Supplementary data of

Novel Thiophene-Thiazole-Schiff Base Hybrids: Design, Synthesis, Antimicrobial and Antioxidant Activity with ADMET Prediction with Molecular Docking and Dynamics Study

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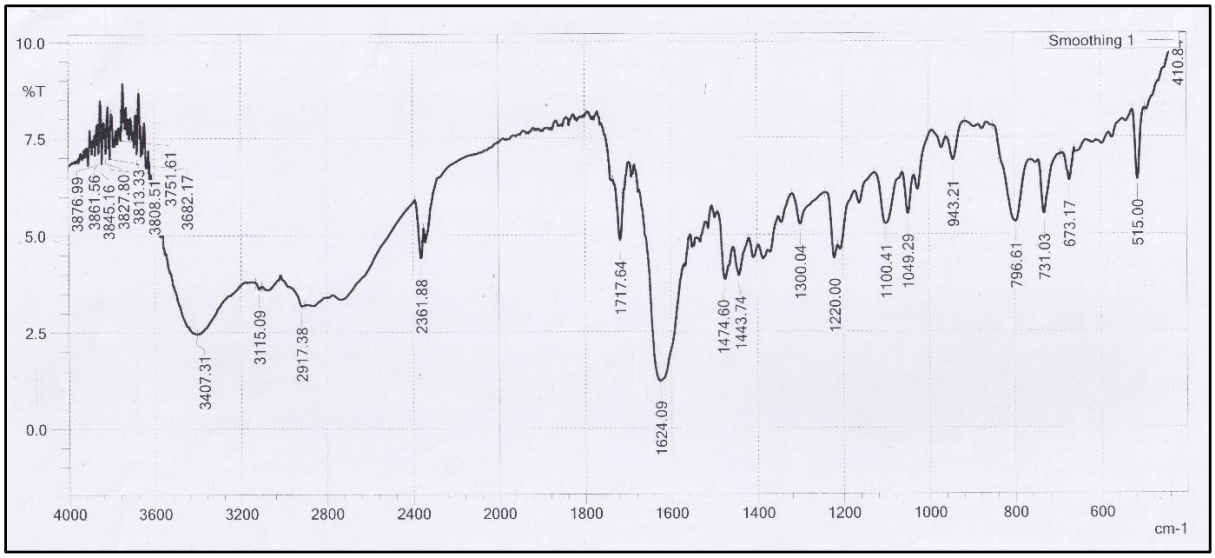


Fig. S1. IR spectrum of **2a.**

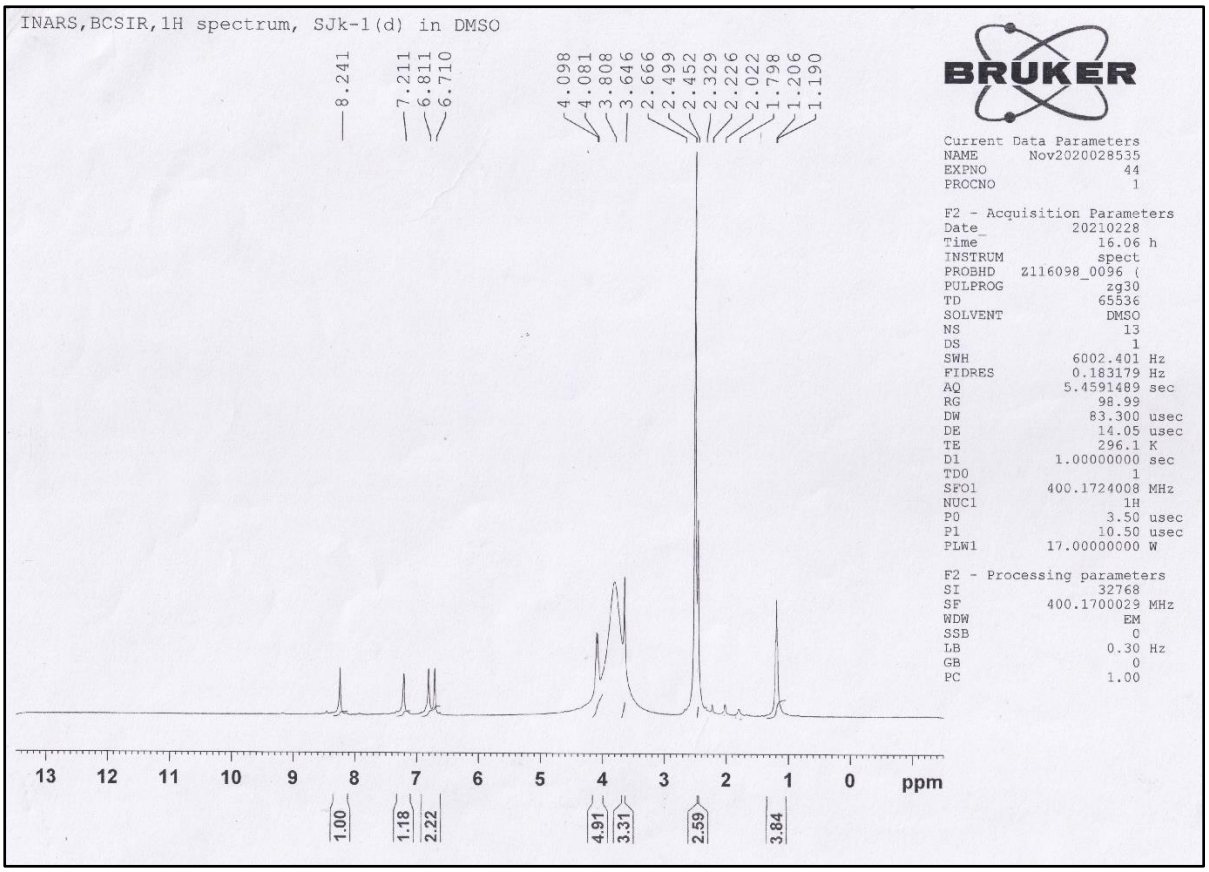
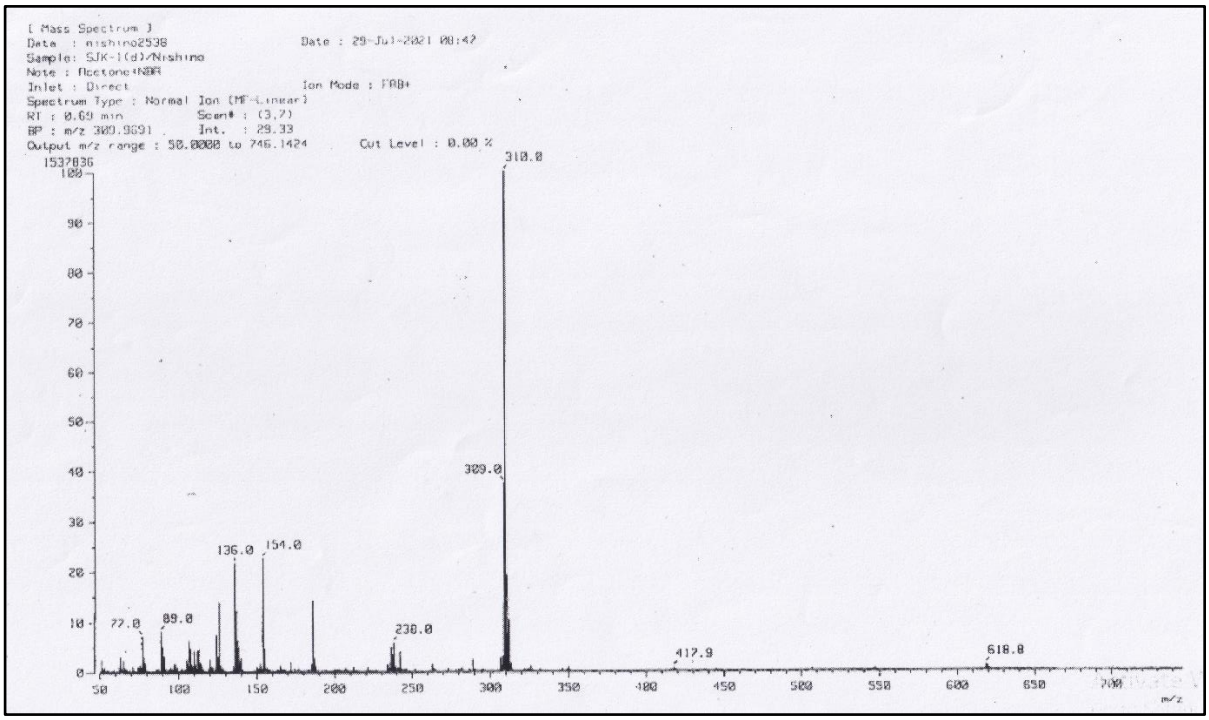


Fig. S2. ^{1}H NMR spectrum of **2a.**



[Elemental Composition]
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Sample: SJK-1(d)/Nishino
Note : Acetone+NBA
Inlet : Direct Ion Mode : FAB+
RT : 5.38 min Scan#: (20,25)
Elements : C 100/0, H 100/0, O 3/1, N 4/2, S 3/1
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
310.0680	100.0	-31.1 / -9.6	13.0	C 17 H 14 O 2 N 2 S
		+9.5 / +2.9	13.5	C 16 H 12 O 2 N 3 S
		-1.4 / -0.4	9.5	C 13 H 16 O 2 N 3 S 2
		-12.3 / -3.8	5.5	C 10 H 20 O 2 N 3 S 3
		+28.3 / +8.8	6.0	C 9 H 18 O 2 N 4 S 3

Fig. S3. HRMS spectrum of **2a.**

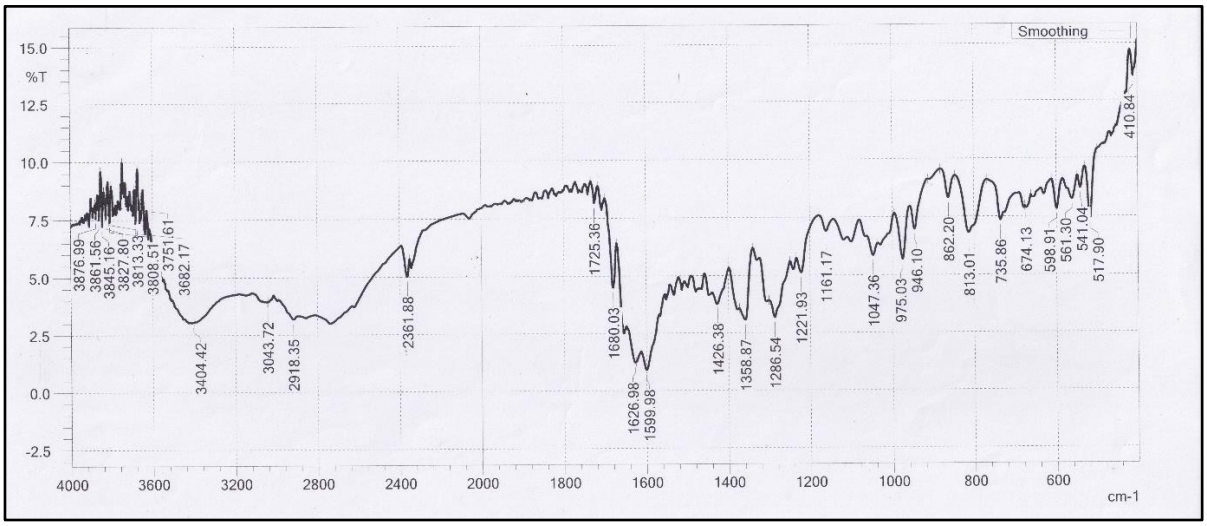


Fig. S4. IR spectrum of **2b.**

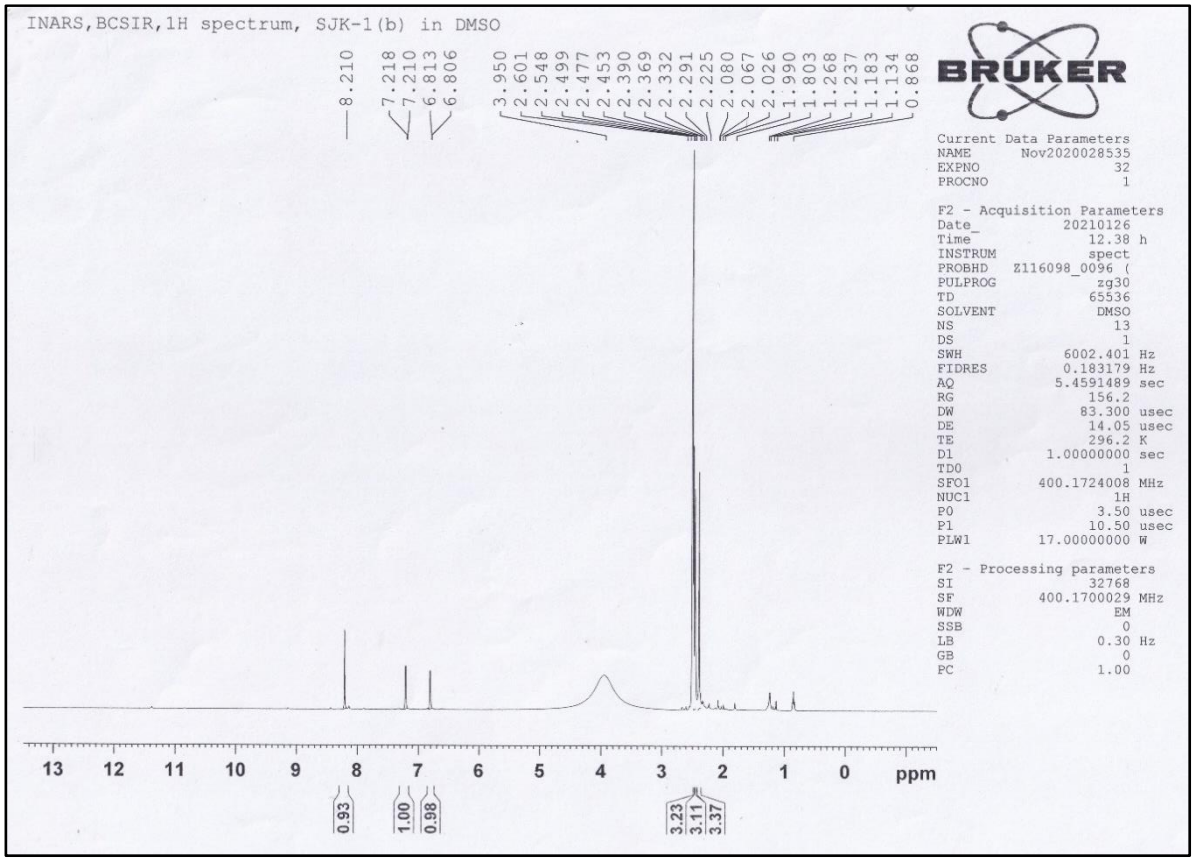
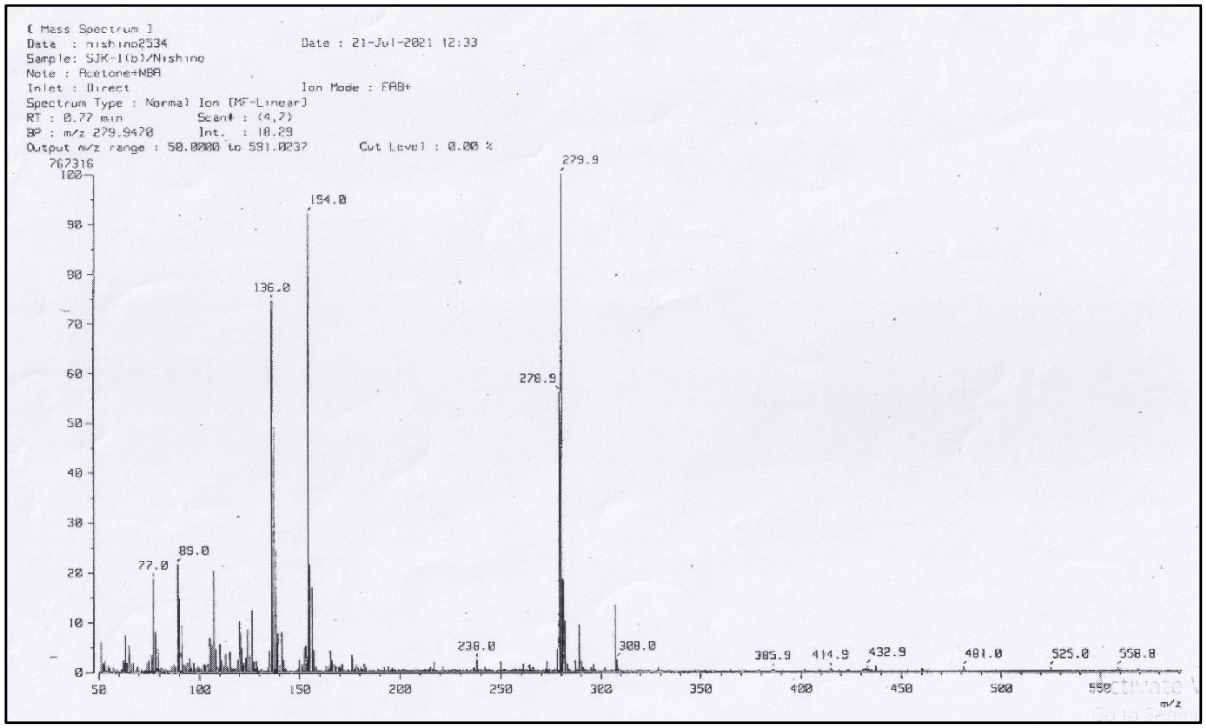


