Original Research

MASS SPECTROMETRIC FRAGMENTATION AND PHARMACOLOGICAL ACTIVITIES OF 1,2,4 TRIAZOLE DERIVATIVES

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ABSTRACT

The mass spectra of several type of 1,2,4 triazole derivatives have been examined and the fragmentation pathway investigated. The fragmentation involves the sequential loss of a number of neutral molectules. Common fragmentation pattern (mass to charge) present in all glucopyranosyl derivatives of 1,2,4-triazole are 331, 127, 109 whereas amino derivatives possess 60 m/z value as common fragmentation pattern.

KEYWORDS: Mass spectrometry, 1,2,4 triazole derivatives, 3-mercaptoacetic acid, Quinoline , Glucopyranosyl

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INTRODUCTION:

Triazoles belong to five-membered ring system containing three nitrogen. It may be 1,2,3-triazole and 1,2,4- triazoles commonly known as v and s triazoles respectively. Bladin was the scientist that defines triazole in 1885 [1]. Due to the prescence of mercapto group at C-3, a renowned class of compounds will develop due to tautomerism. Mercaptotriazole are primarily in thione form as evidence provided by different spectroscopic studies [2]. Aminotriazoles, among the subtituted triazoles are known for its pharmacological activities.

Table 1: List of Pharmacological activities possess by 1, 2, 4- triazole is given under table 1

Pharmacological Activiies	**References**
Anti-fungal	[3][4][5]
Diuretic	[6][7]
Antibacterial	[8]
Hypoglycemic	[9]
Anti-tubercular	[10]
Anti-depressant	[11]
Anti-amoebic	[12]
Antibiotic	[13]
Anti-inflammatory	[14]
Anti-carcinogenic	[15]
Hypnotic	[16]
Sedative	[17]
Plant growth regulators	[18][19]
Insecticidal	[20][21]

In this paper we are discussing about the mass fragmentation pattern and Pharmacological activities of triazole deivatives. Mass spectrum of mercaptoacetic acid, quinoline, Schiff base ligand, Glucopyrnaosyl and amino derivatives of 1,2,4 triazole are discussed.

Mass fragmentation pattern of 1,2,4-triazole-3-mercaptoacetic acid derivatives

5-(2-furyl)-4-ethyl-1,2,4-triazole-3-mercaptoacetic acid hydrazide (1a)

Table 1: Mass spectrum of 5-(2-furyl)-4-ethyl-1,2,4-triazole-3-mercaptoacetic acid hydrazide

A = ion abundance relative to base peak					
m/z	267*	236	208	195	167
A	60	59	5	100**	64

*Molecular ion peak
**Base peak

2-((4-ethyl-5-(furan-2-yl)-4H-1,2,4-triazol-3-yl)thio)-N'-(4-nitrobenzylidene)acetohydrazide (1b)

Table 2: Mass Spectrum of 2-((4-ethyl-5-(furan-2-yl)-4H-1,2,4-triazol-3-yl)thio)-N'-(4-nitrobenzylidene)acetohydrazide

A = ion abundance relative to base peak						
m/z	400*	252	236	209	195	167
A	2	1	8	1	100**	20
m/z	148	77				
A	4	3				

*Molecular ion peak
**Basepeak

2-p-chlorophenyl-3-(50-mercapto-40-phenyl-10,20, 40-triazol-30-yl)-4,5-dihydronaphtho[1,2-c]pyrazol (1c)

Table 3: Mass Spectrum of 2-p-chlorophenyl-3-(50-mercapto-40-phenyl-10,20, 40-triazol-30-yl)-4,5-dihydronaphtho[1,2-c]pyrazol

A = ion abundance relative to base peak						
m/z	455*	280	266	252	177	164
A	1	1	69	2	1	11
m/z	163	150	149	135	109	104
A	11	1	21	4	2	7

m/z	84	77	71	57	56	
A	6	14	9	19	10	

*Molecular ion peak
**Base peak

Pharmacological activities of 1,2,4-triazole-3-mercaptoacetic acid derivatives:
1,2,4-triazole-3-mercaptoacetic acid derivatives were synthesized and evaluated for their antimycobacterial activity[22].

Table 1: Pharmacological activities of compound 1a and 1b

Compound	MIC µ/ml	%Inhibition
1a	>6.25	n.a
1b	>6.25	12

n.a= not active

Mass fragmentation pattern of Quinoline derivative of 1,2,4-triazole

5-(4-(4-(2-Aminoethyl)piperazin-1-yl)-8 (trifluoromethyl)quinolin-3-yl)-4-benzyl-4H-1,2,4-triazole-3-thiol (2a)

Table 1: Mass fragmentation pattern of 5-(4-(4-(2-Aminoethyl)piperazin-1-yl)-8-(trifluoromethyl)quinolin-3-yl)-4-benzyl-4H-1,2,4-triazole-3-thiol

A = ion abundance relative to base peak						
m/z	515	496	470	438	395	353
A	14	19	18	37	37	37
m/z	351	239				
A	100**	18				

*Molecular+2 ion peak
**Base peak

Pharmacological activities of Quinoline derivative of 1,2,4-triazole
Quinoline derivatives are reported to possess antibacterial [23], anti-malarial [24], anti-HIV [25][26], anti-cancer [27], anti-inflammatory [28], anti-convulsant [29] and anti-hypertensive activities [30]. 1,2,4-triazole moiety containing derivatives of quinoline were synthesized and evaluated for antifungal and antimicrobial activity. They showed antimicrobial activity in concentration of 6.25-12.5 µg/ml in DMSO. 2 showed antimicrobial table 3.2(b1) and antifungal table 3.2(b2) activity against different strains.

Table 1: Anti-bacterial activity of compound 2(a)

Bacterial Strain	Compound 2a	Ciprofloxacin*
S. aureus	50(<10)	6.25 (22-30)
E. coli	6.25(20-24)	6.25 (30-40)
P. aeruginosa	50 (<10)	6.25 (25-33)
K. pneumonia	50(<10)	6.25 (23-27)

MIC in mg/mL and zone of inhibition in mm
*standard

Table 2: Antifungal activity of compound 2(a)

Fungal strain	Compound 2(a)	Ciclopiroxol amine*
P. marneffei	50 (<10)	6.25 (20-27)
T. mentagrophytes	50 (<10)	3.125 (27-33)
A. flavus	50 (<10)	3.125 (25-30)
A. fumigatus	50 (<10)	6.25 (25-30)

MIC in mg/mL and zone of inhibition in mm
*standard

1, 2, 4-triazole-derived Schiff base ligand

3,5-diamino-1,2,4-triazole was reacted with 2-hydroxy-1-naphthaldehyde, pyrrole-2-carboxa-ldehyde, pyridine-2-carboxaldehyde and acetyl pyridine-2-carboxaldehyde to yield Schiff base ligands which were complexed with vanadium and evaluated for antimicrobial (table 3a) and

antifungal (table 3b) activity. Vanadium and its complexes are reported to possess antimicrobial [31], [32] and antitumor [33].

Mass fragmentation of 2-((4-ethyl-5-(furan-2-yl)-4H-1,2,4-triazol-3-yl)thio)-N'-(4-nitrobenzylidene)acetohydrazide (3a)

Table 1: Mass Spectrum of 2-((4-ethyl-5-(furan-2-yl)-4H-1, 2, 4-triazol-3-yl)thio)-N'-(4-nitrobenzylidene)acetohydrazide

A = ion abundance relative to base peak						
m/z	407	390	373	252	236	197
A	24	13	15	24	100**	18
m/z	128	170	154	140	127	85
A	28	37	17	16	67	51

*Molecular ion peak
**Base peak

Pharmacological activities of 1, 2 ,4-triazole-derived Schiff base ligand

Table 1: Antibacterial activity of compound 3a

Bacterial strain	Compound 3a	Imipenum*
E. coli	11	29
S. flexenari	13	31
P. aeruginosa	11	30
S. typhi	14	29
S. aureus	12	26
B. subtilis	16	28

MIC in mg/mL and zone of inhibition in mm
Conc. used 1mg/ml of DMSO
*standard

Table 2: Antifungal activity of Compound 3a

Fungal Strain	Compund 3a	Standard*
T. longifucus	49	A
C. albicams	55	B
A.Flavus	47	C
M. canis	41	D
F. solani	38	E
C. glaberata	42	F

*standard A = Miconazole (70 mg/mL: 1.6822×10^{-7} M/mL), B = Miconazole (110.8 mg/mL: 2.6626×10^{-7} M/mL), C = Amphotericin B (20 mg/mL: 2.1642×10^{-8} M/mL), D = Miconazole (98.4 mg/mL: 2.3647×10^{-7} M/mL), E = Miconazole (73.25 mg/mL: 1.7603×10^{-7} M/mL), F = Miconazole (110.8 mg/mL: 2.66266×10^{-7} M/mL).

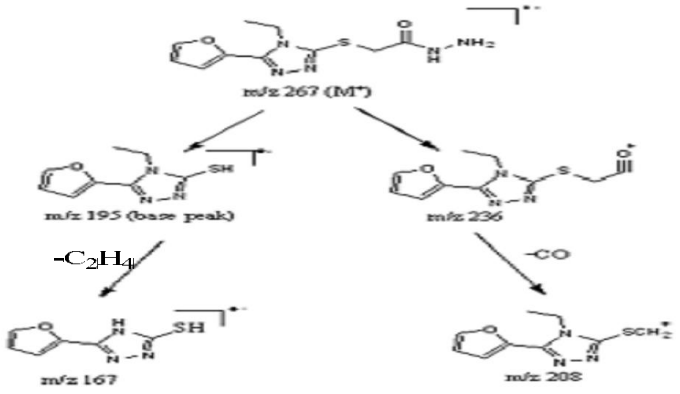

Figure 1: Mass fragmentation pattern of Compound 1(a)

