In-vitro antimicrobial activity and anticancer potential of novel synthesized carbamothioyl-furan-2-carboxamide derivatives

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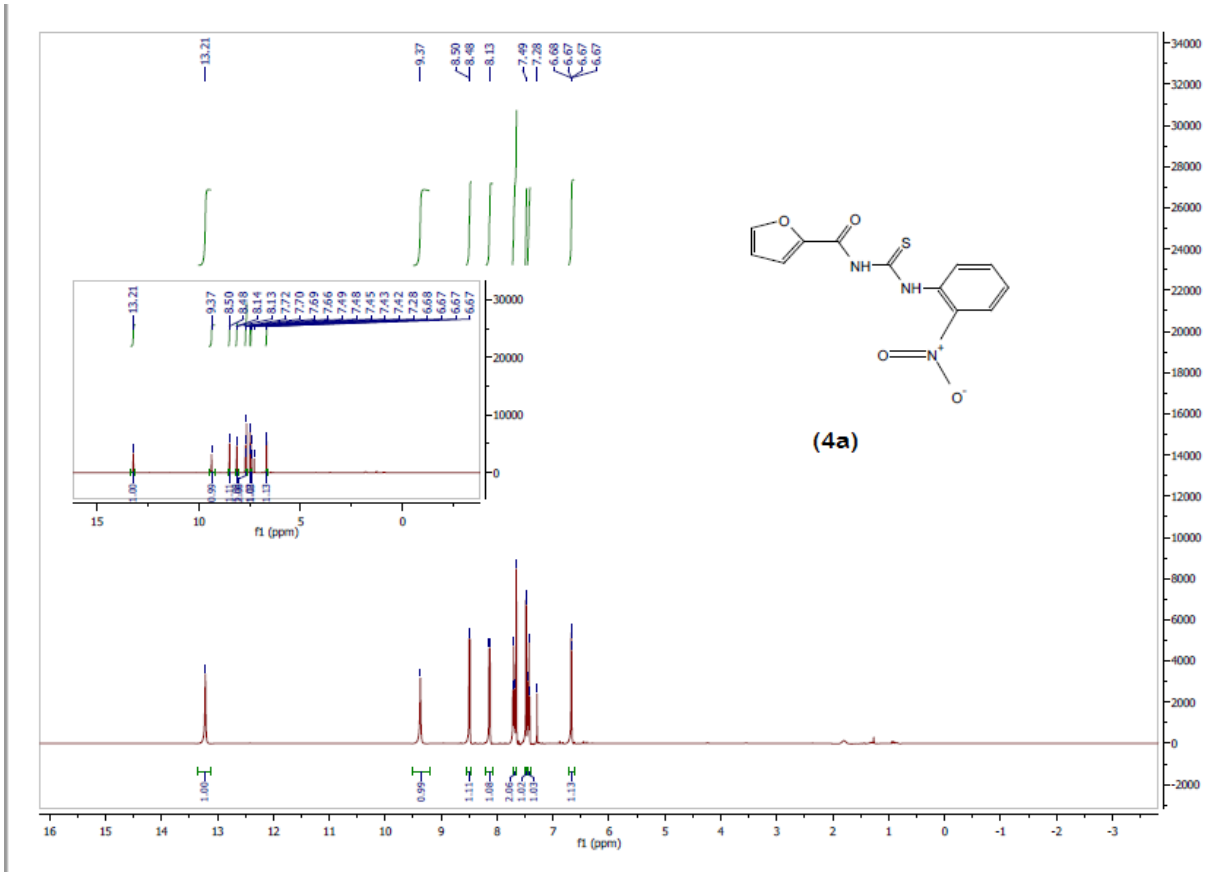
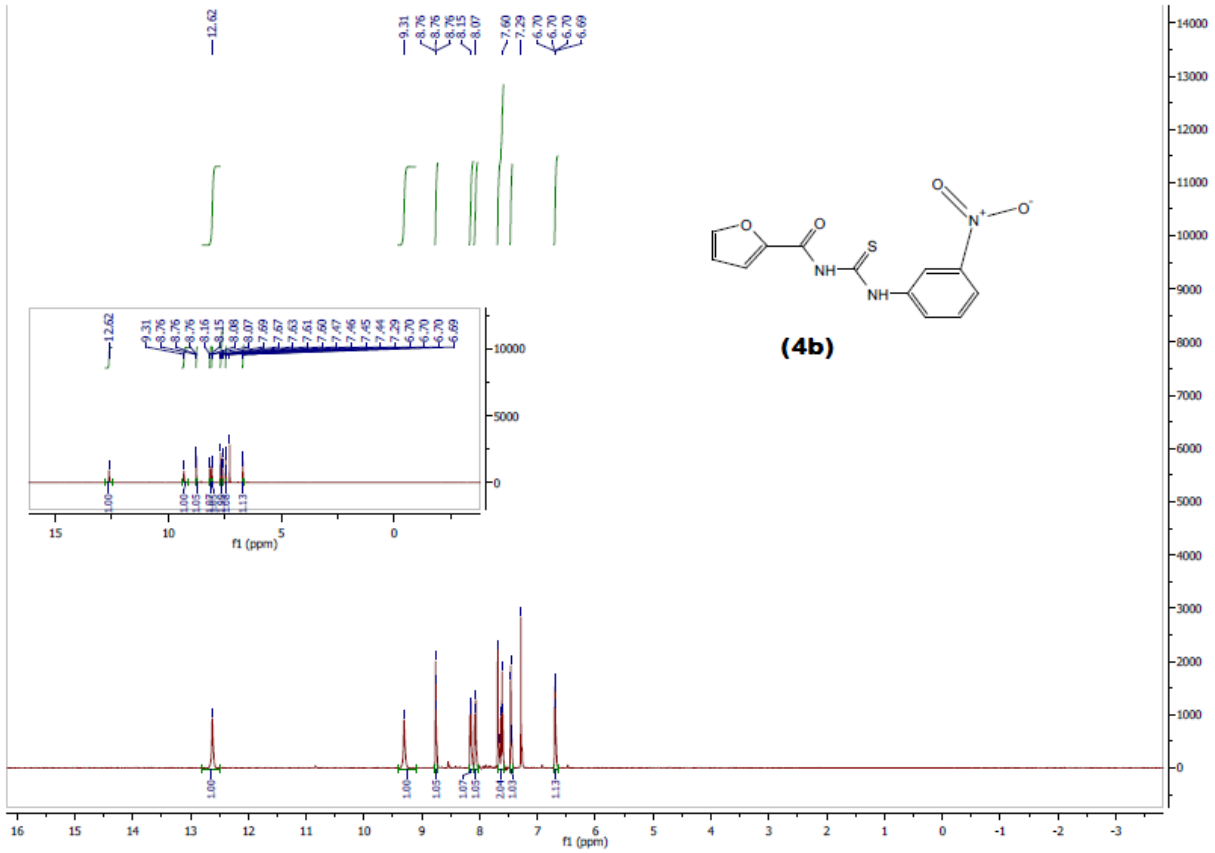
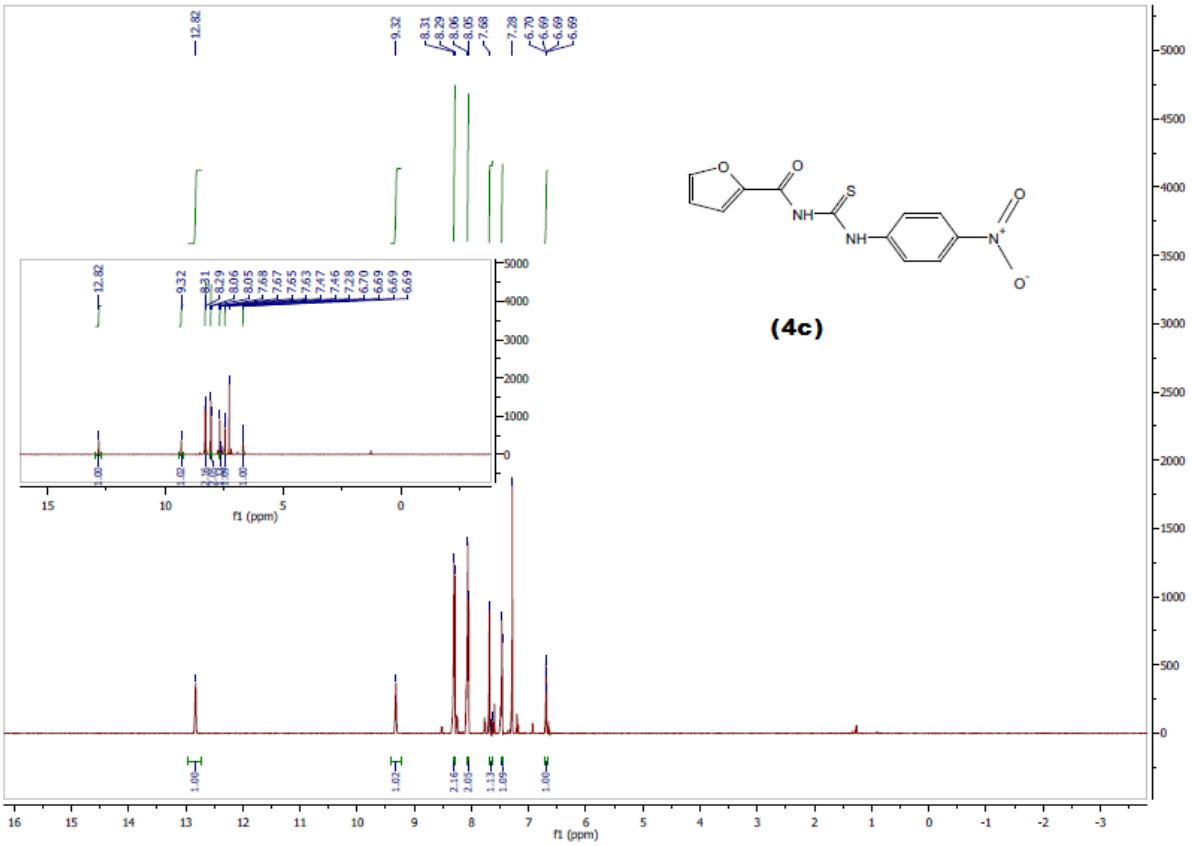