Fig. S5. ^{1}H NMR spectrum of **2b.**



[Elemental Composition]
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Sample: SLJ-1(b)/Nishino
Note : Acetone+NBA
Inlet : Direct Ion Mode : FAB+
RT : 5.38 min Scan#: (19,26)
Elements : C 100/0, H 100/0, O 2/0, N 4/2, S 3/1
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
279.0504	74.4	-31.4 / -8.8	13.5	C 16 H 11 O N 2 S
		+13.7 / +3.8	14.0	C 15 H 9 O N 3 S
		+1.6 / +0.4	10.0	C 12 H 13 O N 3 S 2
		-10.5 / -2.9	6.0	C 9 H 17 O N 3 S 3
		+34.6 / +9.6	6.5	C 8 H 15 O N 4 S 3
280.0576	100.0	-33.7 / -9.4	13.0	C 16 H 12 O N 2 S
		+11.2 / +3.1	13.5	C 15 H 10 O N 3 S
		-0.9 / -0.2	9.5	C 12 H 14 O N 3 S 2
		-12.9 / -3.6	5.5	C 9 H 18 O N 3 S 3
		+32.0 / +9.0	6.0	C 8 H 16 O N 4 S 3

Fig. S6. HRMS spectrum of **2b.**

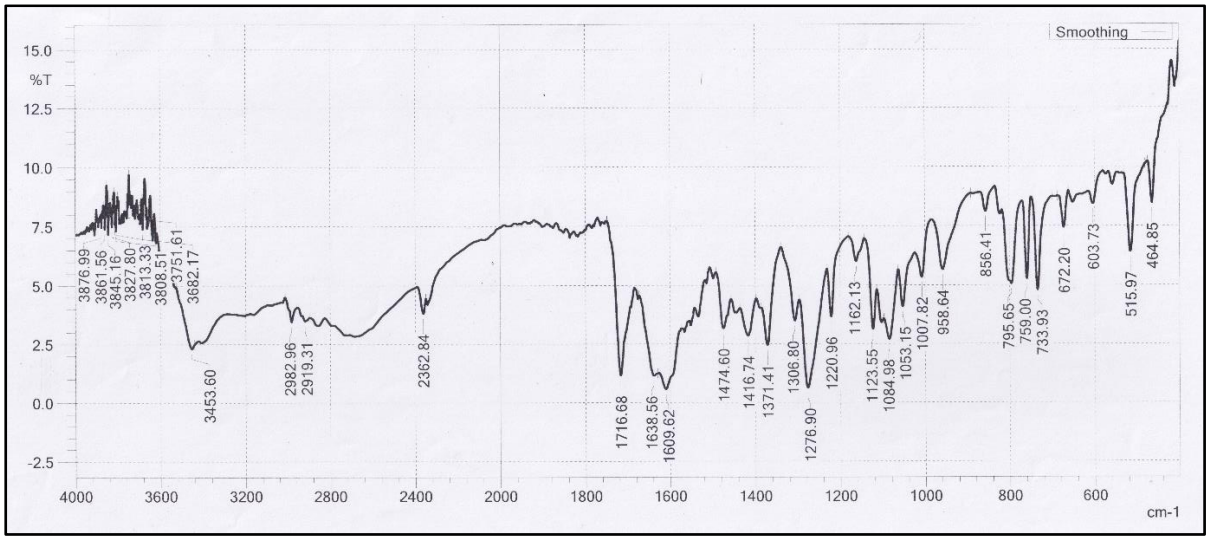


Fig. S7. IR spectrum of **2c.**

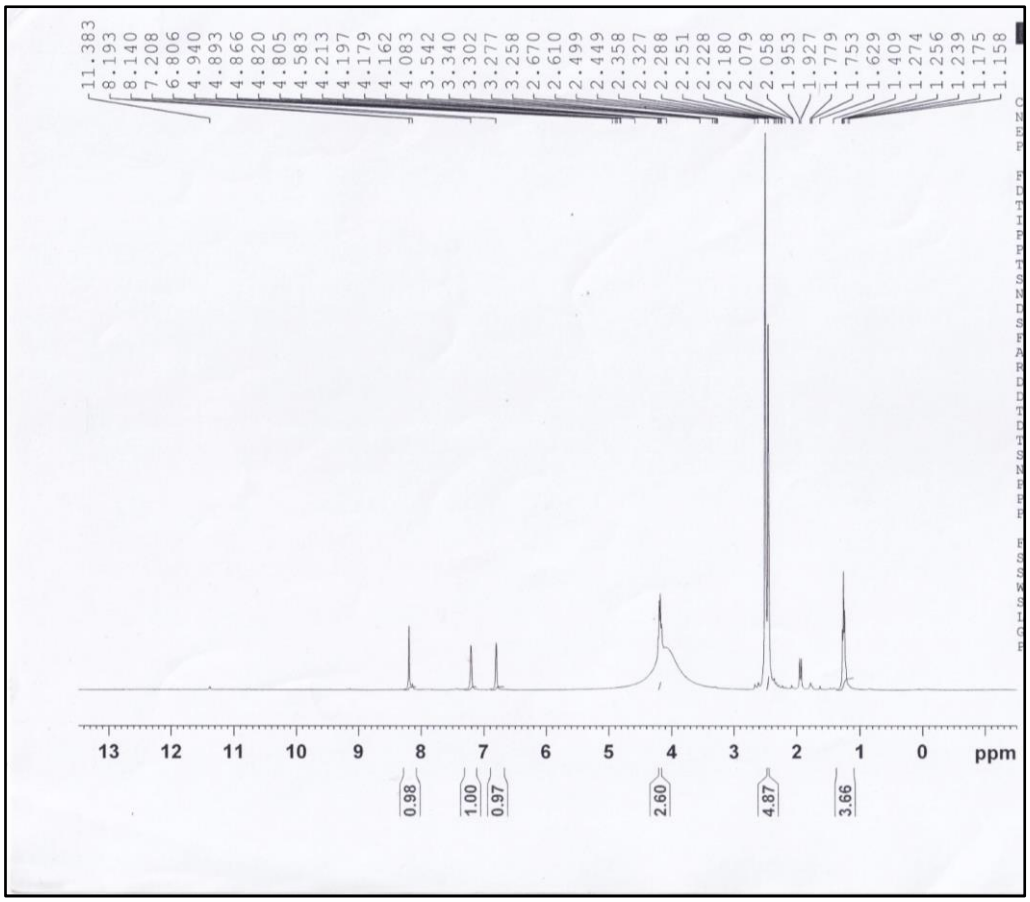
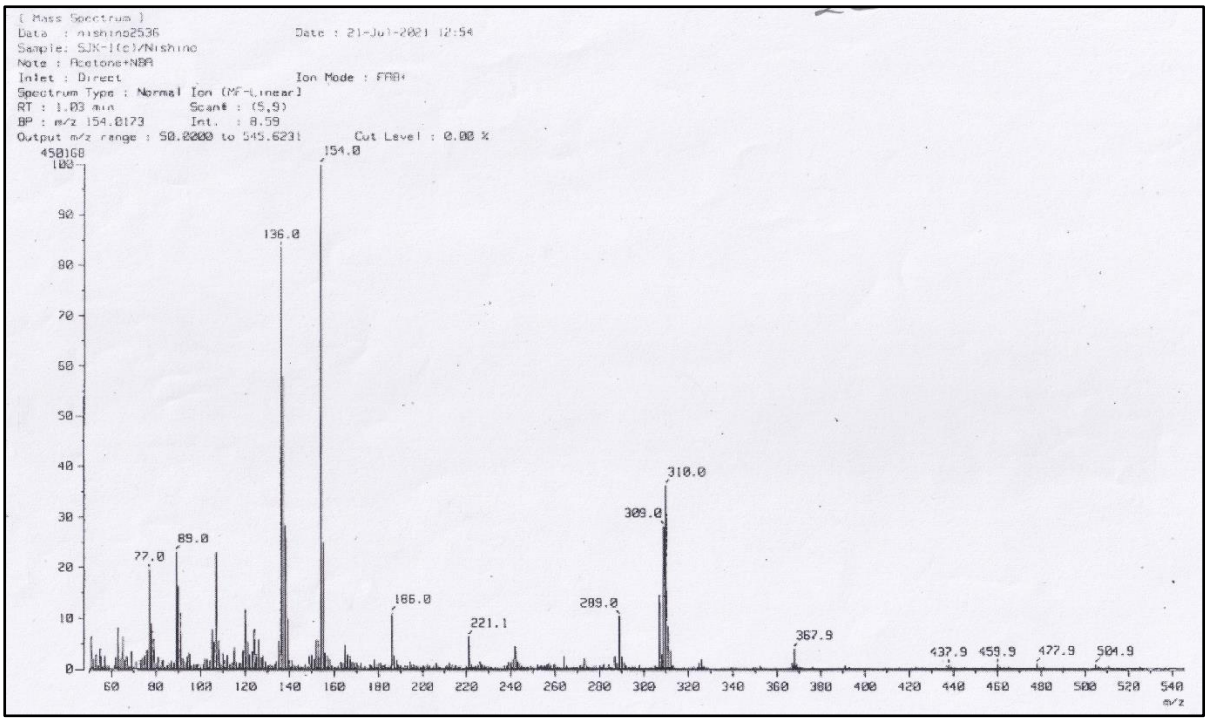


Fig. S8. ^{1}H NMR spectrum of **2c.**



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Data : nishino2537
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Sample: SLJ-1(c)/Nishino
Note : Acetone+NBA
Inlet : Direct
Ion Mode : FAB+
RT : 4.38 min
Scan#: (16,21)
Elements : C 100/0, H 100/0, O 3/1, N 4/2, S 3/1
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
310.0681	62.7	-30.8 / -9.5	13.0	C 17 H 14 O 2 N 2 S
		+9.8 / +3.0	13.5	C 16 H 12 O 2 N 3 S
		-1.1 / -0.3	9.5	C 13 H 16 O 2 N 3 S 2
		-12.0 / -3.7	5.5	C 10 H 20 O 2 N 3 S 3
		+28.6 / +8.9	6.0	C 9 H 18 O 2 N 4 S 3
309.0610	57.1	-28.4 / -8.8	13.5	C 17 H 13 O 2 N 2 S
		+12.3 / +3.8	14.0	C 16 H 11 O 2 N 3 S
		+1.4 / +0.4	10.0	C 13 H 15 O 2 N 3 S 2
		-9.5 / -2.9	6.0	C 10 H 19 O 2 N 3 S 3
		+31.2 / +9.6	6.5	C 9 H 17 O 2 N 4 S 3