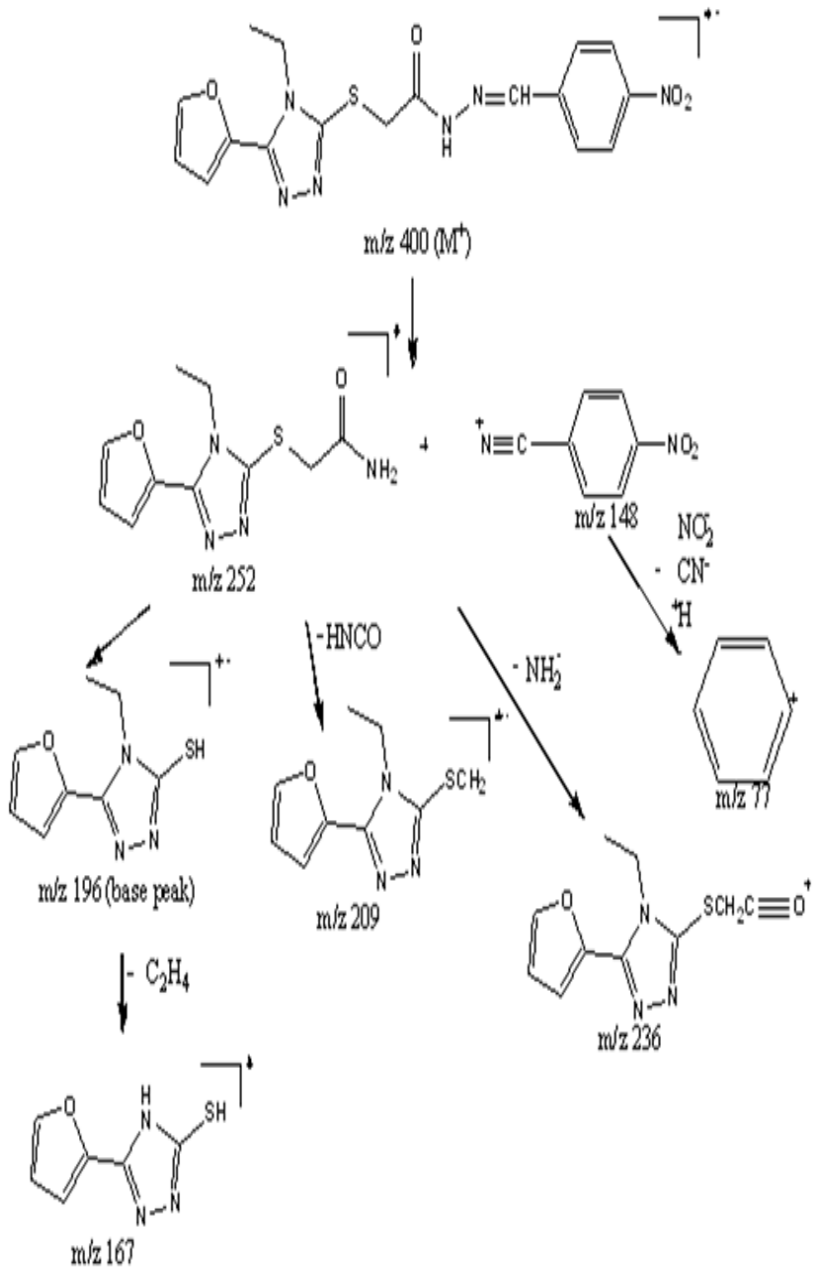

Figure 2: Mass Fragmentation pattern of Compound 1(b)

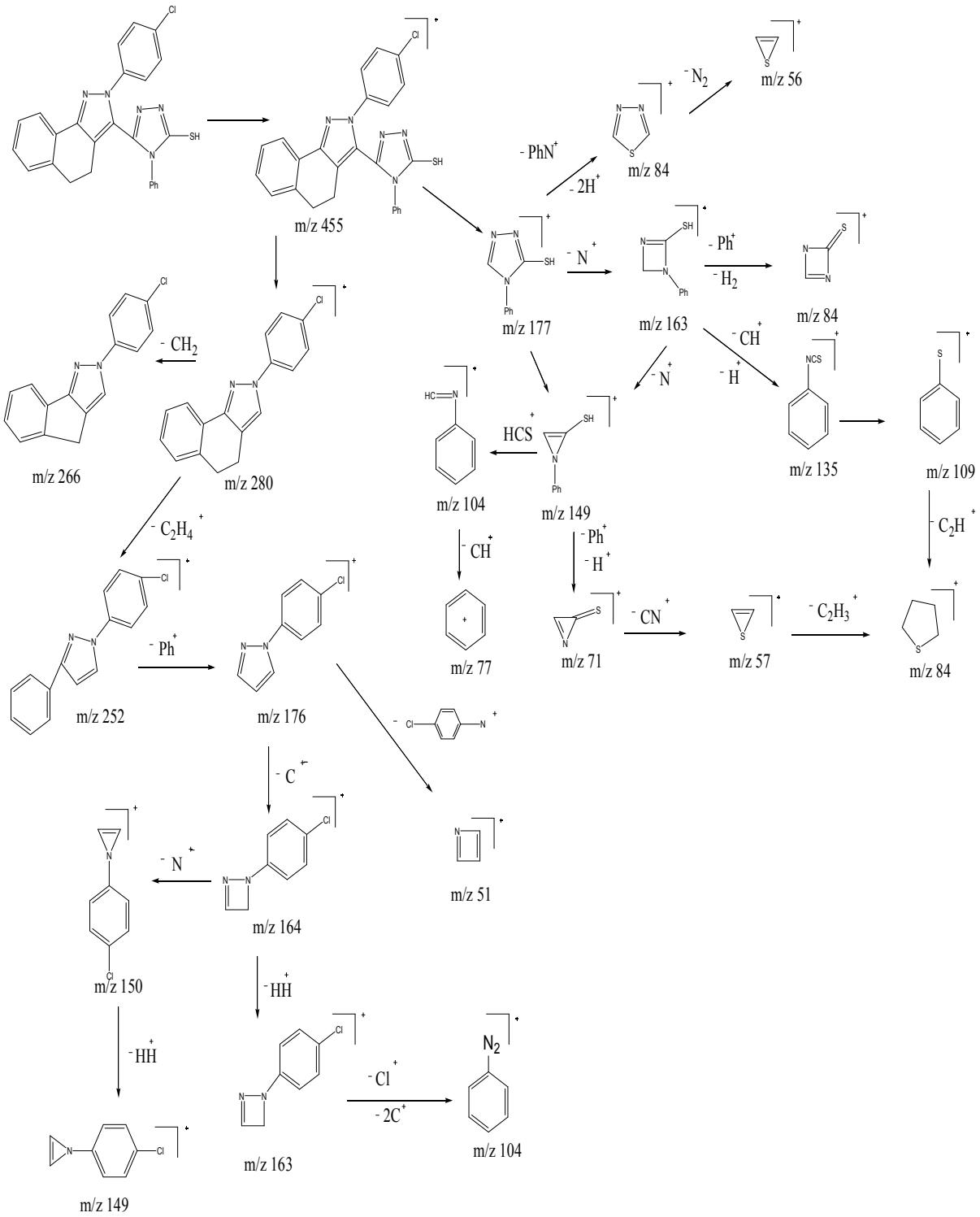

Figure 3: Mass fragmentation pattern of compund 1(c)

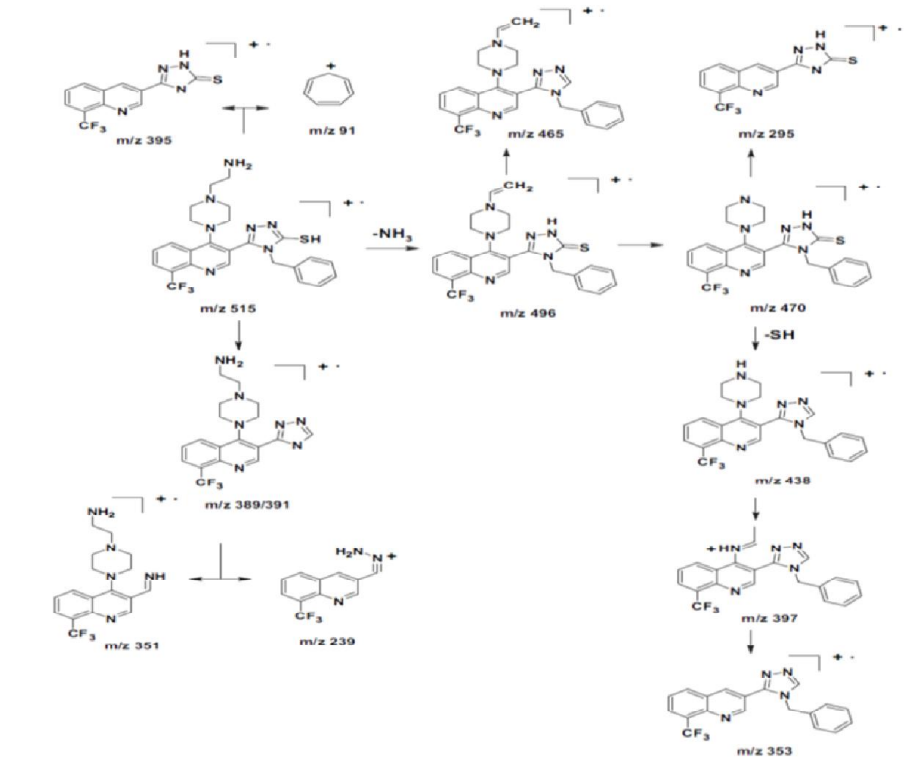

Figure 4: Mass Fragmentation pattern of Compound 2(a)

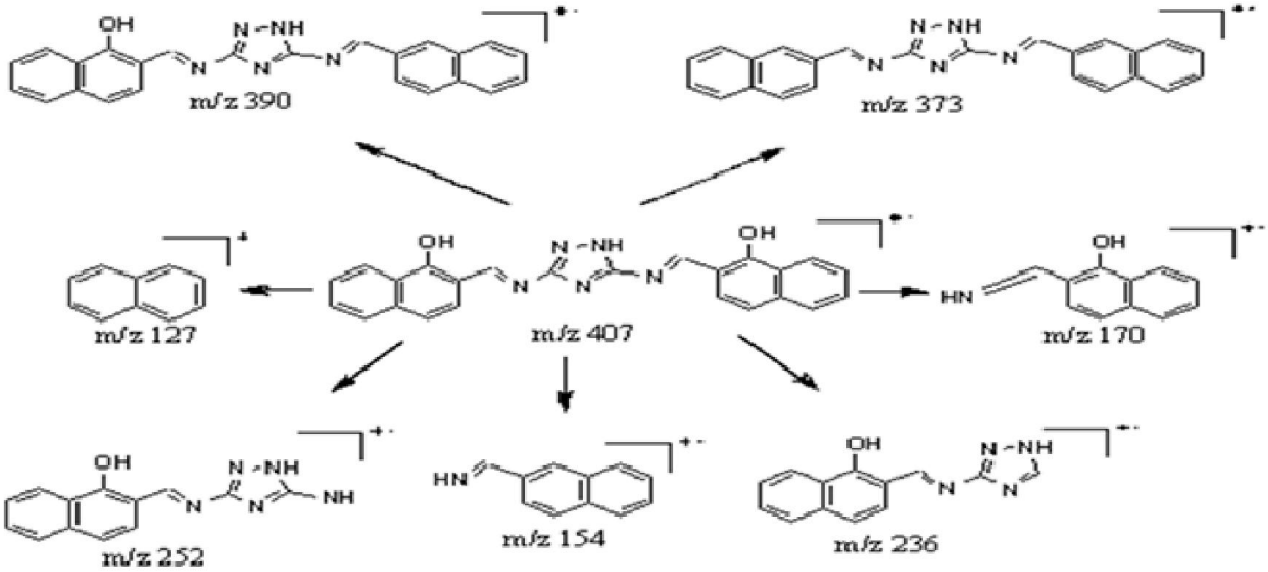

Figure 5: Mass Fragmentation pattern of Compound 3(a)