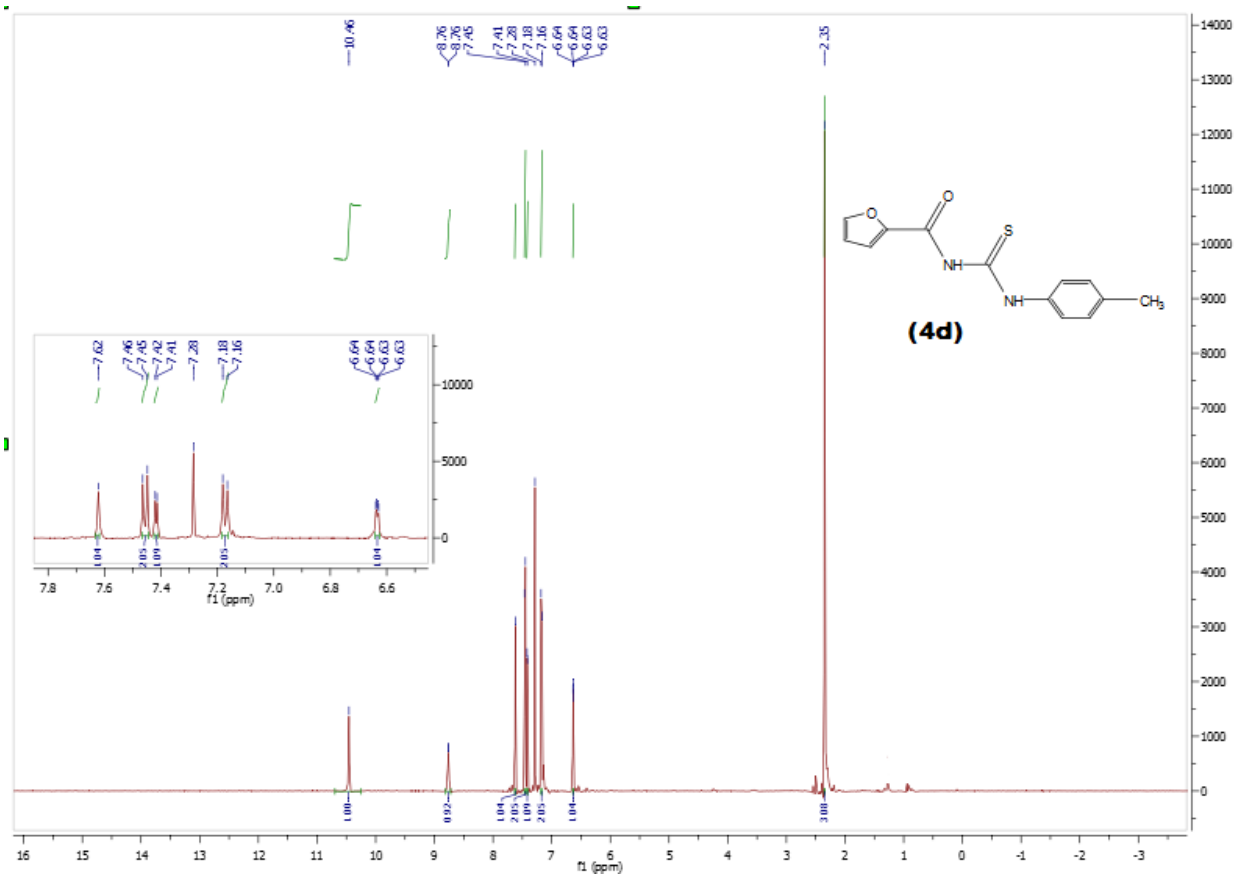
Proton NMR of 4a



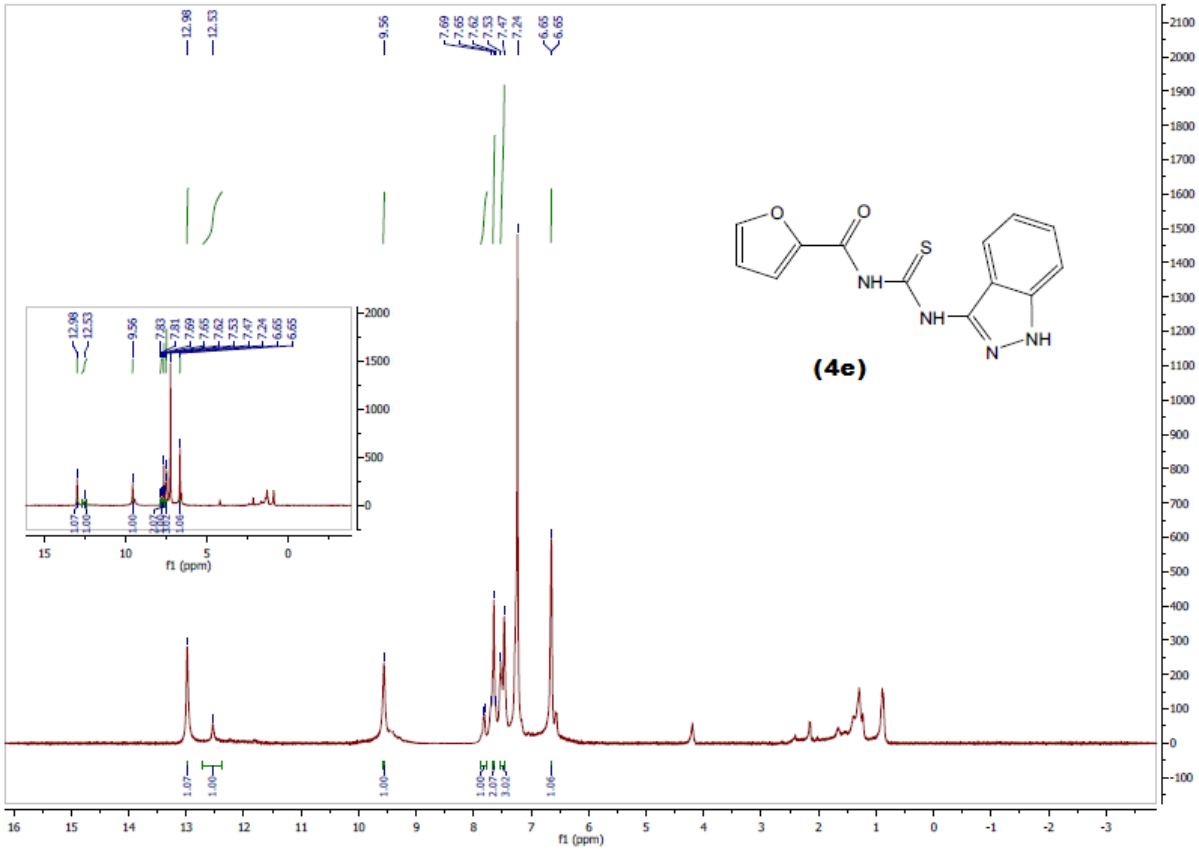
Proton NMR of 4b



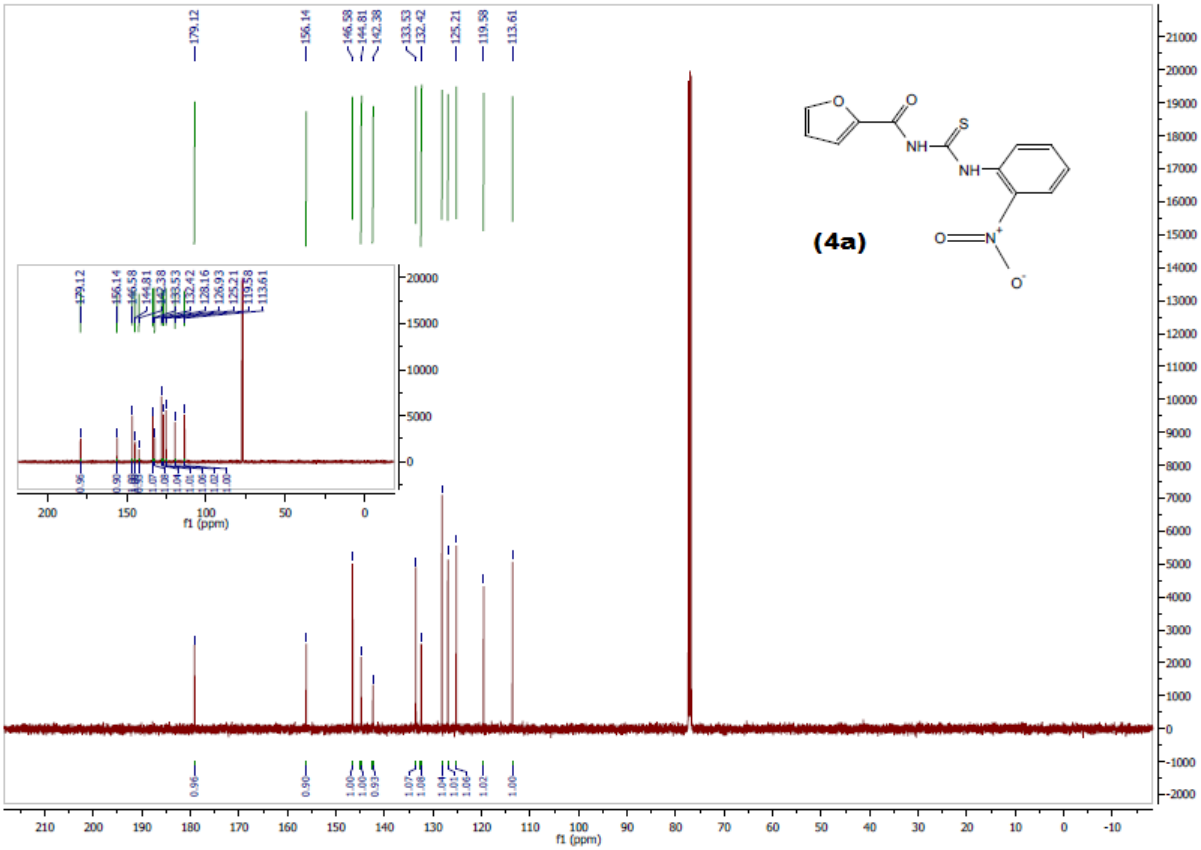
Proton NMR of 4c



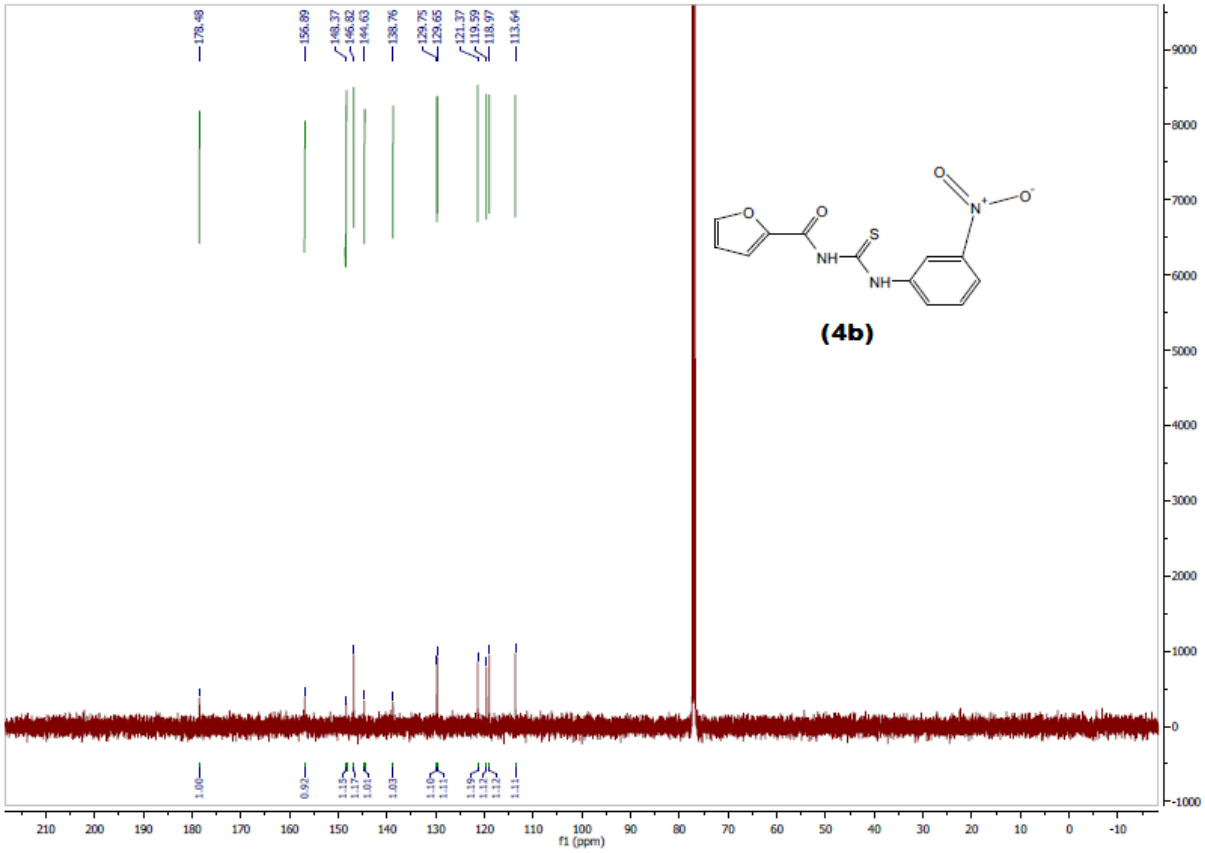
Proton NMR of 4d



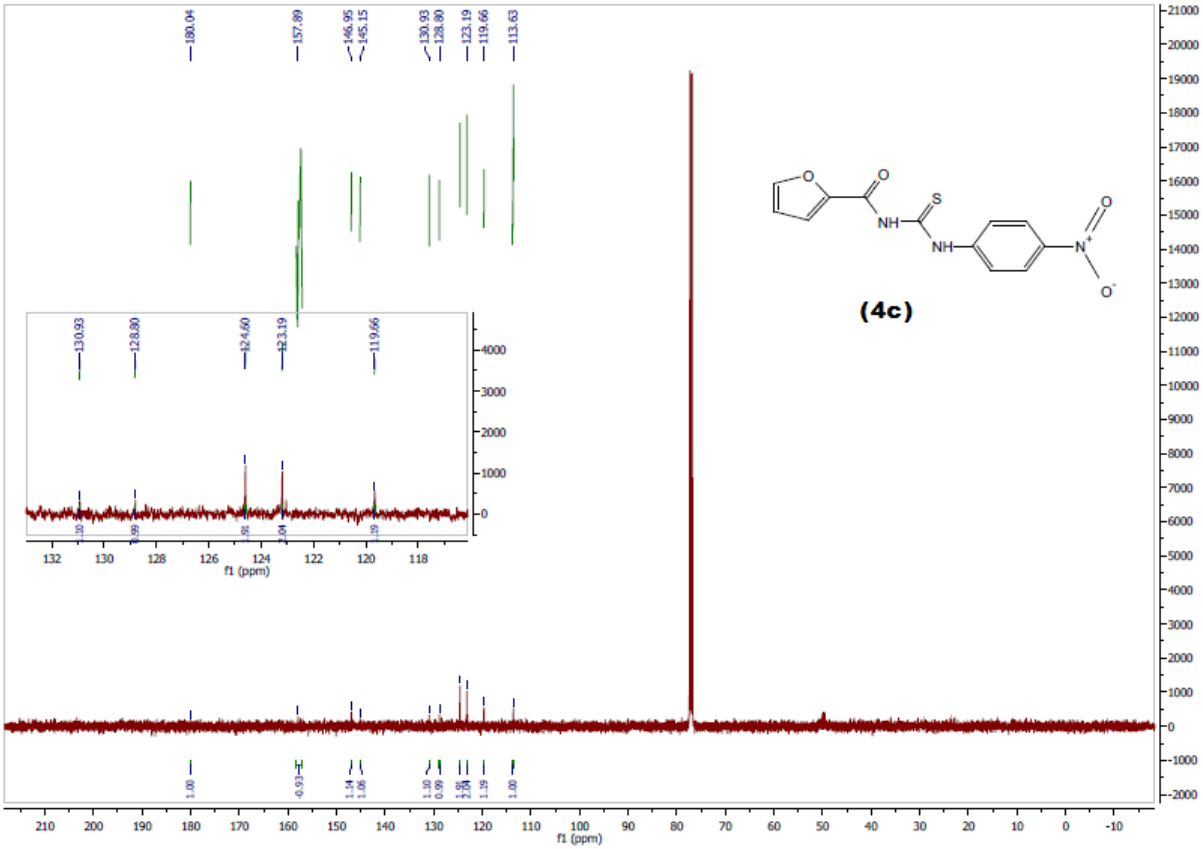