Fig. S9. HRMS spectrum of **2c.**

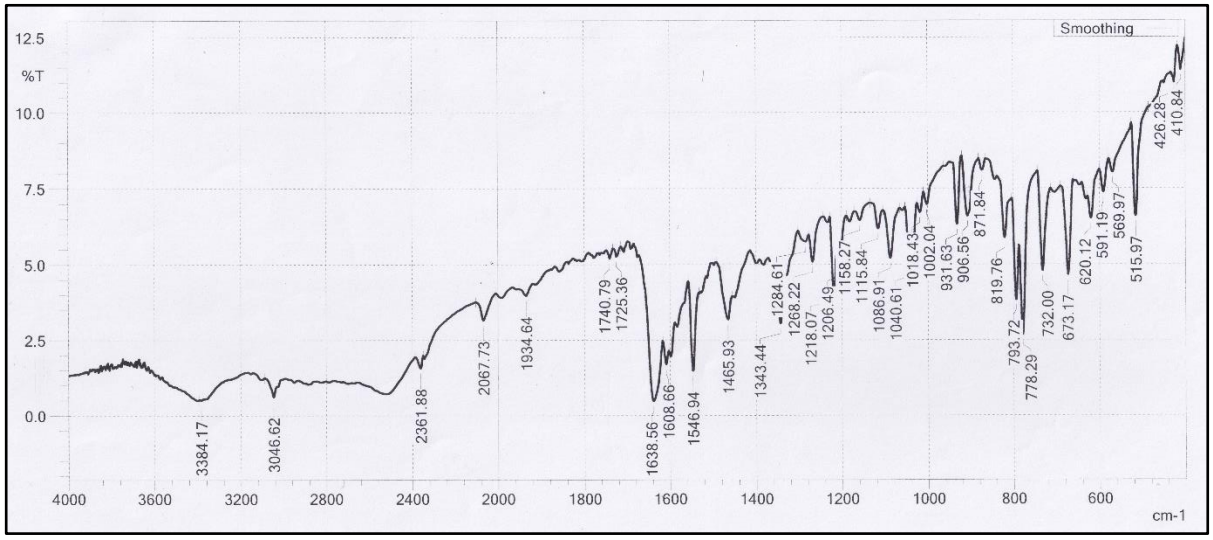


Fig. S10. IR spectrum of **2d.**

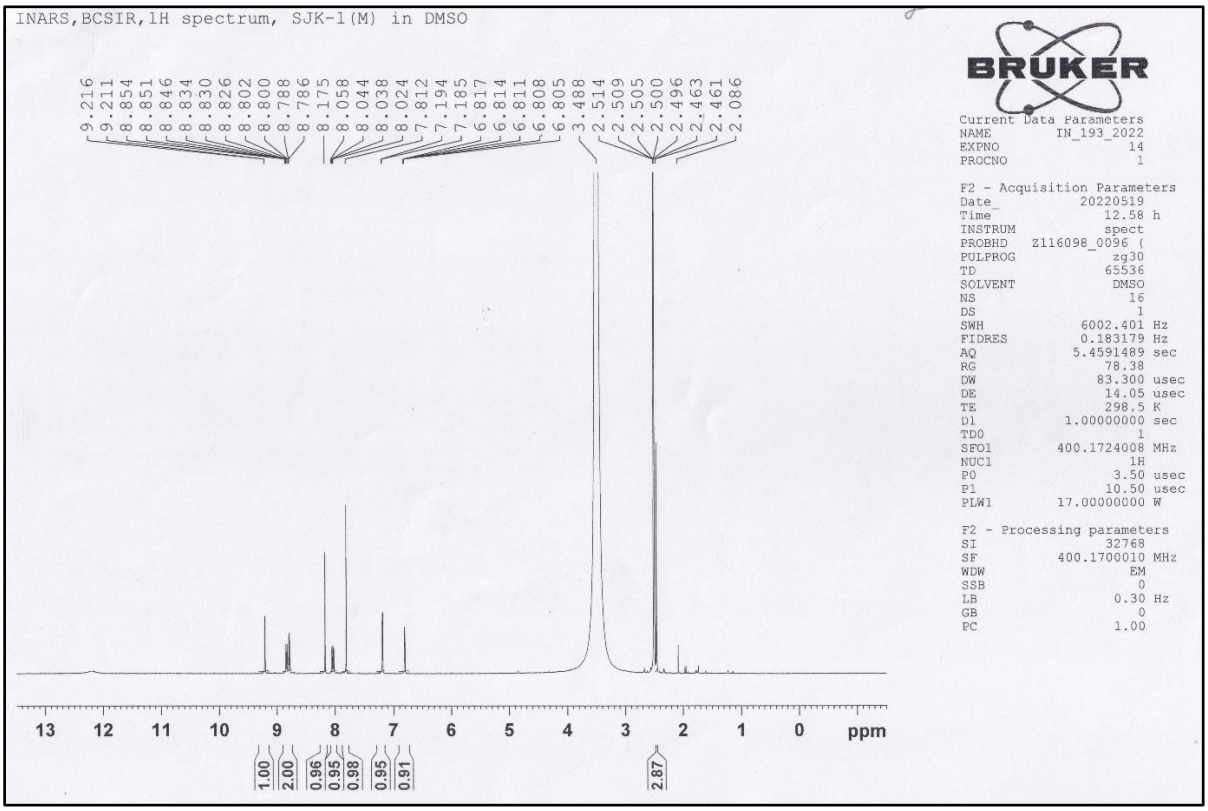
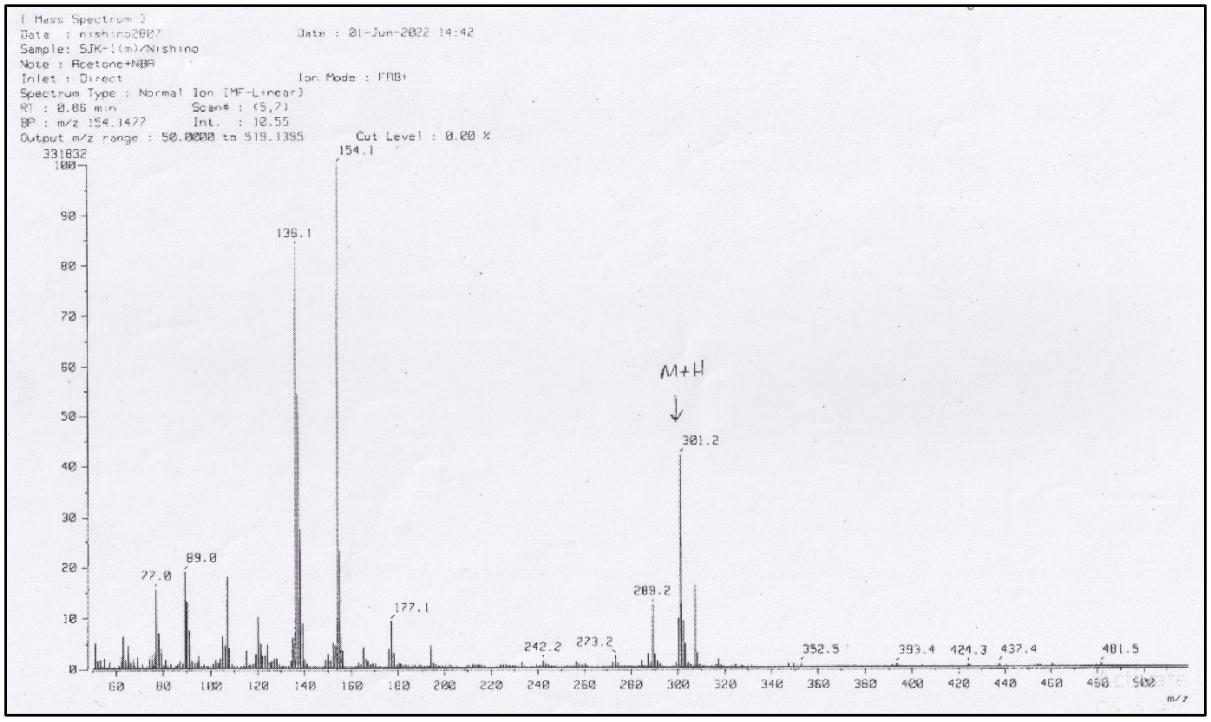


Fig. S11. ^{1}H NMR spectrum of **2d.**



[Elemental Composition]
Data : nishino2808 Date : 01-Jun-2022 14:50
Sample: SJK-1(m)/Nishino
Note : Acetone+NBA
Inlet : Direct Ion Mode : FAB+
RT : 1.75 min Scan#: (6,10)
Elements : C 100/0, H 100/0, N 5/3, S 3/1
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
301.0587	100.0	-28.9 / -8.7	16.0	C 18 H 11 N 3 S
		+12.8 / +3.9	16.5	C 17 H 9 N 4 S
		+1.6 / +0.5	12.5	C 14 H 13 N 4 S 2
		-9.6 / -2.9	8.5	C 11 H 17 N 4 S 3
		+32.2 / +9.7	9.0	C 10 H 15 N 5 S 3

Fig. S12. HRMS spectrum of **2d.**

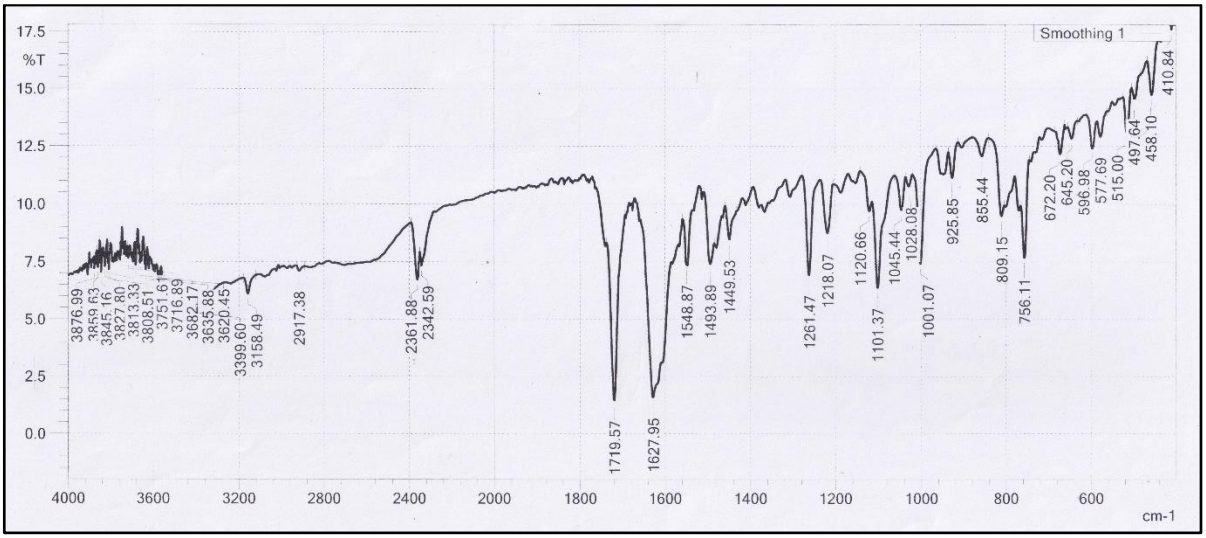


Fig. S13. IR spectrum of **2e.**

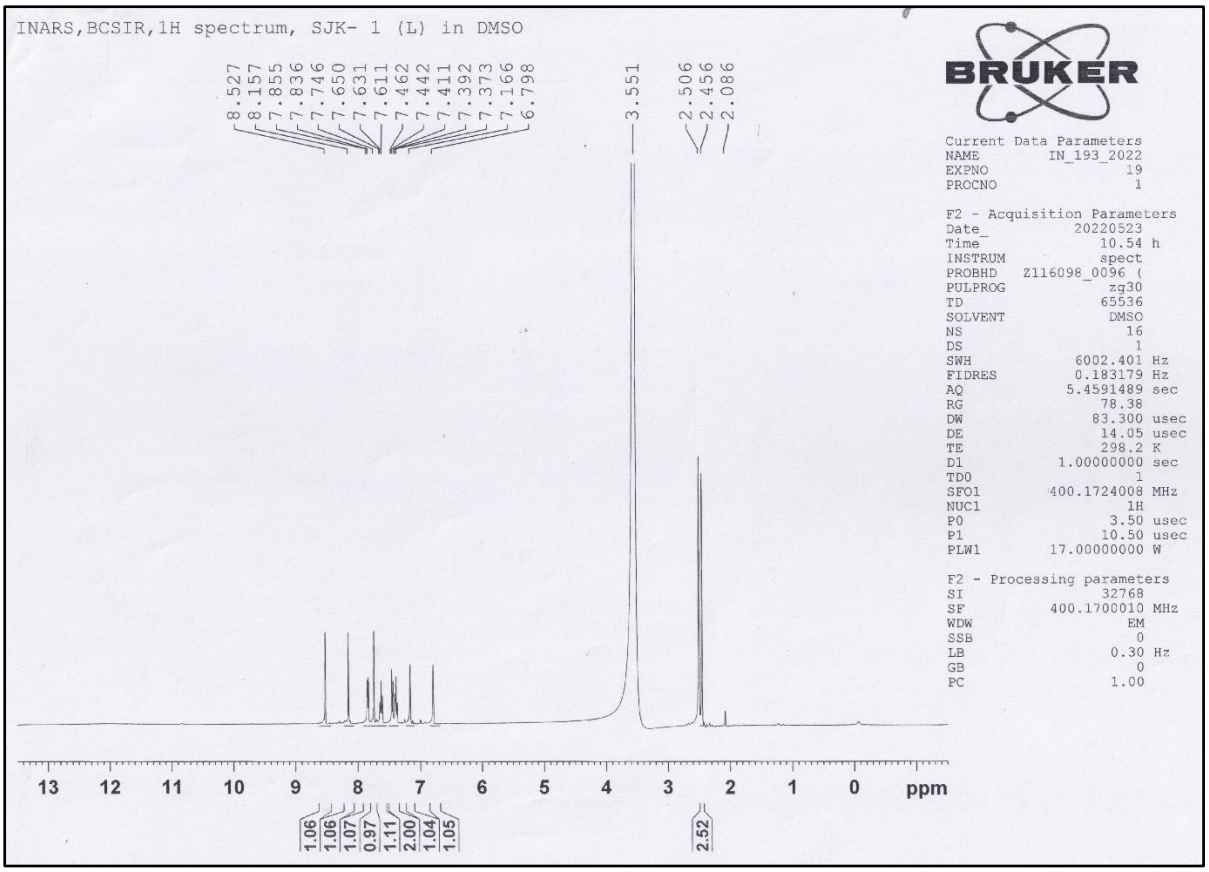
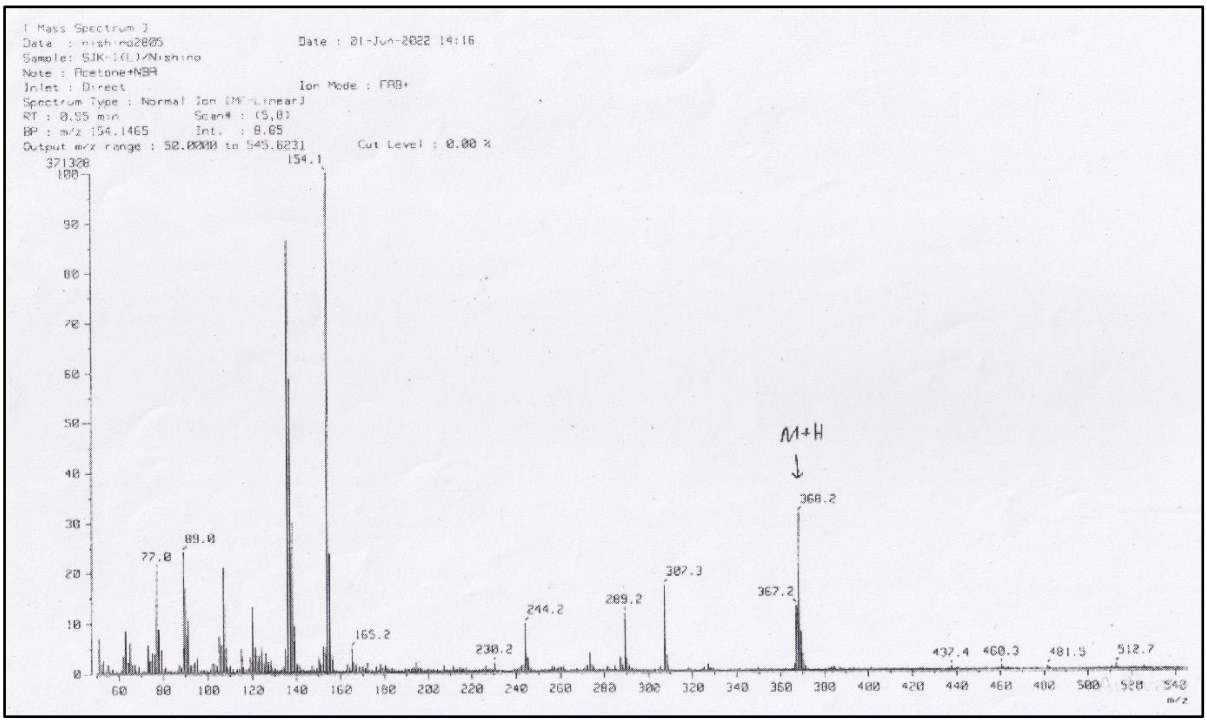


