

Design, synthesis, molecular docking, and dynamics studies of novel thiazole-Schiff base derivatives containing fluorene moiety with the assessment of their antimicrobial and antioxidant activity

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2. Concentration-inhibition curve to determine IC₅₀ values of **2a-2r** and ascorbic acid.

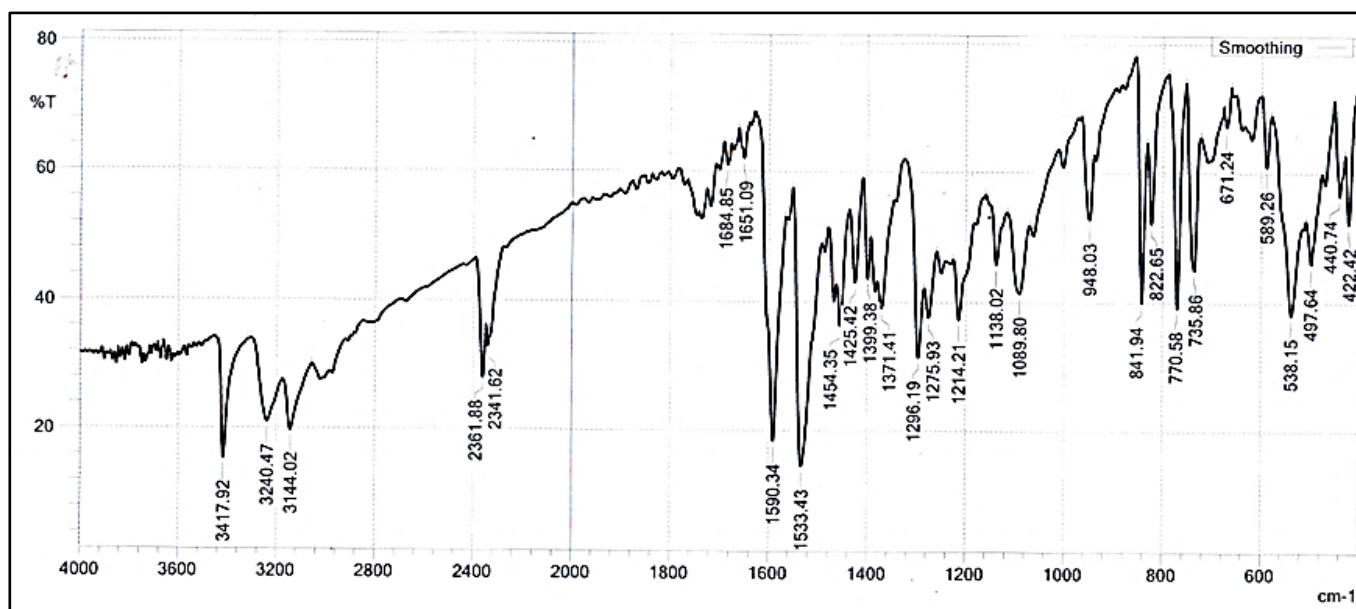


Fig. S1. IR spectrum of **1a**.

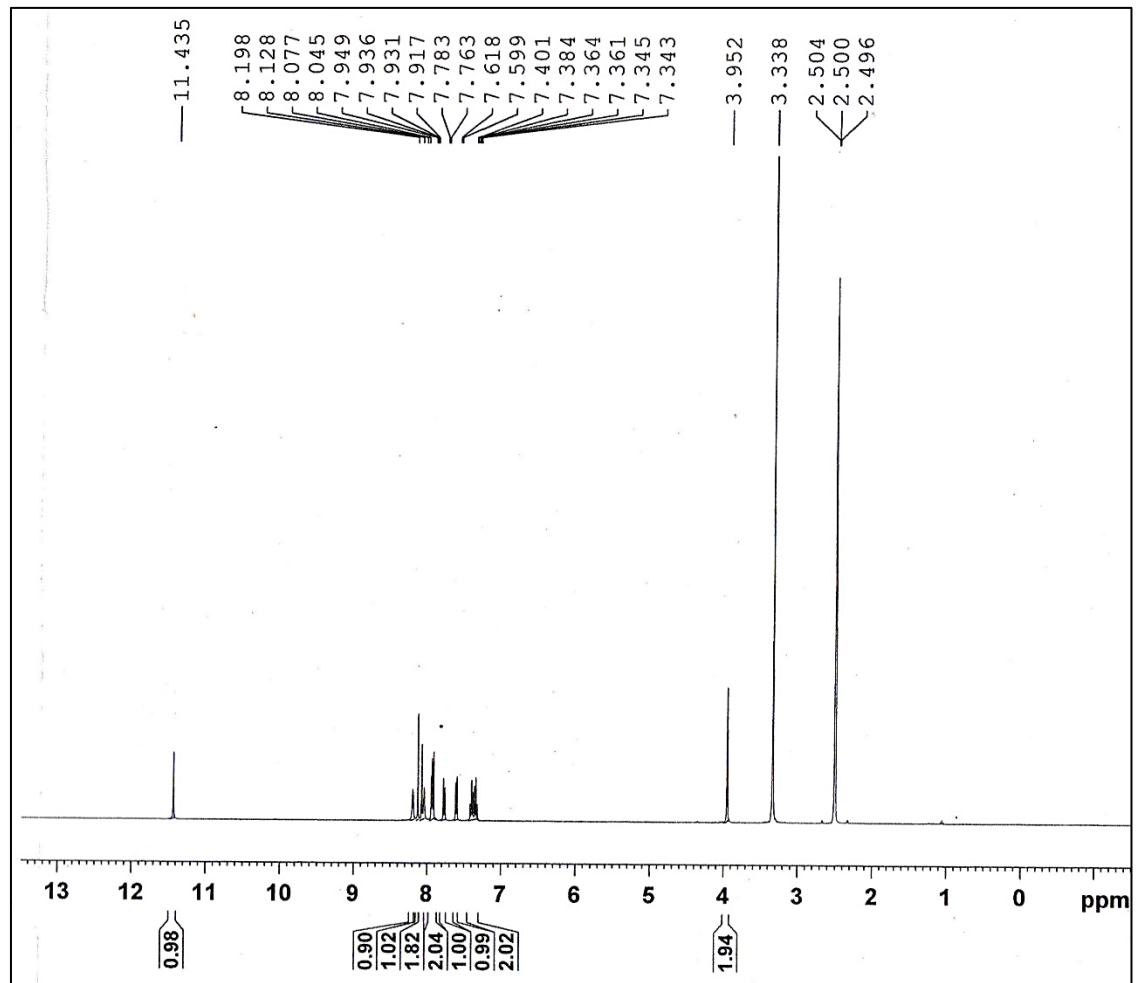
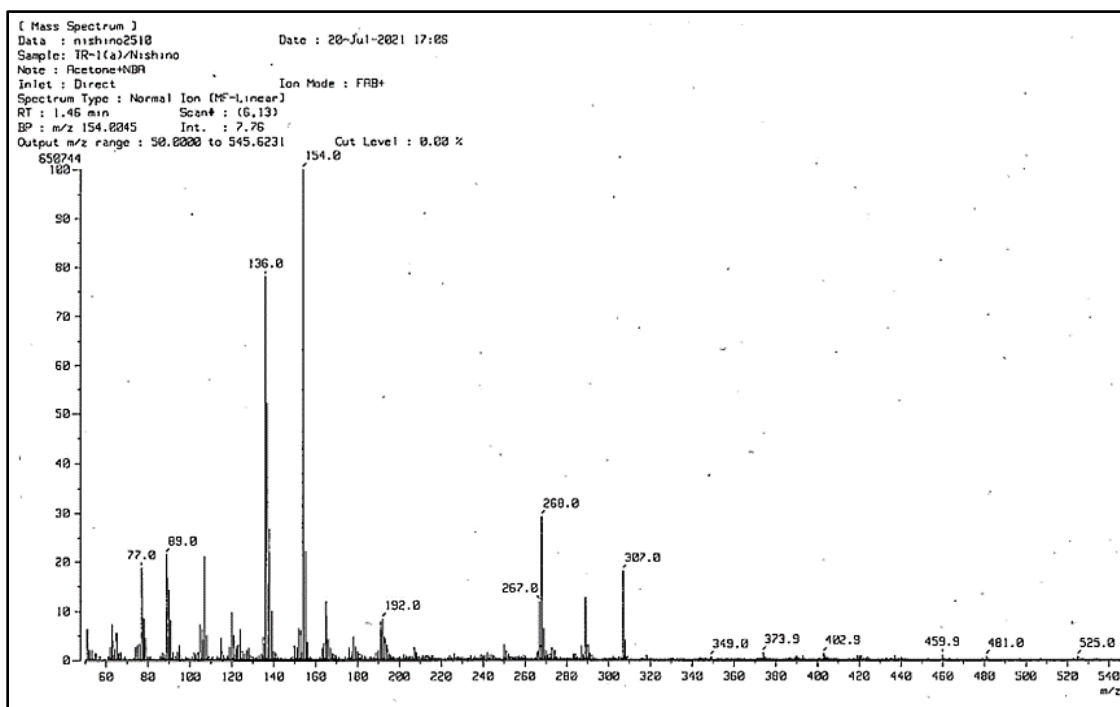


Fig. S2. ^1H NMR spectrum of **1a**.



[Elemental Composition]
 Date : 20-Jul-2021 17:13 Page: 1
 Data : nishino2511
 Sample: TR-1(a)/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 4.38 min Scan# : (16,21)
 Elements : C 100/0, H 100/0, N 4/2, S 2/0
 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
268.0933	14.9	-25.2 / -6.8	15.0	C 19 H 12 N 2
		+21.7 / +5.8	15.5	C 18 H 10 N 3
		+9.1 / +2.4	11.5	C 15 H 14 N 3 S
		-3.4 / -0.9	7.5	C 12 H 18 N 3 S 2

Fig. S3. HRMS spectrum of 1a.

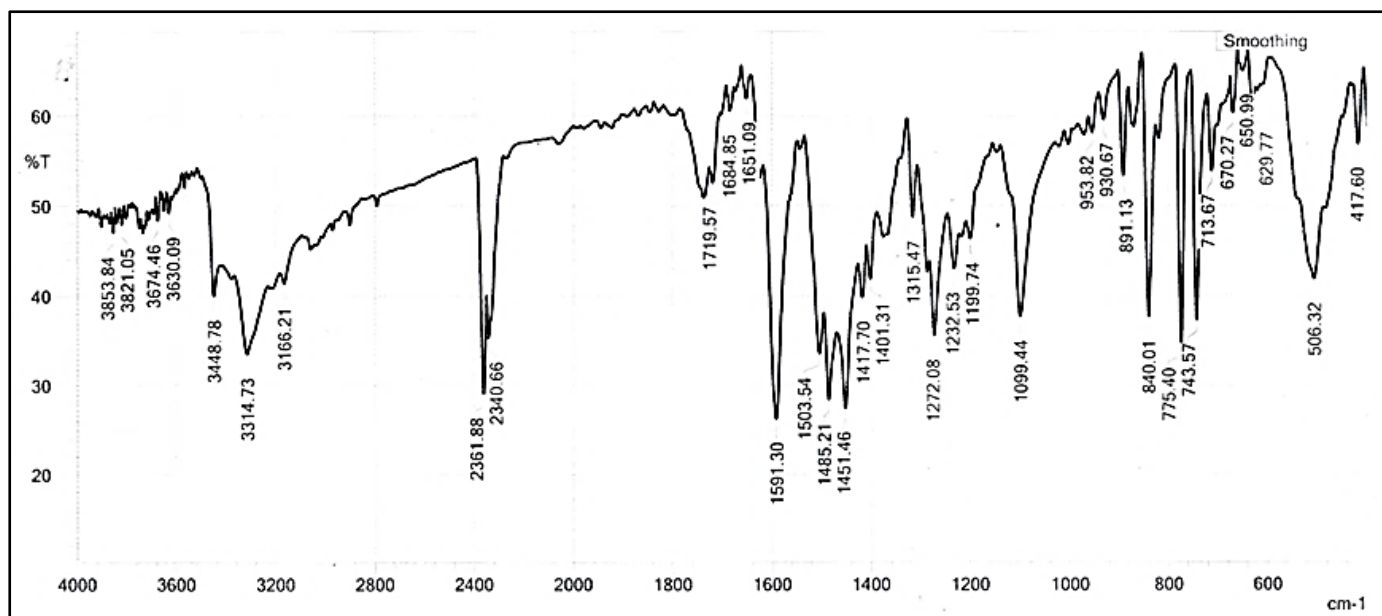


Fig. S4. IR spectrum of 1b.

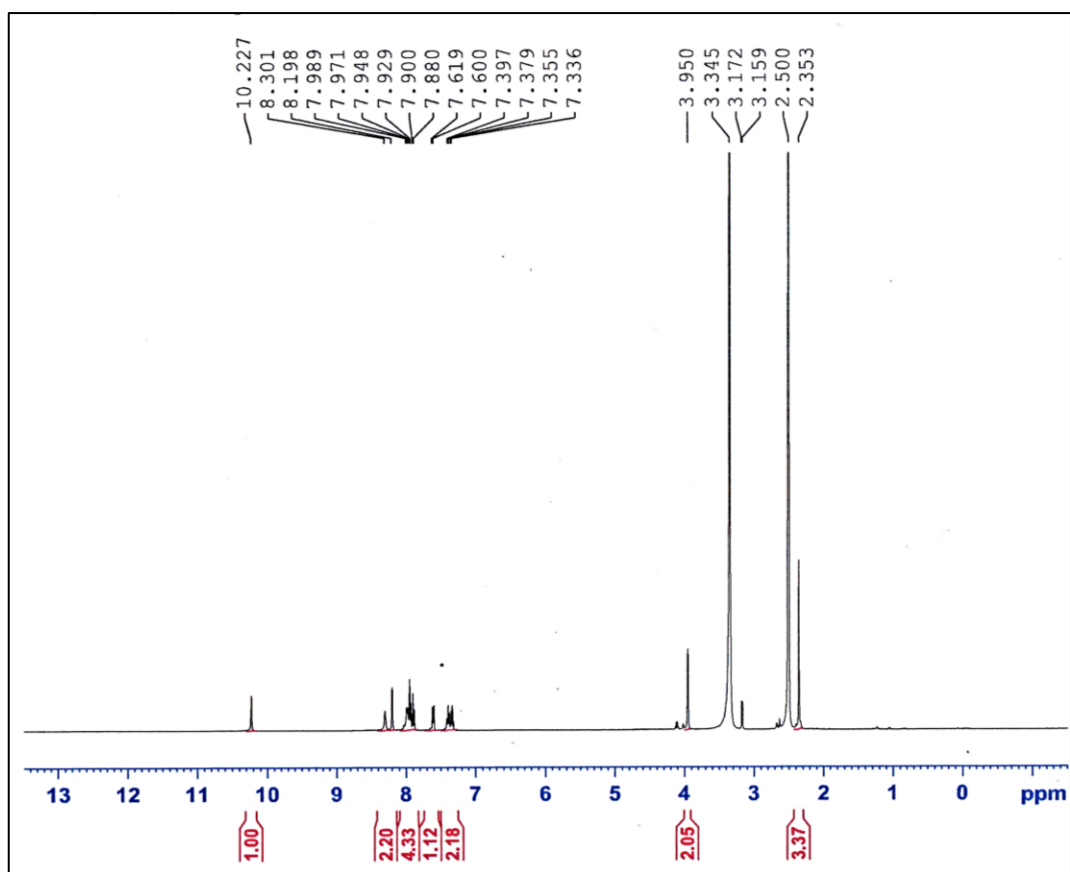
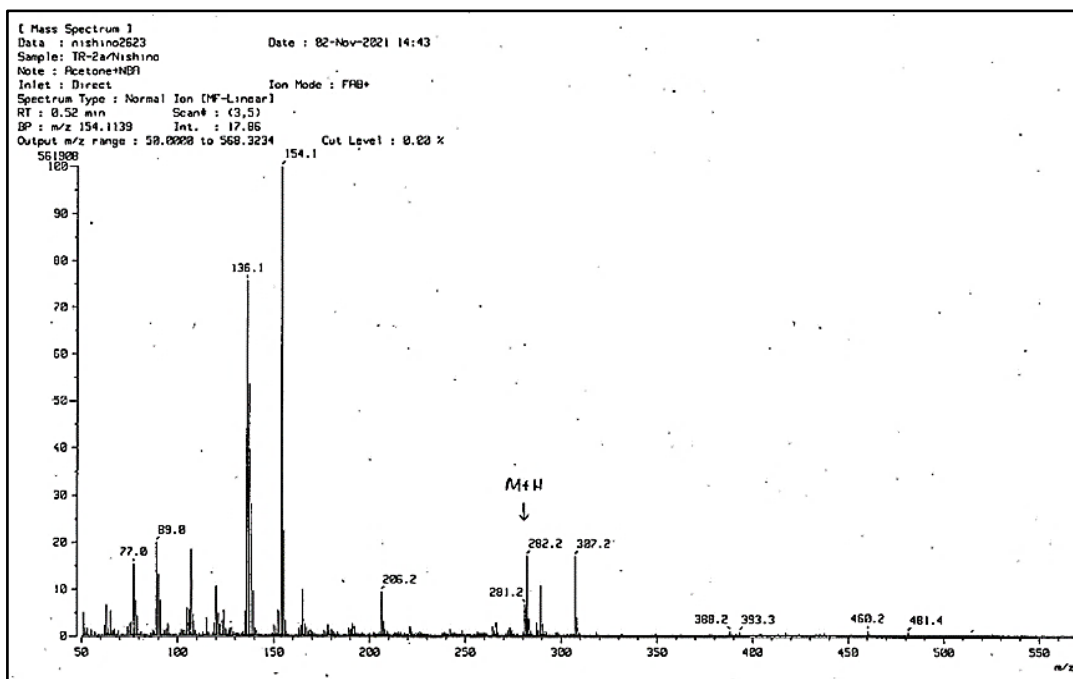


Fig. S5. ^1H NMR spectrum of **1b**.