Proton NMR of 4e



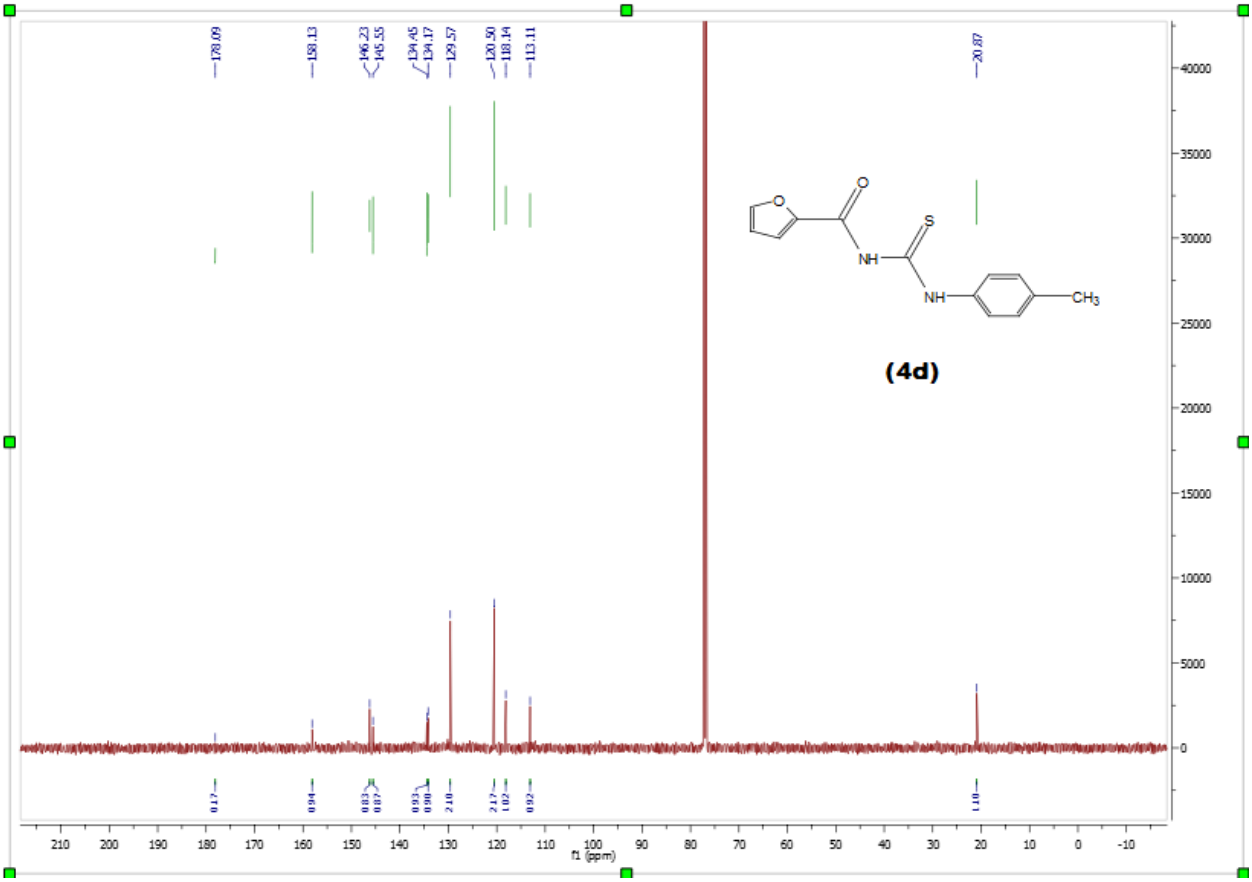
Carbon NMR of 4a



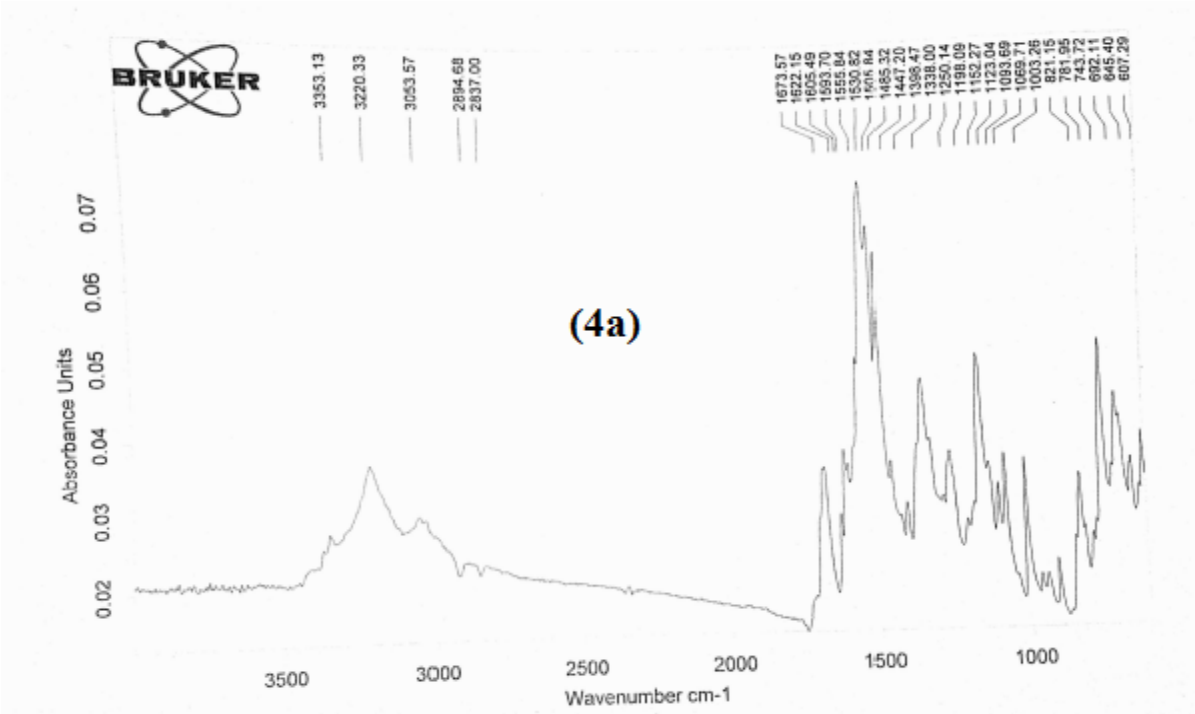
Carbon NMR of 4b



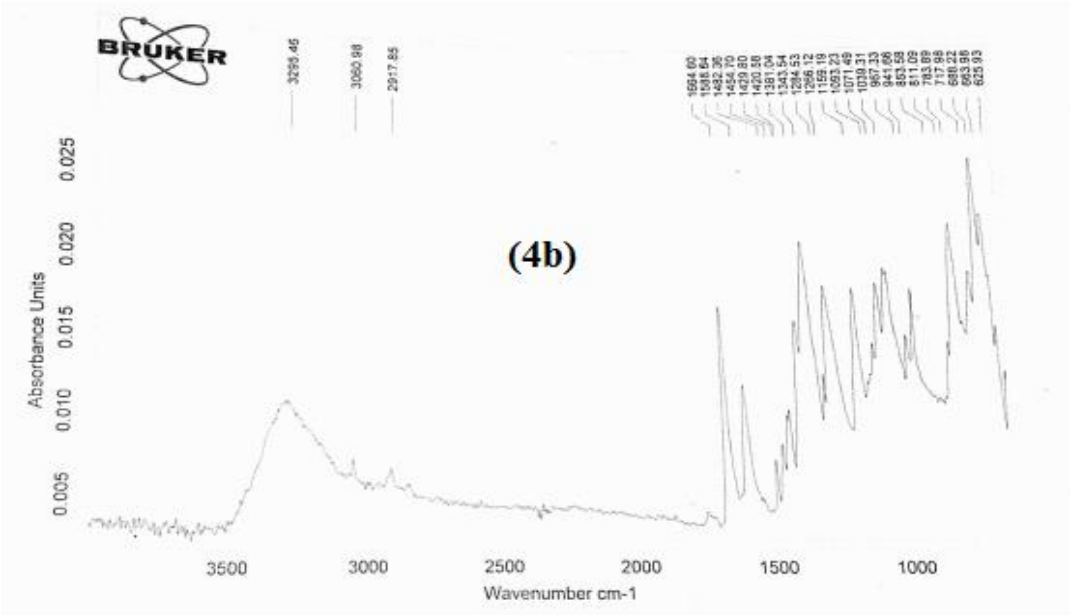
Carbon NMR of 4c



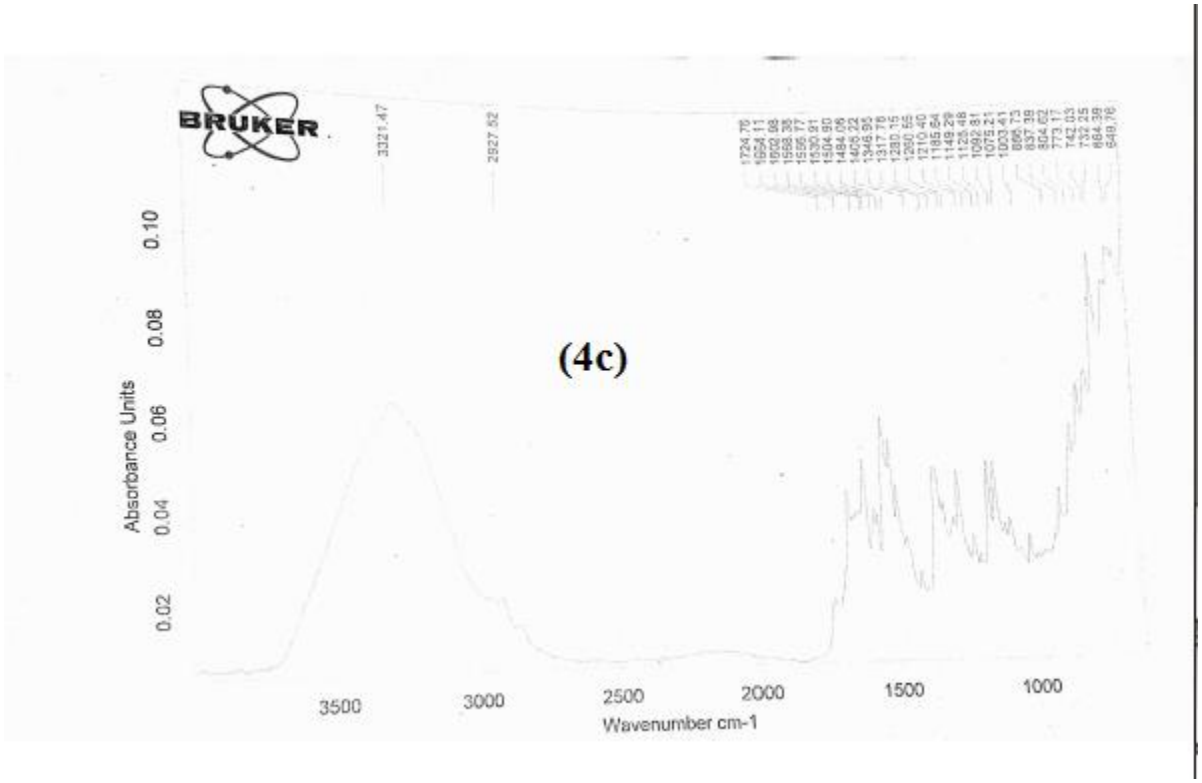
Carbon NMR of 4d



I.R spectrum of 4a