Fig. S14. ^{1}H NMR spectrum of **2e.**



[Elemental Composition]
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Sample: SJK-1(L)/Nishino
Note : Acetone+NBA
Inlet : Direct Ion Mode : FAB+
RT : 1.75 min Scan#: (5,11)
Elements : C 100/0, H 100/0, O 3/1, N 4/2, S 3/1
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
368.0529	100.0	-24.5 / -9.0	19.0	C 22 H 12 O 2 N 2 S
		+9.6 / +3.5	19.5	C 21 H 10 O 2 N 3 S
		+0.5 / +0.2	15.5	C 18 H 14 O 2 N 3 S 2
		-8.7 / -3.2	11.5	C 15 H 18 O 2 N 3 S 3
		+25.5 / +9.4	12.0	C 14 H 16 O 2 N 4 S 3

Fig. S15. HRMS spectrum of **2e.**

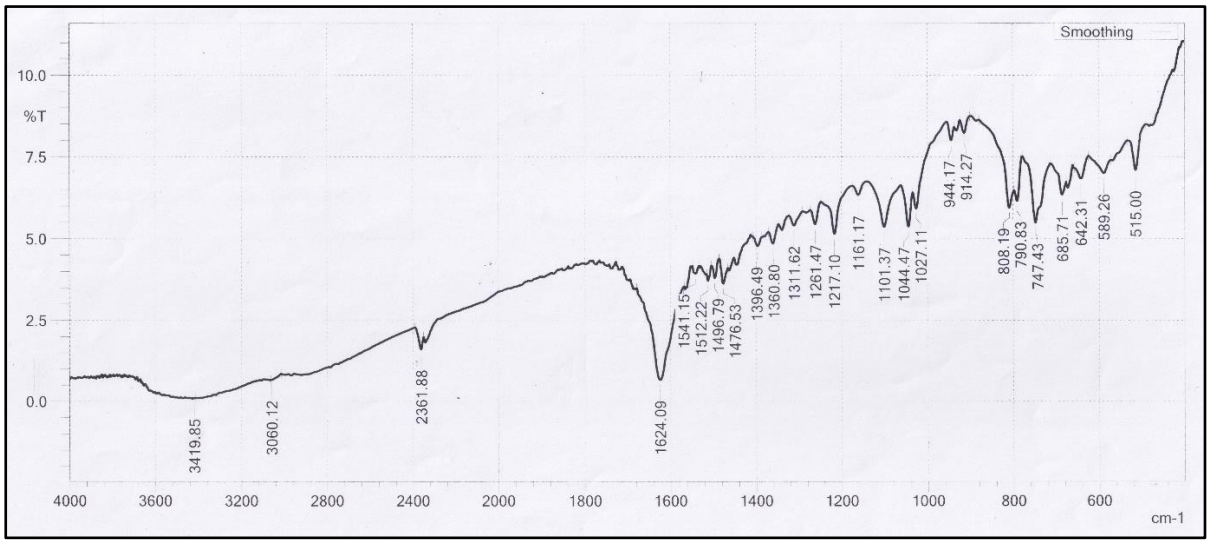


Fig. S16. IR spectrum of **2f.**

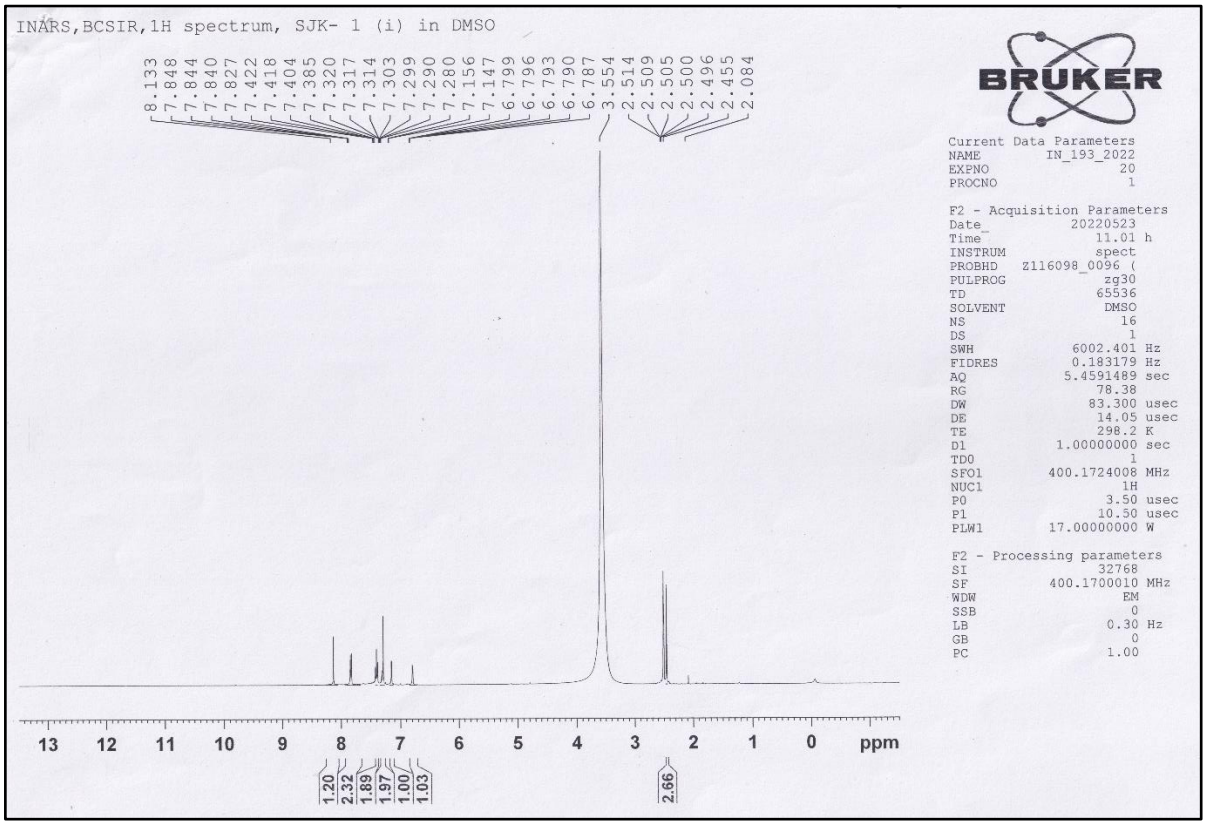
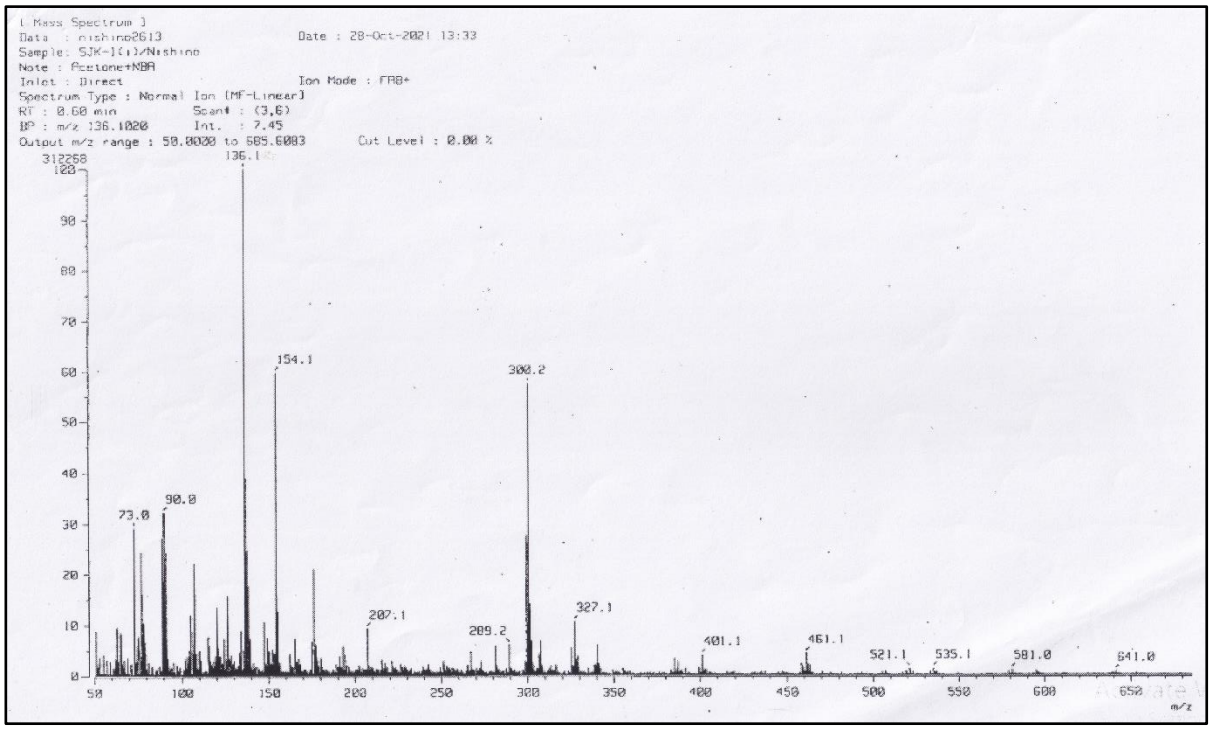


Fig. S17. ^{1}H NMR spectrum of **2f.**



[Elemental Composition]
Data : nishino2615 Date : 28-Oct-2021 13:54
Sample: SJK-1(i)/Nishino
Note : Acetone+NBA
Inlet : Direct Ion Mode : FAB+
RT : 1.75 min Scan#: (6,10)
Elements : C 100/0, H 100/0, N 4/2, S 3/1
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
299.0547	92.4	-32.2 / -9.6	16.5	C 19 H 11 N 2 S
		+9.8 / +2.9	17.0	C 18 H 9 N 3 S
		-1.5 / -0.4	13.0	C 15 H 13 N 3 S 2
		-12.7 / -3.8	9.0	C 12 H 17 N 3 S 3
		+29.3 / +8.8	9.5	C 11 H 15 N 4 S 3
300.0617	100.0	+7.1 / +2.1	16.5	C 18 H 10 N 3 S
		-4.1 / -1.2	12.5	C 15 H 14 N 3 S 2
		-15.4 / -4.6	8.5	C 12 H 18 N 3 S 3
		+26.5 / +8.0	9.0	C 11 H 16 N 4 S 3