[Elemental Composition] Page: 1
 Date : 02-Nov-2021 14:45
 Data : nishino2624
 Sample: TR-2a/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 4.50 min Scan#: (16,22)
 Elements : C 100/0, H 100/0, N 4/2, S 2/0
 Mass Tolerance : 20ppm, 10ppm if m/z < 500, 20ppm if m/z > 1000
 Unsaturation (U.S.) : -0.5 - 50.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
282.1073	44.6	-29.7 / -8.4	15.0	C 20 H 14 N 2
		+14.9 / +4.2	15.5	C 19 H 12 N 3
		+3.0 / +0.8	11.5	C 16 H 16 N 3 S
		-9.0 / -2.5	7.5	C 13 H 20 N 3 S 2

Fig. S6. HRMS spectrum of 1b.

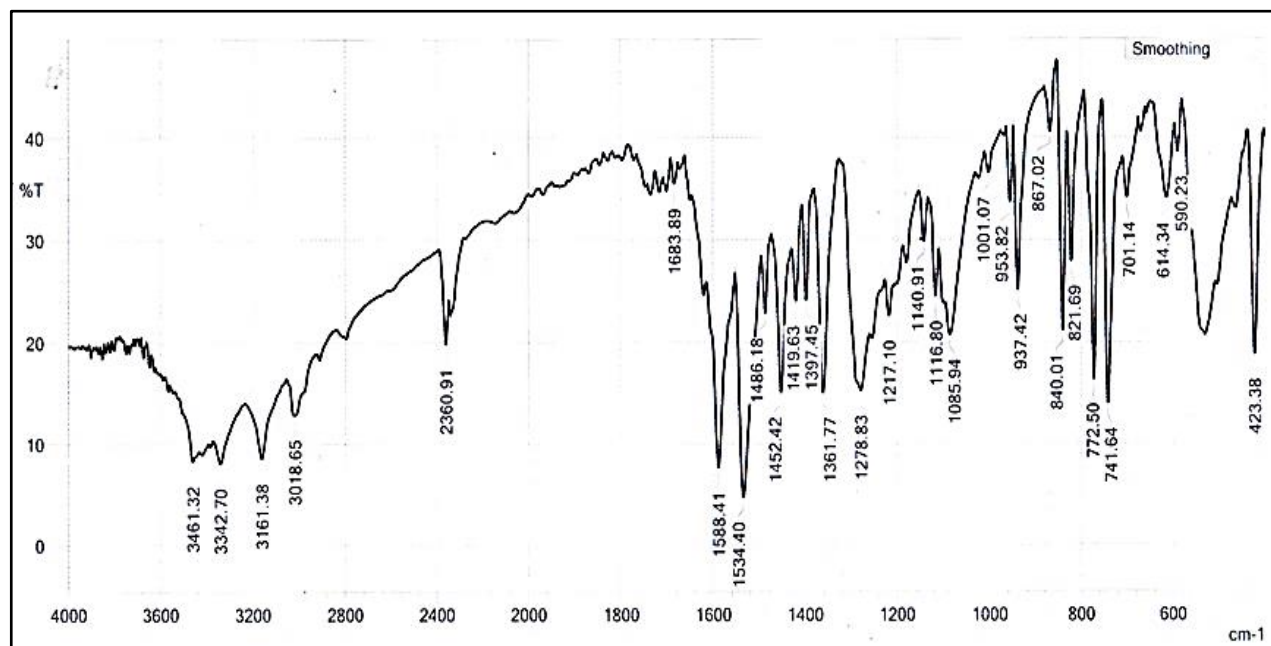


Fig. S7. IR spectrum of 2a.

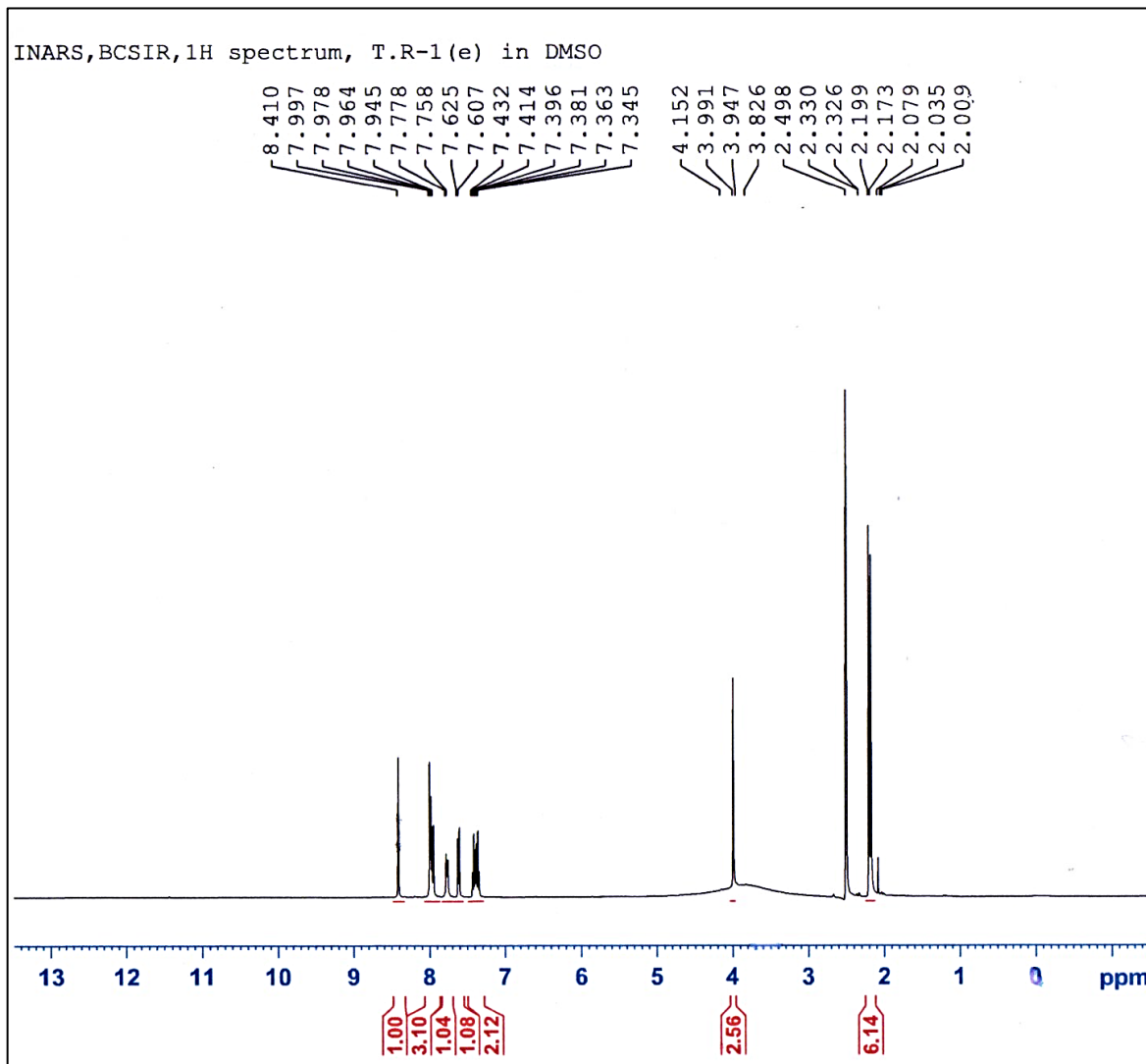
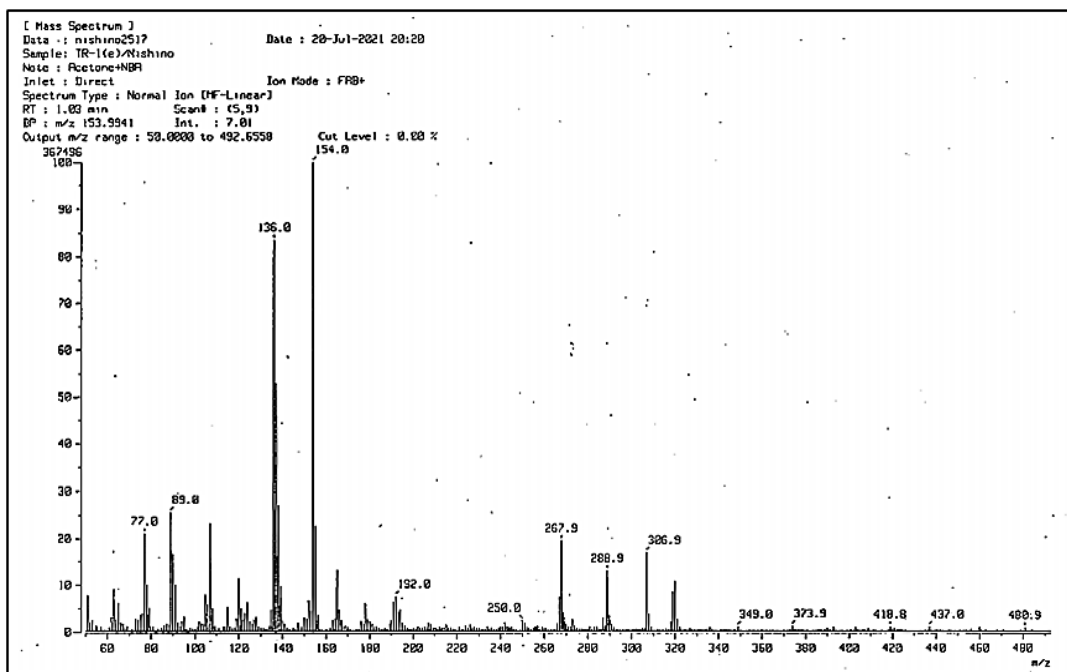


Fig. S8. ^1H NMR spectrum of **2a**.



[Elemental Composition]
 Date : 20-Jul-2021 20:23 Page: 1
 Data : nishino2518
 Sample: TR-1(e)/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 4.63 min Scan#: (16,23)
 Elements : C 100/0, H 100/0, N 4/2, S 2/0
 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
319.1147	64.4	-27.6 / -8.8	17.5	C 23 H 15 N 2
		+11.8 / +3.8	18.0	C 22 H 13 N 3
		+1.2 / +0.4	14.0	C 19 H 17 N 3 S
		-9.3 / -3.0	10.0	C 16 H 21 N 3 S 2
		+30.1 / +9.6	10.5	C 15 H 19 N 4 S 2
320.1212	71.7	+7.7 / +2.5	17.5	C 22 H 14 N 3
		-2.8 / -0.9	13.5	C 19 H 18 N 3 S
		-13.3 / -4.3	9.5	C 16 H 22 N 3 S 2
		+25.9 / +8.3	10.0	C 15 H 20 N 4 S 2

Fig. S9. HRMS spectrum of 2a.

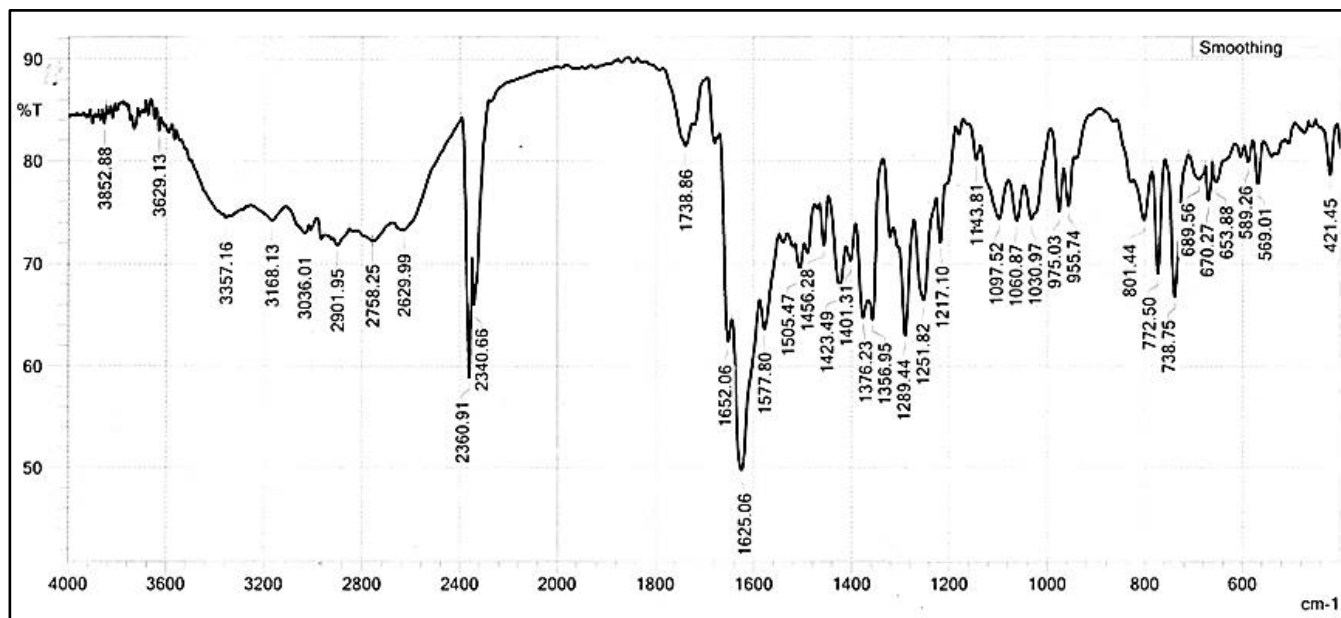


Fig. S10. IR spectrum of **2b**.