I.R spectrum of 4b



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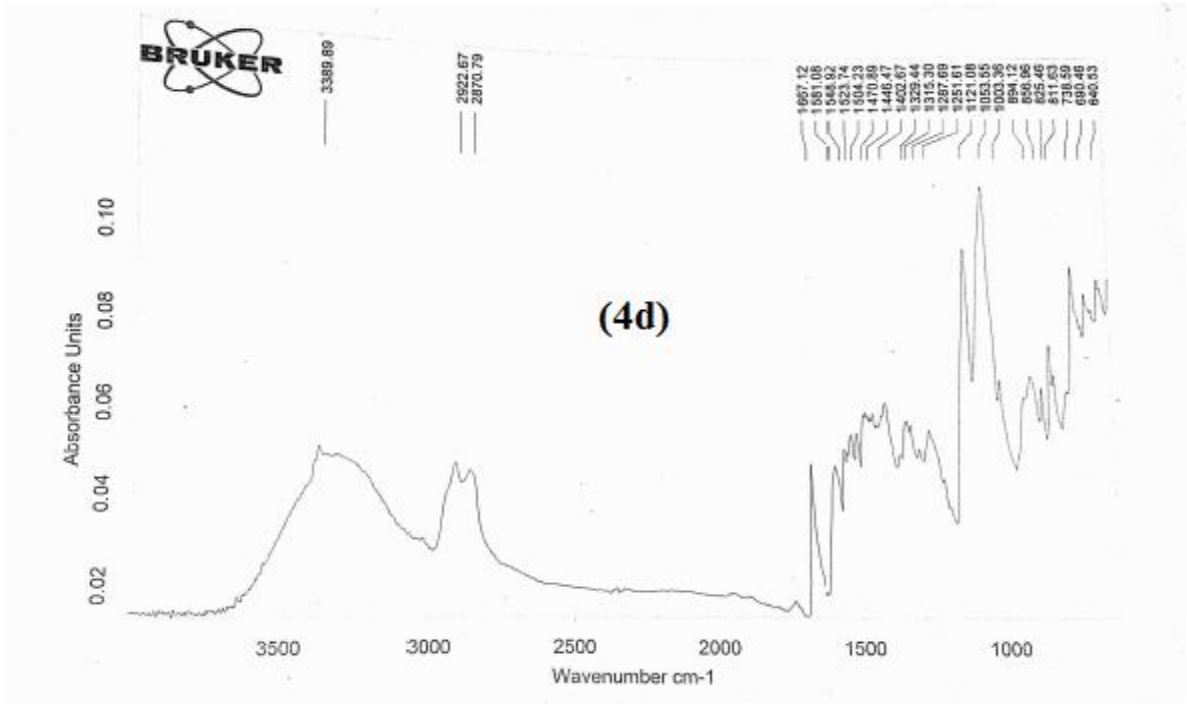

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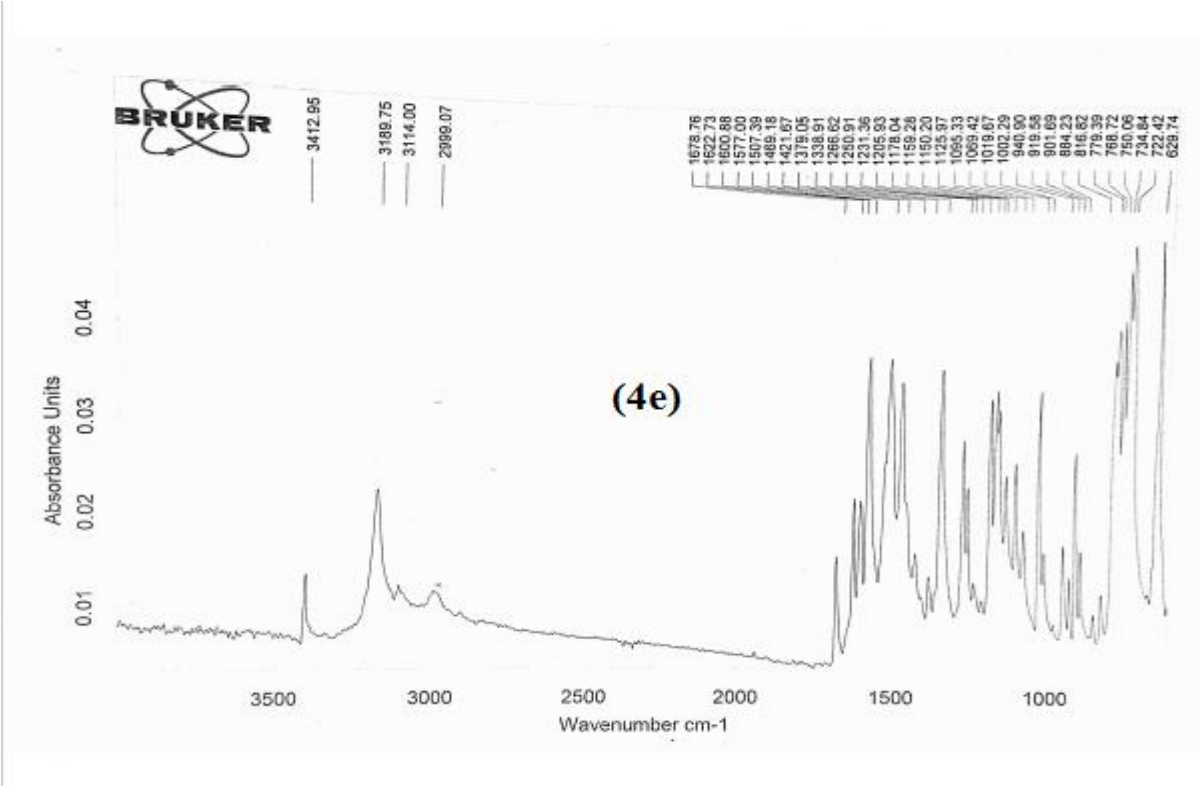
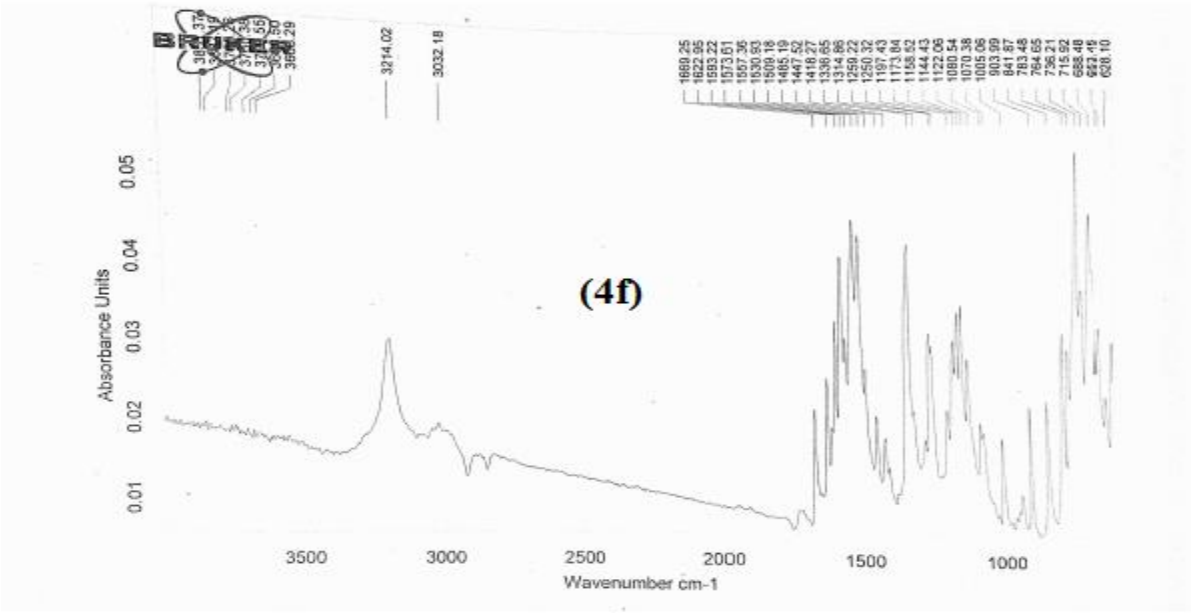
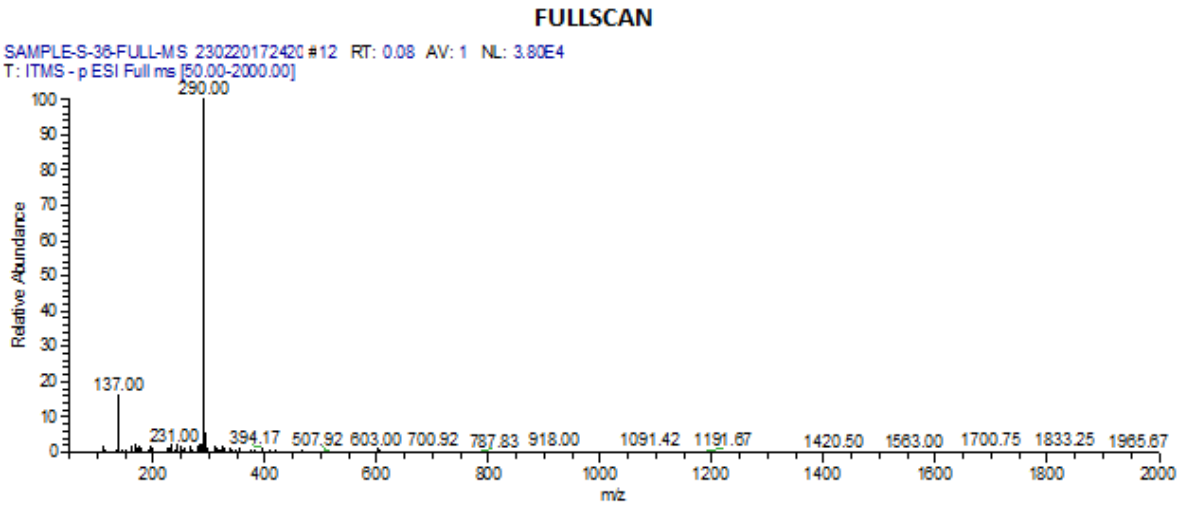