Fig. S18. HRMS spectrum of **2f.**

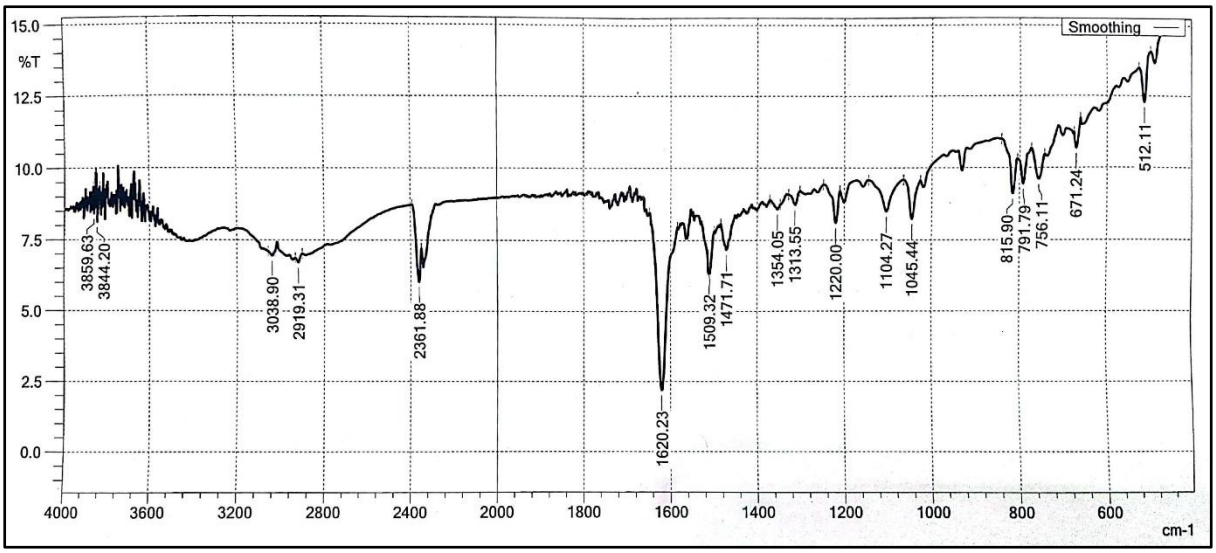


Fig. S19. IR spectrum of **2g.**

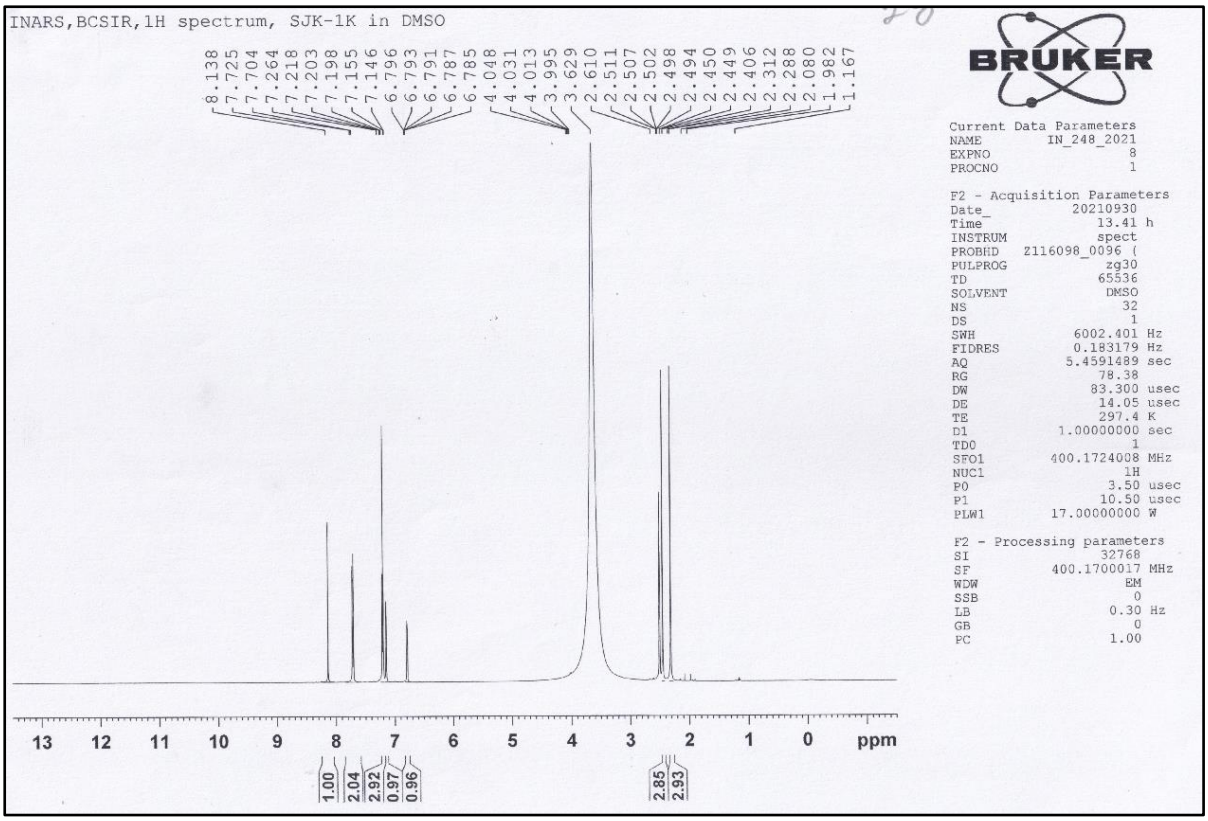
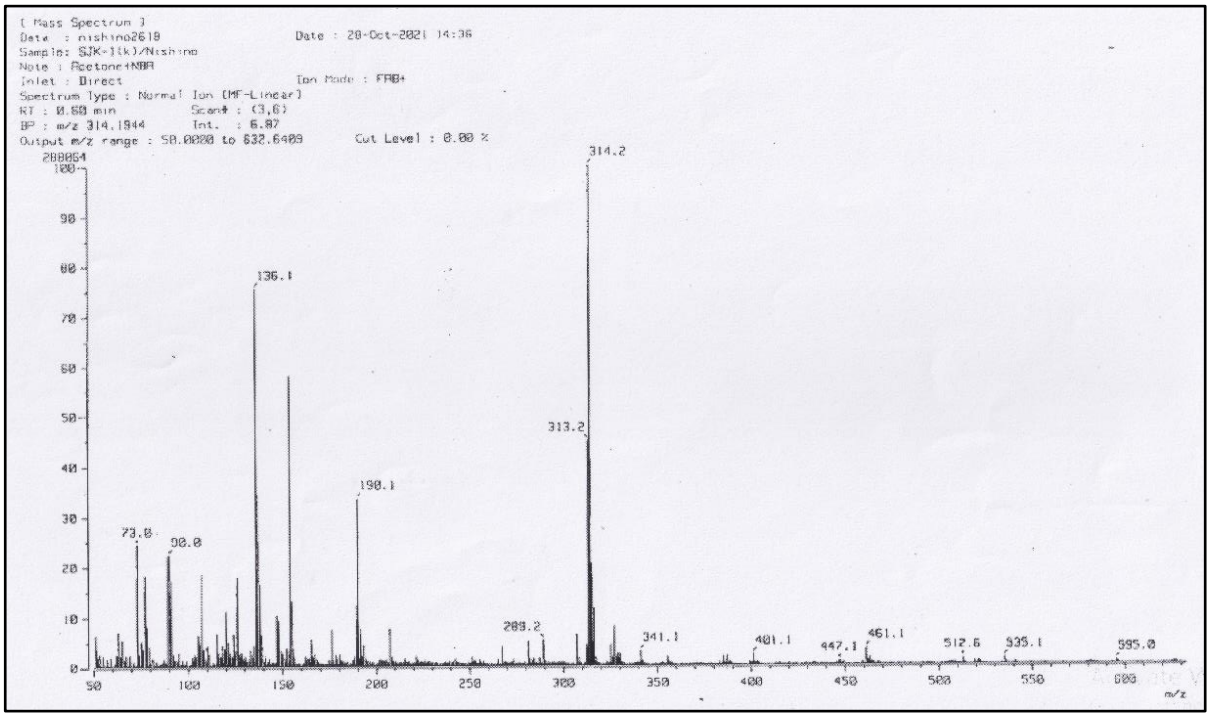


Fig. S20. ^{1}H NMR spectrum of **2g.**

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Sample: SJK-1(k)/Nishino
Note  : Acetone+NBA
Inlet : Direct                         Ion Mode : FAB+
RT : 4.00 min                          Scan#: (15,19)
Elements : C 100/0, H 100/0, N 4/2, S 3/1
Mass Tolerance      : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z  Int%   Err[ppm / mmu]    U.S.  Composition
  313.0716     52.1    -26.8 /  -8.4   16.5  C 20 H 13 N 2 S
                       +13.4 /  +4.2   17.0  C 19 H 11 N 3 S
                        +2.6 /  +0.8   13.0  C 16 H 15 N 3 S 2
                        -8.1 /  -2.5    9.0  C 13 H 19 N 3 S 3

  314.0786    100.0    -29.2 /  -9.2   16.0  C 20 H 14 N 2 S
                       +10.9 /  +3.4   16.5  C 19 H 12 N 3 S
                        +0.1 /  +0.0   12.5  C 16 H 16 N 3 S 2
                       -10.6 /  -3.3    8.5  C 13 H 20 N 3 S 3
                       +29.5 /  +9.3    9.0  C 12 H 18 N 4 S 3
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Fig. S21. HRMS spectrum of **2g.**

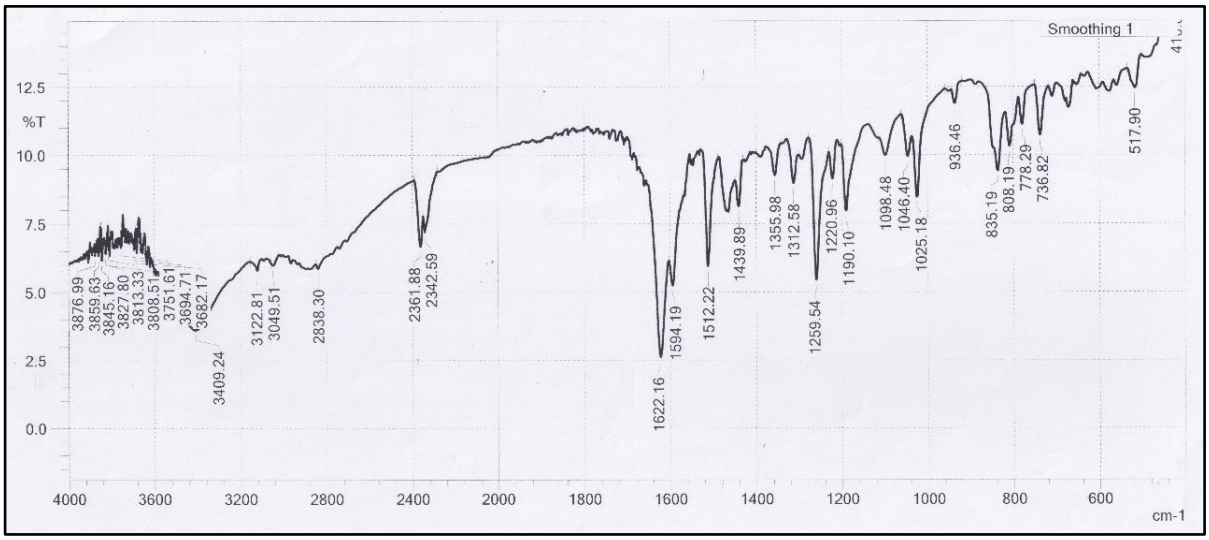


Fig. S22. IR spectrum of **2h.**

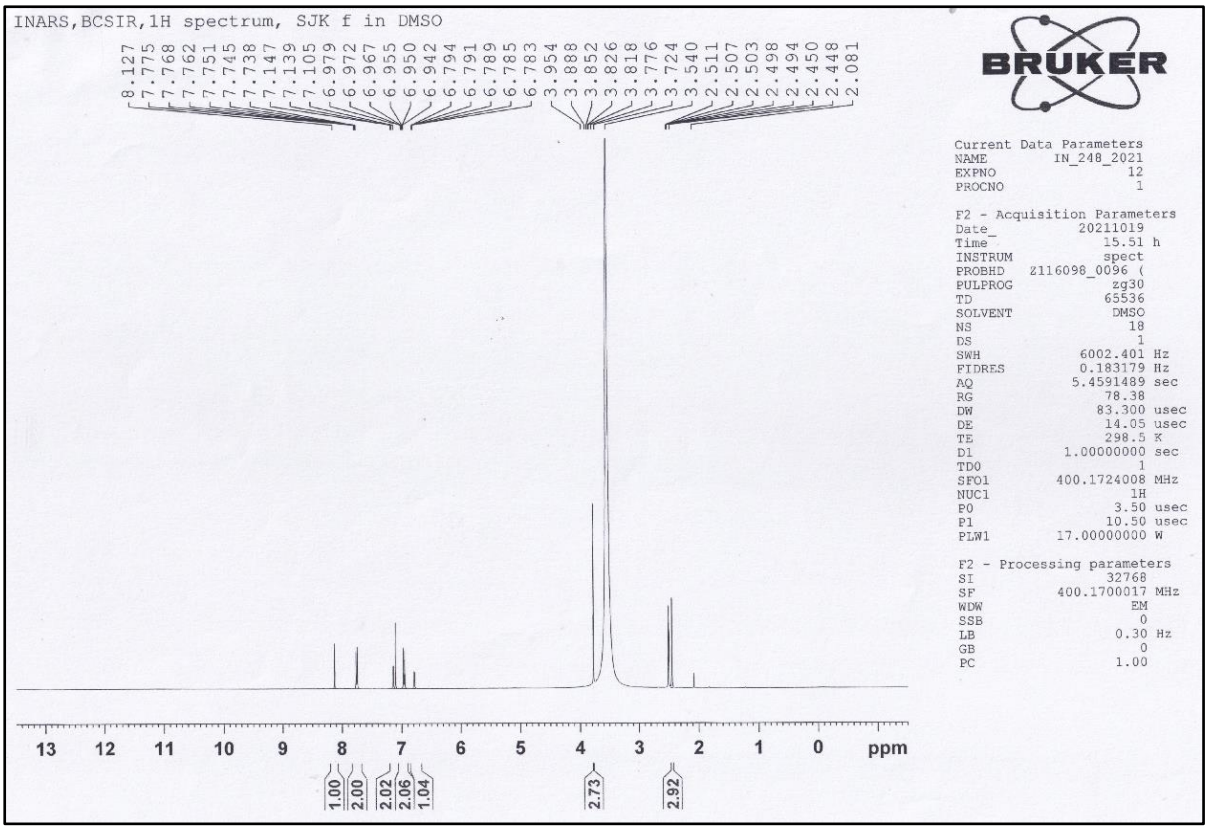
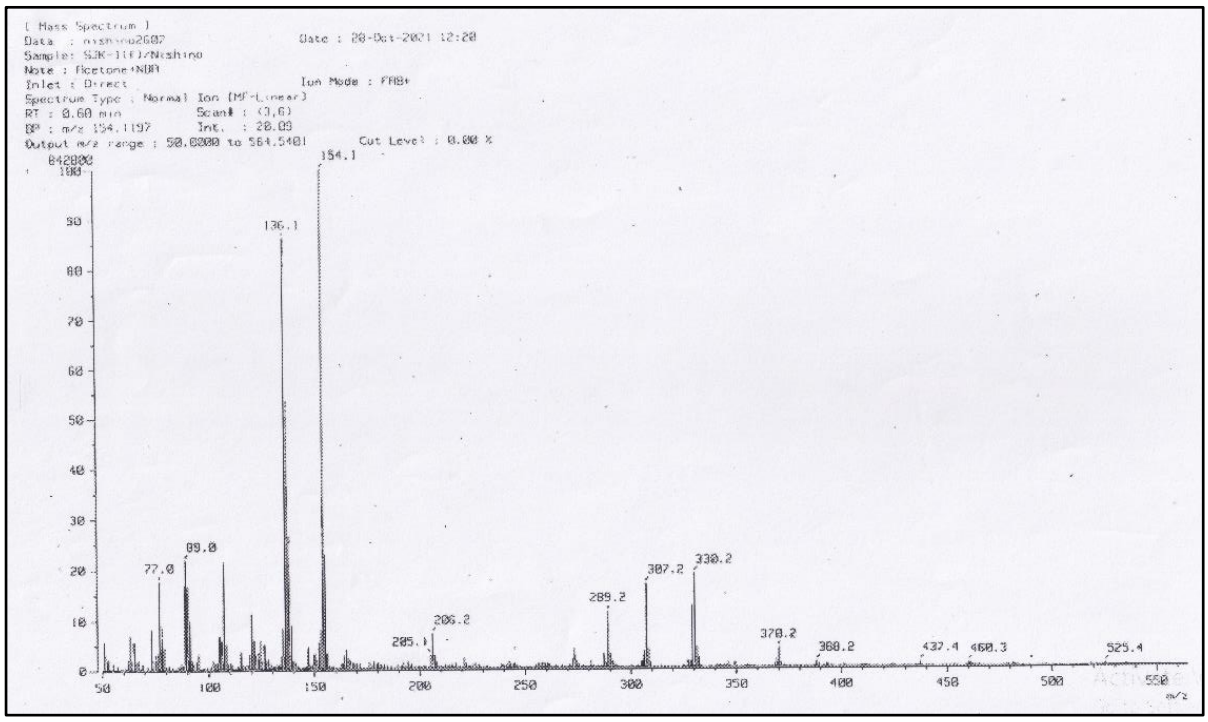


Fig. S23. ^{1}H NMR spectrum of **2h.**

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[ Elemental Composition ]
Data   : nishino2608                    Date : 28-Oct-2021 12:23
Sample: SJK-1(f)/Nishino
Note : Acetone+NBA
Inlet : Direct                          Ion Mode : FAB+
RT : 4.63 min                           Scan#: (17,22)
Elements : C 100/0, H 100/0, O 2/0, N 4/2, S 3/1
Mass Tolerance       : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z Int%   Err[ppm / mmu]    U.S.  Composition
  329.0678    59.5    -21.4 /  -7.0   16.5  C 20 H 13 O N 2 S
                      +16.8 /  +5.5   17.0  C 19 H 11 O N 3 S
                       +6.5 /  +2.2   13.0  C 16 H 15 O N 3 S 2
                       -3.7 /  -1.2    9.0  C 13 H 19 O N 3 S 3