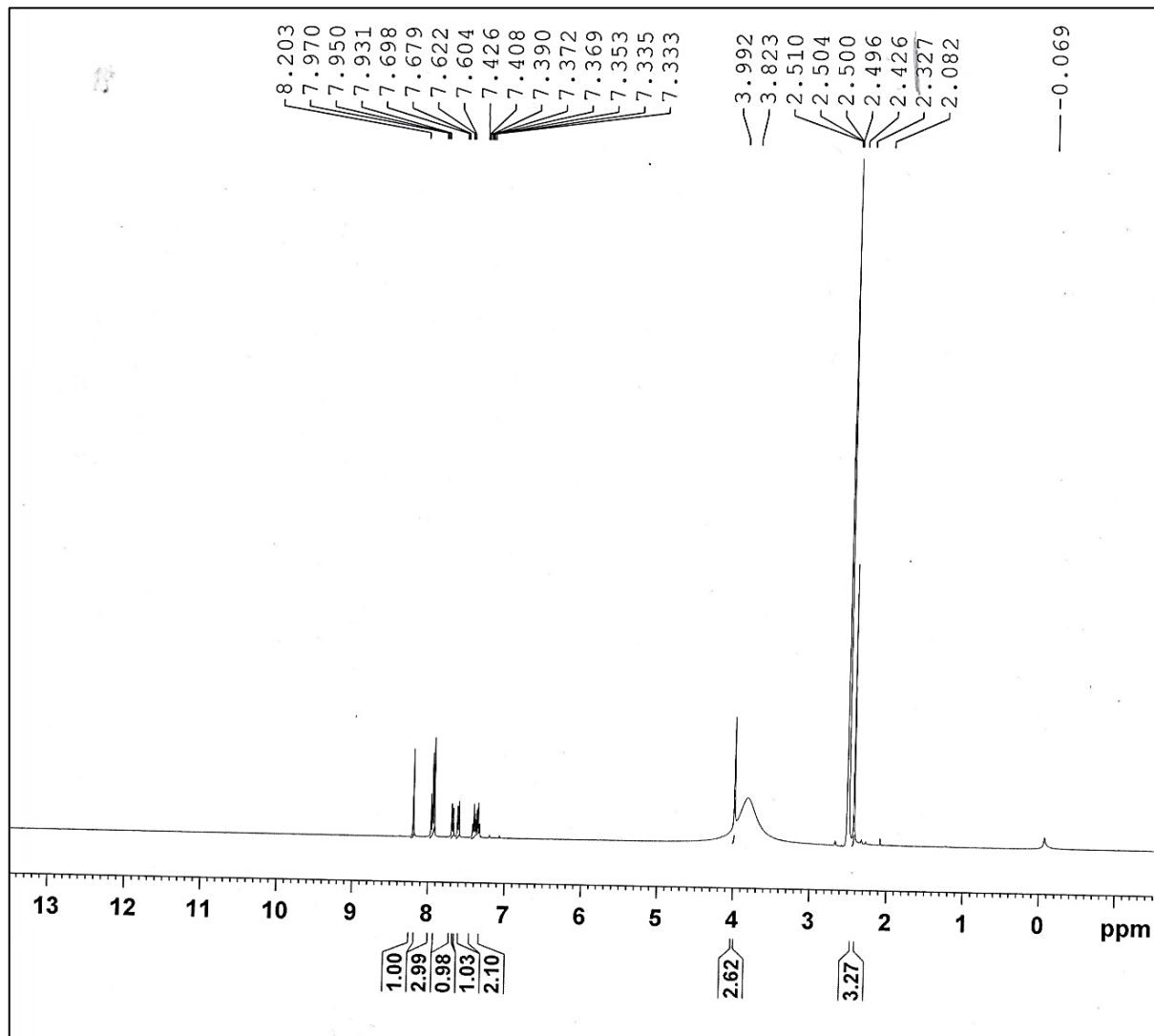
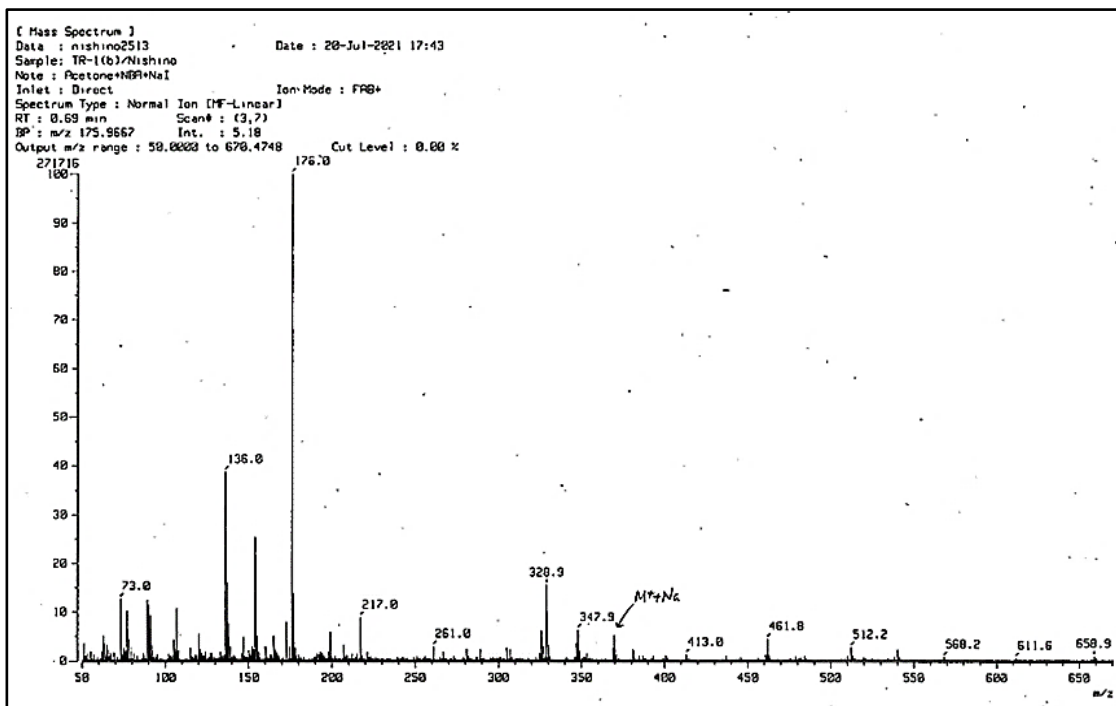


Fig. S11. ^1H NMR spectrum of **2b**.



[Elemental Composition]
 Data : nishino2514 Date : 20-Jul-2021 17:50 Page: 1
 Sample: TR-1(b)/Nishino
 Note : Acetone+NBA+NaI
 Inlet : Direct Ion Mode : FAB+
 RT : 1.13 min Scan#: (3,8)
 Elements : C 100/0, H 100/0, O 2/0, N 4/2, S 2/0, Na 1/1
 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
370.1021	100.0	-16.6 / -6.2	18.0	C 24 H 15 O N 2 Na
		+17.3 / +6.4	18.5	C 23 H 13 O N 3 Na
		-25.7 / -9.5	14.0	C 21 H 19 O N 2 S Na
		+8.2 / +3.0	14.5	C 20 H 17 O N 3 S Na
		-0.9 / -0.3	10.5	C 17 H 21 O N 3 S 2 Na

Fig. S12. HRMS spectrum of 2b.

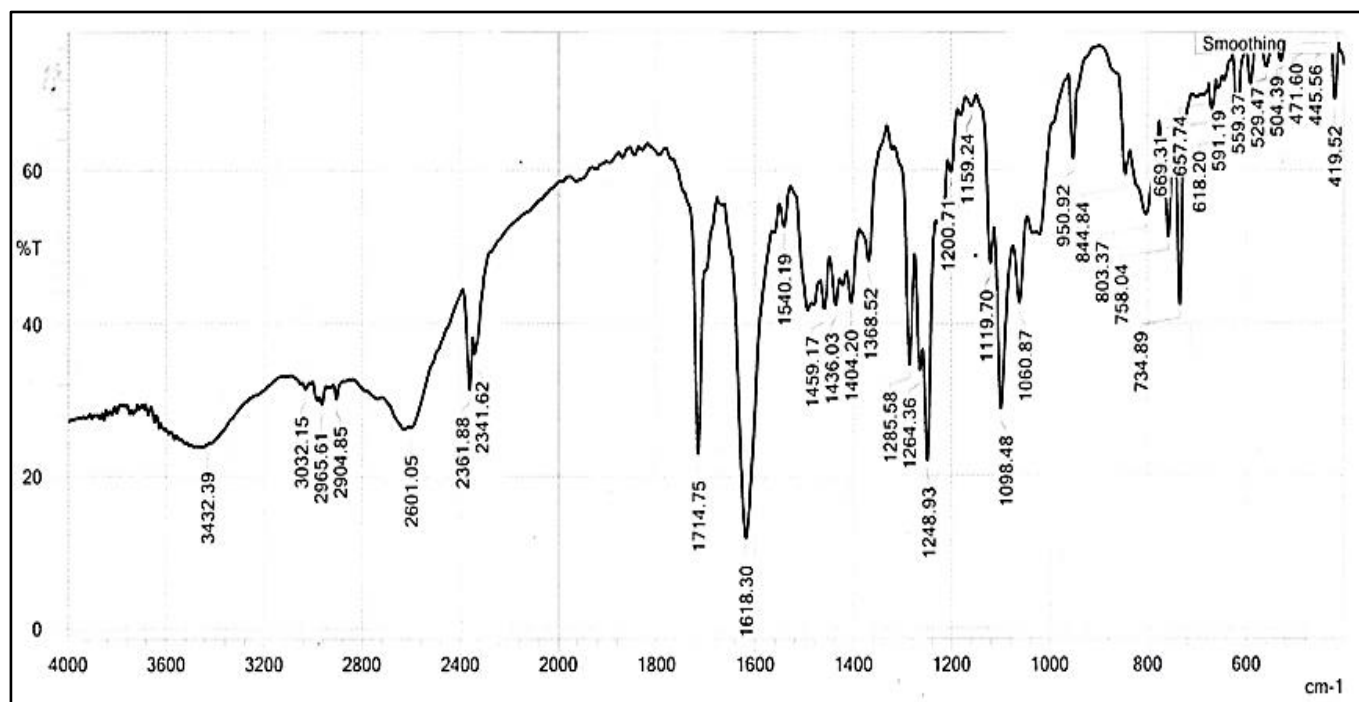


Fig. S13. IR spectrum of 2c.

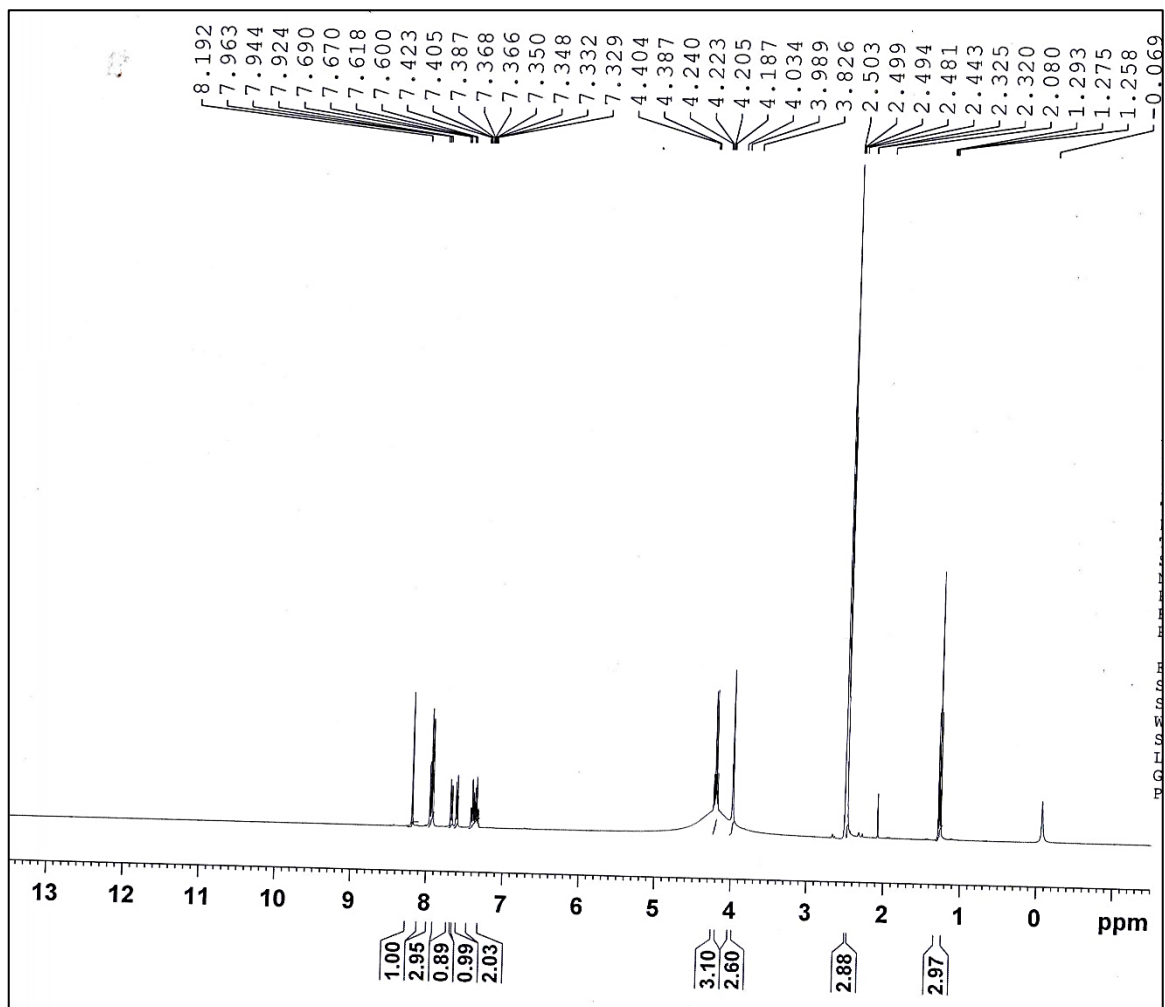
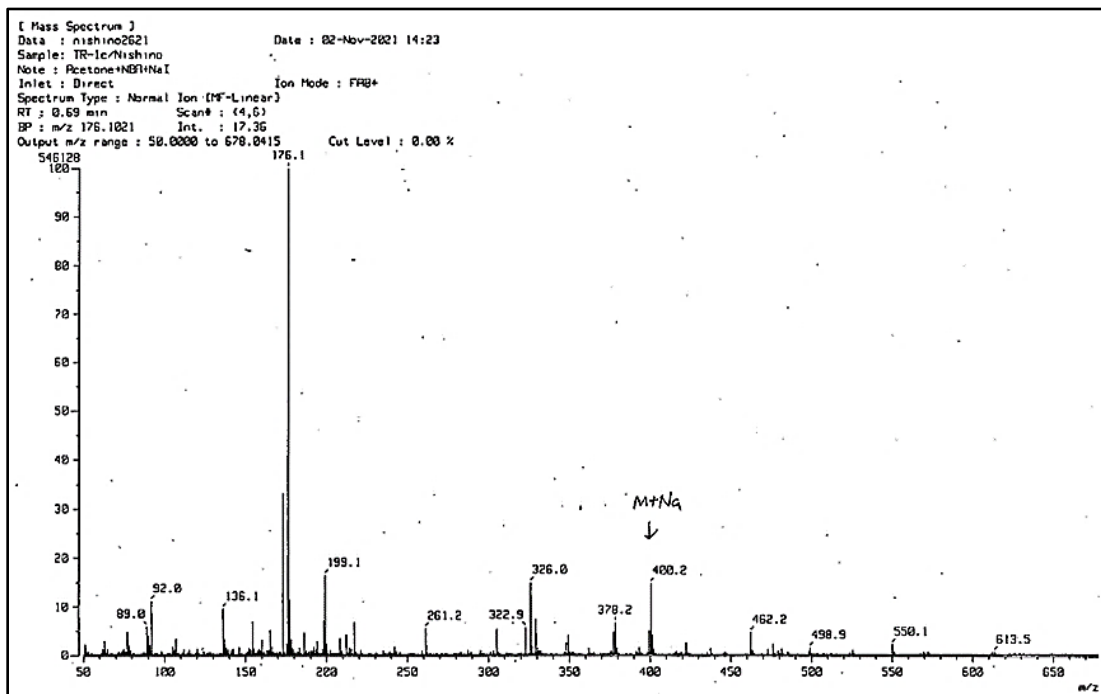


Fig. S14. ^1H NMR spectrum of **2c**.



[Elemental Composition]
 Date : 02-Nov-2021 14:25 Page: 1
 Data : nishino2622
 Sample: TR-1c/Nishino
 Note : Acetone+NBA+NaI
 Inlet : Direct Ion Mode : FAB+
 RT : 4.75 min Scan# : (18,22)
 Elements : C 100/0, H 100/0, O 3/1, N 4/2, S 2/0, Na 1/1
 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
400.1101	14.4	-21.6 / -8.6	18.0	C 25 H 17 O 2 N 2 Na
		+9.9 / +3.9	18.5	C 24 H 15 O 2 N 3 Na
		+1.4 / +0.6	14.5	C 21 H 19 O 2 N 3 S Na
		-7.0 / -2.8	10.5	C 18 H 23 O 2 N 3 S 2 Na
		+24.4 / +9.8	11.0	C 17 H 21 O 2 N 4 S 2 Na

Fig. S15. HRMS spectrum of 2c.

