
(10.68)		4-(CH ₁),C ₂ H,OCH ₁ -	Cl-	C2H5O-	52.4	130	C26H25CIN4O2S2	10.56	12.08
		,,+,	;					(10.68)	(12.20)

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1/(Calcd.)	S	15.20	(15.31)	14.03	(14.14)	13.96	(13.85)	14.25	(14.14)	13.03	(13.14)	12.74	(12.89)	15.72	(15.84)	14.46	(14.59)	14.40	(14.29)	14.70	(14.59)	13.40	(13.53)	13.15	(13.26)	
% Found/(Calcd.)	z	13.29	(13.39)	12.26	(12.38)	12.02	(12.12)	12.28	(12.38)	11.41	(11.50)	11.17	(11.28)	13.74	(13.86)	12.63	(12.77)	12.38	(12.50)	12.65	(12.77)	11.69	(11.84)	11.50	(11.61)	
Molecular	tormula	C22H18N4OS2		C22H17CIN4OS2		C24H22N4O2S2		C11H12CIN4OS1		C22H16Cl2N4OS2		C24H21CIN4O2S2		C1H16N4OS2		C11H15CIN,OS2		C23H20N4O2S2		C21H13CIN4OS2		C21H14Cl2N4OS2		C13H19CIN1O2S2		
M.pt.	၃	195		157		147		188		180		204		272		266		260		289		283		249		
%	rieid	63.4		52.4		62.3		65.6		74.5		77.5		67.9		53.6		59.2		55.2		55.6		59.1		
R.		H-		<u>-</u>	1	C2H5O-		H.	į	디		C2H5O-		H-	i	급	·	C2H,0-		H-	į	<u>-</u>		C ₂ H ₅ O-		
R.		Н-		H-	,	H		占	į	占	i	占	!	H-		H-	i	H-	i	다 당	,	占	i	占		
x		4-CH ₃ O.C ₆ H ₄ -		4-CH ₃ O.C ₆ H ₄ -		4-CH3O.C6H4-		4-CH3O.C4H4-		4-CH3O.C6H4-		4-CH ₃ O.C ₆ H ₄ -	1	4-OH.C6H4-	!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!	4-OH.C,H4-		4-OH.C ₆ H ₄ -	•	4-OH.C ₆ H ₆ -	1	4-OH.C,H,-		4-OH. C.H.		
Compd.	No.	37		38	;	39		9	;	41	. :	42	:	£3	;	4	;	45	;	4	,	47	\$	œ œ		

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The fungus was planted in agar growth media mixed with test compounds. The diameter of the fungus colony was measured at three different concentrations, viz. 1000, 100 and 10 ppm. The inhibition of the fungus growth was determined as the difference in growth between the control plate and those treated with the test compound. The activity of the test compounds was compared with commercial fungicide Carbendazim under similar conditions. The number of replications in each case was three. The percentage inhibition was calculated as:

Percentage inhibition =
$$\frac{(C-T)}{C} \times 100$$

C = diameter of fungus colony (in mm) in the control plate after 96 hrs.

T = diameter of fungus colony (in mm) in the treated plate after 96 hrs.

RESULTS AND DISCUSSION

The results show* that all the compounds under investigation were fairly toxic against both the fungi at 1000 ppm, but their toxicity decreased markedly on dilution at 1000 ppm and 100 ppm. They were, however, more toxic against *H. oryzae* than *A. niger*. Dithiocarbamates displayed good level of toxicity than other compounds screened. Further, alkyl sulphides, bis-triazolyl disulphides and bis-triazolyl ethylene disulphides displayed nearly the same level of fungitoxicity and they showed better toxicity than their parent triazoles. Compounds 30 and 36 were found to be more fungitoxic against both the fungi and the toxicity displayed by them was quite comparable with commercial fungicide, carbendazim at 1000 ppm. In general, the aryloxy derivatives were more potent than aryl derivatives and compounds with methoxy and/or chlorine groups displayed better fungitoxicity.

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^{*}Details can be obtained from author on request.

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Heteroatom Chemistry

III INTERNATIONAL CONFERENCE ON HETEROATOM CHEMISTRY

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