Mass fragmentation pattern of Glucopyranosyl derivatives of 1,2,4-triazole

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)-4,5-diphenyl-3H-1,2,4-triazole-3-thione (4a)

Table 1: Mass spectrum of N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)-4,5-diphenyl-3H-1,2,4-triazole-3-thione

A = ion abundance relative to base peak						
m/z	583*	524	464	331	253	211
A	3	2	6	28	16	10
m/z	220	229	194	176	187	169
A	4	2	5	20	3	100**
m/z	127	109	117	103	75	43
A	4	69	10	5	6	60

*Molecular ion peak
**Base peak

N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucopyranosyl)-4-phenyl-5-(2-pyridyl)1,2,4-triazole-3-thione (4b)

Table 2: Mass Spectrum of N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucopyranosyl)-4-phenyl-5-(2-pyridyl)1,2,4-triazole-3-thione

A = ion abundance relative to base peak						
m/z	584*	524	465	405	367	365
A	8	3	7	4	2	10
m/z	331	297	279	255	254	221
A	3	19	1	100**	17	2
m/z	181	169	127	109	78	43
A	3	22	4	12	1	17

*Molecular ion peak
**Base peak

3.4.3 N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucopyranosyl)-4-phenyl-5-(3-pyridyl)1,2,4-triazole-3-thione (4c)

Table 3: Mass spectrum of N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucopyranosyl)-4-phenyl-5-(3-pyridyl)1,2,4-triazole-3-thione

A = ion abundance relative to base peak						
m/z	584*	541	524	481	465	405
A	4	0.1	2	0.1	3	2
m/z	365	331	297	255	254	221
A	7	3	18	100**	16	1
m/z	181	169	127	109	78	43
A	3	21	4	9	2	15

*Molecular+2 ion peak
**Base peak

N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucopyranosyl)-4-phenyl-5-(4-pyridyl)1,2,4-triazole-3-thione (4d)

Table 4: Mass Spectrum of N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucopyranosyl)-4-phenyl-5-(4-pyridyl)1,2,4-triazole-3-thione

A = ion abundance relative to base peak						
m/z	584	524	465	405	365	331
A	3	2	3	1	6	7
m/z	297	255	221	181	169	127
A	13	100**	1	2	19	4
m/z	109	78	43			
A	8	2	16			

*Molecular ion peak
**Base peak

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-phenyl-5-(4-methylphenyl)-1,2,4-Triazole-3-thione (4e)

Table 5: Mass Spectrum of N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-phenyl-5-(4-methylphenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	597*	582	554	539	479	331
A	2	3	5	1	2	12
m/z	267	252	211	229	190	187

A	17	5	4	1	7	13
m/z	150	135	169	127	109	75
A	2	6	100**	24	72	2

N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucopyranosyl)-4-phenyl-5-benzyl-1,2,4-triazole-3-thione (4f)

Table 6: Mass Spectrum of N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucopyranosyl)-4-phenyl-5-benzyl-1,2,4-triazole-3-thione

A = ion abundance relative to base peak						
m/z	597	554	538	494	331	267
A	3	6	4	2	19	15
m/z	271	229	211	208	187	176
A	1	3	5	17	2	11
m/z	150	169	127	117	109	91
A	7	72	2	5	32	100**
m/z	77					
A	1					

*Molecular ion peak
**Base peak

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-phenyl-1,2,4-Triazole-3-thione (4g)

Table 7: Mass spectrum of N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-phenyl-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	601*	542	523	482	331	272
A	7	3	1	6	10	62
m/z	271	238	212	176	169	127
A	16	2	4	1	100**	5
m/z	109	103	75	43		
A	61	1	3	20		

*Molecular ion peak
**Base peak

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-(2-pyridyl)-3H-1,2,4-Triazole-3-thione (4h)

Table 8: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-(2-pyridyl)-3H-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	602*	524	484	483	423	383
A	9	4	2	6	3	8
m/z	331	315	273	239	199	169
A	7	42	100**	2	4	62
m/z	139	127	109	78	43	
A	3	5	37	3	63	

*Molecular ion peak
**Base peak

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-(3-pyridyl)-1,2,4-Triazole-3-thione (4i)

Table 9: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-(3-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	602	559	542	483	441	423
A	6	0.1	3	4	0.2	2
m/z	383	331	273	199	169	139
A	5	4	100**	2	63	2
m/z	127	109	78	43		
A	**4**	**33**	**5**	**65**		

*Molecular ion peak
**Base peak

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-(4-pyridyl)-1,2,4-Triazole-3-thione (4j)

Table 10: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-(4-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak

m/z	602*	542	483	423	383	331
A	6	3	4	2	6	5
m/z	273	239	119	169	139	127
A	100**	1	3	62	2	6
m/z	109	78	43			
A	36	3	42			

*Molecular ion peak
**Base peak

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-(4-methylphenyl)-1,2,4-Triazole-3-thione (4k)

Table 11: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-fluoro-phenyl)-5-(4-methylphenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	615*	600	572	556	496	331
A	6	1	3	7	2	29
m/z	289	285	270	211	229	190
A	1	32	3	12	6	10
m/z	187	169	168	153	145	127
A	9	100**	35	16	1	13
m/z	109	117	90	75		
A	49	22	5	3		

*Molecular ion peak
**Base peak

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 5-benzyl-4-(4-fluorophenyl)-1,2,4-Triazole-3-thione (4l)

Table 12: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 5-benzyl-4-(4-fluorophenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	615*	572	556	331	285	211
A	14	2	8	19	18	3
m/z	226	194	169	168	131	127
A	3	2	75	20	1	25
m/z	117	109	91	77		
A	5	45	100**	3		

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-chlorophenyl)-5-phenyl-1,2,4-Triazole-3-thione (4m)

Table 13: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-chlorophenyl)-5-phenyl-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	617*	558	498	311	288	211
A	3	6	2	51	100**	4
m/z	229	187	254	228	151	169
A	2	4	6	115	41	72
m/z	127	109	75	43		
A	10	38	2	47		

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-chlorophenyl)-5-(2-pyridyl)-1,2,4-Triazole-3-thione (4n)

Table 14: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-chlorophenyl)-5-(2-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	618*	559	499	439	399	331
A	5	3	4	1	6	42
m/z	289	217	229	215	183	169
A	100**	1.2	1	2	0.5	65
m/z	139	127	109	78	43	
A	2	6	40	3	61	

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-chlorophenyl)-5-(3-

pyridyl)-1,2,4-Triazole-3-thione (4o)

Table 15: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-chlorophenyl)-5-(3-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	619	618	559	499	439	399
A	2	4	3	2	1	5
m/z	331	289	229	215	183	169
A	39	100**	5	4	1	69
m/z	139	127	109	78	43	
A	5	7	40	5	25	

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-chlorophenyl)-5-(4-pyridyl)-1,2,4-Triazole-3-thione (4p)

Table 16: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-chlorophenyl)-5-(4-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	618*	559	449	438	399	331
A	4	3	4	2	1	41
m/z	289	229	215	169	139	127
A	100**	2	3	7	2	6
m/z	109	78	43			
A	34	3	56			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 5-(4-methylphenyl)-1,2,4-Triazole-3-thione (4q)

Table 17: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 5-(4-methylphenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	631*	616	588	572	512	331
A	9	2	5	11	3	41
m/z	301	287	271	211	169	187
A	66	28	2	15	100**	6
m/z	184	190	127	109	117	91
A	16	25	12	81	4	5
m/z	76	43				
A	3	2				

N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucanosyl)-5-benzyl-4-(4-chlorophenyl)-1,2,4-triazole-3-thione (4r)

Table 18: Mass Spectrum Mass fragmentation of N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucanosyl)-5-benzyl-4-(4-chlorophenyl)-1,2,4-triazole-3-thione

A = ion abundance relative to base peak						
m/z	631*	588	572	528	331	301
A	12	2	7	3	11	33
m/z	271	242	210	187	184	169
A	1	15	2	3	4	92
m/z	127	117	109	91	77	
A	2	1	12	100**	1	

*Molecular ion peak
**Base peak

N-(2',3',4',6'-tetra-O-acetyl)-β-D-glucopyranosyl)-4-(4-bromophenyl)-5-phenyl-3H-1,2,4-triazole-3-thione (4s)

Table 19: Mass Spectrum of N-(2',3',4',6'-tetra-O-acetyl)-BETA-D-glucopyranosyl)-4-(4-bromophenyl)-5-phenyl-3H-1,2,4-triazole-3-thione

A = ion abundance relative to base peak						
m/z	662*	603	543	332	331	299
A	7	2	6	100**	61	3
m/z	271	273	229	196	187	176
A	1	11	1	5	4	2
m/z	169	145	109	103	75	43
A	62	3	51	1	2	21

*Molecular ion peak
**Base peak

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-bromophenyl)-5-(2-pyridyl)-1,2,4-Triazole-3-thione (4t)

Table 20: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-bromophenyl)-5-(2-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	663*	664	603	560	334	333
A	9	2	3	1	100**	12
m/z	331	271	270	268	211	229
A	25	1	4	3	2	34
m/z	214	274	169	133	127	109
A	10	5	65	2	11	45
m/z	104	78				
A	1	3				

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-bromophenyl)-5-(3-pyridyl)-1,2,4-Triazole-3-thione (4u)

Table 21: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-bromophenyl)-5-(3-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	663*	664	603	334	333	332
A	11	2	1	100**	6	19
m/z	331	274	268	229	214	211
A	28	5	3	13	6	3
m/z	169	187	127	109	104	78
A	72	2	1	42	2	3