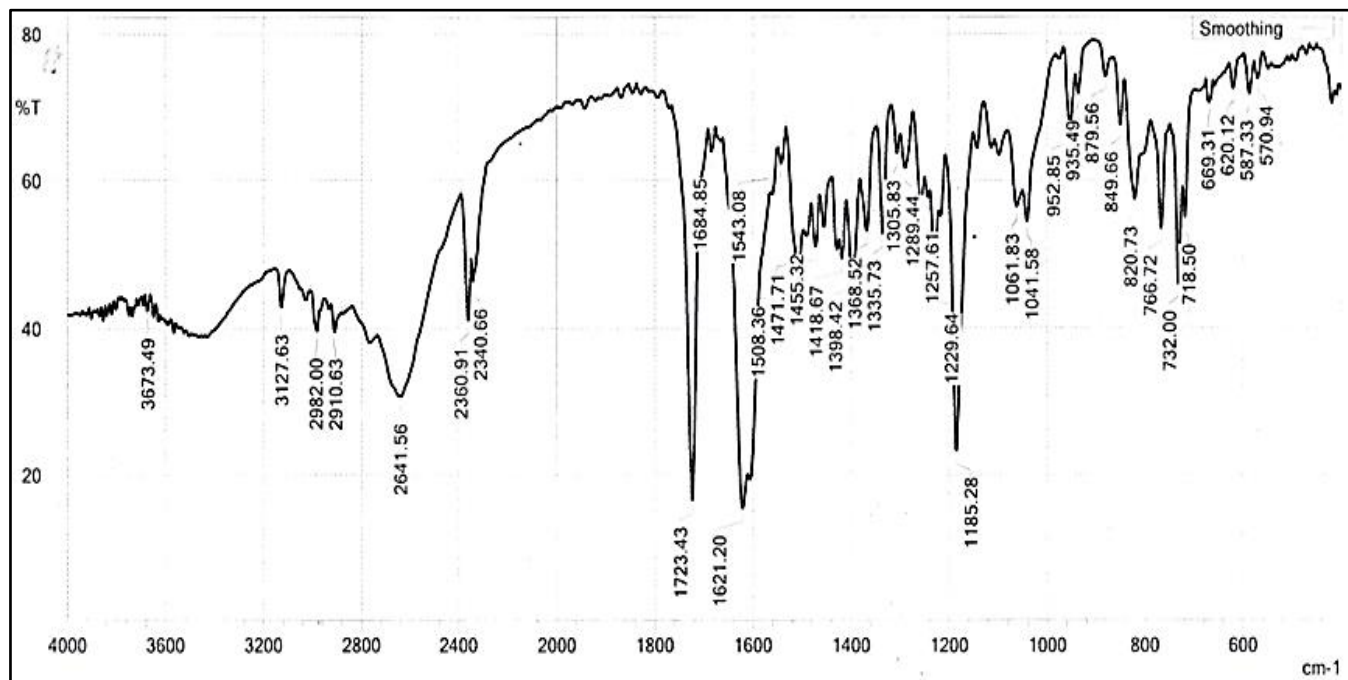


Fig. S16. IR spectrum of 2d.

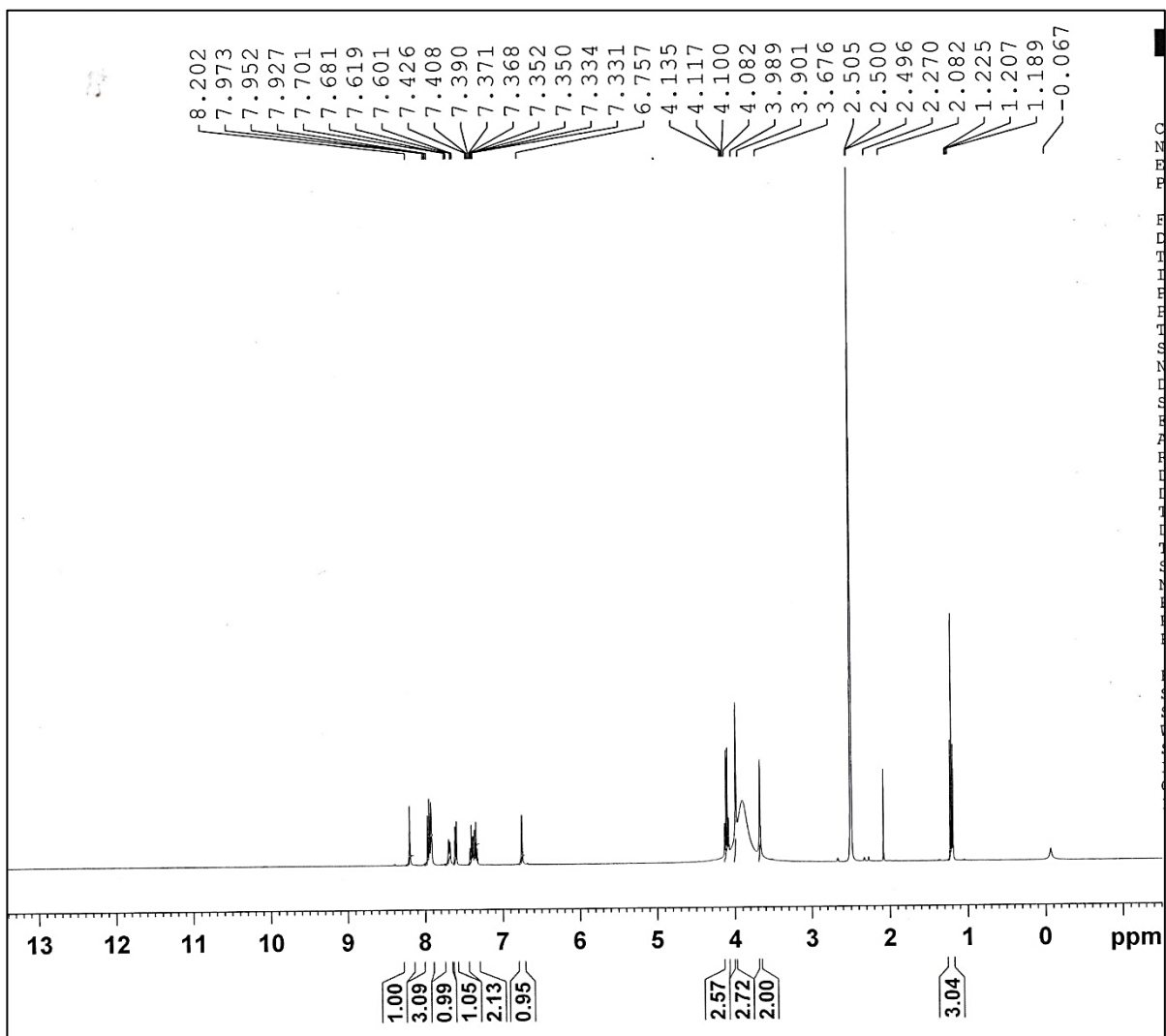
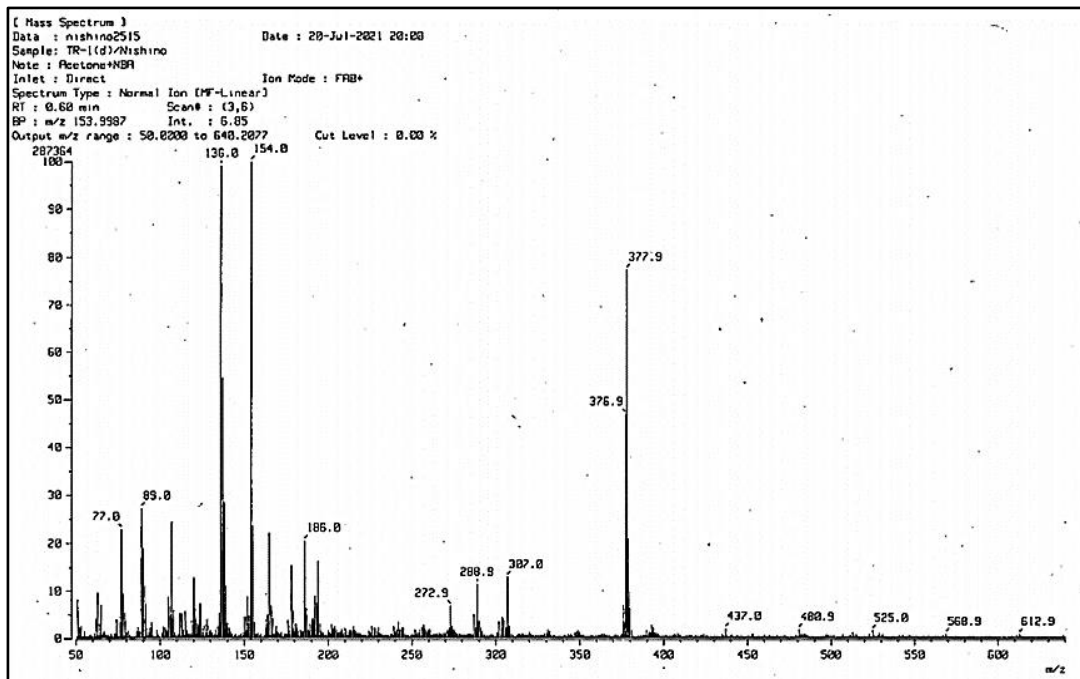


Fig. S17. ¹H NMR spectrum of **2d**.



[Elemental Composition]
 Date : 20-Jul-2021 20:02 Page: 1
 Data : nishino2516
 Sample: TR-1(d)/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 4.25 min Scan# : (15,21)
 Elements : C 100/0, H 100/0, O 3/1, N 4/2, S 2/0
 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
378.1281	72.7	-23.0 / -8.7	18.0	C 25 H 18 O 2 N 2
		+10.3 / +3.9	18.5	C 24 H 16 O 2 N 3
		+1.4 / +0.5	14.5	C 21 H 20 O 2 N 3 S
		-7.5 / -2.9	10.5	C 18 H 24 O 2 N 3 S 2
		+25.7 / +9.7	11.0	C 17 H 22 O 2 N 4 S 2

Fig. S18. HRMS spectrum of 2d.

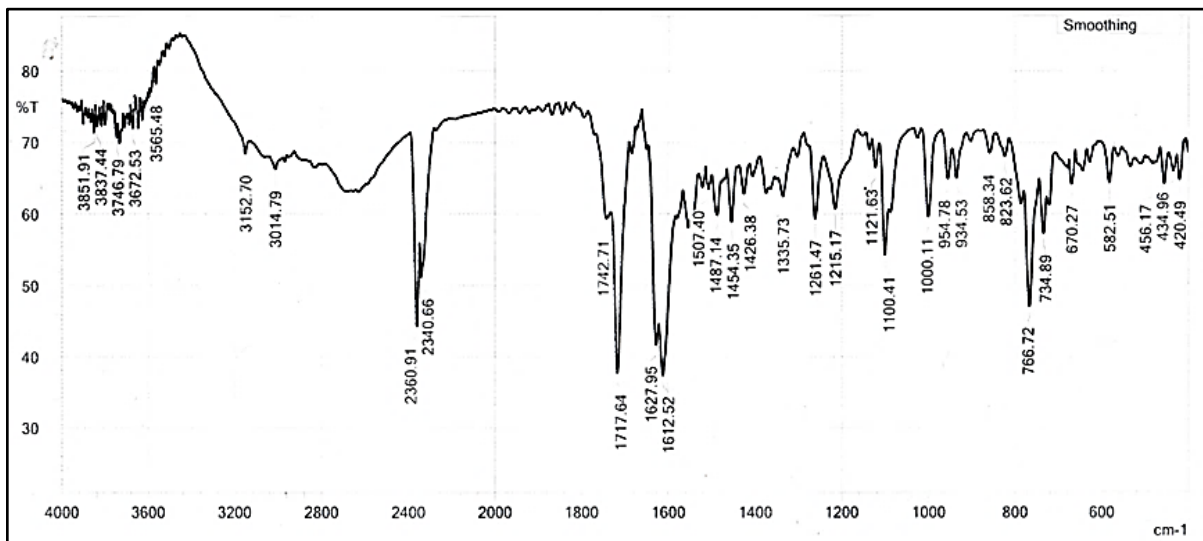


Fig. S19. IR spectrum of **2e**.

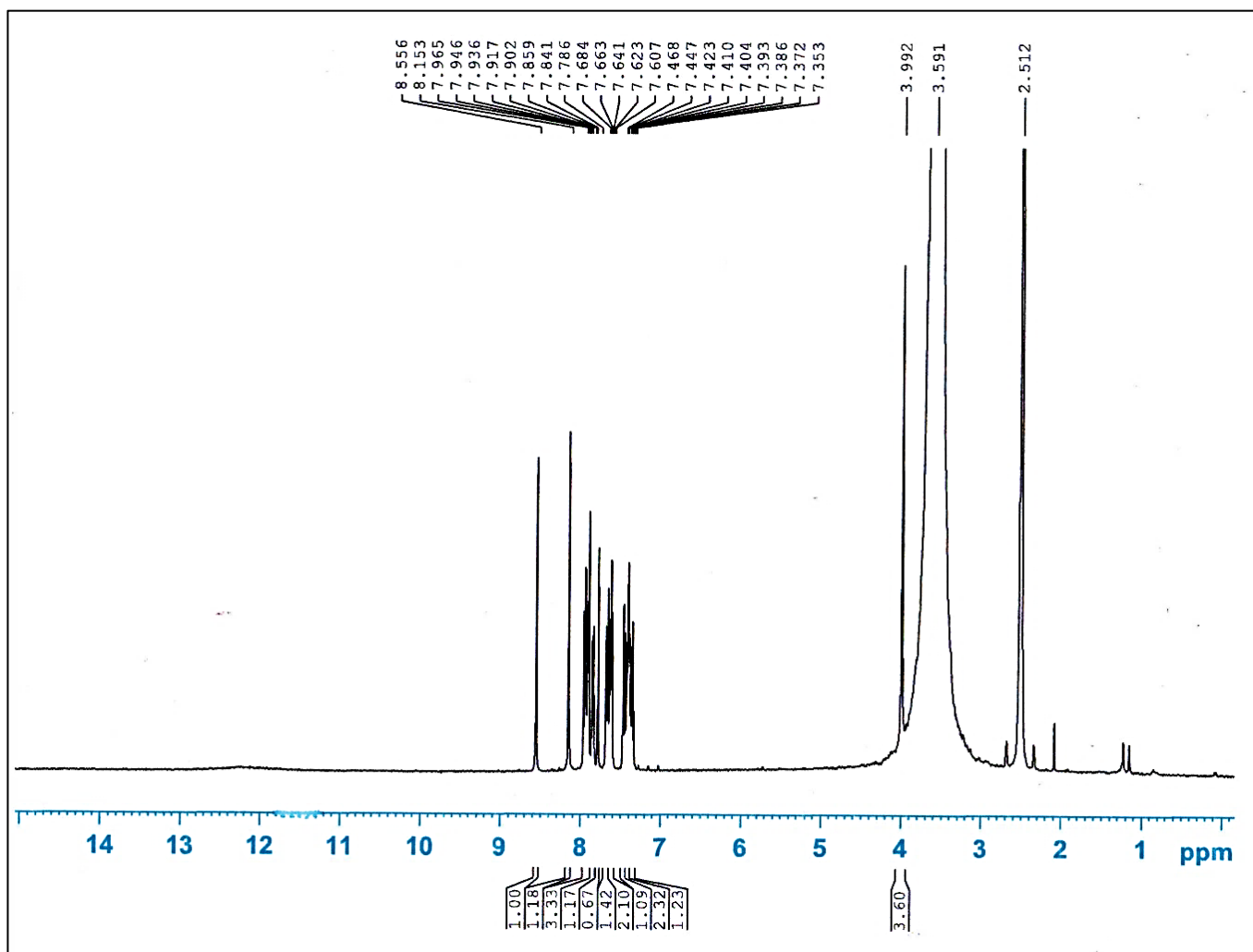
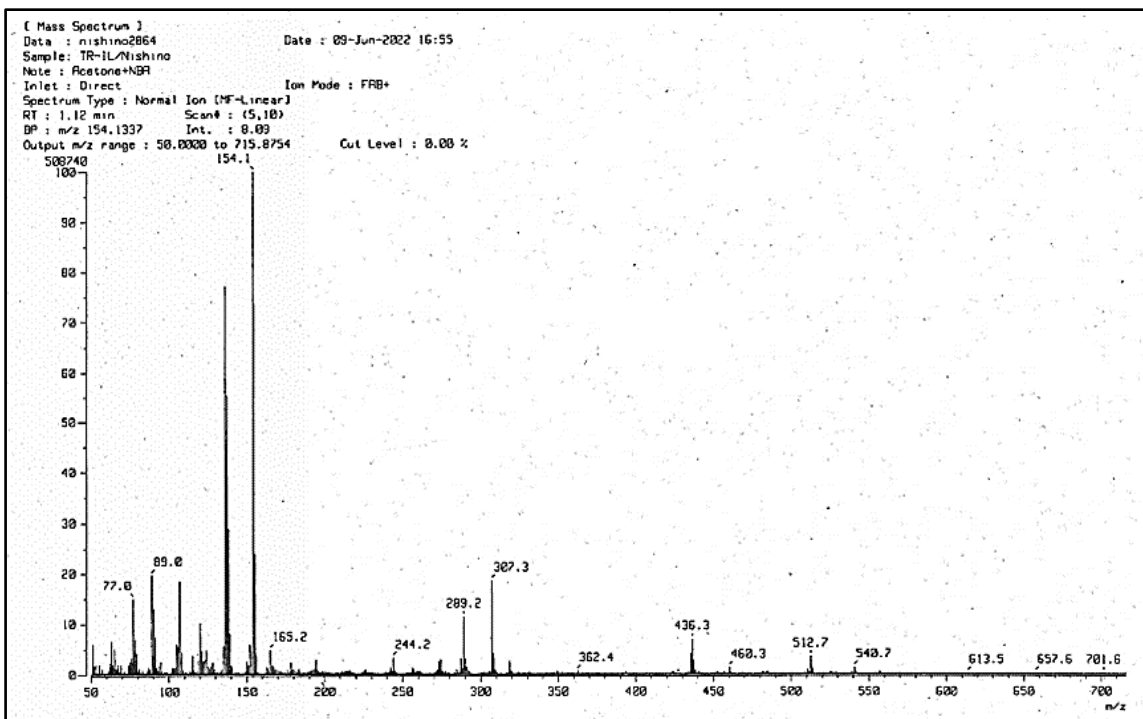


Fig. S20. ^1H NMR spectrum of 2e.