  330.0749    56.2    -23.6 /  -7.8   16.0  C 20 H 14 O N 2 S
                      +14.5 /  +4.8   16.5  C 19 H 12 O N 3 S
                       +4.3 /  +1.4   12.5  C 16 H 16 O N 3 S 2
                       -5.9 /  -2.0    8.5  C 13 H 20 O N 3 S 3
```

Fig. S24. HRMS spectrum of **2h.**

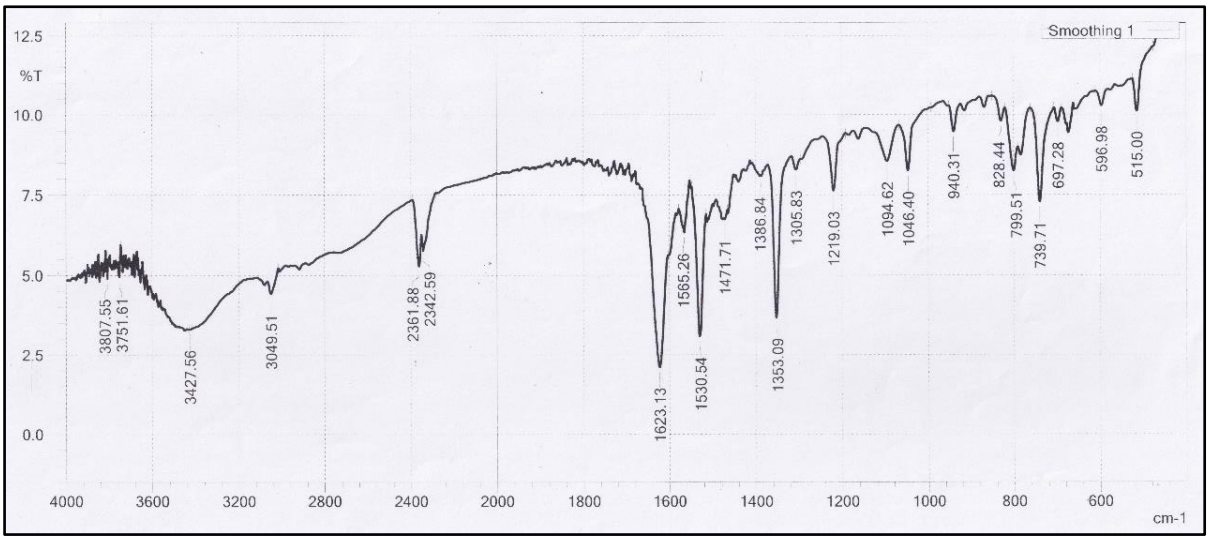


Fig. S25. IR spectrum of **2i.**

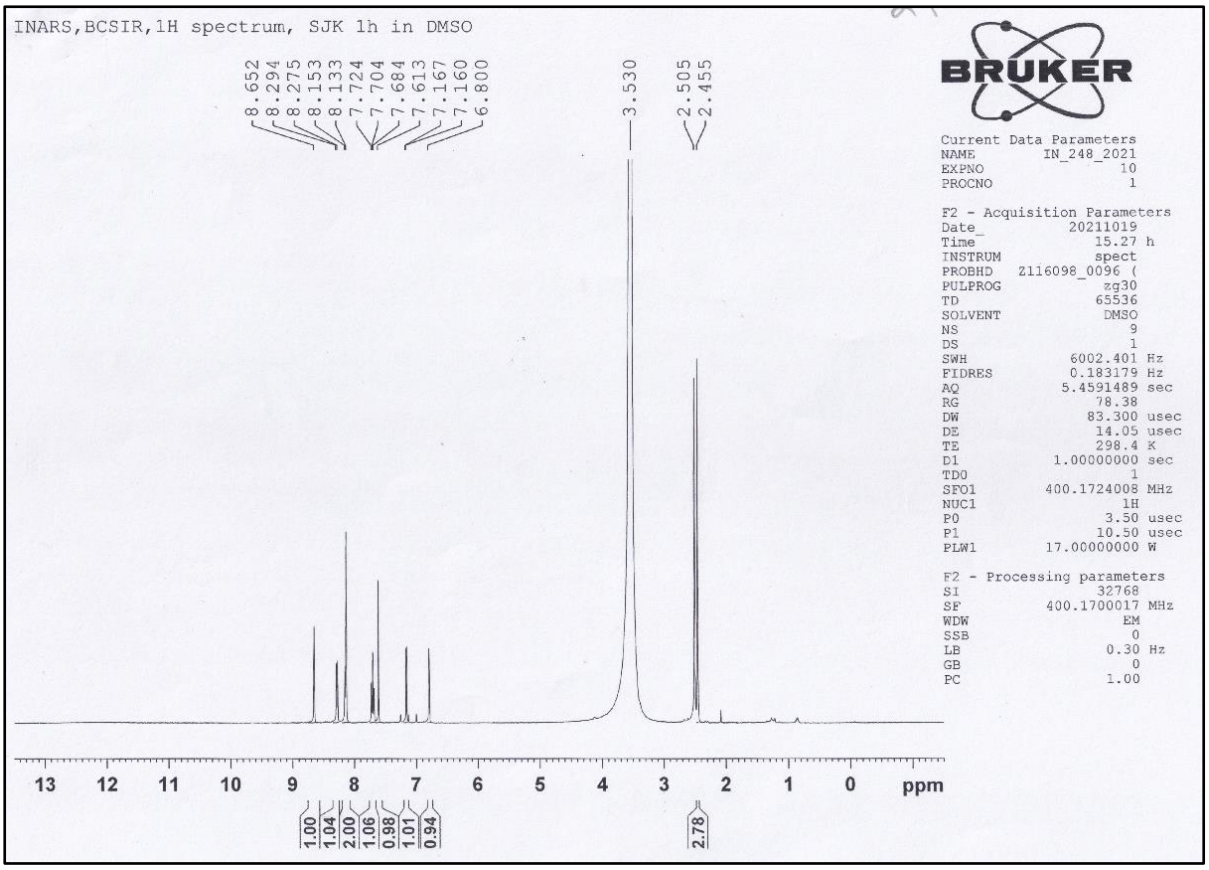
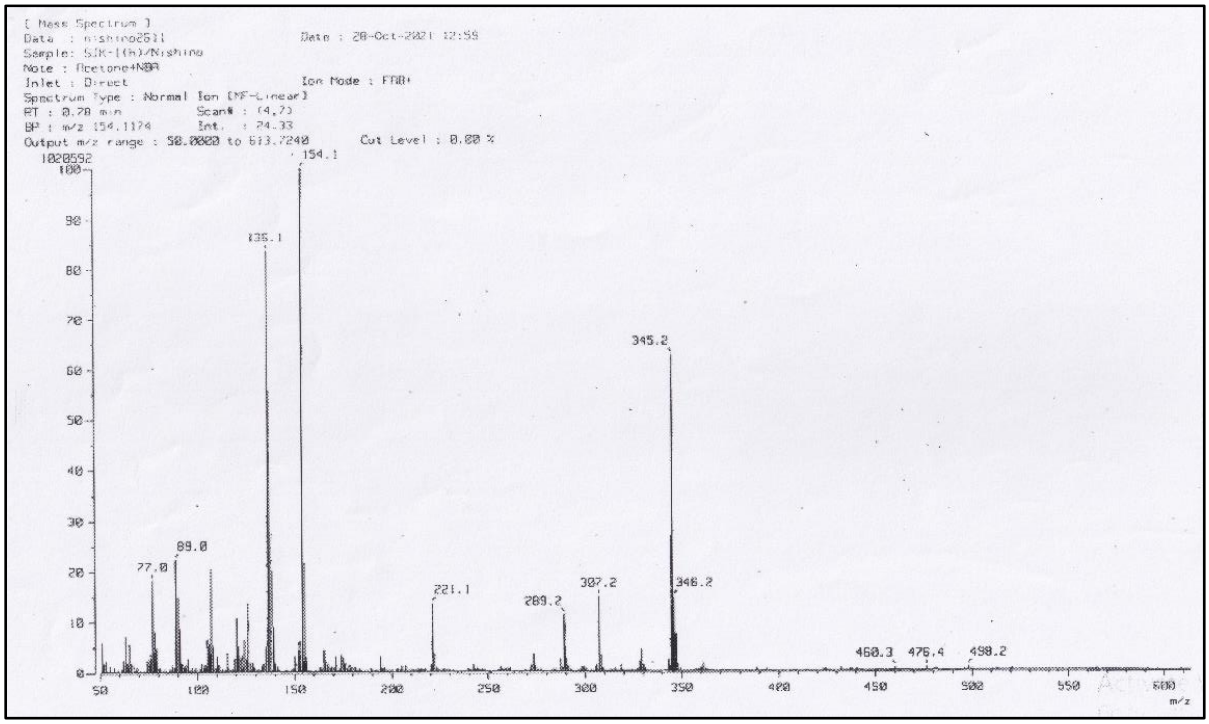


Fig. S26. ^{1}H NMR spectrum of **2i.**



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Note : Acetone+NBA
Inlet : Direct Ion Mode : FAB+
RT : 4.25 min Scan#: (16,20)
Elements : C 100/0, H 100/0, O 3/1, N 5/3, S 3/1
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
344.0402	78.8	-26.7 / -9.2	17.5	C 19 H 10 O 2 N 3 S
		+9.9 / +3.4	18.0	C 18 H 8 O 2 N 4 S
		+0.1 / +0.0	14.0	C 15 H 12 O 2 N 4 S 2
		-9.7 / -3.3	10.0	C 12 H 16 O 2 N 4 S 3
		+26.8 / +9.2	10.5	C 11 H 14 O 2 N 5 S 3
345.0471	100.0	+7.1 / +2.5	17.5	C 18 H 9 O 2 N 4 S
		-2.6 / -0.9	13.5	C 15 H 13 O 2 N 4 S 2
		-12.4 / -4.3	9.5	C 12 H 17 O 2 N 4 S 3
		+24.0 / +8.3	10.0	C 11 H 15 O 2 N 5 S 3

Fig. S27. HRMS spectrum of **2i.**

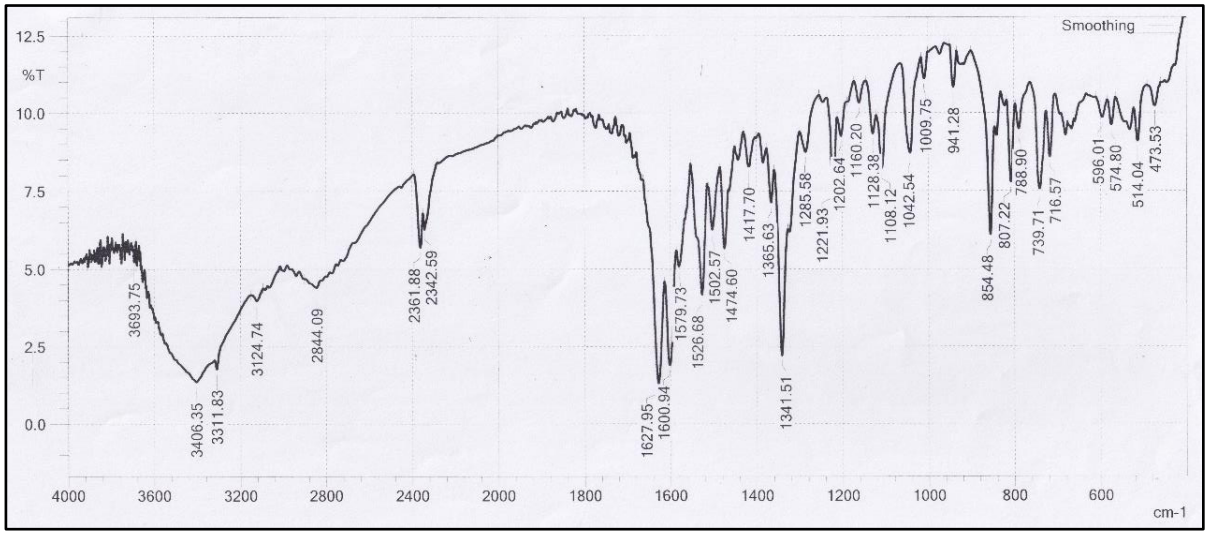


Fig. S28. IR spectrum of **2j.**

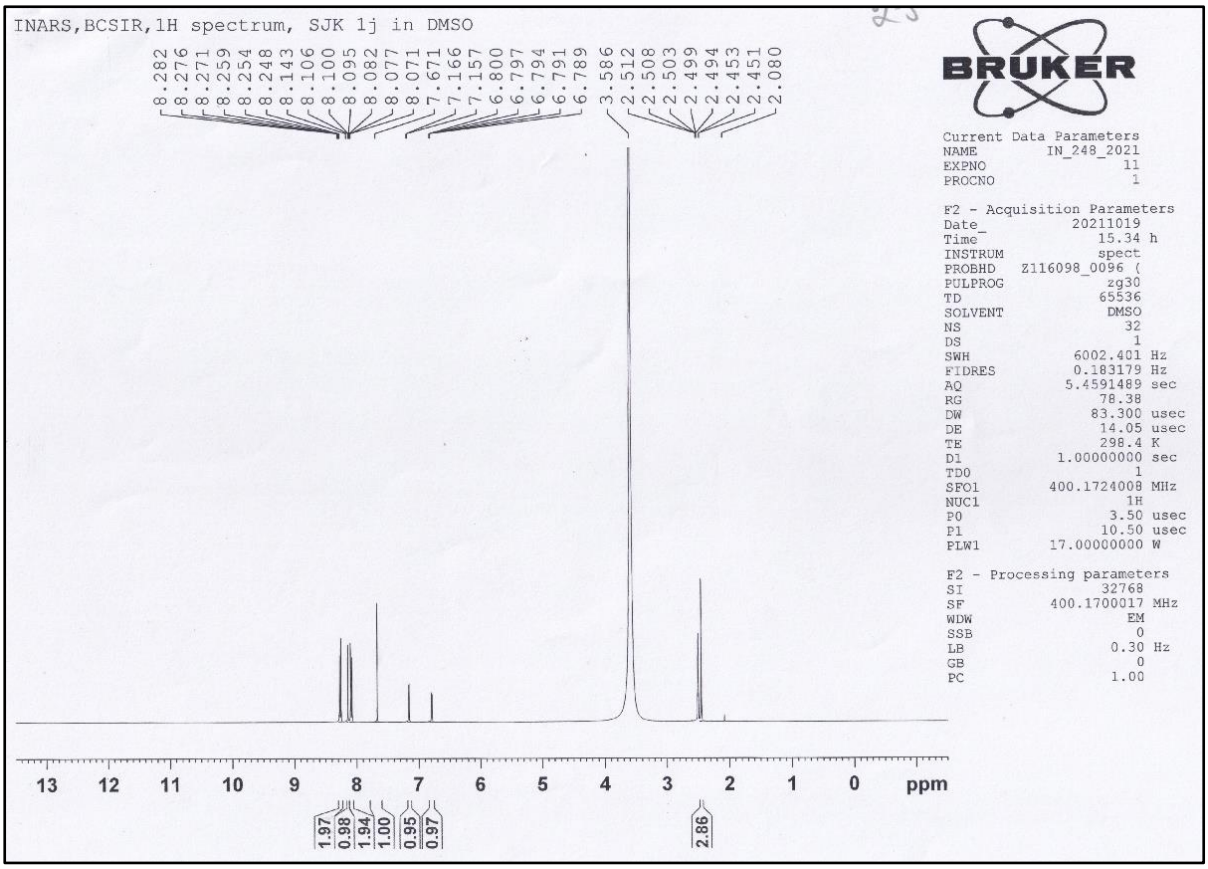
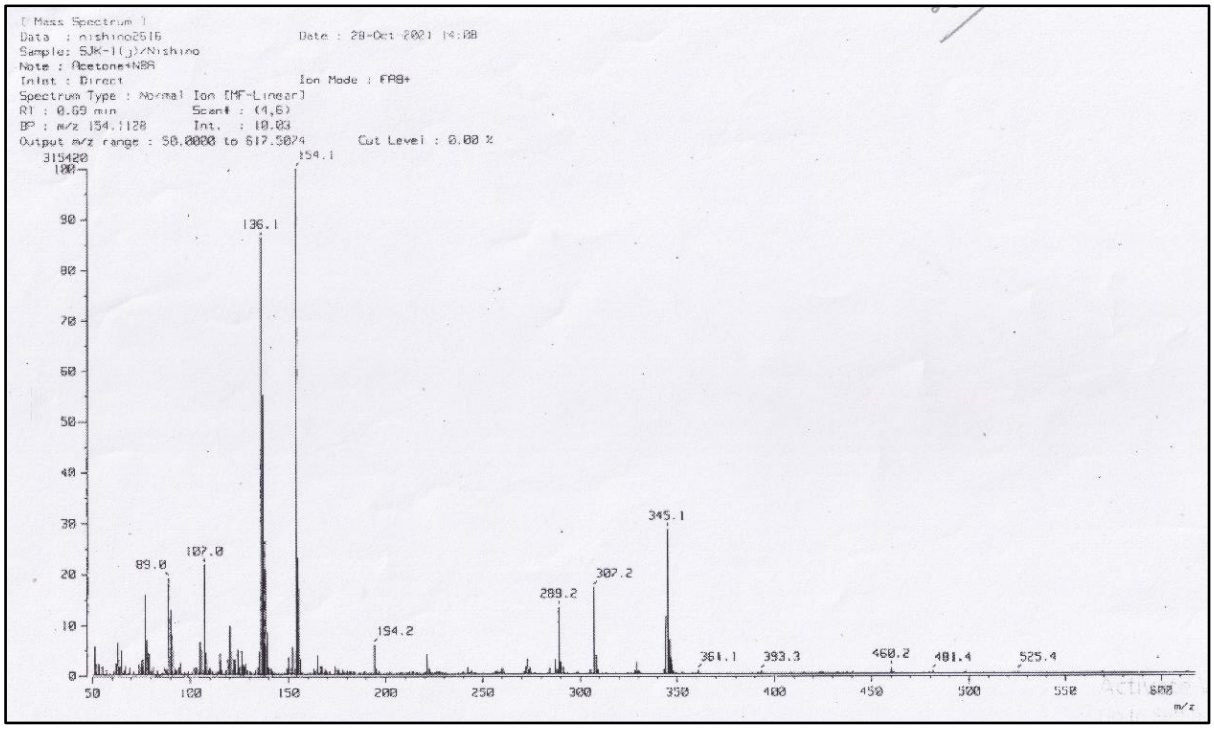


Fig. S29. ^{1}H NMR spectrum of **2j.**