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-bromophenyl)-5-(4-pyridyl)-1,2,4-Triazole-3-thione (4v)

Table 22: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-bromophenyl)-5-(4-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	663*	664	334	333	331	274
A	8	1	100**	61	38	12
m/z	271	229	214	211	187	169
A	1	6	2	1	8	45
m/z	133	127	109	104	78	
A	5	8	60	5	2	

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-bromophenyl)-5-(4-methylphenyl)-1,2,4-Triazole-3-thione (4w)

Table 23: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-(4-bromophenyl)-5-(4-methylphenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	676*	661	633	617	557	346
A	11	3	9	5	2	17
m/z	331	289	271	229	214	190
A	60	3	1	24	8	7
m/z	187	169	127	117	109	90
A	3	100	13	4	53	17
m/z	76	43				
A	2	1				

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-phenyl-1,2,4-Triazole-3-thione (4x)

Table 24: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-phenyl-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	535*	475	374	331	317	271
A	10	2	4	5	12	1
m/z	261	206	177	169	136	127
A	3	100**	8	73	2	5
m/z	109	103	77	43		
A	40	2	2	60		

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-(2-pyridyl)-1,2,4-Triazole-3-thione (4y)

Table 25: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-(2-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	536*	493	476	417	357	331
A	12	0.1	3	5	3	4
m/z	317	275	249	211	207	179
A	14	1	25	1	100**	7

m/z	169	139	127	109	105	78
A	81	2	6	43	8	2
m/z	43					
A	63					

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-(3-pyridyl)-1,2,4-Triazole-3-thione (4z)

Table 26: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-(3-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak							
m/z	536*	493	476	433	417	357	331
A	10	0.1	2	0.1	5	1	4
m/z	275	249	211	207	179	169	127
A	2	21	2	100**	6	75	5
m/z	109	105	78	43			
A	52	3	3	57			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-(4-pyridyl)-1,2,4-Triazole-3-thione (4aa)

Table 27: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-(4-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	536*	476	417	375	331	317
A	9	3	5	0.1	6	8
m/z	249	207	179	169	139	127
A	22	100**	5	79	2	4
m/z	109	105	78	43		
A	45	3	5	35		

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-(4-methylphenyl)-1,2,4-Triazole-3-thione (4ab)

Table 28: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-ethyl-5-(4-methylphenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	549	489	430	331	`219	211
A	9	2	7	5	6	2
m/z	187	191	169	127	117	109
A	10	7	100**	8	2	50
m/z	96	91	75			
A	2	32	2			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-hexyl-5-(2-pyridyl)-1,2,4-Triazole-3-thione (4ac)

Table 29: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-hexyl-5-(2-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	592*	577	533	331	330	262
A	52	3	1	28	16	42
m/z	234	229	211	206	187	184
A	2	5	6	4	1	10
m/z	169	177	152	145	109	78
A	100**	9	5	2	67	11

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-hexyl-5-(3-pyridyl)-1,2,4-Triazole-3-thione (4ad)

Table 30: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-hexyl-5-(3-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	592*	533	331	262	234	206
A	2	3	11	67	2	1
m/z	229	211	187	178	177	169
A	13	4	6	8	3	92
m/z	156	145	127	109	78	
A	4	2	40	100**	3	

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-hexyl-5-(4-pyridyl)-1,2,4-Triazole-3-thione (4ae)

Table 31: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-hexyl-5-(4-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	592	331	330	271	211	262
A	2	10	2	1	6	32

m/z	261	206	229	177	169	127
A	15	5	2	1	100**	5
m/z	109	78	65			
A	72	5	1			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-hexyl-5-(3,4,5-trimethoxyphenyl)-1,2,4-Triazole-3-thione (4af)

Table 32: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-hexyl-5-(3,4,5-trimethoxyphenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	681	666	622	595	331	351
A	3	1	4	2	16	9
m/z	323	295	271	267	252	229
A	12	5	2	8	4	3
m/z	193	187	169	167	152	137
A	11	7	100**	2	3	1
m/z	127	109	75			
A	3	54	5			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-benzyl-5-(2-pyridyl)-1,2,4-Triazole-3-thione (4ag)

Table 33: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-benzyl-5-(2-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	598*	539	479	437	419	379
A	13	8	17	4	7	16
m/z	330	310	269	268	235	211
A	19	15	7	32	11	7
m/z	187	169	128	109	91	78
A	4	52	25	38	100 **	10

N-(β-D-Galactopyranosyl)-4-benzyl-5-(3-pyridyl)-1,2,4-Triazole-3-thione (4ah)

Table 34: N-(β-D-Galactopyranosyl)-4-benzyl-5-(3-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak

m/z	523	193	456	453	331	271
A	5	5	2	1	12	2
m/z	229	211	194	169	145	127
A	2	4	5	100**	6	30
m/z	109	98	78			
A	80	12	5			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)-4-amino-5-(3-pyridyl)-1,2,4-Triazole-3-thione (4ai)

Table 35: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)-4-amino-5-(3-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	523	456	331	271	236	211
A	2	1	15	5	7	4
m/z	202	193	169	145	128	109
A	4	12	100**	1	9	77
m/z	99	78	60			
A	4	5	21			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(4-pyridyl)-1,2,4-Triazole-3-thione (4aj)

Table 36: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(4-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	523*	456	453	331	271	236
A	3	2	1	14	3	4
m/z	229	211	202	194	193	169
A	2	3	3	20	8	100**
m/z	145	128	109	98	78	60
A	7	32	92	13	3	20

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(4-fluorophenyl)-1,2,4-Triazole-3-thione (4ak)

Table 37: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(4-fluorophenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	540*	331	271	211	229	187
A	3	29	6	4	13	1
m/z	169	209	210	138	151	128
A	100**	5	7	10	5	46
m/z	111	95	75			
A	2	1	3			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(4-chlorophenyl)-1,2,4-Triazole-3-thione (4al)

Table 38: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(4-chlorophenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	556*	331	269	229	227	226
A	1	24	7	13	27	12
m/z	211	169	155	145	127	109
A	4	100**	2	6	21	64
m/z	99					
A	2					

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(4-bromophenyl)-1,2,4-Triazole-3-thione (4am)

Table 39: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(4-bromophenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	601*	331	271	211	229	199
A	3	8	10	2	3	4
m/z	212	156	156	169	127	145
A	2	7	7	100**	90	1
m/z	109	99	75			
A	60	3	2			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(2-naphthyl)-1,2,4-Triazole-3-thione (4an)

Table 40: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(2-naphthyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	572*	512	469	331	271	288
A	6	3	2	16	4	9
m/z	242	229	226	211	194	169
A	5	2	4	4	1	100**
m/z	153	127	126	139	109	103
A	8	33	4	2	73	1

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(1-naphthyl)-1,2,4-Triazole-3-thione (4ao)

Table 41: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-glucopyranosyl)- 4-amino-5-(1-naphthyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	572*	512	469	331	288	271
A	3	1	2	19	3	6
m/z	242	229	211	194	169	153
A	4	3	7	3	100**	16
m/z	127	126	109	103		
A	92	62	85	2		

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)- 4-amino-5-(2-phenoxymethyl)-1,2,4-Triazole-3-thione (4ap)

Table 42: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)- 4-amino-5-(2-phenoxymethyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	552*	492	433	331	271	269
A	1	2	1	35	3	2
m/z	222	211	229	192	176	169
A	0.9	10	6	64	8	83
m/z	129	144	127	109	107	94
A	2	5	1	100**	3	41

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(2-chlorophenoxymethyl)-1,2,4-Triazole-3-thione(4aq)

Table 43: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(2-

chlorophenoxymethyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	586.5	556	527	496	331	271
A	n.a	10	2	3	41	1
m/z	256	229	226	211	169	144
A	1	3	3	5	100**	5
m/z	128	127	116	129	112	91
A	8	3	2	4	1	11

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(3-chlorophenoxymethyl)-1,2,4-Triazole-3-thione (4ar)

Table 44: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(3-chlorophenoxymethyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	586.5*	556	496	331	271	256
A	n.a	9	3	22	3	1
m/z	241	211	169	144	141	128
A	2	15	78	3	1	5
m/z	127	116	109	91		
A	3	2	100**	42		

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(4-chlorophenoxymethyl)-1,2,4-Triazole-3-thione (4as)

Table 45: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(4-chlorophenoxymethyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	556*	496	331	271	256	241
A	0.5	2	38	2	2	5
m/z	211	169	144	141	128	127
A	19	72	2	3	3	5
m/z	116	109	91			
A	1	100**	52			

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(4-bromophenoxymethyl)-1,2,4-Triazole-3-thione (4at)

Table 46: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(4-bromophenoxymethyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	631*	601	571	331	301	271
A	1	4	2	12	1	21
m/z	255	211	229	187	186	173
A	3	9	2	1	4	2
m/z	169	144	129	127	109	
A	100**	2	1	7	48	

N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(4-methylphenoxymethyl)-1,2,4-Triazole-3-thione (4au)

Table 47: N-(2',3',4',6'-Tetra-O-acetyl)-β-D-galactopyranosyl)-4-amino-5-(4-methylphenoxymethyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	566*	536	506	331	271	236
A	n.a	2	1	28	7	1
m/z	211	206	190	169	144	127
A	3	15	10	100**	1	3
m/z	109	108				
A	63	43				

Pharmacological activity of Glucopyranosyl derivatives of 1,2,4-triazole

Table 1: Anti-bacterial activities of selected compounds

Compounds	Bacillus subtiles	Staphylococcus aureus	Escherichia colai	Shigella flexnari	Pseudomonas aeruginosa	Salmonella typhi
4b	10	17	18	9	16	13
4h	21	18	20	16	26	11

4n	18	15	25	10	20	12
4t	20	20	23	17	28	17
4y	n.a	n.a	n.a	n.a	9	n.a
4ac	15	n.a	15	n.a	16	n.a
4e	10	n.a	9	n.a	n.a	n.a
4k	10	n.a	n.a	n.a	13	n.a
4q	17	17	21	n.a	18	20
4w	15	10	22	n.a	10	18
4ab	24	15	13	n.a	24	20
4aj	22	15	13	20	20	n.a
4am	19	15	n.a	n.a	24	n.a
4al	9	10	9	10	12	13
4an	12	n.a	10	n.a	10	n.a
Standard*	33	33	30	27	24	25

Concentration used 3.00 mg/mL of DMSO
Standard drug = Imipenem
n.a = No activity
Size of well = 6mm (dia)