[Elemental Composition]
 Date : 09-Jun-2022 17:03 Page: 1
 Data : nishino2865
 Sample: TR-1L/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 2/0
 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
436.1117	100.0	-21.8 / -9.5	24.0	C 30 H 16 O 2 N 2
		+7.0 / +3.1	24.5	C 29 H 14 O 2 N 3
		-0.7 / -0.3	20.5	C 26 H 18 O 2 N 3 S
		-8.4 / -3.7	16.5	C 23 H 22 O 2 N 3 S 2
		+20.4 / +8.9	17.0	C 22 H 20 O 2 N 4 S 2

Fig. S21. HRMS spectrum of 2e.

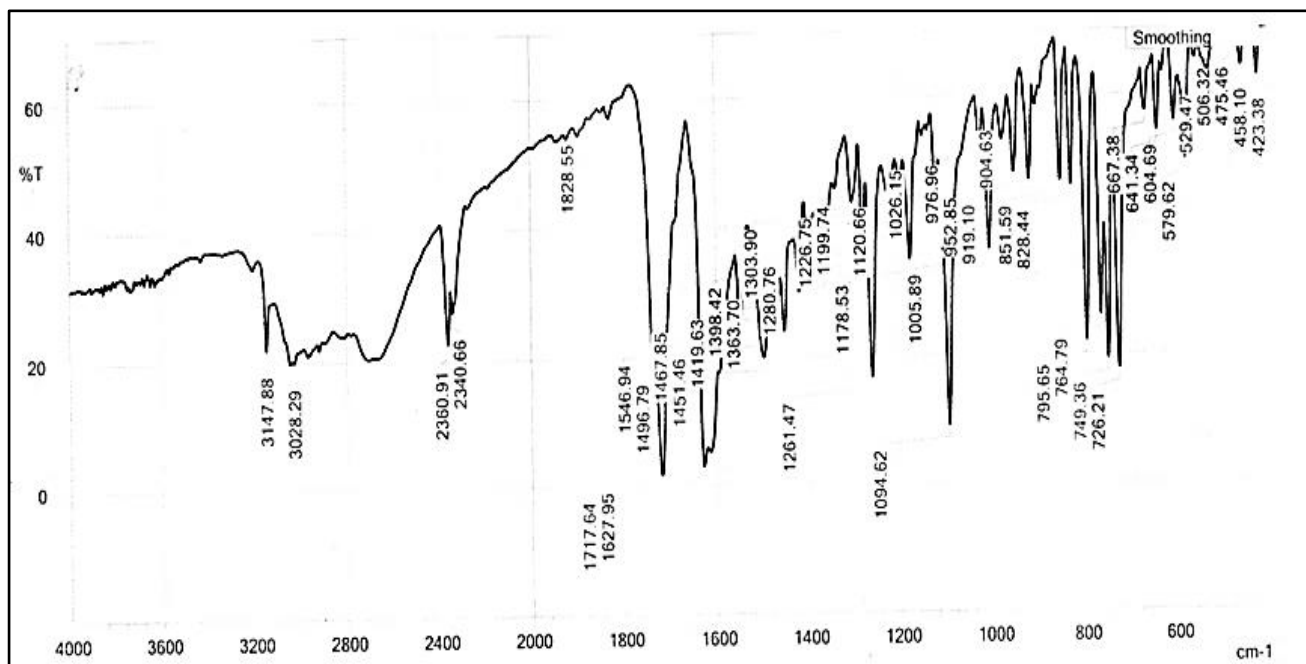


Fig. S22. IR spectrum of 2f.

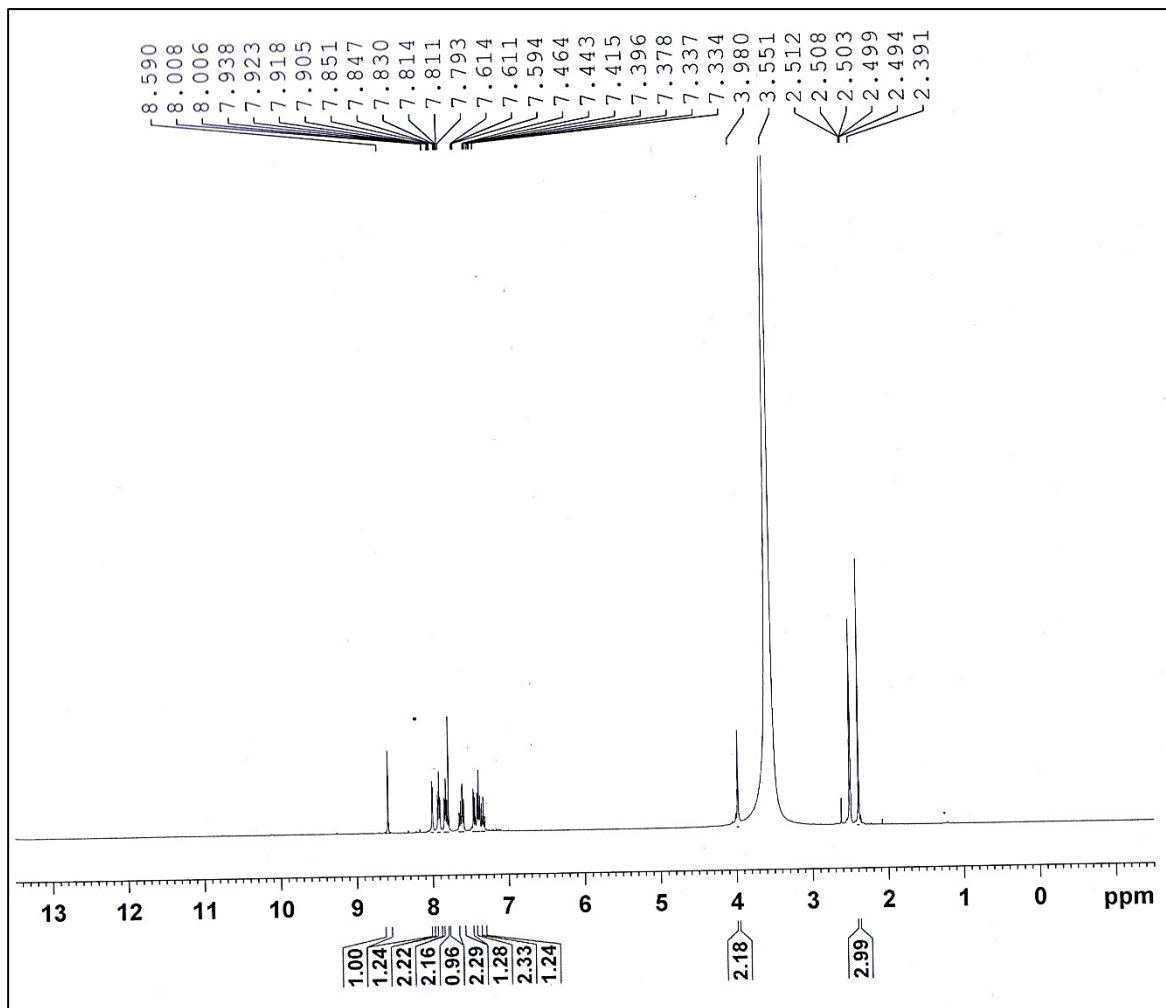
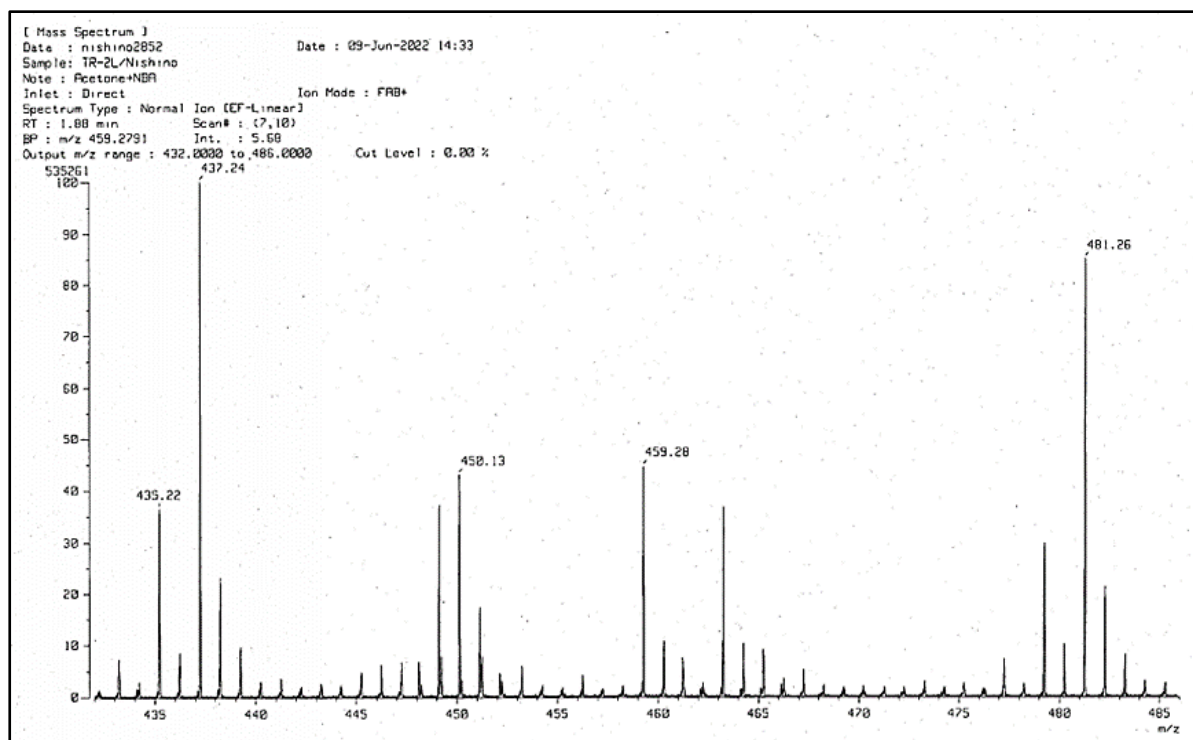


Fig. S23. ^1H NMR spectrum of **2f**.



[Elemental Composition] Page: 1

Data : nishino2852 Date : 09-Jun-2022 14:33
 Sample: TR-2L/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.88 min Scan# : (7,10)
 Elements : C 100/0, H 100/0, O 3/1, N 4/2, S 2/0
 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
450.1266	96.6	+5.1 / +2.3	24.5	C 30 H 16 O 2 N 3
		-2.4 / -1.1	20.5	C 27 H 20 O 2 N 3 S
		-9.9 / -4.4	16.5	C 24 H 24 O 2 N 3 S 2
		+18.1 / +8.1	17.0	C 23 H 22 O 2 N 4 S 2

Fig. S24. HRMS spectrum of 2f.

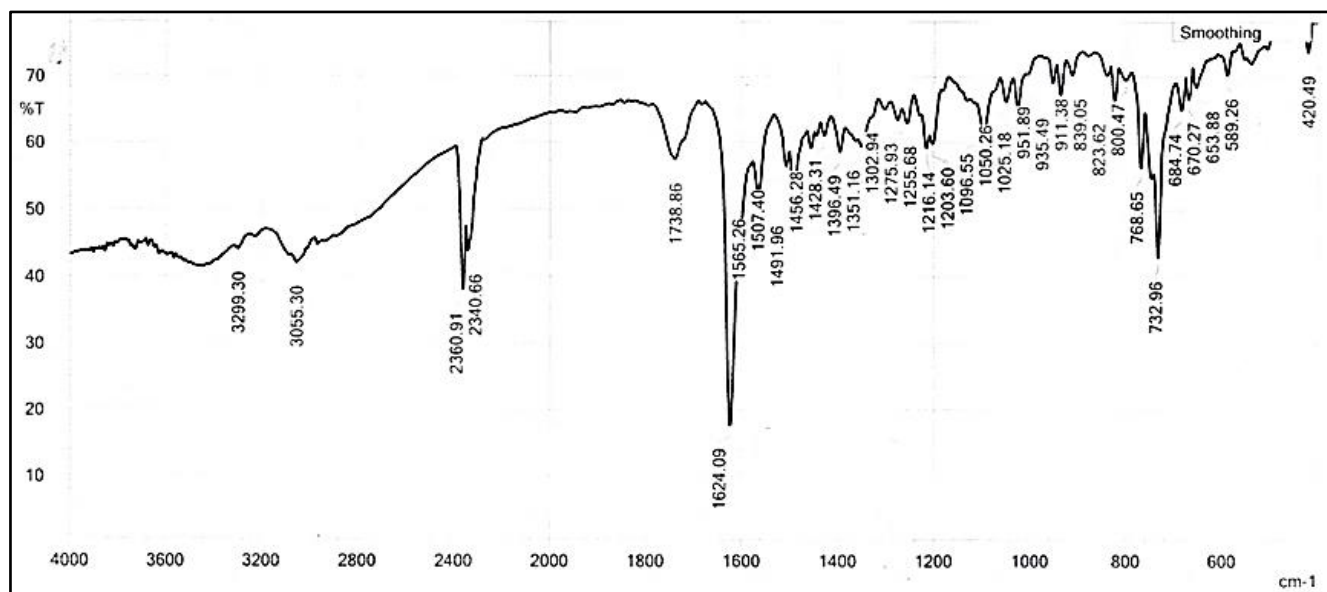


Fig. S25. IR spectrum of **2g**.