```
[ Elemental Composition ]
Data   : nishino2617                    Date : 28-Oct-2021 14:11
Sample: SJK-1(j)/Nishino
Note   : Acetone+NBA
Inlet  : Direct                         Ion Mode : FAB+
RT     : 4.50 min                       Scan#: (17,21)
Elements : C 100/0, H 100/0, O 3/1, N 5/3, S 3/1
Mass Tolerance      : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z  Int%   Err[ppm / mmu]     U.S.   Composition
  344.0405    20.6     -25.7 /  -8.8    17.5   C 19 H 10 O 2 N 3 S
                       +10.8 /  +3.7    18.0   C 18 H 8 O 2 N 4 S
                        +1.0 /  +0.4    14.0   C 15 H 12 O 2 N 4 S 2
                        -8.8 /  -3.0    10.0   C 12 H 16 O 2 N 4 S 3
                       +27.8 /  +9.6    10.5   C 11 H 14 O 2 N 5 S 3

  345.0473    17.6     -28.6 /  -9.9    17.0   C 19 H 11 O 2 N 3 S
                        +7.9 /  +2.7    17.5   C 18 H 9 O 2 N 4 S
                        -1.9 /  -0.7    13.5   C 15 H 13 O 2 N 4 S 2
                       -11.7 /  -4.0     9.5   C 12 H 17 O 2 N 4 S 3
                       +24.8 /  +8.5    10.0   C 11 H 15 O 2 N 5 S 3
```

Fig. S30. HRMS spectrum of **2j.**

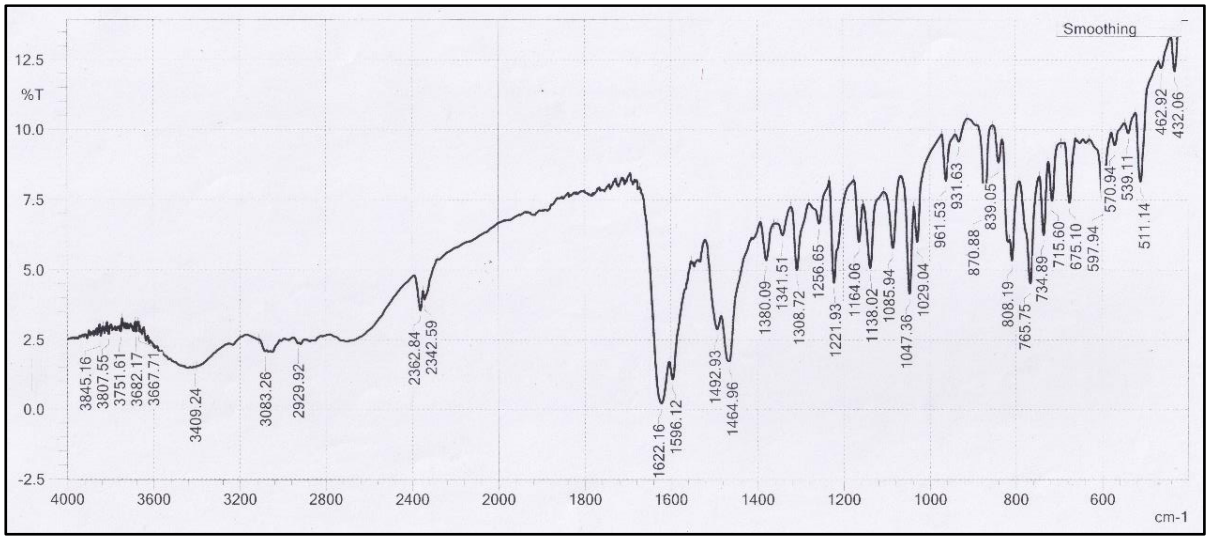


Fig. S31. IR spectrum of **2k.**

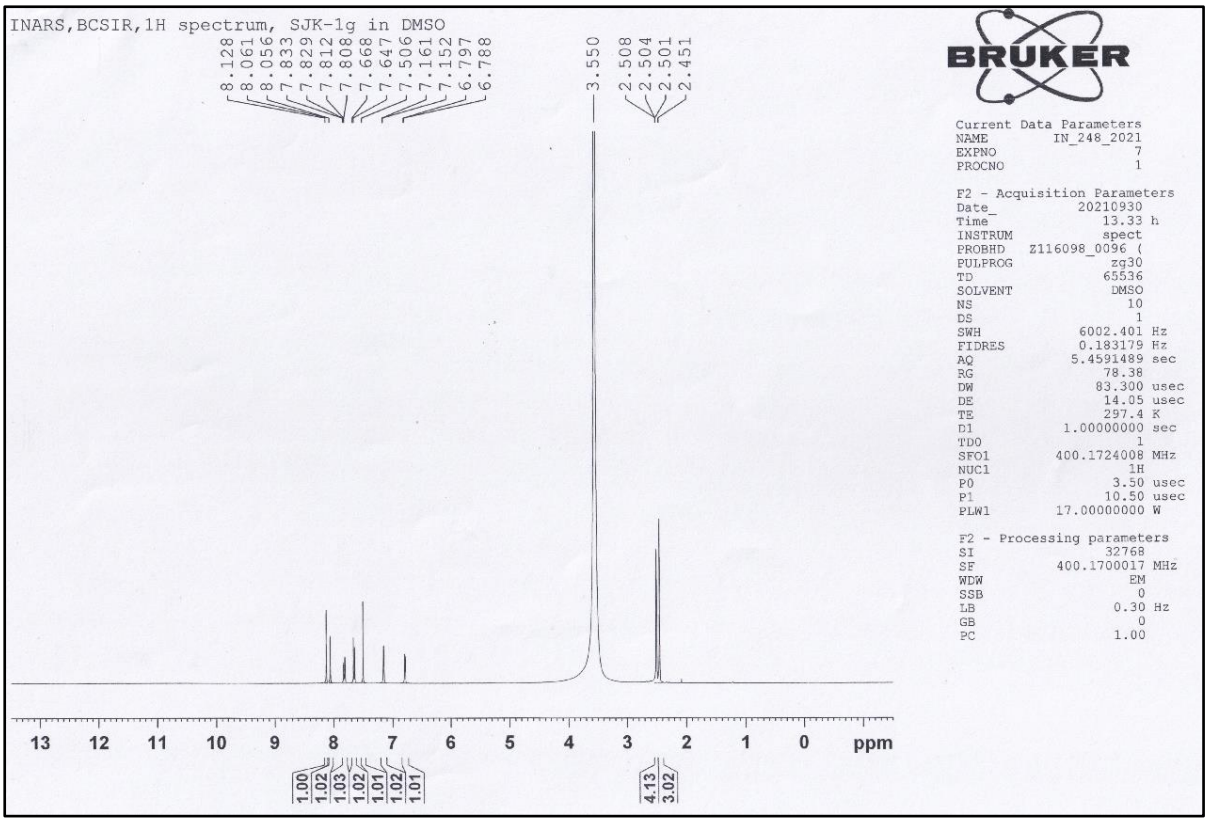
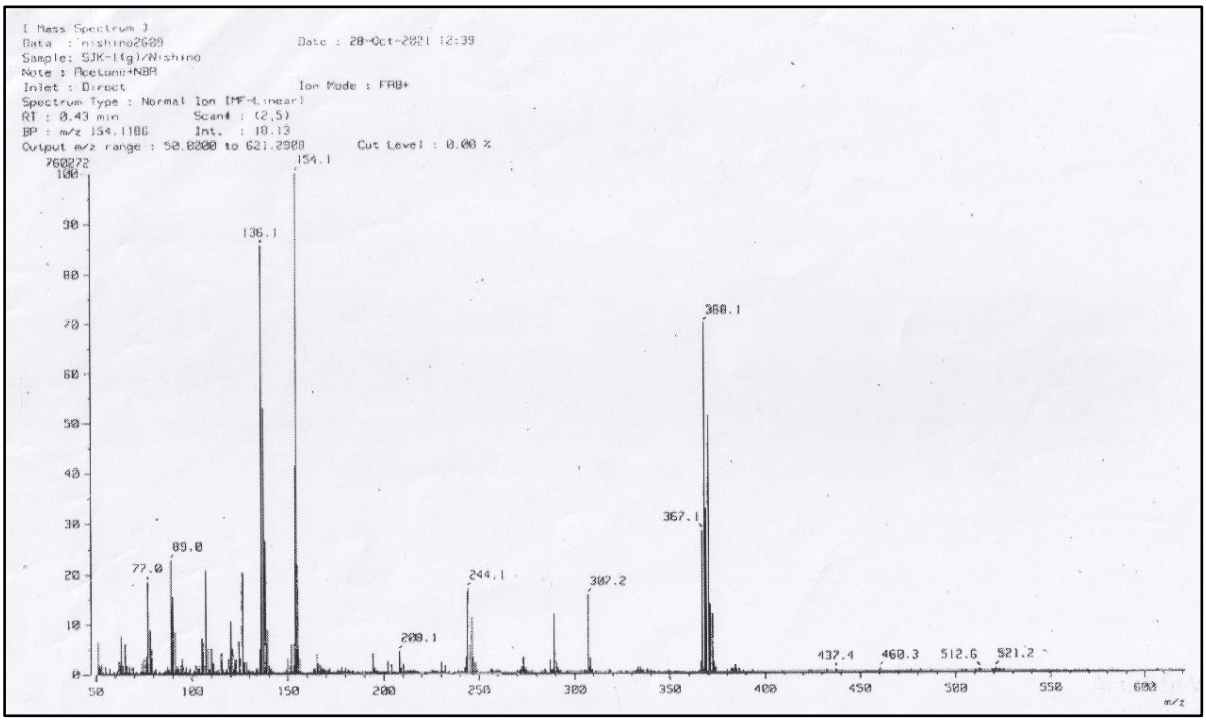


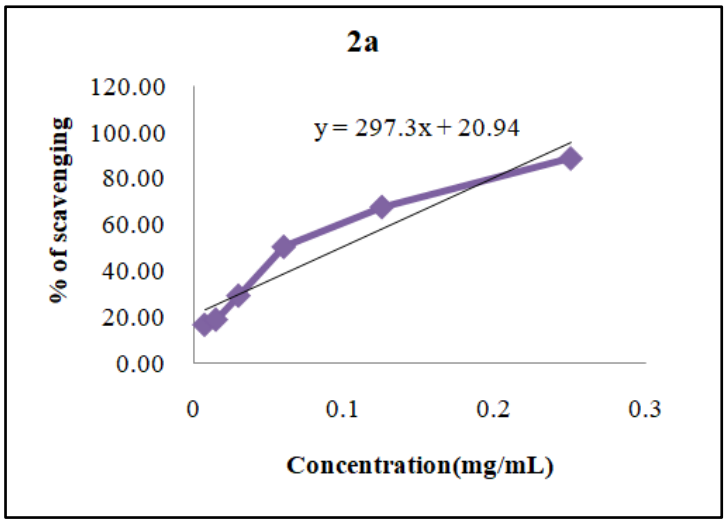
Fig. S32. ^{1}H NMR spectrum of **2k.**

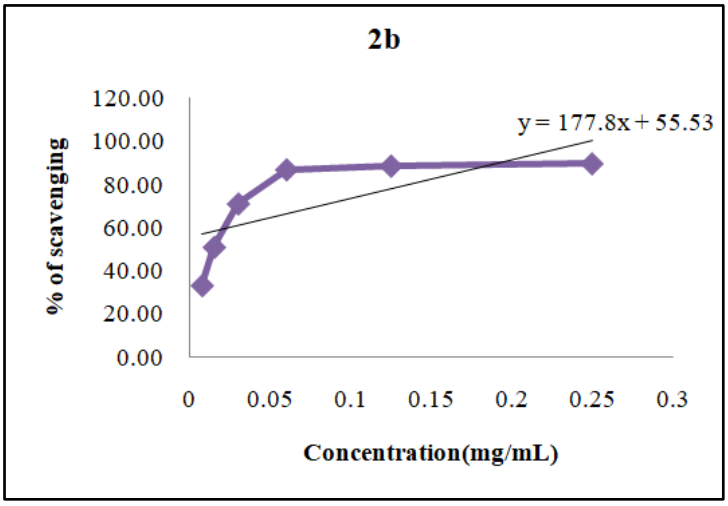


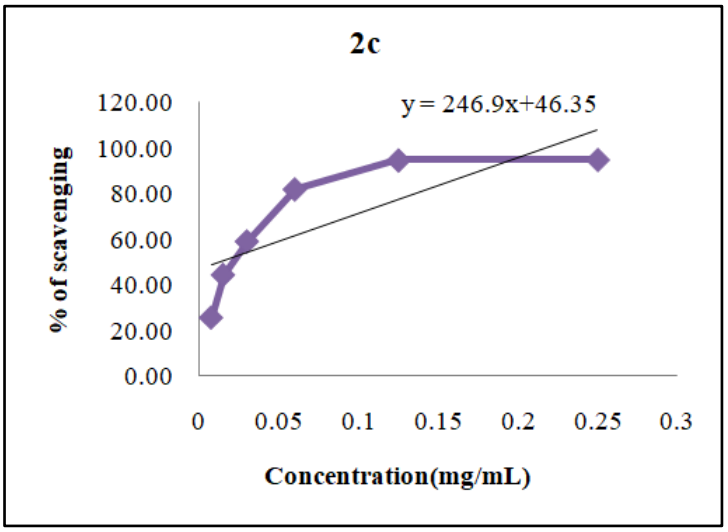
[Elemental Composition]
Data : nishino2610 Date : 28-Oct-2021 12:41
Sample: SJK-1(g)/Nishino
Note : Acetone+NBA
Inlet : Direct Ion Mode : FAB+
RT : 4.13 min Scan#: (16,19)
Elements : C 100/0, H 100/0, N 4/2, Cl 3/1, S 3/1
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 50.0

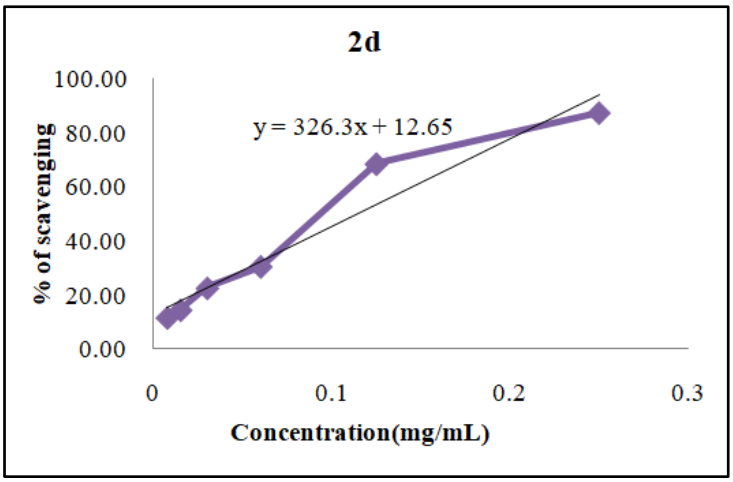
Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
366.9783	65.0	-16.9 / -6.2	21.5	C 20 H 4 N 4 Cl S
		-21.8 / -8.0	16.5	C 19 H 9 N 2 Cl 2 S
		+12.4 / +4.6	17.0	C 18 H 7 N 3 Cl 2 S
		-26.1 / -9.6	17.5	C 17 H 8 N 4 Cl S 2
		+3.2 / +1.2	13.0	C 15 H 11 N 3 Cl 2 S 2
		-6.0 / -2.2	9.0	C 12 H 15 N 3 Cl 2 S 3
		+23.3 / +8.6	4.5	C 10 H 18 N 2 Cl 3 S 3