Table 2: Anti-fungal activities of selected compounds

Compounds	Trichophyton longifusus	Candida albicans	Aspergiilus flavus	microsporum canis	Fusarium solani	Candida glabbrata
4d	60	0	0	45	0	40
4j	70	65	0	55	0	50
4p	0	0	0	40	0	0
4v	45	0	0	65	0	40
4aa	60	0	0	45	0	0
4ae	65	0	0	60	0	30

Conc of sample = 200µg/mL of DMSO
Incubation time = 27C
Incubation period = 7 days

Table 3: Phytotoxic activity of selected compounds

Conc of compound µg/mL	4a	4g	4m	4s	4x	Conc of std Drug µg/mL
100	64.4	64.44	66.67	100	100	0.015
50	11.11	11.11	33.33	100	91.11	
5	6.66	6.66	11.11	77.78	33.33	

Name of plant: Lemna minor
Standard drug: Paraquat

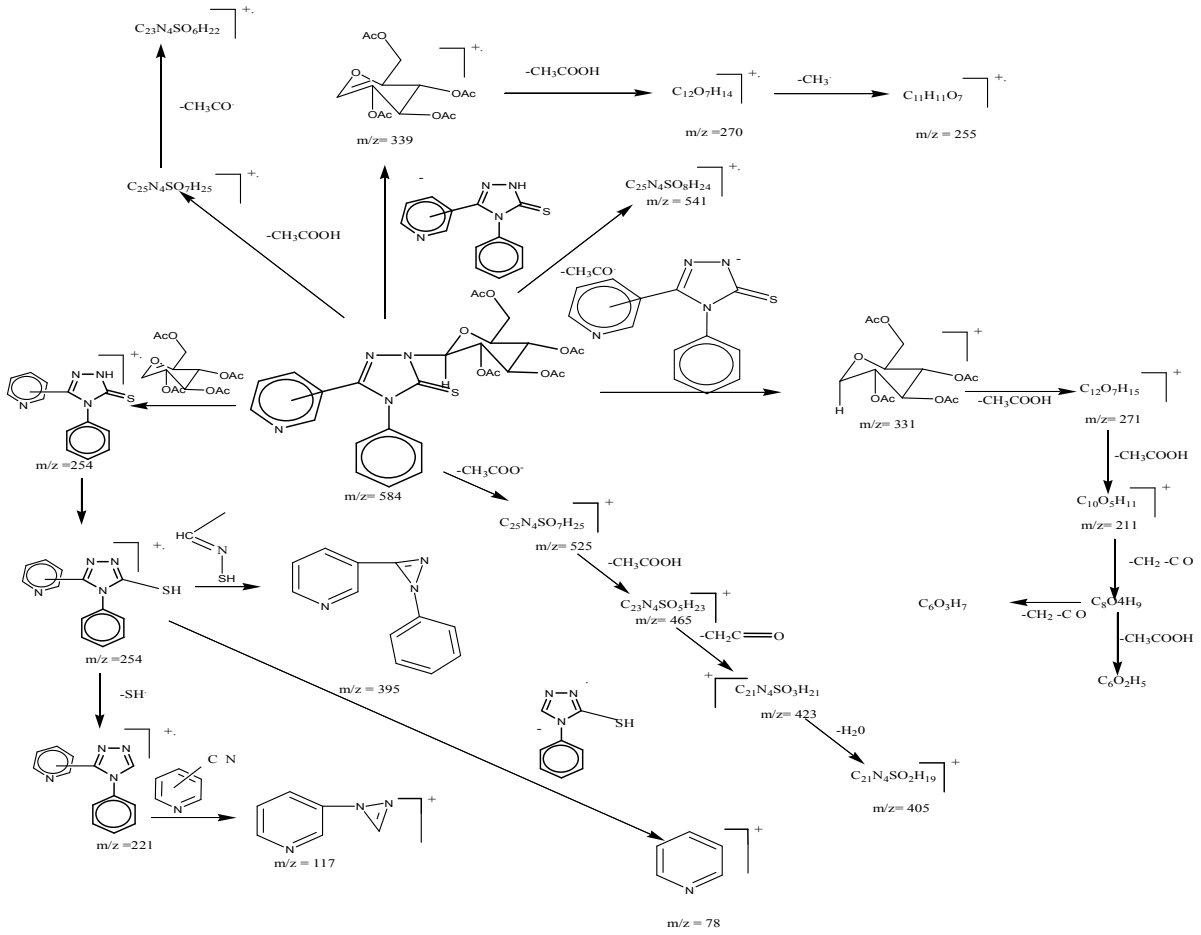

Figure 1: Mass Fragmentation pattern of Compound 4(b)(c)(d)

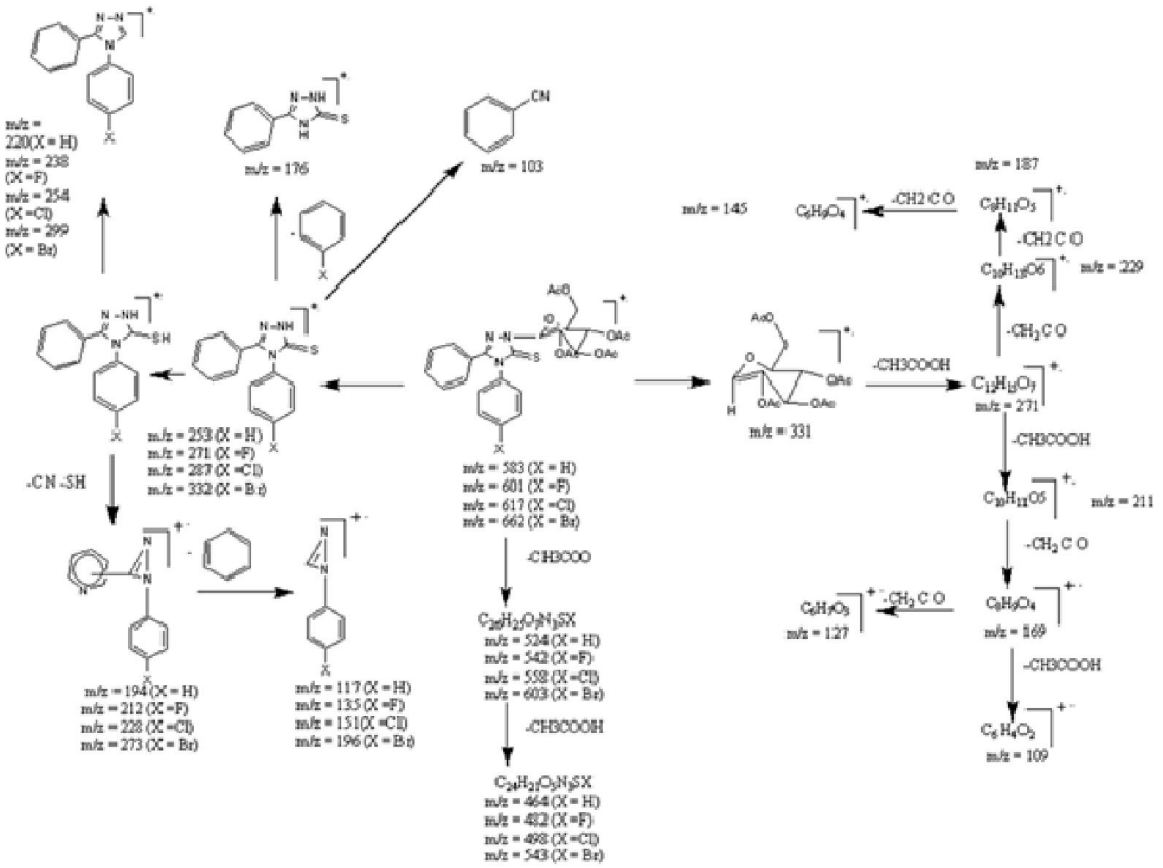

Figure 2: Mass Fragmentation pattern of Compound 4(a)(s)

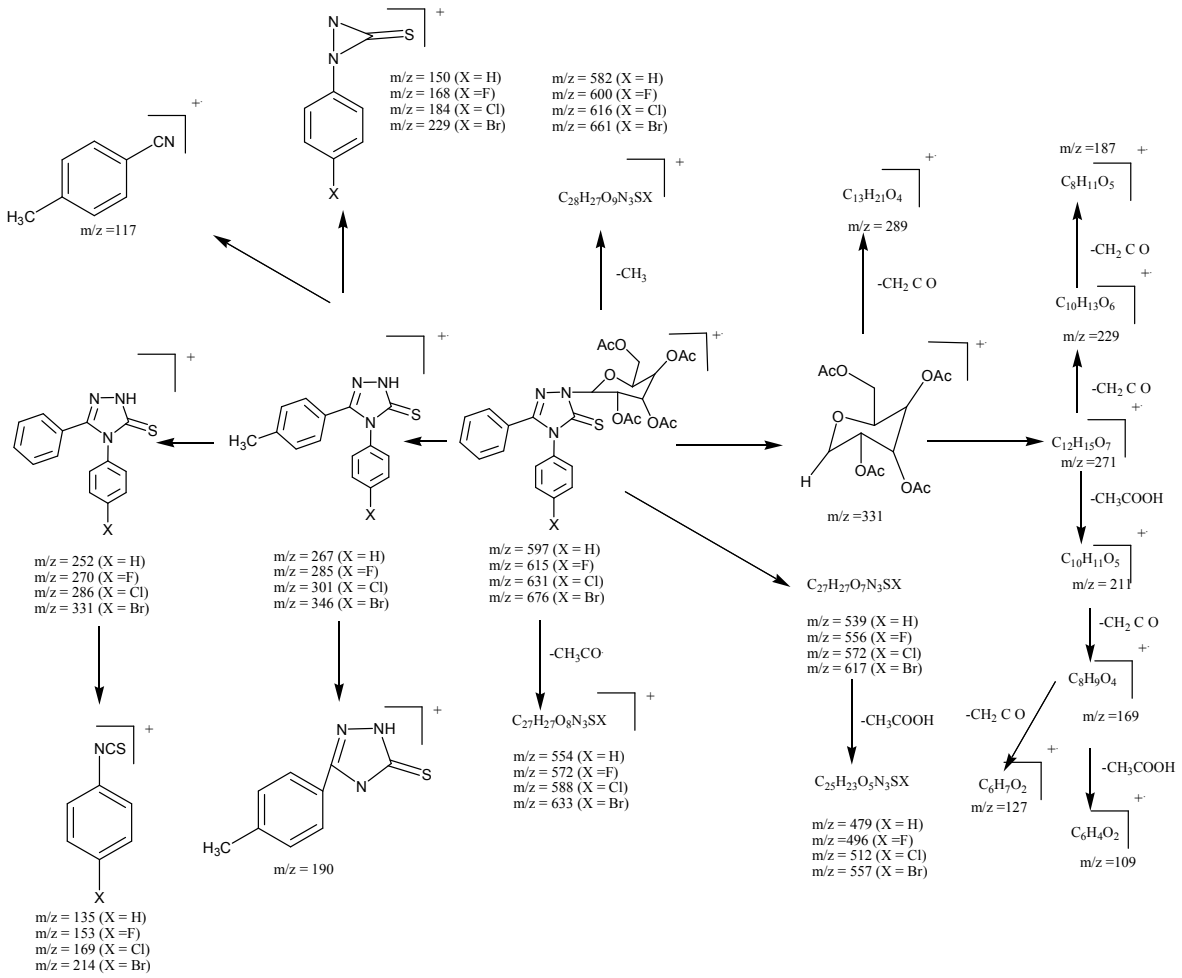

Figure 3: Mass Fragmentation pattern of Compound 4(e)(k)