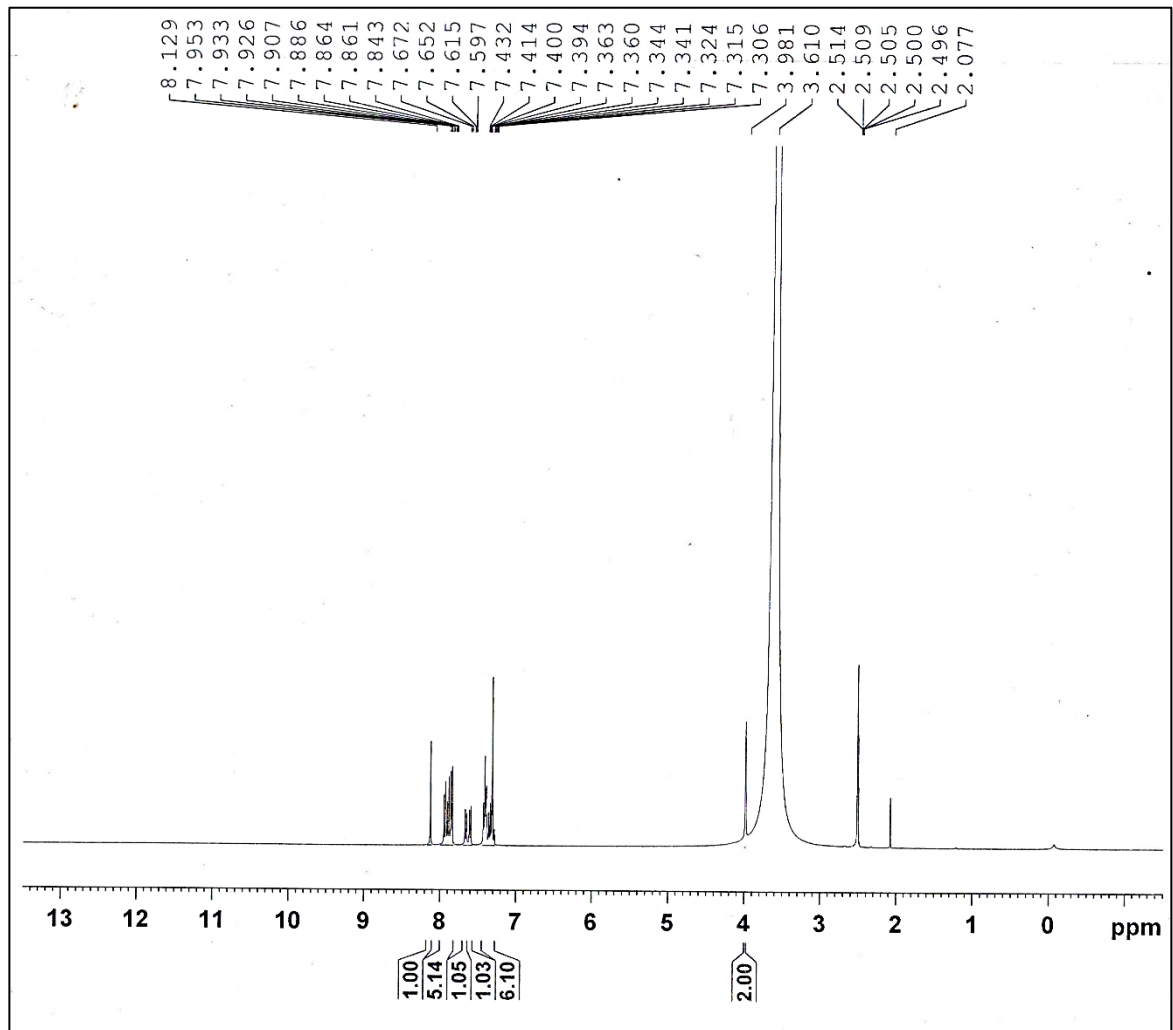
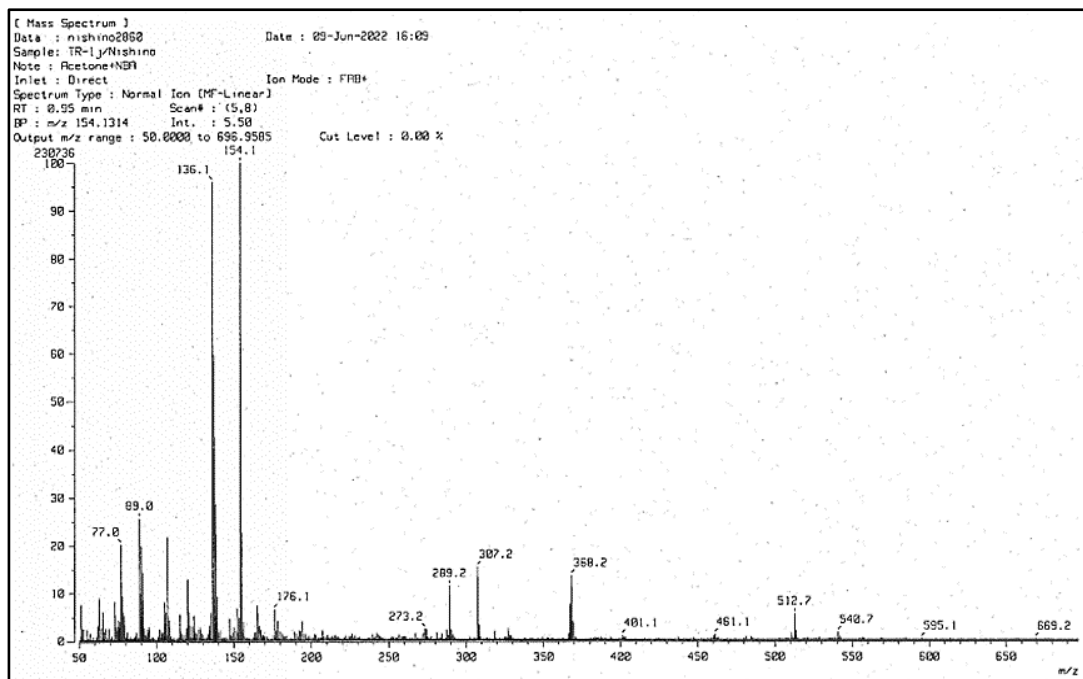


Fig. S26. ^1H NMR spectrum of **2g**.



[Elemental Composition]
 Date : 09-Jun-2022 16:17 Page: 1
 Data : nishino2861
 Sample: TR-1j/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.13 min Scan# : (4,7)
 Elements : C 100/0, H 100/0, N 4/2, S 2/0
 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
368.1220	56.9	-25.3 / -9.3	21.0	C 27 H 16 N 2
		+8.9 / +3.3	21.5	C 26 H 14 N 3
		-0.3 / -0.1	17.5	C 23 H 18 N 3 S
		-9.4 / -3.5	13.5	C 20 H 22 N 3 S 2
		+24.7 / +9.1	14.0	C 19 H 20 N 4 S 2

Fig. S27. HRMS spectrum of 2g.

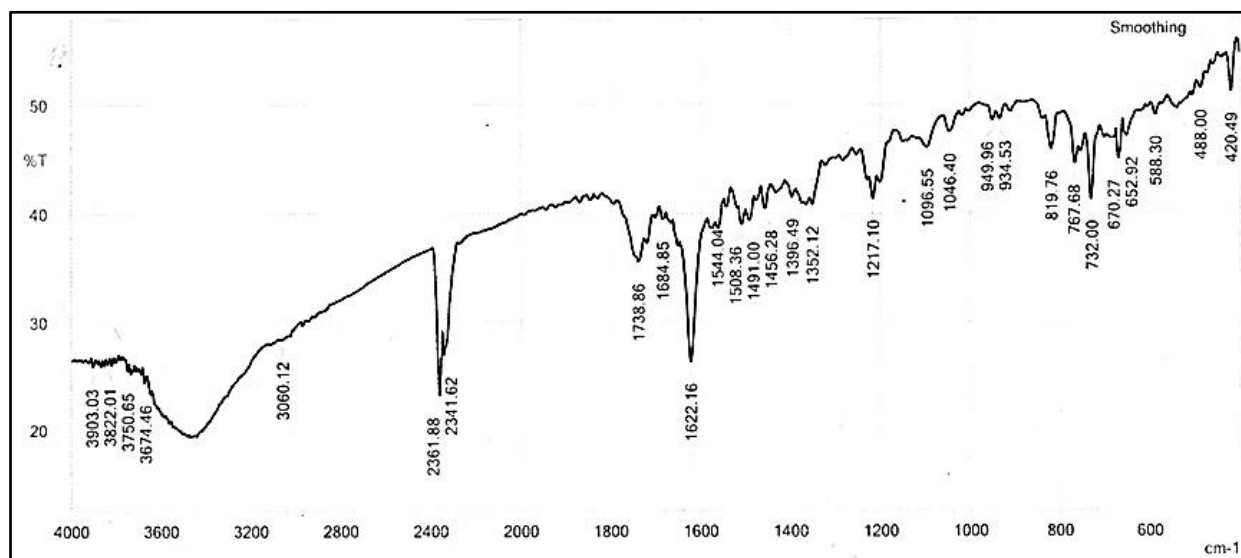


Fig. S28. IR spectrum of 2h.

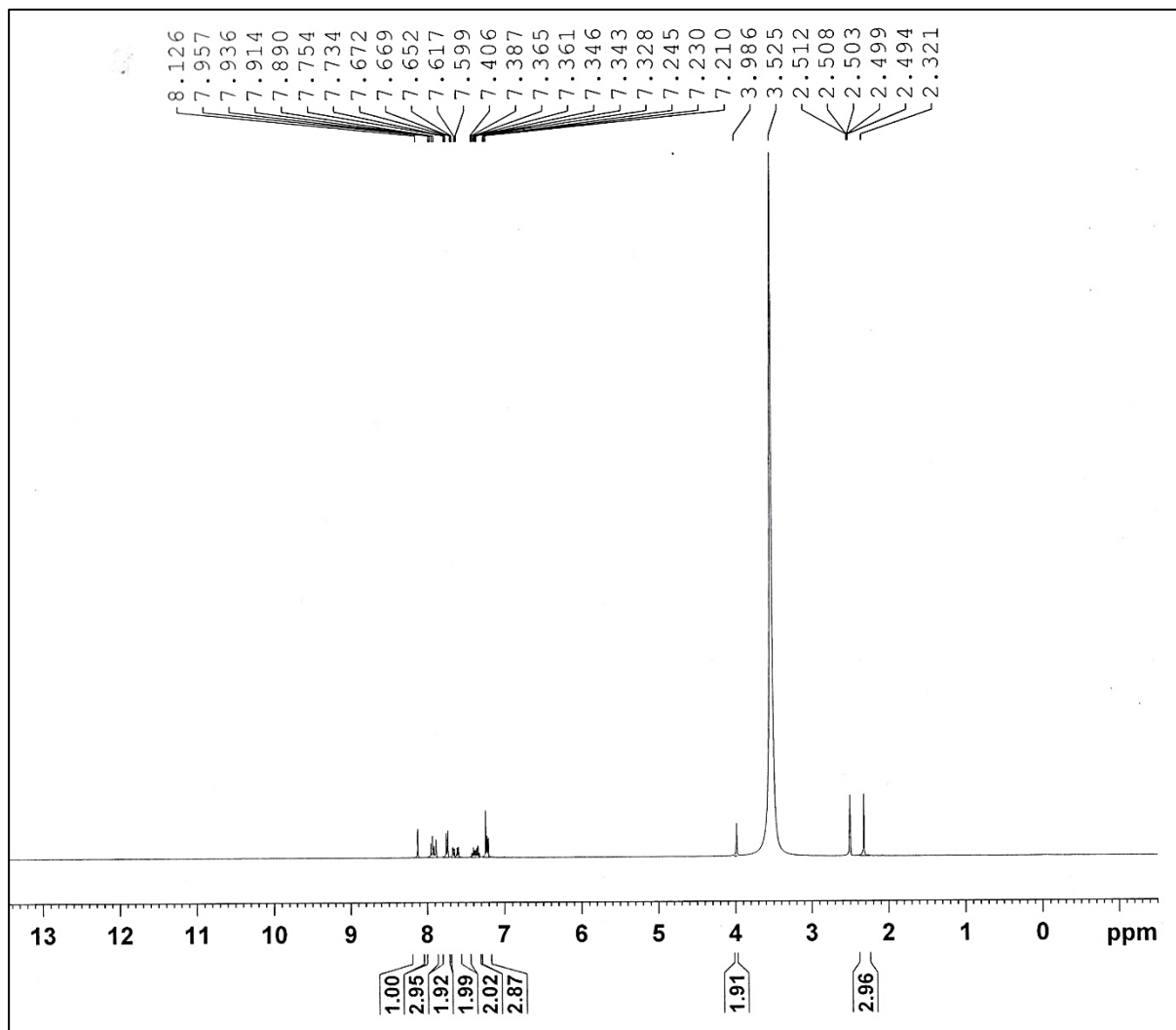
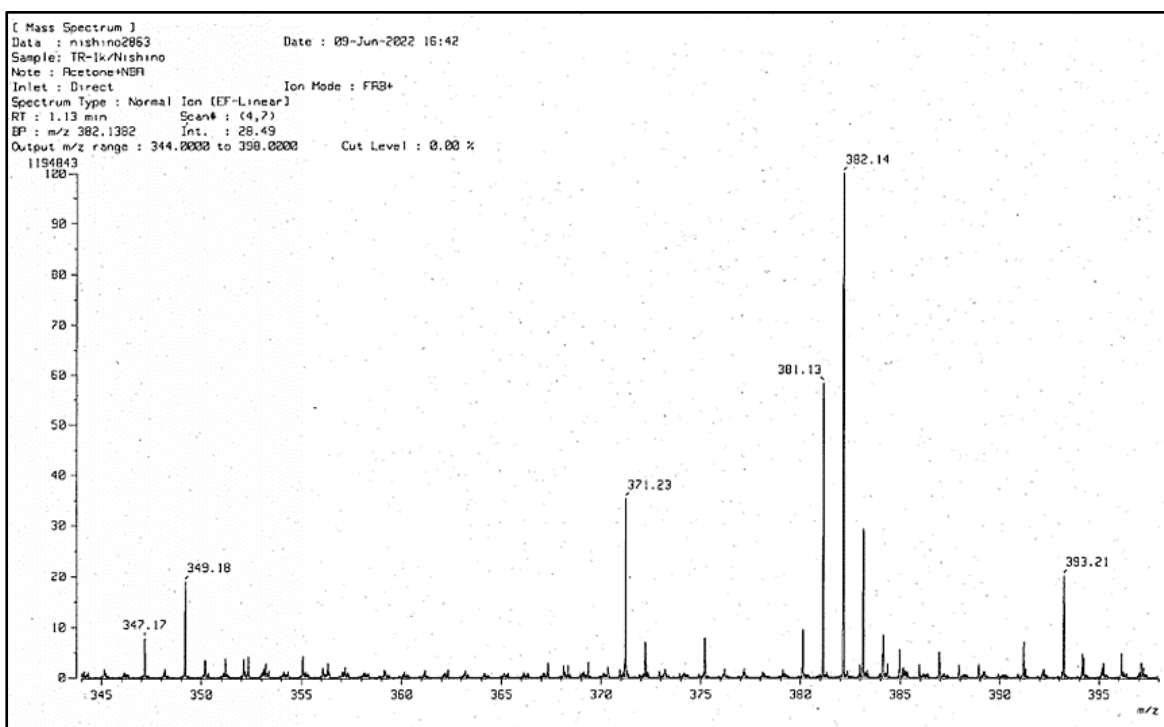


Fig. S29. ^1H NMR spectrum of **2h**.



[Elemental Composition]
 Date : 09-Jun-2022 16:42 Page: 1
 Data : nishino2863
 Sample: TR-1k/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.13 min Scan# : (4,7)
 Elements : C 100/0, H 100/0, N 4/2, S 2/0
 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
382.1382	100.0	-23.1 / -8.8	21.0	C 28 H 18 N 2
		+9.8 / +3.8	21.5	C 27 H 16 N 3
		+1.0 / +0.4	17.5	C 24 H 20 N 3 S
		-7.8 / -3.0	13.5	C 21 H 24 N 3 S 2
		+25.1 / +9.6	14.0	C 20 H 22 N 4 S 2

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

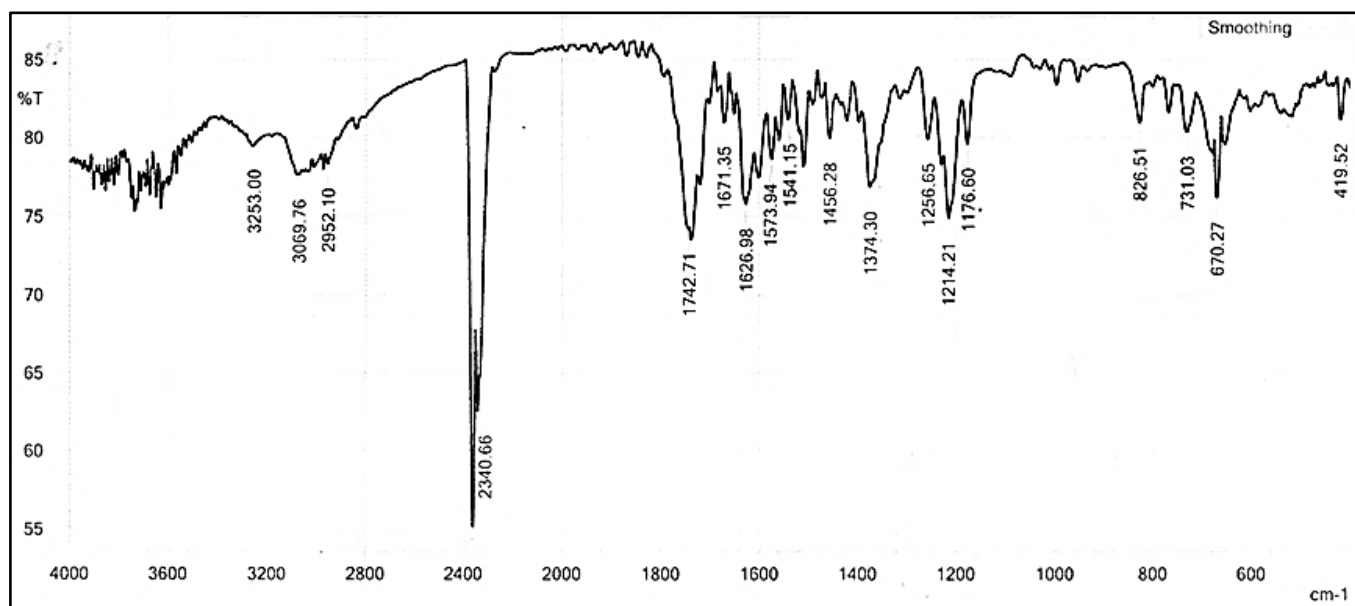


Fig. S31. IR spectrum of 2i.