I.R spectrum of 4e

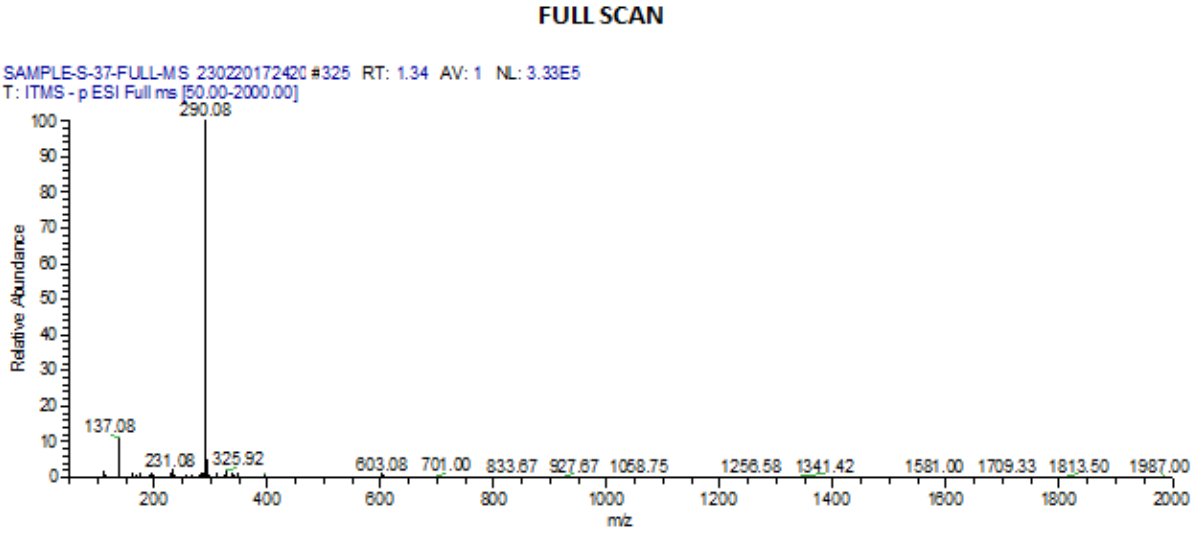


I.R spectrum of 4f

LC/MS Spectra of synthesized molecules

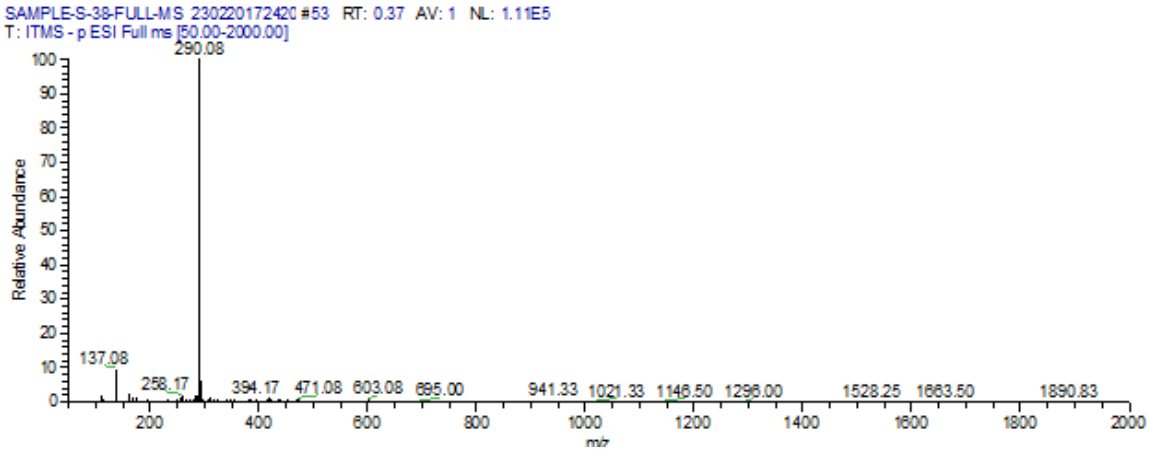


LC/MS Spectra of 4a



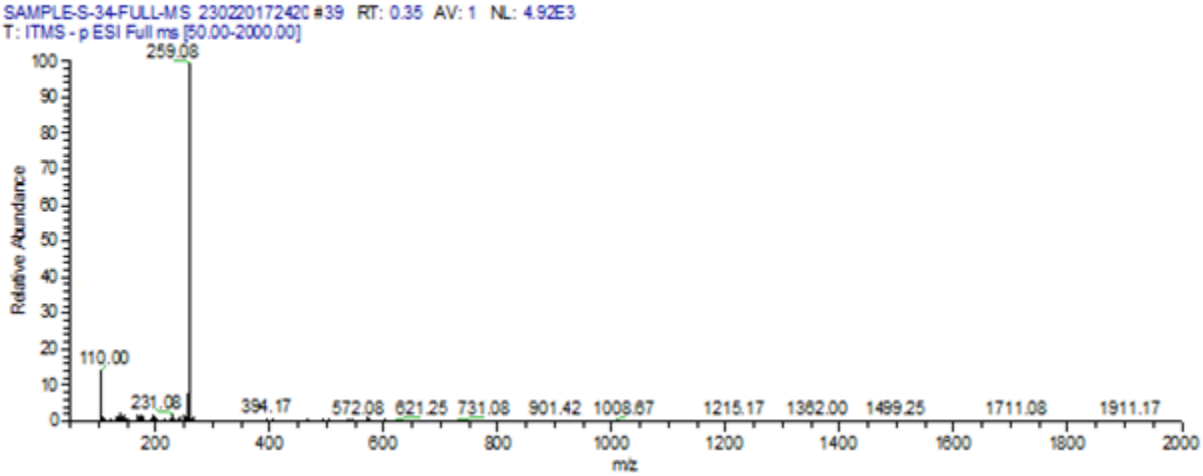
LC/MS Spectra of 4b

FULL SCAN

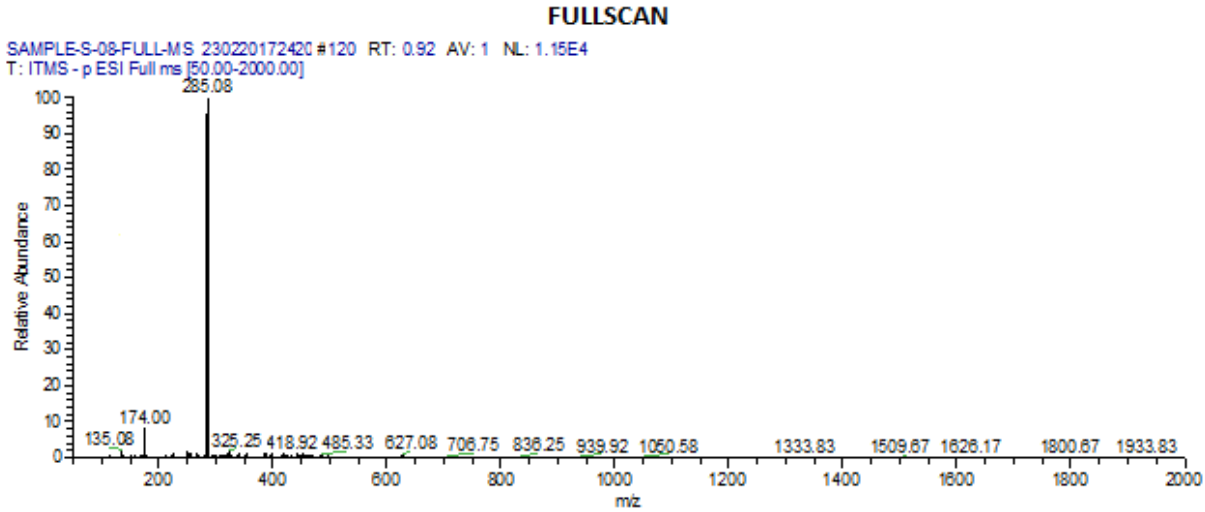


LC/MS Spectra of 4c

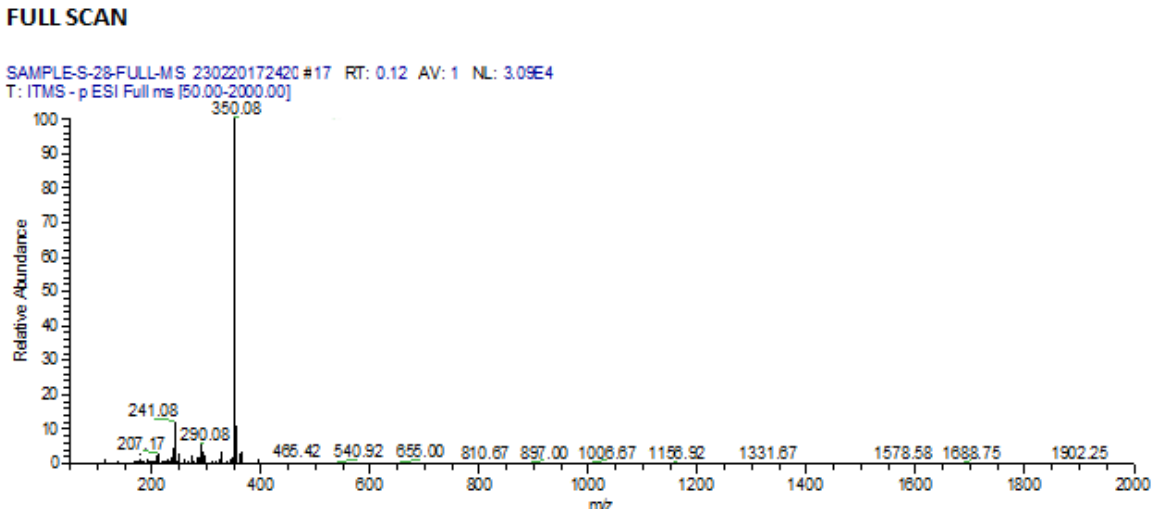
FULLSCAN



LC/MS Spectra of 4d



LC/MS Spectra of 4e



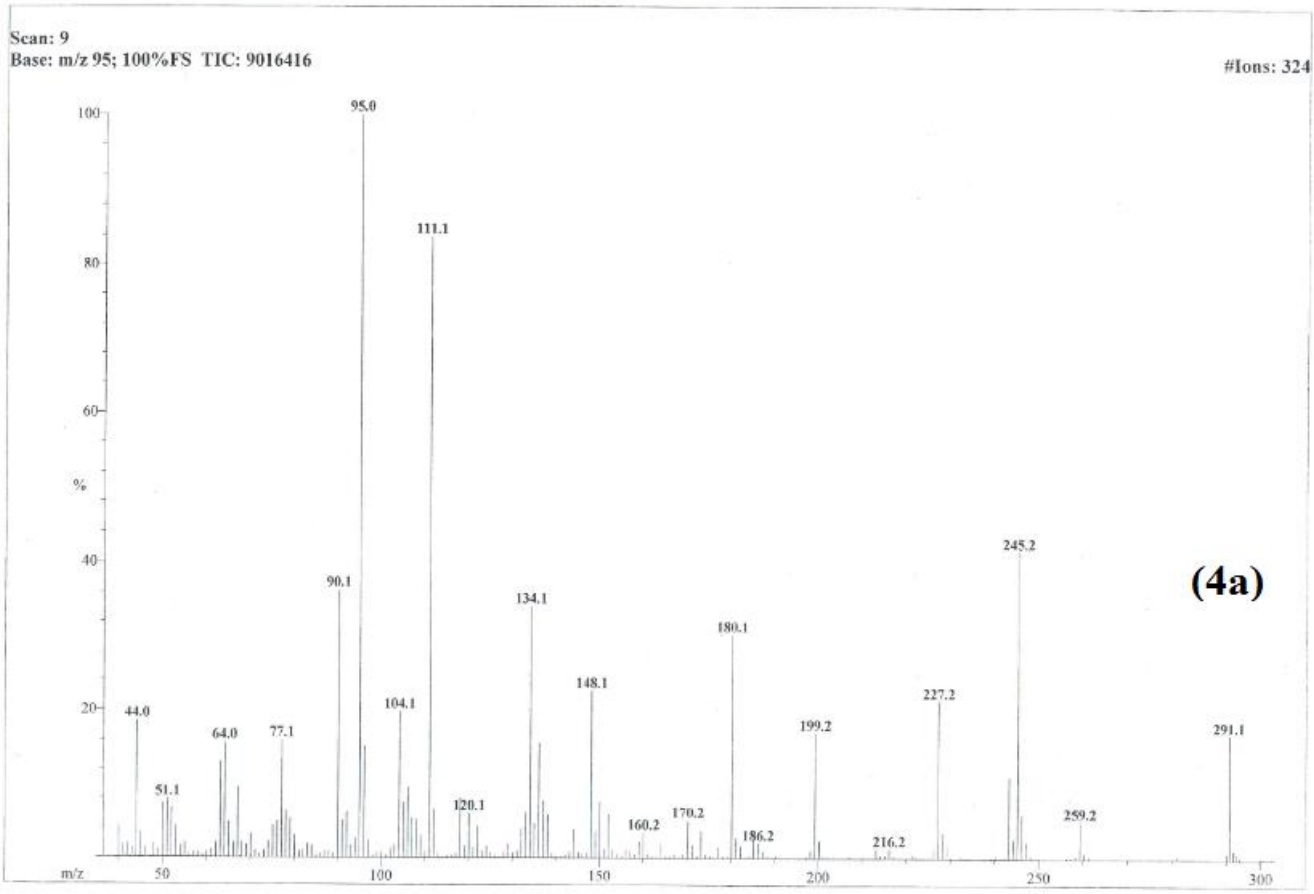
LC/MS Spectra of 4f

EI-HR-MS data of synthesized molecules

Instrument: JEOL JMS 600H-1
Inlet: Direct Probe

Ionization mode: EI+

Run By: MASS LAB 104

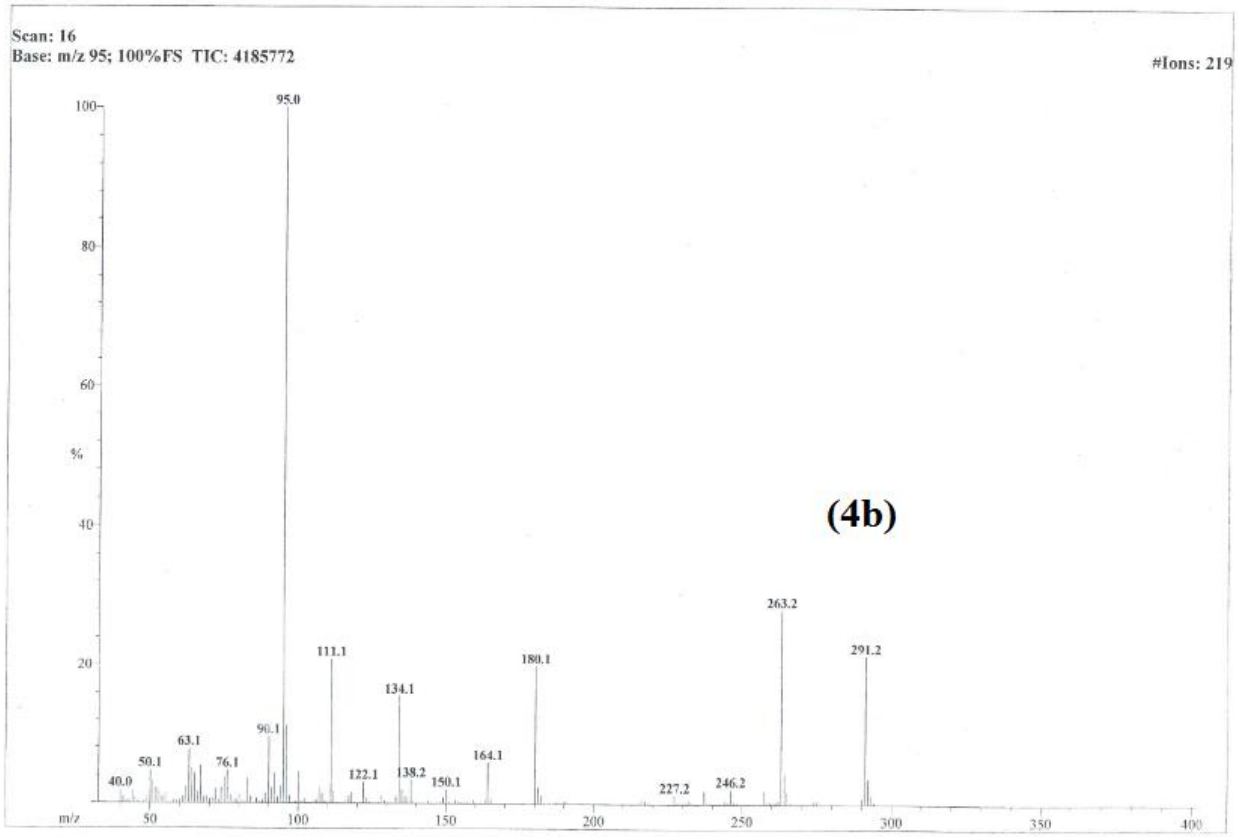


Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
290.0161	0.1	290.0157	1.4	0.4	24.0	$C_{24}H_2$
		290.0150	3.7	1.1	15.0	$C_{16}H_6O_2N_2S_1$
		290.0190	-10.2	-3.0	19.0	$C_{21}H_6S_1$
		290.0202	-14.2	-4.1	15.5	$C_{15}H_4O_4N_3$
291.0297	1.9	291.0314	-5.8	-1.7	10.0	$C_{12}H_9O_4N_3S_1$
		291.0280	5.8	1.7	15.0	$C_{15}H_5O_4N_3$
		291.0320	-8.0	-2.3	19.0	$C_{20}H_5O_2N_1$
		291.0268	9.8	2.9	18.5	$C_{21}H_7S_1$

Instrument: JEOL JMS 600H-1
Inlet: Direct Probe

Ionization mode: EI+

Run By: MASS LAB 104

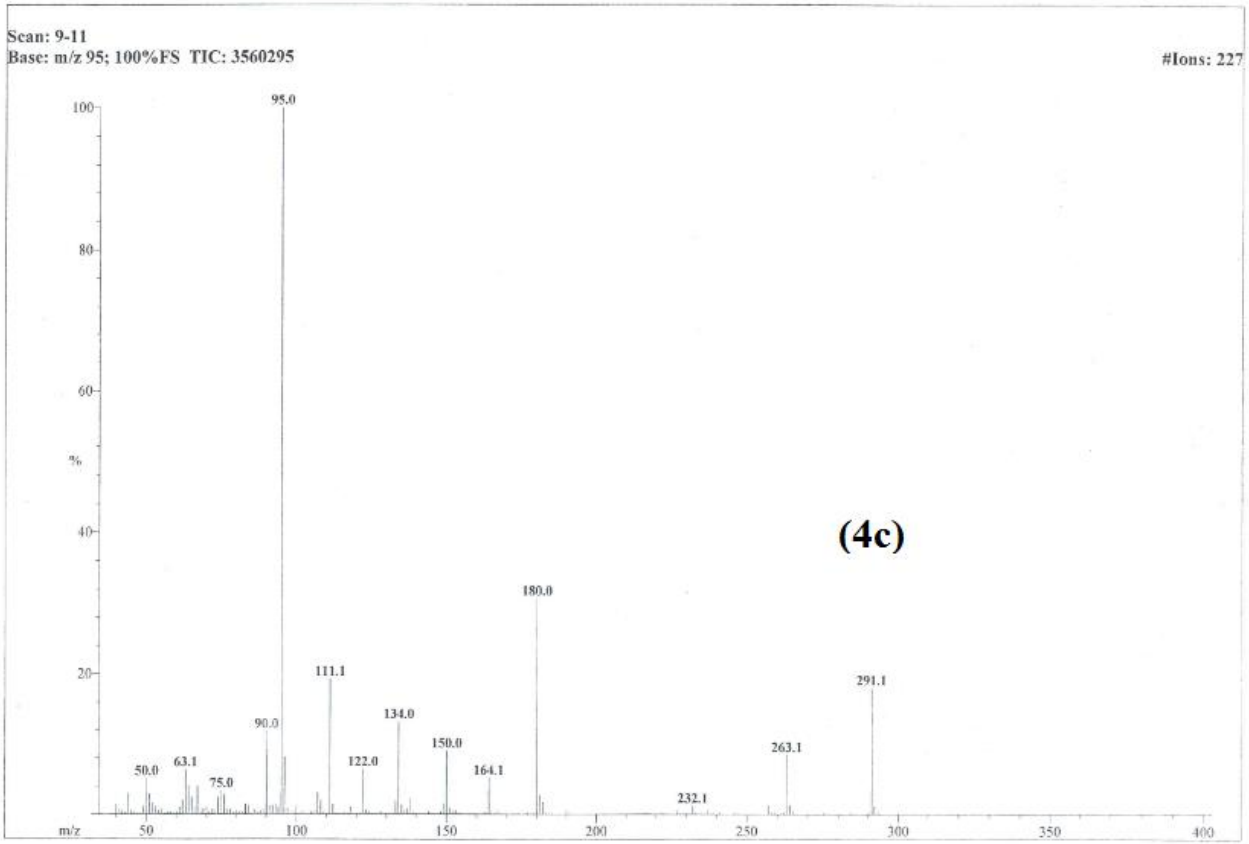


Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		232.0181	-5.8	-1.3	9.5	$C_{10}H_6O_2N_3S_1$
		232.0187	-8.6	-2.0	18.5	$C_{18}H_2N_1$