367.9835	100.0	-24.0 / -8.8	21.0	C 20 H 5 N 4 Cl S
		+5.2 / +1.9	16.5	C 18 H 8 N 3 Cl 2 S
		-3.9 / -1.5	12.5	C 15 H 12 N 3 Cl 2 S 2
		+25.3 / +9.3	8.0	C 13 H 15 N 2 Cl 3 S 2
		-13.1 / -4.8	8.5	C 12 H 16 N 3 Cl 2 S 3
		+21.1 / +7.8	9.0	C 11 H 14 N 4 Cl 2 S 3
		+16.1 / +5.9	4.0	C 10 H 19 N 2 Cl 3 S 3

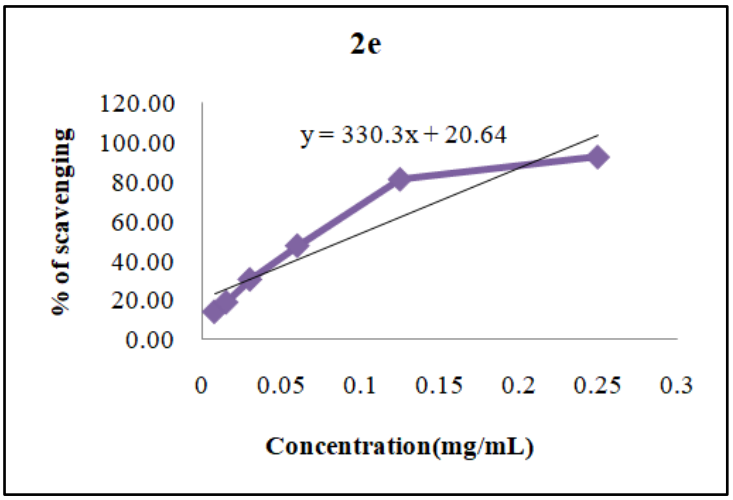
Fig. S33. HRMS spectrum of **2k.**

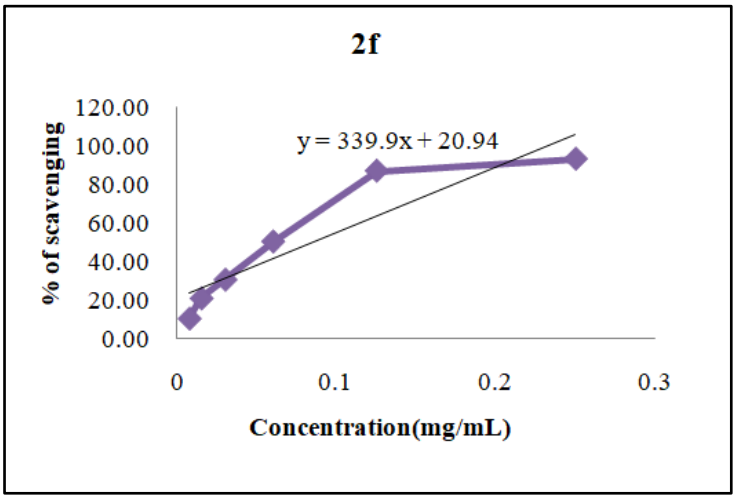

2a
120.00
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 297.3x + 20.94
0
0.1
0.2
0.3
Concentration(mg/mL)

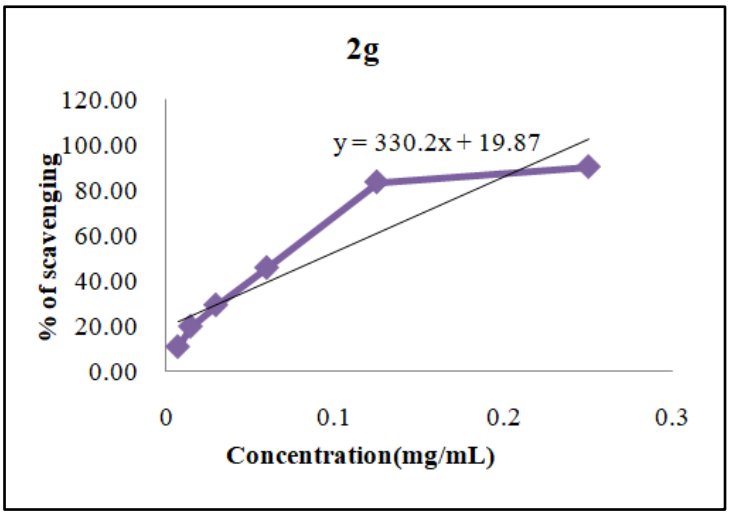

2b
120.00
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 177.8x + 55.53
0
0.05
0.1
0.15
0.2
0.25
0.3
Concentration(mg/mL)

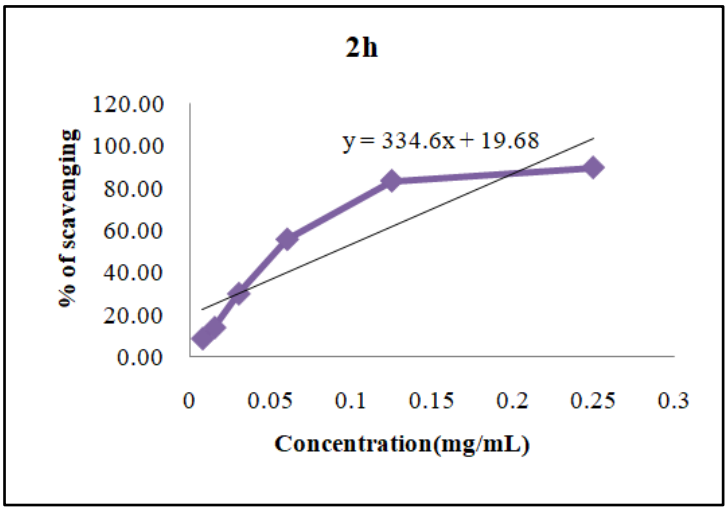

2c
120.00
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 246.9x+46.35
0
0.05
0.1
0.15
0.2
0.25
0.3
Concentration(mg/mL)

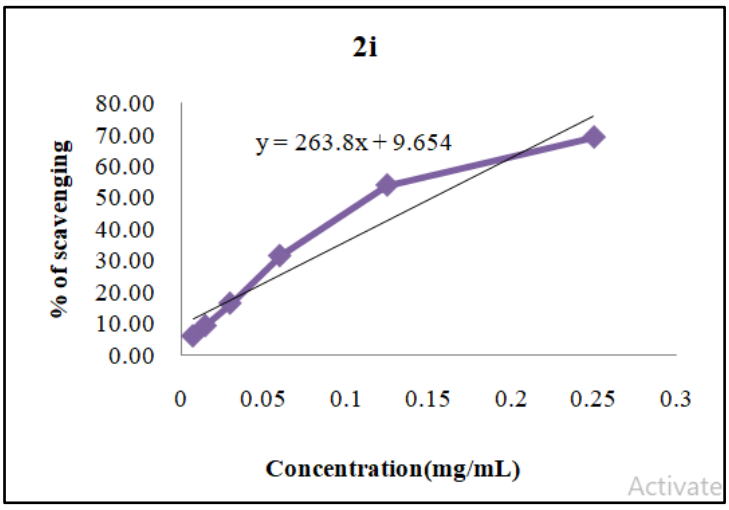

2d
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 326.3x + 12.65
0
0.1
0.2
0.3
Concentration(mg/mL)

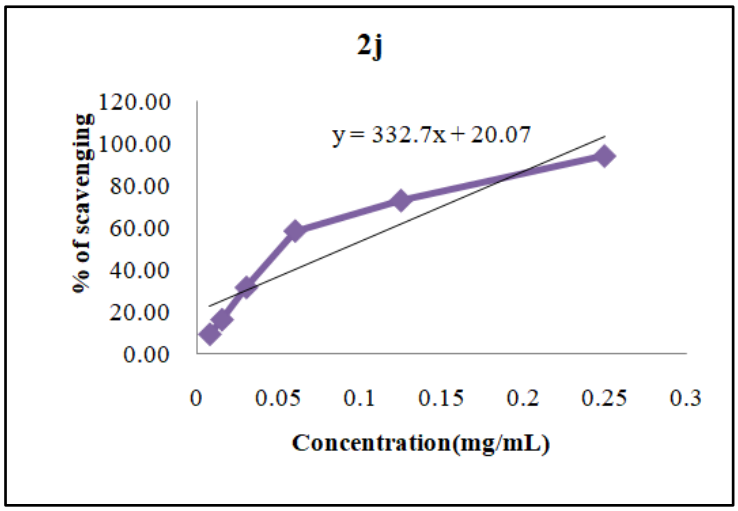

2e
120.00
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 330.3x + 20.64
0
0.05
0.1
0.15
0.2
0.25
0.3
Concentration(mg/mL)

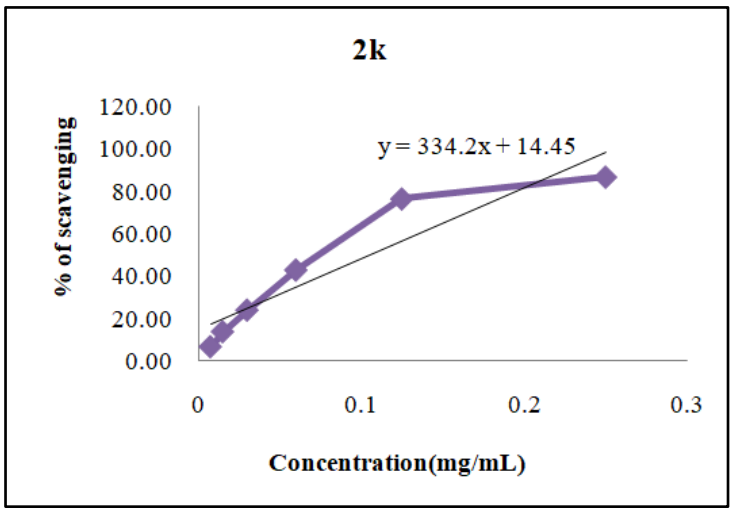

2f
120.00
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 339.9x + 20.94
0
0.1
0.2
0.3
Concentration(mg/mL)


2g
120.00
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 330.2x + 19.87
0
0.1
0.2
0.3
Concentration(mg/mL)


2h
120.00
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 334.6x + 19.68
0
0.05
0.1
0.15
0.2
0.25
0.3
Concentration(mg/mL)


2i
80.00
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
% of scavenging
y = 263.8x + 9.654
0
0.05
0.1
0.15
0.2
0.25
0.3
Concentration(mg/mL)
Activate


2j
120.00
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 332.7x + 20.07
0
0.05
0.1
0.15
0.2
0.25
0.3
Concentration(mg/mL)


2k
120.00
100.00
80.00
60.00
40.00
20.00
0.00
% of scavenging
y = 334.2x + 14.45
0
0.1
0.2
0.3
Concentration(mg/mL)

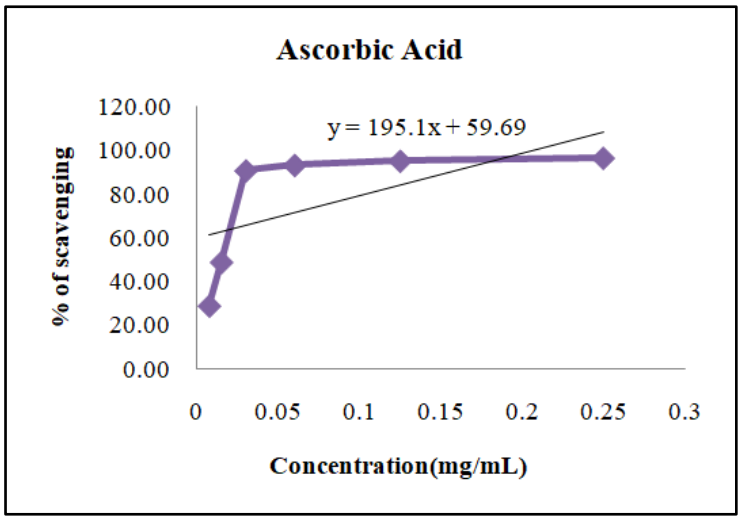


Fig. S34. Concentration-inhibition curves of synthesized compounds **2a-2k** and ascorbic acid.