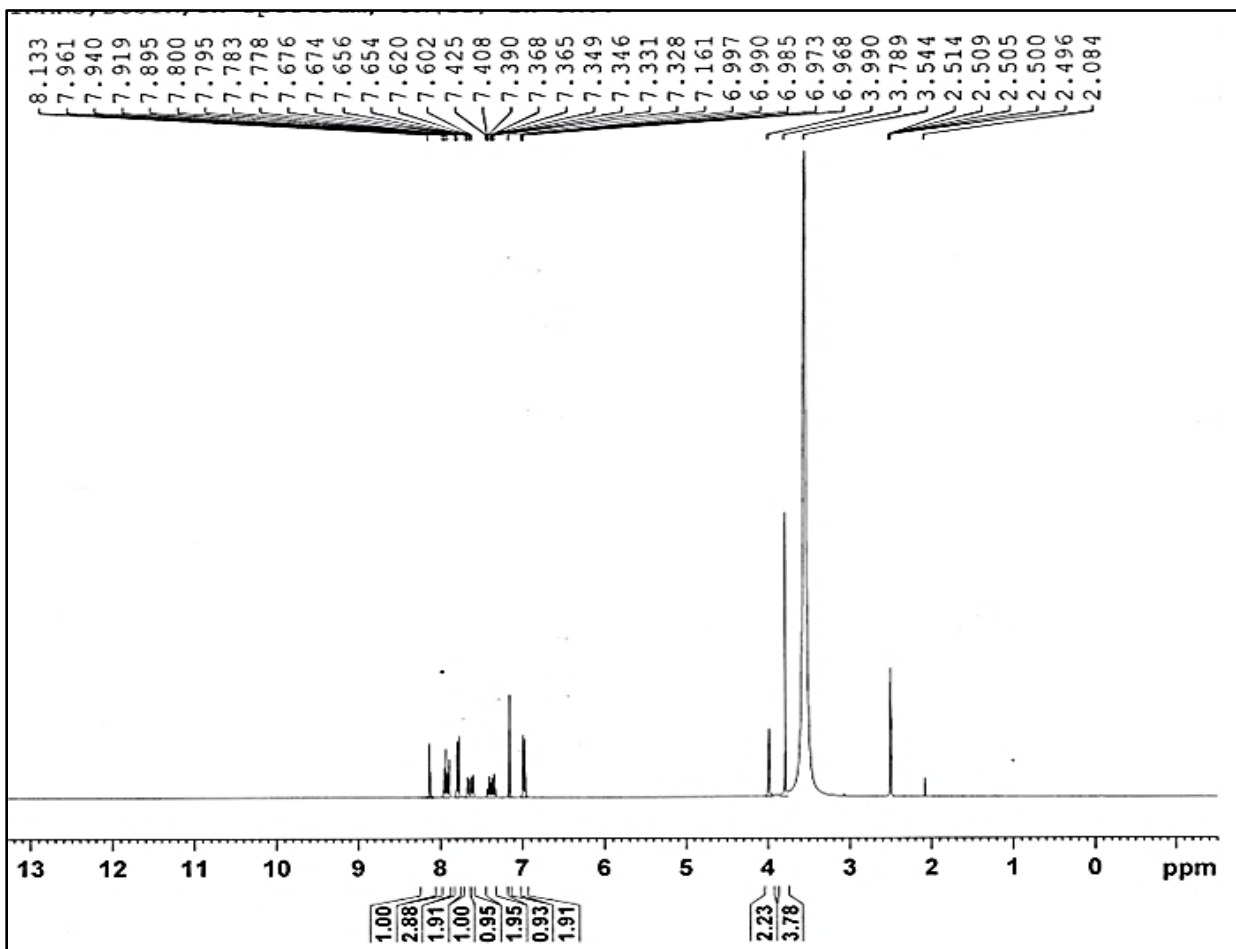
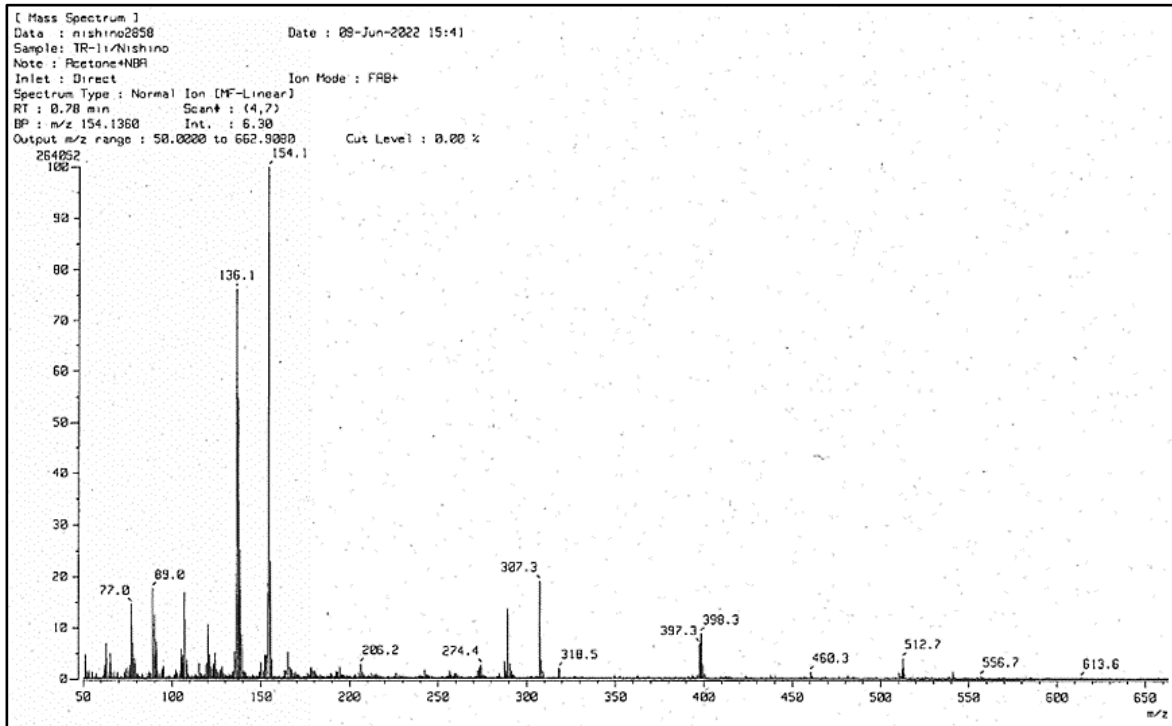


Fig. S32. ^1H NMR spectrum of **2i**.



[Elemental Composition] Page: 1
 Date : 09-Jun-2022 15:48
 Data : nishino2859
 Sample: TR-1i/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.38 min Scan#: (4,9)
 Elements : C 100/0, H 100/0, O 2/0, N 4/2, S 2/0
 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
398.1311	50.6	+4.4 / +1.7	21.5	C 27 H 16 O N 3
		-4.1 / -1.6	17.5	C 24 H 20 O N 3 S
		-12.6 / -5.0	13.5	C 21 H 24 O N 3 S 2
		+19.0 / +7.6	14.0	C 20 H 22 O N 4 S 2

Fig. S33. HRMS spectrum of 2i.

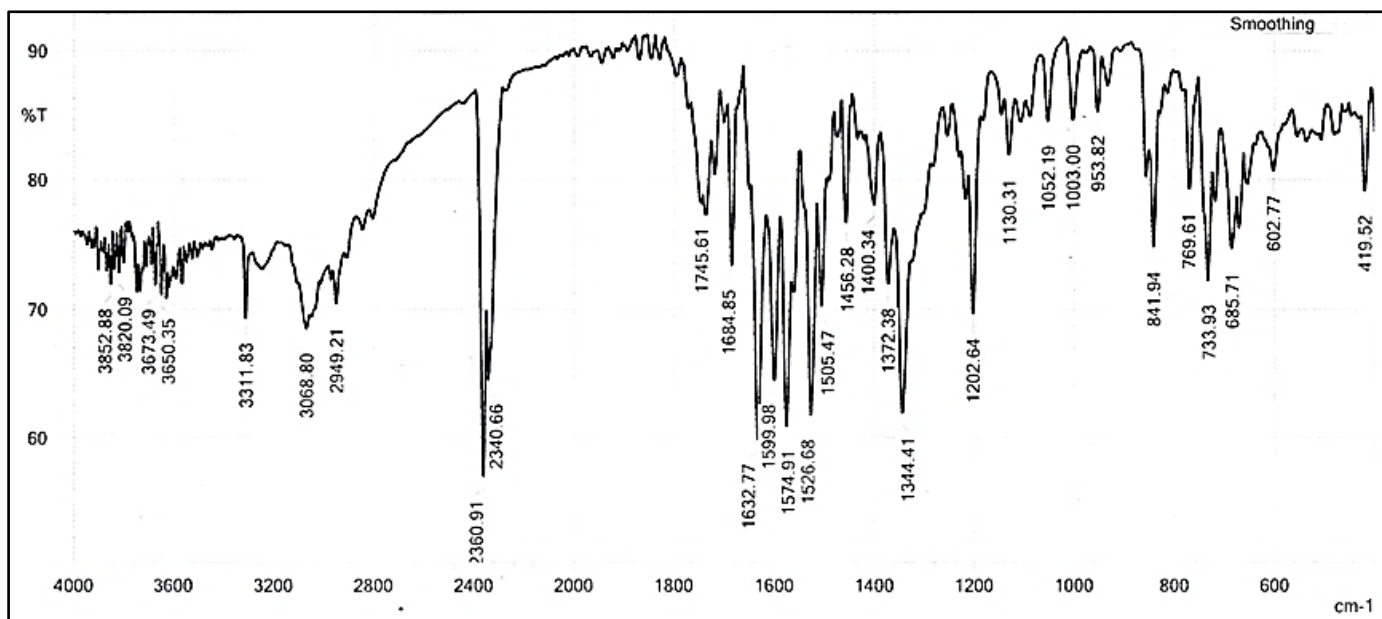


Fig. S34. IR spectrum of 2j.

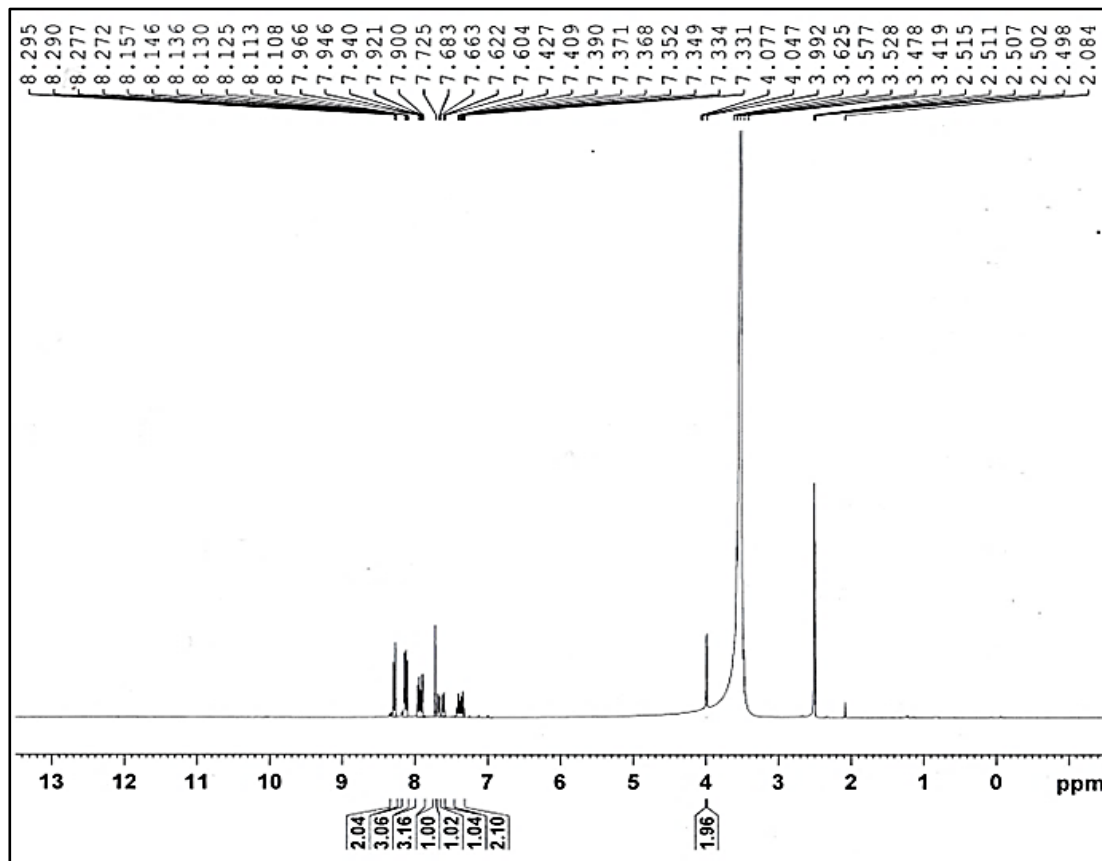
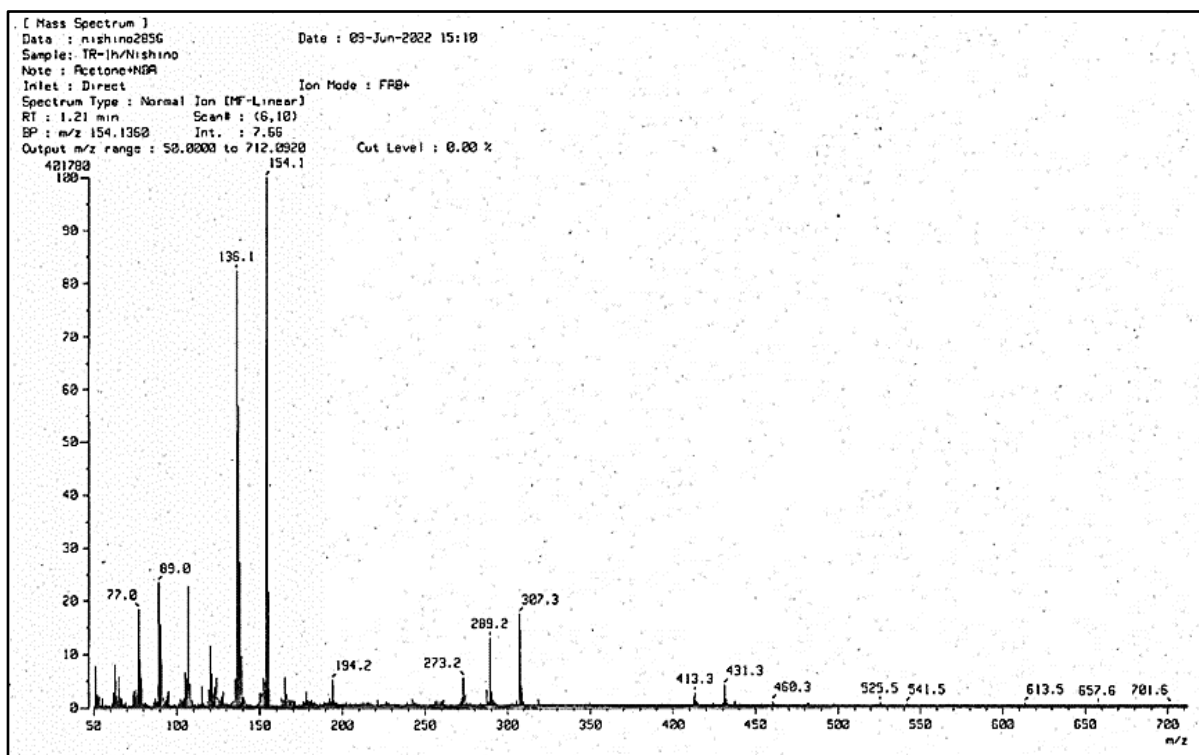


Fig. S35. ^1H NMR spectrum of **2j**.