		232.0147	8.8	2.0	14.5	$C_{13}H_2O_2N_3$
237.0129	0.8	237.0123	2.8	0.7	12.5	$C_{13}H_5O_1N_2S_1$
		237.0096	14.1	3.3	8.0	$C_{10}H_7O_4N_1S_1$
		237.0089	17.0	4.0	17.5	$C_{16}H_1O_1N_2$
		237.0174	-19.0	-4.5	13.0	$C_{12}H_3O_3N_3$
246.0340	0.6	246.0337	1.0	0.3	9.5	$C_{11}H_8O_2N_3S_1$
		246.0344	-1.6	-0.4	18.5	$C_{19}H_4N_1$
		246.0351	-4.4	-1.1	9.0	$C_{13}H_{10}O_3S_1$
		246.0317	9.3	2.3	14.0	$C_{16}H_6O_3$
263.0365	5.4	263.0365	0.3	0.1	9.0	$C_{11}H_9O_3N_3S_1$
		263.0371	-2.1	-0.6	18.0	$C_{19}H_5O_1N_1$
		263.0378	-4.8	-1.3	8.5	$C_{13}H_{11}O_4S_1$
		263.0344	8.0	2.1	13.5	$C_{16}H_7O_4$
264.0375	0.7	264.0357	6.8	1.8	13.0	$C_{15}H_8O_1N_2S_1$
		264.0409	-12.8	-3.4	13.5	$C_{14}H_6O_3N_3$
		264.0331	17.0	4.5	8.5	$C_{12}H_{10}O_4N_1S_1$
		264.0423	-17.9	-4.7	13.0	$C_{16}H_8O_4$
279.1622	2.6	279.1623	-0.2	-0.1	10.0	$C_{19}H_{21}O_1N_1$
		279.1617	2.1	0.6	1.0	$C_{11}H_{25}O_3N_3S_1$
		279.1630	-2.7	-0.8	0.5	$C_{13}H_{27}O_4S_1$
		279.1596	9.4	2.6	5.5	$C_{16}H_{23}O_4$
291.0326	3.7	291.0320	2.0	0.6	19.0	$C_{20}H_5O_2N_1$
		291.0314	4.3	1.2	10.0	$C_{12}H_9O_4N_3S_1$
		291.0354	-9.5	-2.8	14.0	$C_{17}H_9O_2N_1S_1$
		291.0280	15.9	4.6	15.0	$C_{15}H_5O_4N_3$
292.0261	0.5	292.0273	-4.0	-1.2	19.0	$C_{10}H_4O_5N_2$
		292.0221	13.8	4.0	18.5	$C_{20}H_6N_1S_1$
		292.0306	-15.5	-4.5	14.0	$C_{16}H_8O_2N_2S_1$
		292.0313	-17.7	-5.2	23.0	$C_{24}H_4$