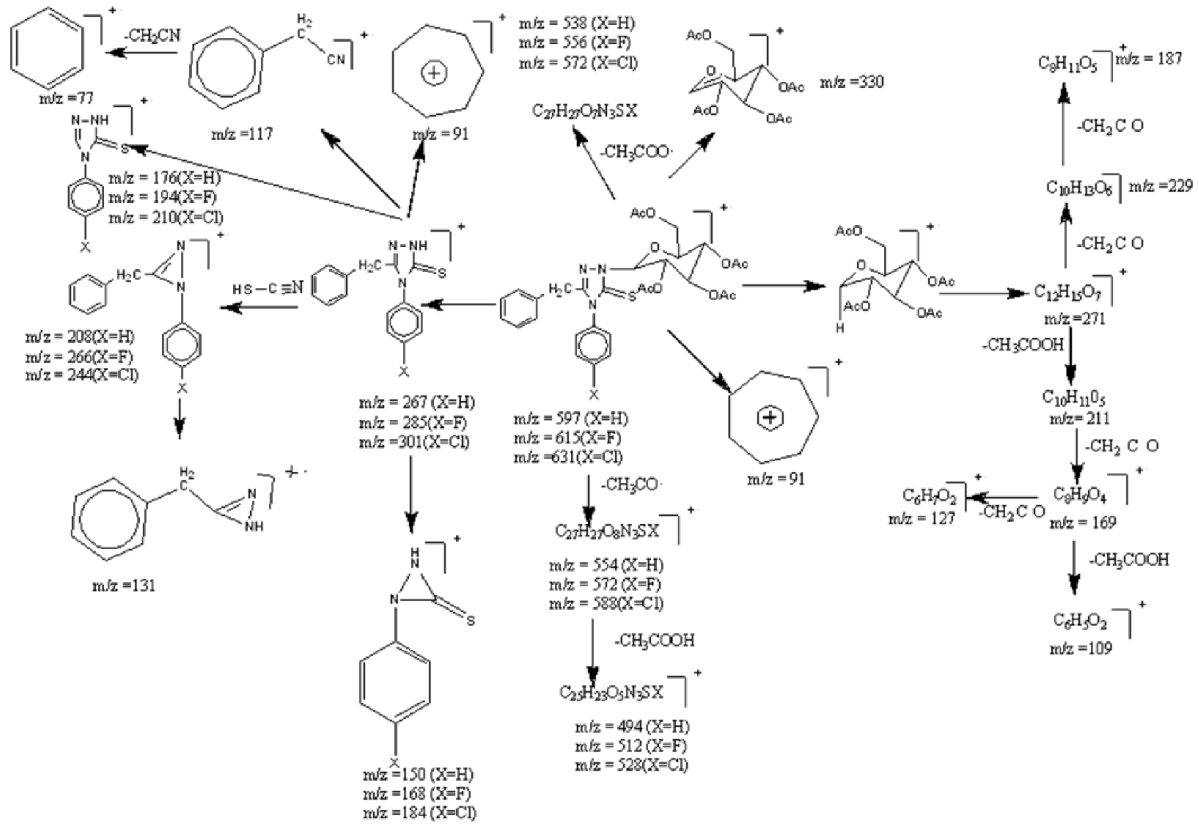

Figure 4: Mass Fragmentation pattern of Compound 4(f)(r)

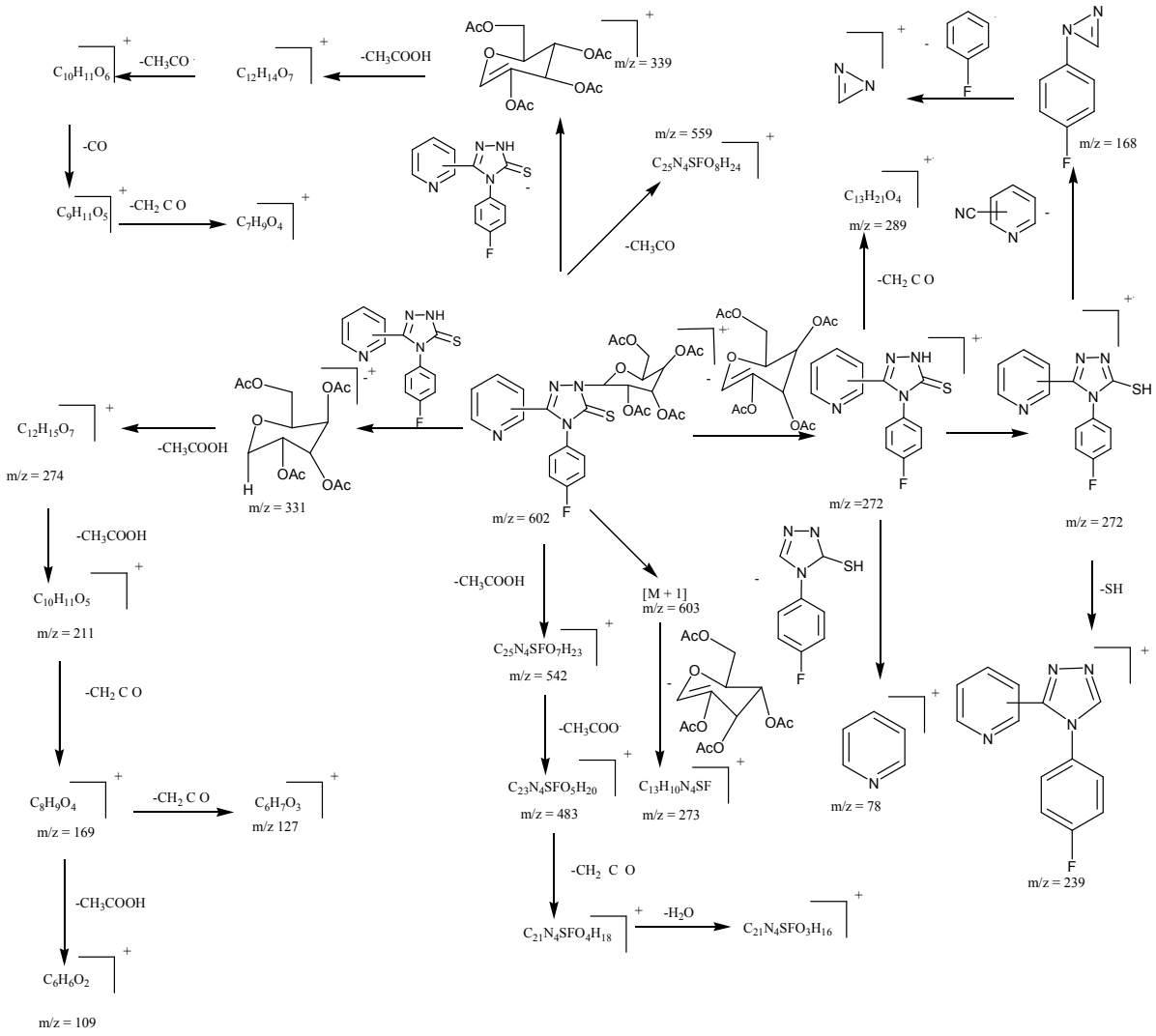

Figure 5: Mass Fragmentation pattern of Compound 4(h)(i)(j)