Instrument: JEOL JMS 600H-1
Inlet: Direct Probe

Ionization mode: EI+

Run By: MASS LAB 104

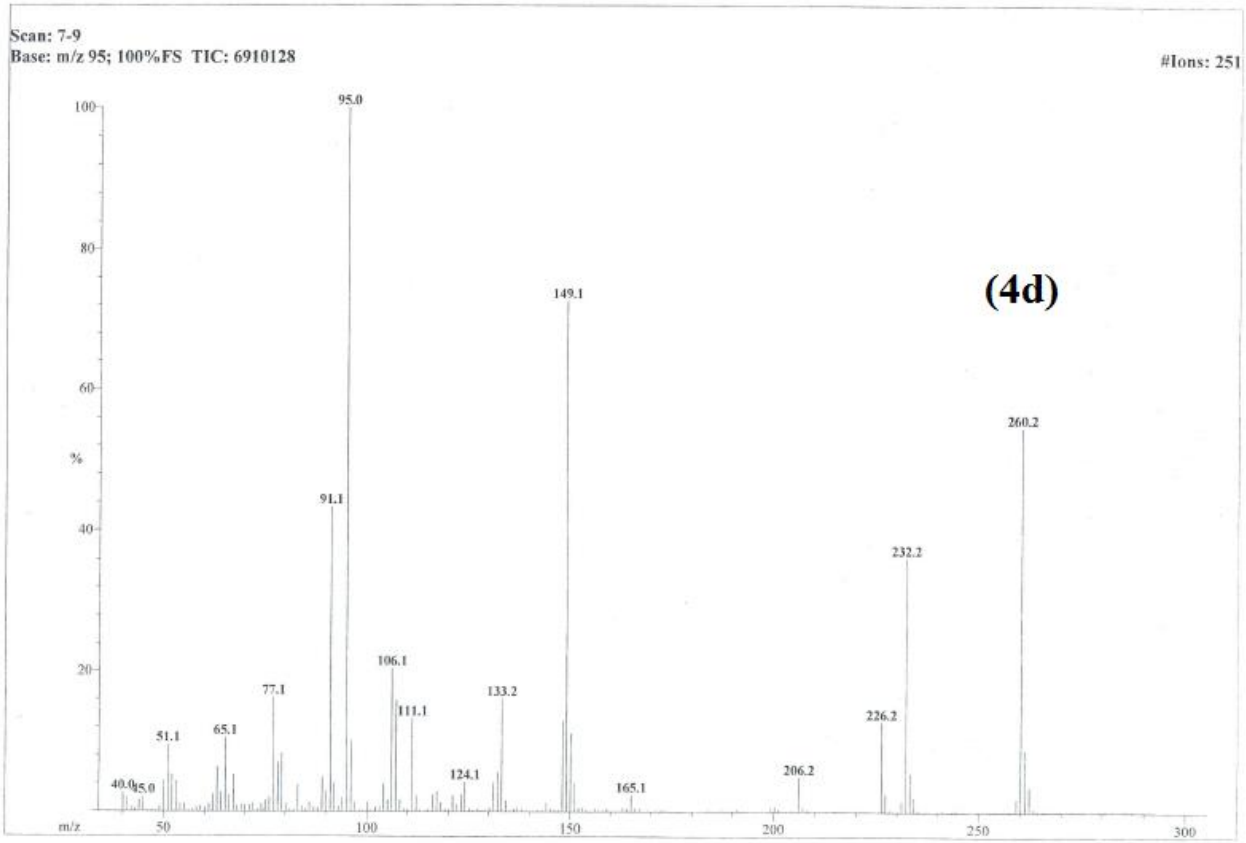


Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		232.0518	-18.5	-4.3	4.0	$C_8 H_{12} O_4 N_2 S_1$
		232.0524	-21.3	-4.9	13.0	$C_{16} H_8 O_2$
		232.0545	-30.0	-7.0	8.5	$C_{11} H_{10} O_1 N_3 S_1$
263.0362	8.9	263.0365	-1.2	-0.3	9.0	$C_{11} H_9 O_3 N_3 S_1$
		263.0371	-3.6	-1.0	18.0	$C_{19} H_5 O_1 N_1$
		263.0378	-6.3	-1.6	8.5	$C_{13} H_{11} O_4 S_1$
		263.0344	6.5	1.7	13.5	$C_{16} H_7 O_4$
		263.0331	11.6	3.1	14.0	$C_{14} H_5 O_3 N_3$
		263.0405	-16.5	-4.3	13.0	$C_{16} H_9 O_1 N_1 S_1$
264.0365	1.3	264.0357	2.7	0.7	13.0	$C_{15} H_8 O_1 N_2 S_1$
		264.0331	12.9	3.4	8.5	$C_{12} H_{10} O_4 N_1 S_1$
		264.0324	15.5	4.1	18.0	$C_{18} H_4 O_1 N_2$
		264.0409	-16.9	-4.5	13.5	$C_{14} H_6 O_3 N_3$
		264.0423	-22.0	-5.8	13.0	$C_{16} H_8 O_4$
		264.0297	25.7	6.8	13.5	$C_{15} H_6 O_4 N_1$
291.0297	6.8	291.0314	-5.6	-1.6	10.0	$C_{12} H_9 O_4 N_3 S_1$
		291.0280	5.9	1.7	15.0	$C_{15} H_5 O_4 N_3$
		291.0320	-7.9	-2.3	19.0	$C_{20} H_5 O_2 N_1$
		291.0268	9.9	2.9	18.5	$C_{21} H_7 S_1$
		291.0354	-19.5	-5.7	14.0	$C_{17} H_9 O_2 N_1 S_1$
		291.0235	21.5	6.3	23.5	$C_{24} H_3$
292.0332	1.0	292.0347	-5.0	-1.5	18.0	$C_{21} H_8 S_1$
		292.0313	6.5	1.9	23.0	$C_{24} H_4$
		292.0306	8.8	2.6	14.0	$C_{16} H_8 O_2 N_2 S_1$
		292.0358	-9.0	-2.6	14.5	$C_{15} H_6 O_4 N_3$
		292.0273	20.3	5.9	19.0	$C_{19} H_4 O_2 N_2$
		292.0392	-20.5	-6.0	9.5	$C_{12} H_{10} O_4 N_3 S_1$

Instrument: JEOL JMS 600H-1
Inlet: Direct Probe

Ionization mode: EI+

Run By: MASS LAB 104

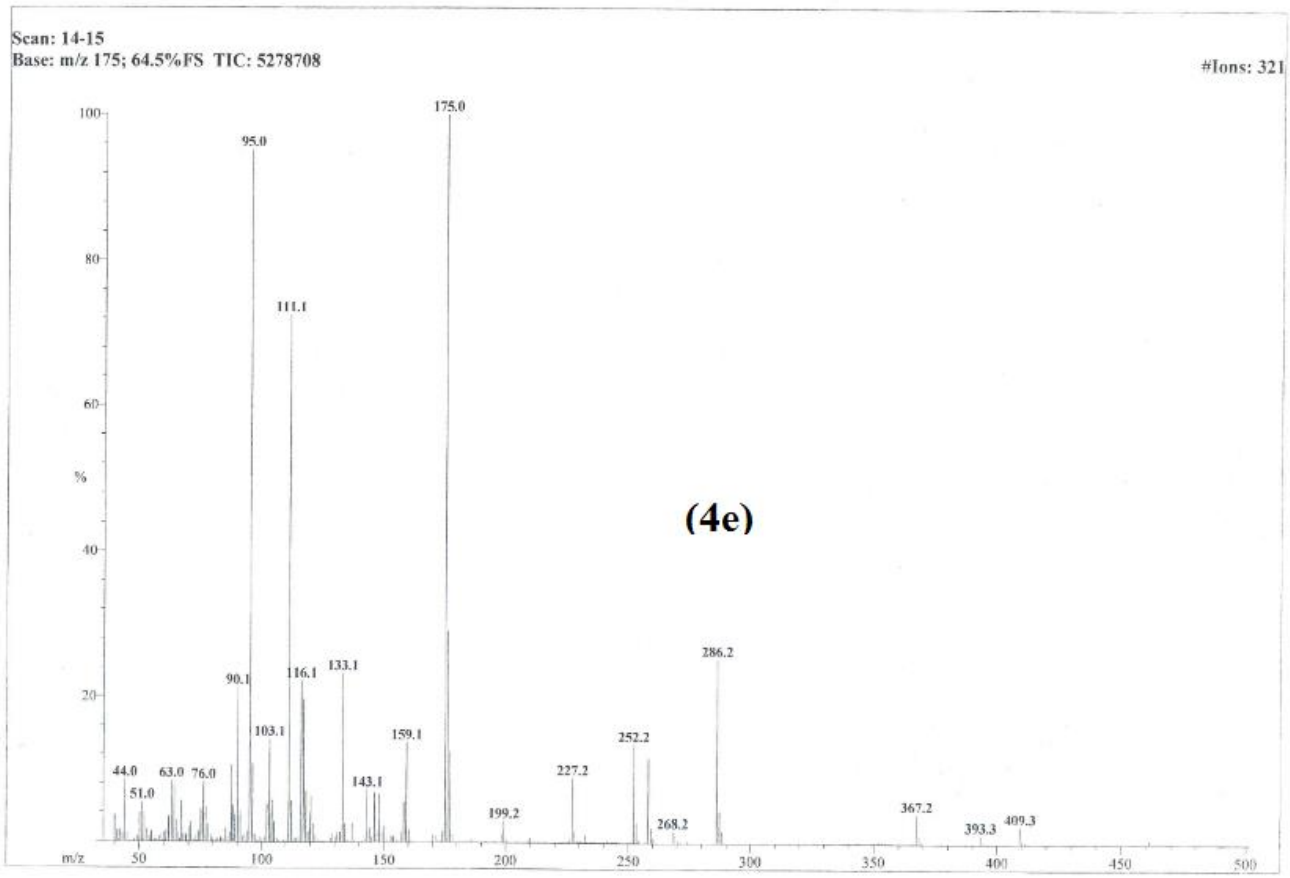


Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		150.0344	-16.7	-2.5	10.5	$C_{11} H_4 N_1$
		150.0351	-21.3	-3.2	1.0	$C_5 H_{10} O_3 S_1$
		150.0377	-39.1	-5.9	5.5	$C_8 H_6 N_1 S_1$
151.0237	1.4	151.0218	13.0	2.0	5.5	$C_8 H_7 O_1 S_1$
		151.0269	-21.3	-3.2	6.0	$C_7 H_5 O_3 N_1$
		151.0184	35.3	5.3	10.5	$C_{11} H_3 O_1$
		151.0296	-39.0	-5.9	10.5	$C_{10} H_3 N_2$
200.0937	1.4	200.0950	-6.5	-1.3	8.0	$C_{12} H_{12} O_1 N_2$
		200.0923	6.9	1.4	3.5	$C_9 H_{14} O_4 N_1$
		200.0983	-23.3	-4.7	3.0	$C_9 H_{16} O_1 N_2 S_1$
		200.0871	32.8	6.6	3.0	$C_{10} H_{14} O_2 S_1$
206.0502	1.1	206.0514	-5.6	-1.1	7.0	$C_{10} H_{10} O_1 N_2 S_1$
		206.0487	7.4	1.5	2.5	$C_7 H_{12} O_4 N_1 S_1$
		206.0480	10.8	2.2	12.0	$C_{13} H_6 O_1 N_2$
		206.0453	23.8	4.9	7.5	$C_{10} H_8 O_4 N_1$
226.0741	6.4	226.0742	-0.7	-0.2	10.0	$C_{13} H_{10} O_2 N_2$
		226.0776	-15.6	-3.5	5.0	$C_{10} H_{14} O_2 N_2 S_1$
		226.0783	-18.5	-4.2	14.0	$C_{18} H_{10}$
		226.0690	22.2	5.0	9.5	$C_{14} H_{12} N_1 S_1$
227.0740	1.5	227.0742	-0.8	-0.2	4.5	$C_{11} H_{15} O_3 S_1$
		227.0735	2.3	0.5	14.0	$C_{17} H_9 N_1$
		227.0769	-12.6	-2.9	9.0	$C_{14} H_{13} N_1 S_1$
		227.0708	14.1	3.2	9.5	$C_{14} H_{11} O_3$
232.0649	9.7	232.0644	2.5	0.6	3.5	$C_9 H_{14} O_4 N_1 S_1$
		232.0637	5.4	1.3	13.0	$C_{15} H_8 O_1 N_2$
		232.0670	-9.1	-2.1	8.0	$C_{12} H_{12} O_1 N_2 S_1$
		232.0610	17.0	3.9	8.5	$C_{12} H_{10} O_4 N_1$
233.0688	1.4	233.0688	0.0	0.0	8.0	$C_{12} H_{11} O_4 N_1$
		233.0715	-11.5	-2.7	12.5	$C_{15} H_9 O_1 N_2$
		233.0722	-14.4	-3.4	3.0	$C_9 H_{15} O_4 N_1 S_1$
		233.0636	22.3	5.2	7.5	$C_{13} H_{13} O_2 S_1$
260.0624	13.1	260.0626	-0.6	-0.2	18.0	$C_{21} H_8$
		260.0619	1.9	0.5	9.0	$C_{13} H_{12} O_2 N_2 S_1$
		260.0660	-13.6	-3.5	13.0	$C_{18} H_{12} S_1$
		260.0586	14.8	3.9	14.0	$C_{16} H_8 O_2 N_2$
261.0678	2.1	261.0664	5.2	1.4	13.5	$C_{16} H_9 O_2 N_2$
		261.0698	-7.7	-2.0	8.5	$C_{13} H_{13} O_2 N_2 S_1$
		261.0704	-10.2	-2.7	17.5	$C_{21} H_9$
		261.0738	-23.1	-6.0	12.5	$C_{18} H_{13} S_1$