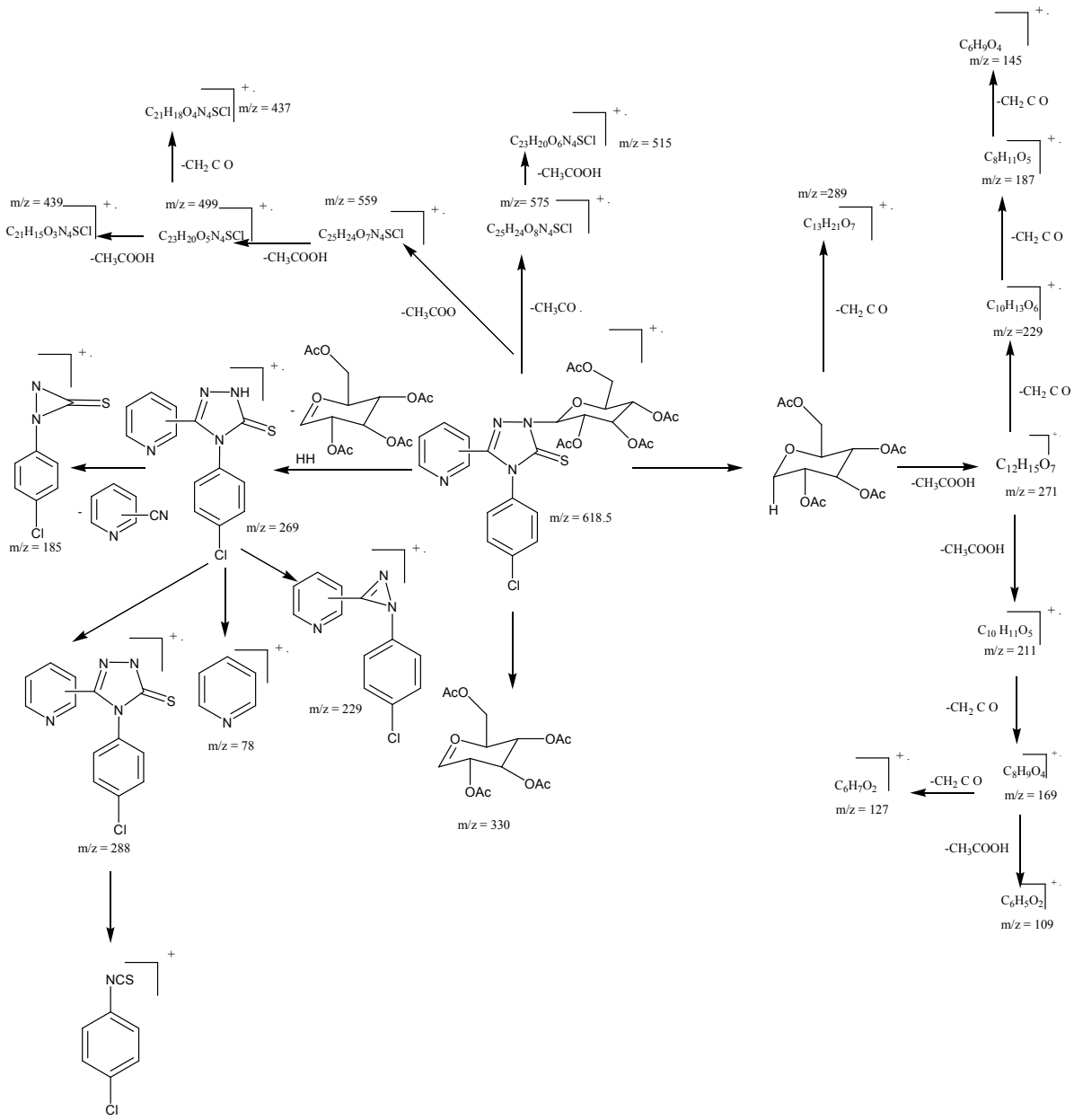

Figure 6: Mass Fragmentation pattern of Compound 4(n)(o)(p)

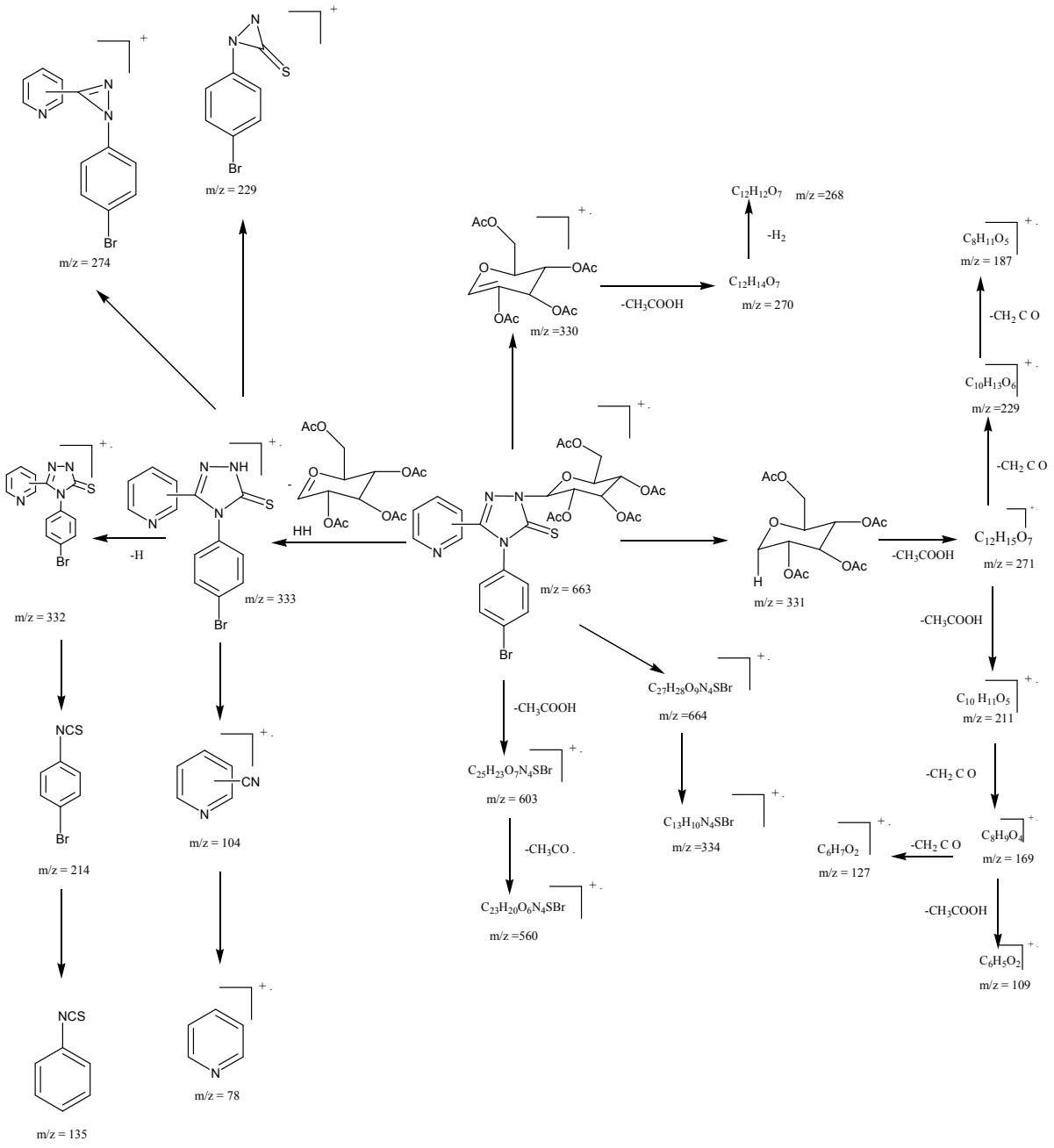

Figure 7: Mass Fragmentation pattern of Compound 4(t)(u)(v)

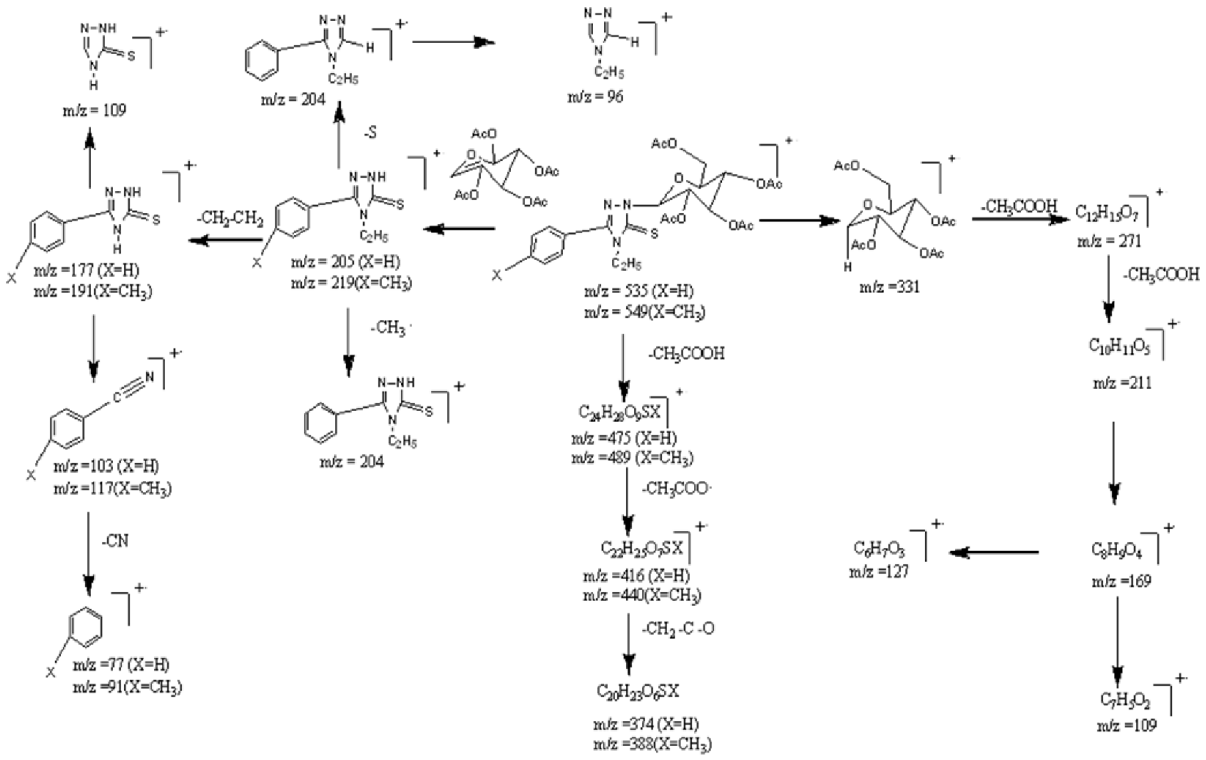

Figure 8: Mass Fragmentation pattern of Compound 4(x)(ab)

Mass fragmentation pattern of Amino derivatives of 1,2,4-triazole

4-amino-5-(2-pyridyl)-1,2,4-Triazole-3-thione (5a)

Table 1: Mass Spectrum of N-(2',3',4',6'-tetra-O-acetyl)-BETA-D-glucopyranosyl)-4-ethyl-5-(4-methylphenyl)-1,2,4-triazole-3-thione

A = ion abundance relative to base peak						
m/z	193*	162	122	119	111	105
A	100**	6.2	10.3	33.2	3.0	20.3
m/z	92	91	85	83	78	60
A	10.1	4.0	15.9	25.3	36.6	34.6

*Molecular ion peak
**Base peak

4-amino-5-(3-pyridyl)-1,2,4-Triazole-3-thione (5b)

Table 2: Mass Spectrum of 4-amino-5-(3-pyridyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	193*	162	135	122	118	105
A	100**	4.46	8.74	12.80	8.96	19.37
m/z	91	85	83	78	60	
A	5.39	13.15	20.2	23.4	34.9	

*Molecular ion peak
**Base peak

5-(4-Pyridyl)-4-amino-1,2,4-triazole-3-thione (5c)

Table 3: Mass Spectrum of 5-(4-Pyridyl)-4-amino-1,2,4-triazole-3-thione

A = ion abundance relative to base peak						
m/z	193*	162	122	119	111	105
A	100**	7.2	6.3	57	3	27.3
m/z	91	85	83	78	60	56
A	2	46.9	5.3	36.6	6.7	`8.6

*Molecular ion peak
**Base peak

4-amino-5-(4-methylphenyl)-1,2,4-Triazole-3-thione (5d)

Table 4: Mass Spectrum of 4-amino-5-(4-methylphenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	206*	191	175	160	135	132
A	100**	1.94	2.94	1.83	47.33	7.79
m/z	118	117	102	91	78	77
A	46.92	29.92	7.31	26.47	2.66	4.89
m/z	75	65	60	51		
A	1.76	14.47	29.14	6.73		

*Molecular ion peak
**Base peak

4-amino-5-(3,4,5-trimethoxyphenyl)-1,2,4-Triazole-3-thione (5e)

Table 5: Mass Spectrum of 4-amino-5-(3,4,5-trimethoxyphenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	296*	281	235	249	218	193
A	100**	36.70	5.31	1.72	2.16	21.49
m/z	178	150	135	120	118	105
A	19.34	10.23	10.35	11.69	6.57	1.51
m/z	103	93	90	77	74	64
A	15.50	2.80	3.23	3.39	8.62	8.43
m/z	60	50				
A	75.88	1.84				

*Molecular ion peak
**Base peak

4-amino-5-(4-fluorophenyl)-1,2,4-Triazole-3-thione (5f)

Table 6: Mass Spectrum of 4-amino-5-(4-fluorophenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	210*	209	194	180	178	138
A	100**	1.1	2.8	4.1	2.7	33.4
m/z	121	108	102	89	75	60
A	39.51	10.2	20.3	7.8	32.1	56.4

*Molecular ion peak
**Base peak

4-amino-5-(4-chlorophenyl)-1,2,4-Triazole-3-thione (5g)

Table 7: Mass Spectrum of 4-amino-5-(4-chlorophenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	226*	211	195	157	155	138
A	100**	1.16	3.70	14.56	40.92	38.91
m/z	137	127	125	113	111	102
A	35.47	2.17	7.04	11.14	22.80	26.85
m/z	95	89	76	75	60	50
A	3.68	9.52	11.01	29.27	54.81	17.83

*Molecular ion peak
**Base peak

4-amino-5-(4-bromophenyl)-1,2,4-Triazole-3-thione (5h)

Molecular ion peak and base peak for 4-amino-5-(4-bromophenyl)-1,2,4-Triazole-3-thione is m/z 270. Removal of amine from parent compound will give to m/z 255. Loss of N_2H_2 moiety will give to m/z 241. Elimination of Sulphur will produce m/z 239. Exclusion of 3H-diazirine-3-thione will produce m/z 199. Second most abandance of 4-amino-5-(4-bromophenyl)-1,2,4-Triazole-3-thione is methanethioimidic acid having m/z 60

Table 8: Mass Spectrum of 4-amino-5-(4-bromophenyl)-1,2,4-Triazole-3-thione

A = ion abundance relative to base peak						
m/z	271	270*	255	241	239	199
A	38	100**	2.6	1.2	4.5	42.7
m/z	182	142	155	102	75	60
A	15.3	16.8	2.7	31.2	67.8	73.2

*Molecular ion peak
**Base peak

Pharmacological activities of Amino derivatives of 1,2,4-triazole

Compound 5(c), 5(d) and 5(g) are least affective anti-bacterial having only active against Shigella flexnari and Pseudomonas aeruginosa.

Table 1: Anti-bacterial activities of selected compounds

Compounds	Bacillus subtiles	Staphylococcus aureus	Escherichia colai	Shigella flexnari	Pseudomonas aeruginosa	Salmonella typhi
5a	12	n.a	11	n.a	22	n.a
5b	n.a	n.a	10	19	20	n.a
5c	n.a	n.a	n.a	16	10	n.a
5d	n.a	n.a	n.a	18	17	n.a
5e	10	n.a	12	15	21	n.a
5g	n.a	n.a	n.a	11	22	n.a
5h	12	n.a	15	10	12	n.a
Standard*	33	33	30	27	24	25

Concentration used 3.00 mg/mL of DMSO
Standard drug = Imipenem
n.a = No activity
Size of well = 6mm (dia)

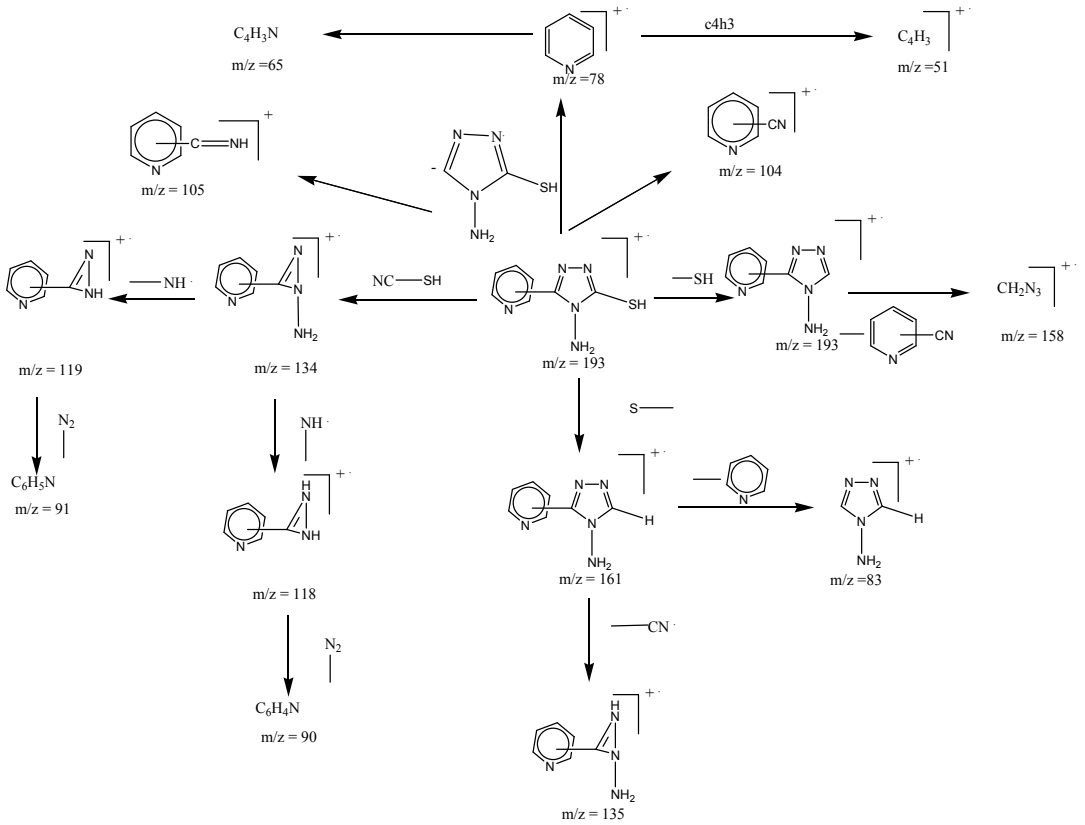

Figure 1: Mass Fragmentation pattern of Compound 5(a), 5(b), 5(c)

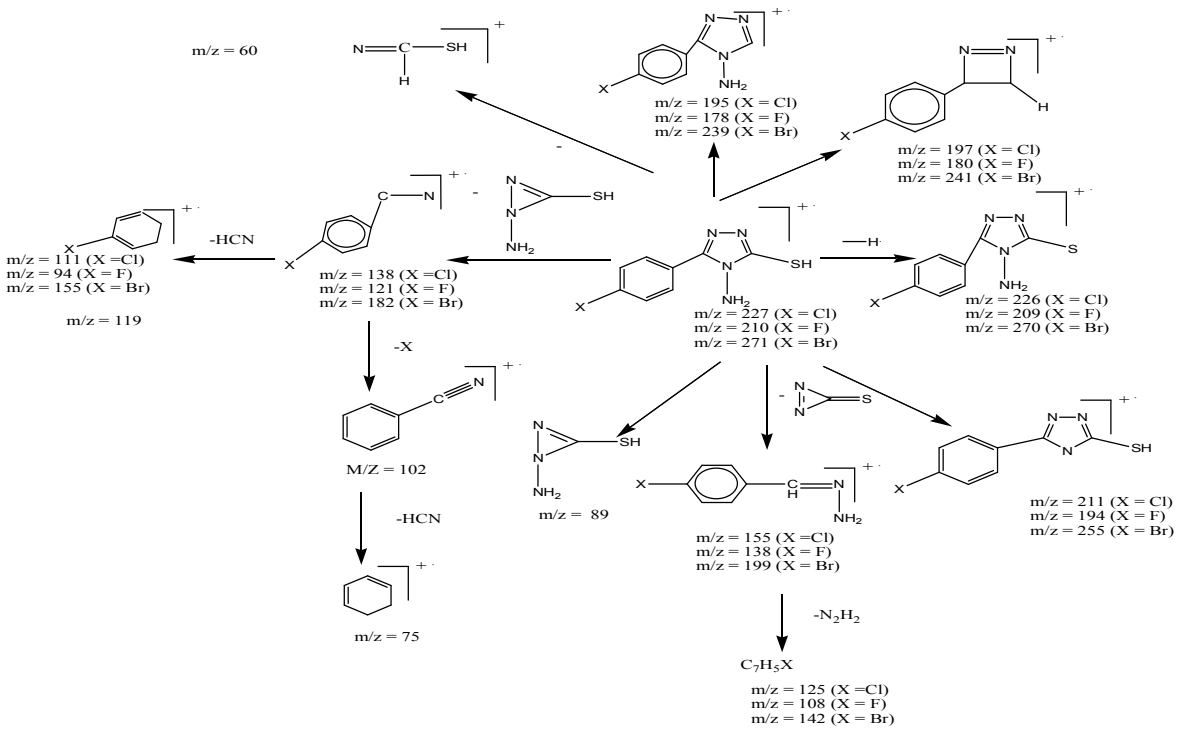

Figure 2: Mass Fragmentation pattern of 5(f), 5(g), 5(h)

CONCLUSION:

We have documented Mass Spectrometric Fragmentation and Pharmacological activities of 1,2,4 triazole derivatives. Triazole is pharmacologically active compounds containing numurous activities such as antifungal [3][4][5], diuretic [6][7],anti-bacterial [8], hypoglycemic [9], antitubular [10], anti-depressant [11], anti-amoebic [12], anti-biotic [13], anti- inflammatory [14], anti-carcinogenic [15], hypnotic [16] and sedative [17]. We conclude Mass spectrum of mercaptoacetic acid, quinoline, Schiff base ligand, Glucopyrnaosyl and amino derivatives of 1,2,4 triazole .

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