Instrument: JEOL JMS 600H-1
Inlet: Direct Probe

Ionization mode: EI+

Run By: MASS LAB 104

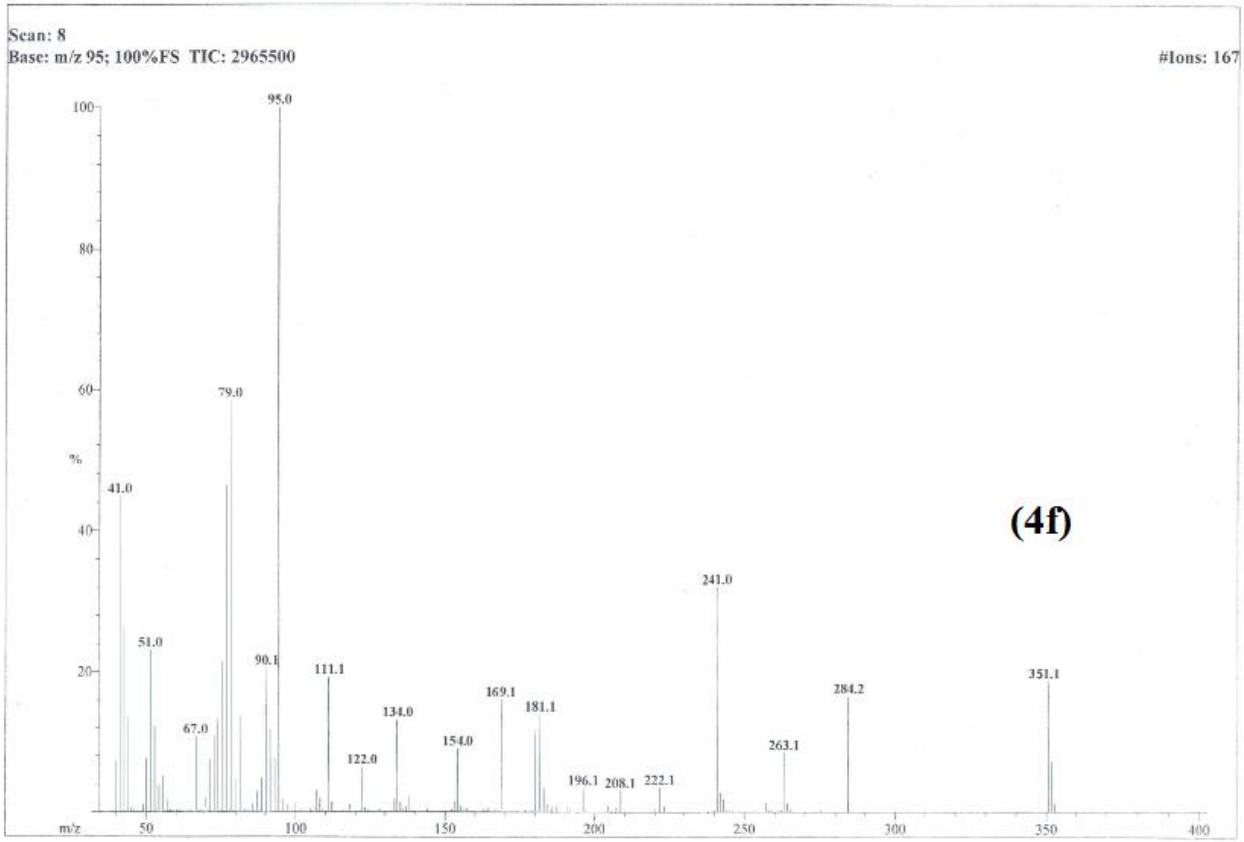


Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		262.1477	10.1	2.6	1.5	$C_{12}H_{24}O_3N_1S_1$
		262.1470	12.7	3.3	11.0	$C_{18}H_{18}N_2$
		262.1463	15.2	4.0	2.0	$C_{10}H_{22}O_2N_4S_1$
279.1571	45.5	279.1583	-4.3	-1.2	6.0	$C_{14}H_{21}O_3N_3$
		279.1610	-13.9	-3.9	10.5	$C_{17}H_{19}N_4$
		279.1531	14.3	4.0	5.5	$C_{15}H_{23}O_1N_2S_1$
		279.1617	-16.4	-4.6	1.0	$C_{11}H_{25}O_3N_3S_1$
280.1637	7.0	280.1661	-8.7	-2.4	5.5	$C_{14}H_{22}O_3N_3$
		280.1609	9.8	2.7	5.0	$C_{15}H_{24}O_1N_2S_1$
		280.1688	-18.3	-5.1	10.0	$C_{17}H_{20}N_4$
		280.1695	-20.7	-5.8	0.5	$C_{11}H_{26}O_3N_3S_1$
281.1651	1.0	281.1654	-1.0	-0.3	9.5	$C_{16}H_{21}O_1N_2$
		281.1647	1.3	0.4	0.5	$C_{10}H_{25}O_3N_4S_1$
		281.1688	-13.0	-3.6	4.5	$C_{15}H_{25}O_1N_2S_1$
		281.1614	13.3	3.7	5.5	$C_{13}H_{21}O_3N_4$
286.0531	3.7	286.0531	-0.0	-0.0	20.0	$C_{21}H_6N_2$
		286.0524	2.3	0.6	11.0	$C_{13}H_{10}O_2N_4S_1$
		286.0538	-2.4	-0.7	10.5	$C_{15}H_{12}O_3N_1S_1$
		286.0504	9.4	2.7	15.5	$C_{18}H_8O_3N_1$
287.0602	0.6	287.0603	-0.1	-0.0	10.5	$C_{13}H_{11}O_2N_4S_1$
		287.0609	-2.3	-0.7	19.5	$C_{21}H_7N_2$
		287.0616	-4.8	-1.4	10.0	$C_{15}H_{13}O_3N_1S_1$
		287.0582	7.0	2.0	15.0	$C_{18}H_9O_3N_1$

Instrument: JEOL JMS 600H-1
Inlet: Direct Probe

Ionization mode: EI+

Run By: MASS LAB 104

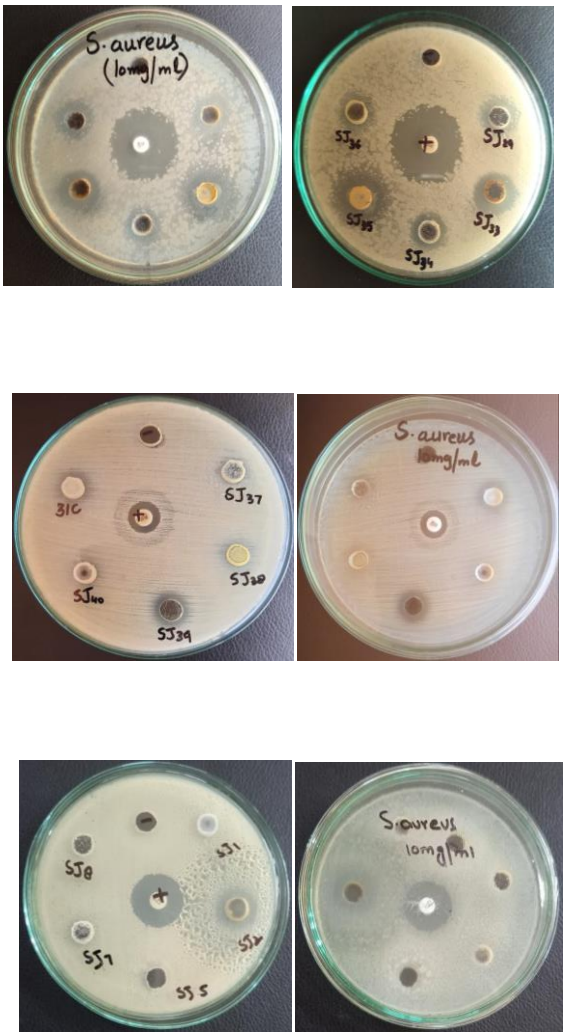


Strain: ***E.coli***

Front ***Back***

Strain***: S.aureus***

Front ***Back***



Note=S-J-36 (4a), S-J-37 (4b), S-J-38 (4c), S-J-34 (4d), S-J-8 (4e), S-J-35 (4f)

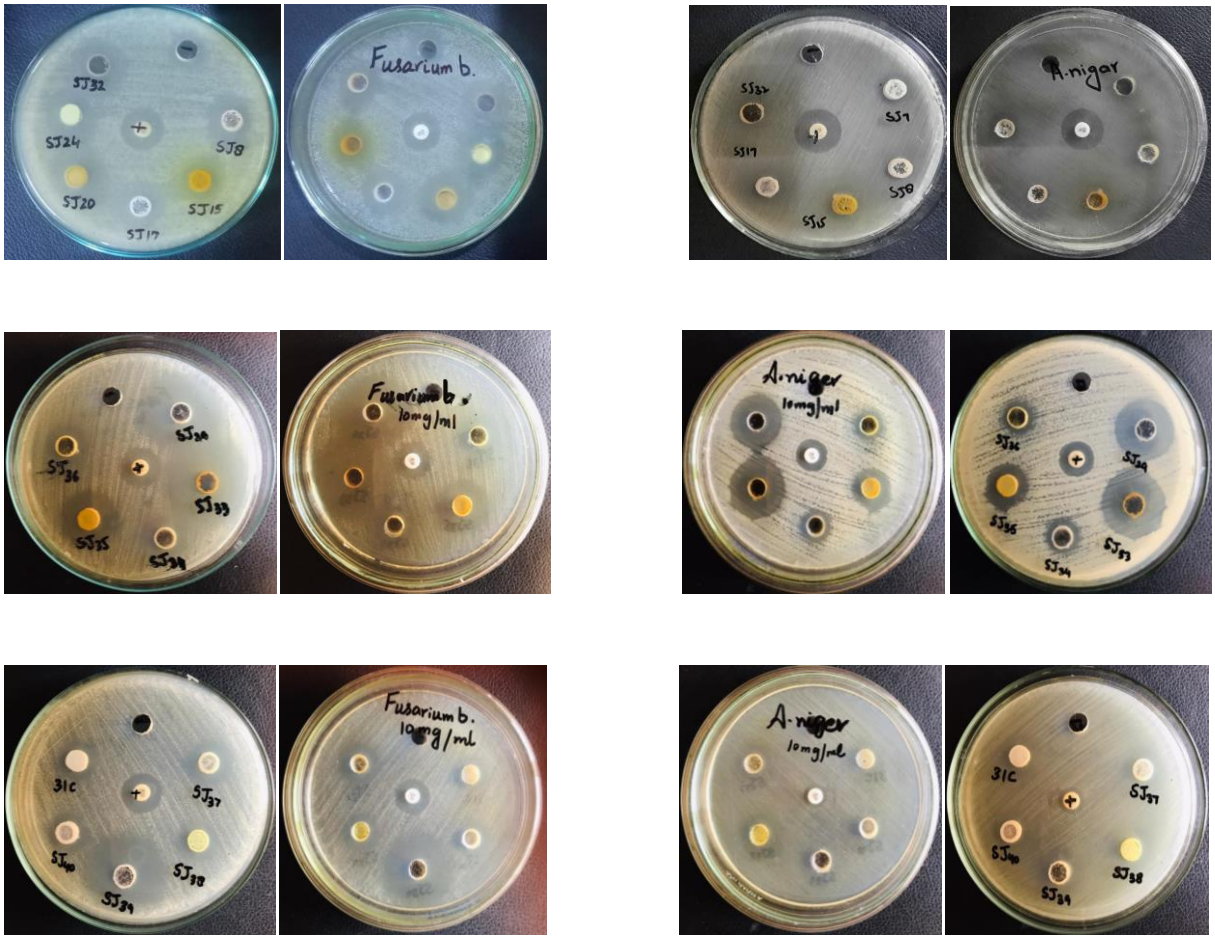
Figure S1. Antibacterial activity of the synthesized compounds (4a-4f) by well diffusion method.

Strain: *F. bracchygibossum*

Front ***Back***

Strain***: A. niger***

Front ***Back***



Note=S-J-36 (4a), S-J-37 (4b), S-J-38 (4c), S-J-34 (4d), S-J-8 (4e), S-J-35 (4f)

Figure S2. Antifungal activity of the synthesized compounds (4a-4f) by well diffusion method.

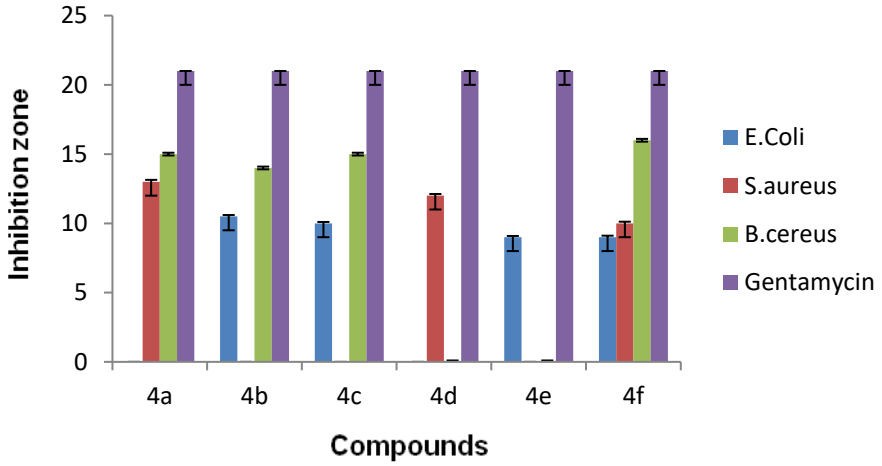


Figure S3: Antibacterial activity of the synthesized compounds (4a-4f) by well diffusion method.

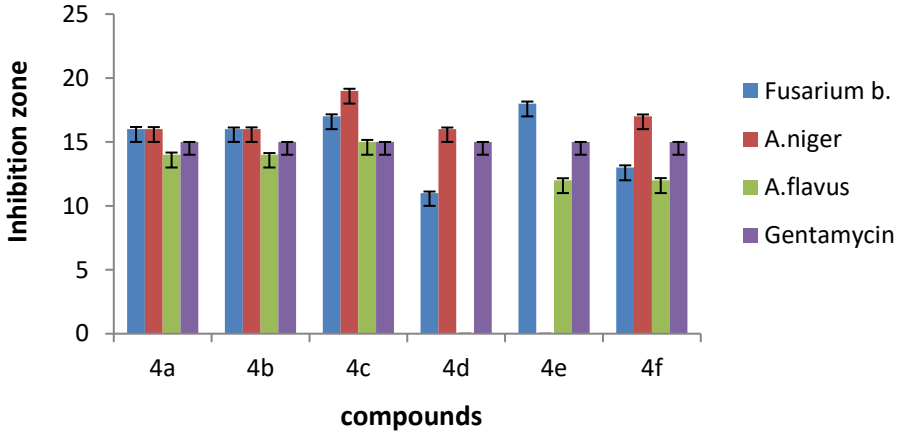


Figure S4: Antifungal activity of the synthesized compounds (4a-4h) by well diffusion method.