[Elemental Composition]
 Date : 09-Jun-2022 15:19 Page: 1
 Data : nishino2857
 Sample: TR-1h/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 2.50 min Scan# : (9,13)
 Elements : C 100/0, H 100/0, O 3/1, N 5/3, S 2/0
 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
413.1068	22.0	-23.3 / -9.6	22.0	C 27 H 15 O 2 N 3
		+7.1 / +2.9	22.5	C 26 H 13 O 2 N 4
		-1.1 / -0.4	18.5	C 23 H 17 O 2 N 4 S
		-9.2 / -3.8	14.5	C 20 H 21 O 2 N 4 S 2
		+21.2 / +8.8	15.0	C 19 H 19 O 2 N 5 S 2

Fig. S36. HRMS spectrum of 2j.

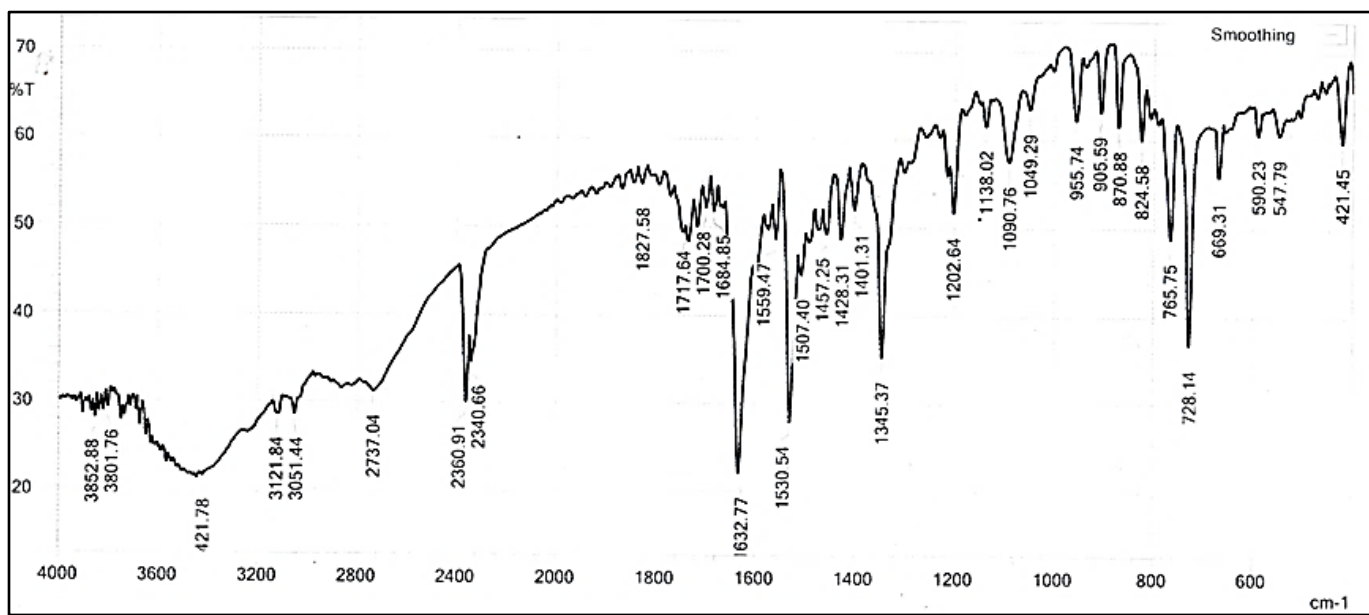


Fig. S37. IR spectrum of 2k.

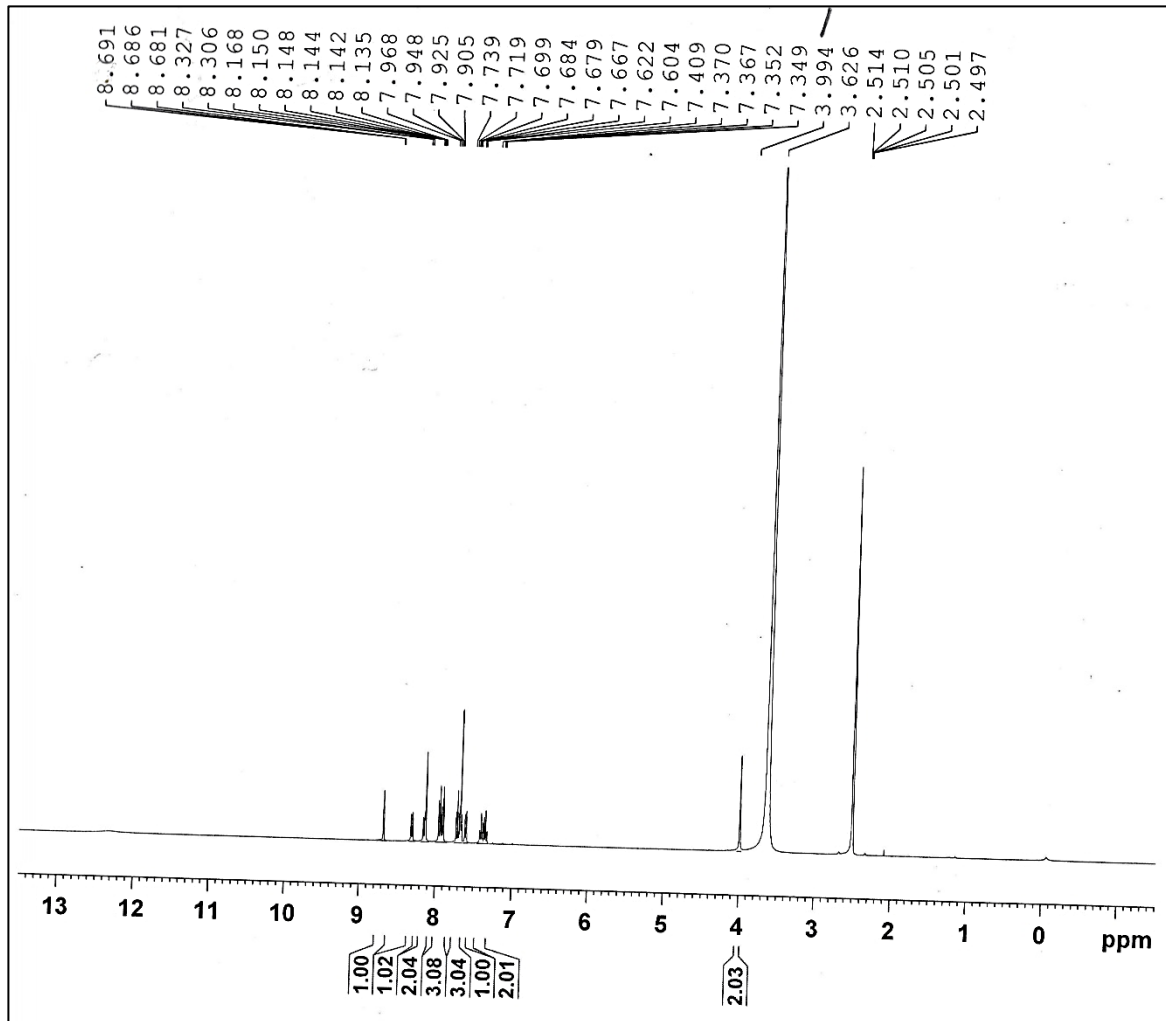
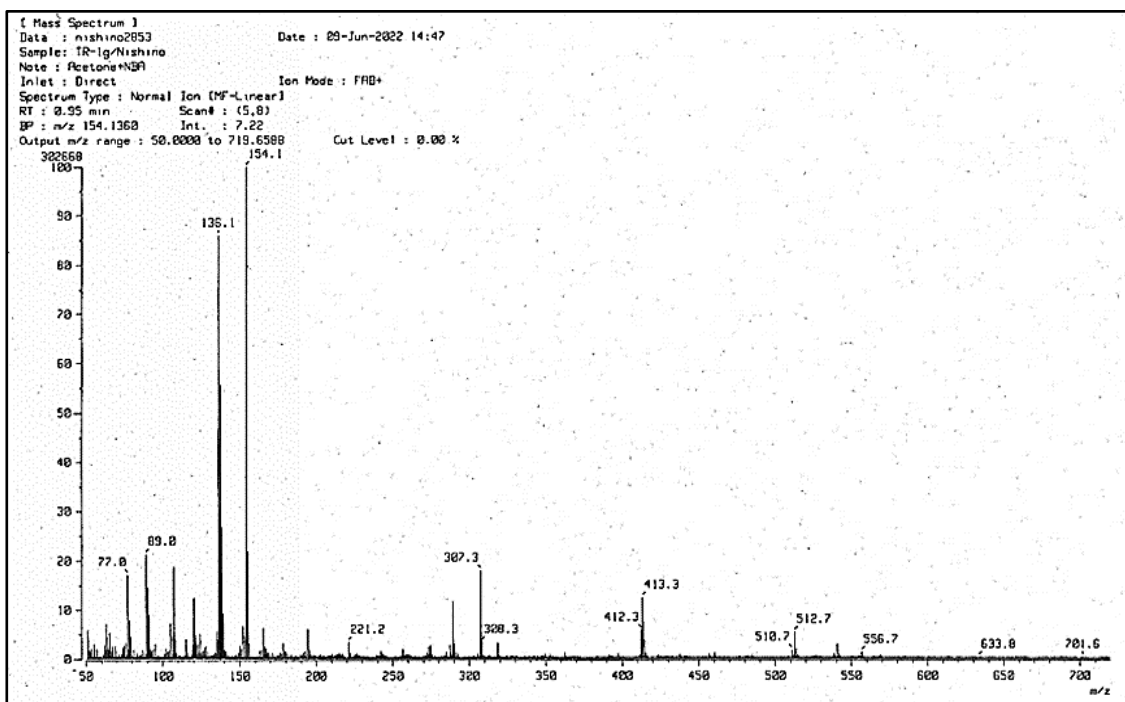


Fig. S38. ^1H NMR spectrum of **2k**.



[Elemental Composition] Page: 1
 Date : 09-Jun-2022 14:55
 Data : nishino2854
 Sample: TR-1g/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.38 min Scan# : (5,8)
 Elements : C 100/0, H 100/0, O 3/1, N 5/3, S 2/0
 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
413.1080	100.0	-20.3 / -8.4	22.0 C 27 H 15 O 2 N 3
		+10.1 / +4.2	22.5 C 26 H 13 O 2 N 4
		+2.0 / +0.8	18.5 C 23 H 17 O 2 N 4 S
		-6.2 / -2.6	14.5 C 20 H 21 O 2 N 4 S 2

Fig. S39. HRMS spectrum of 2k.

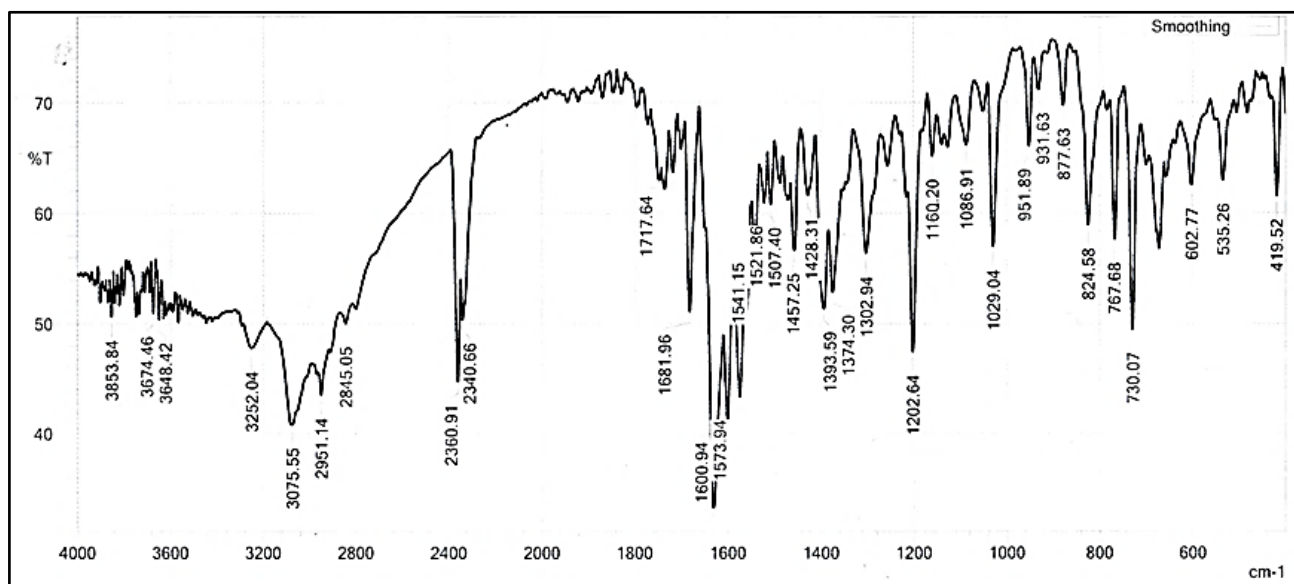


Fig. S40. IR spectrum of **2l**.

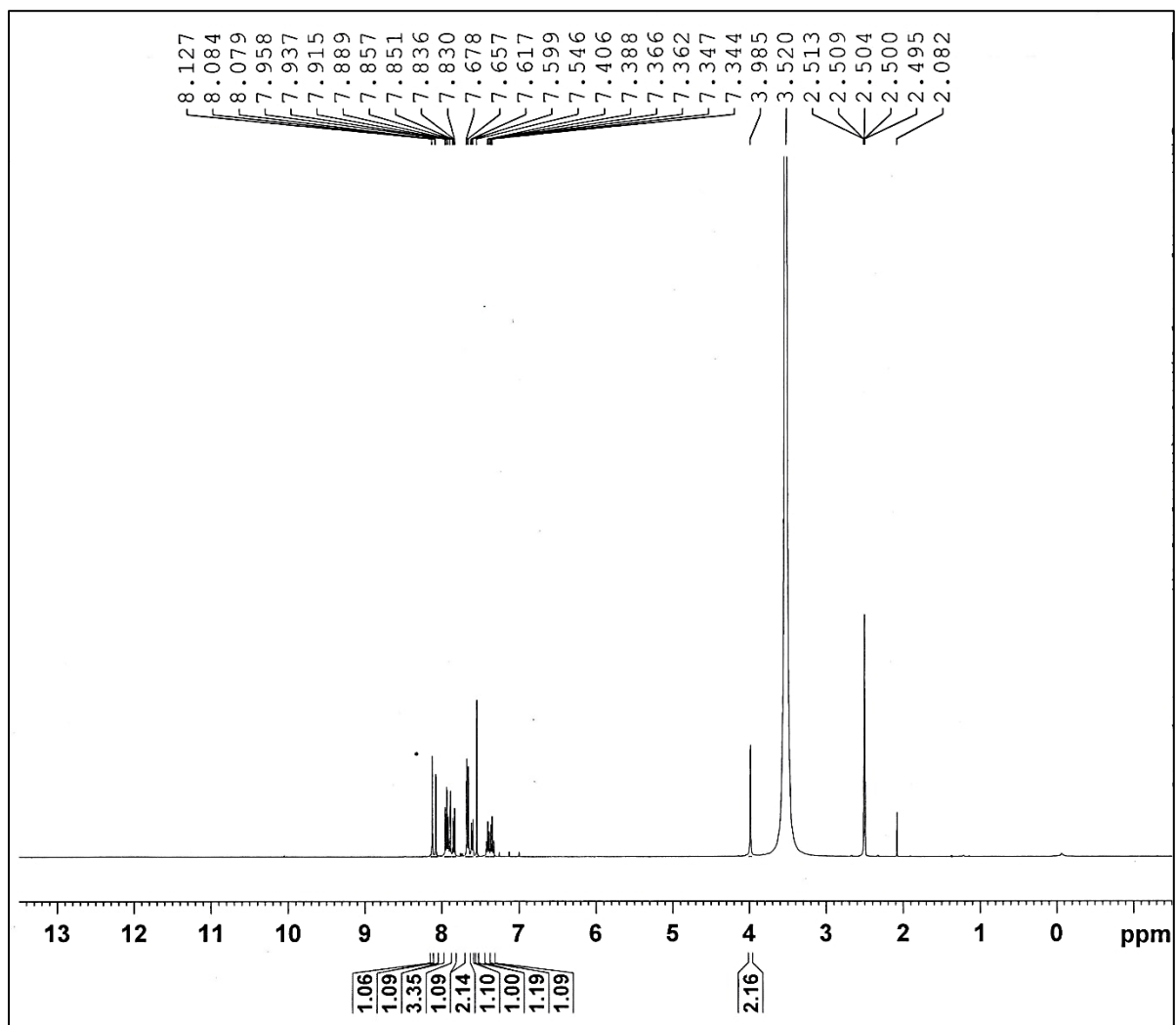
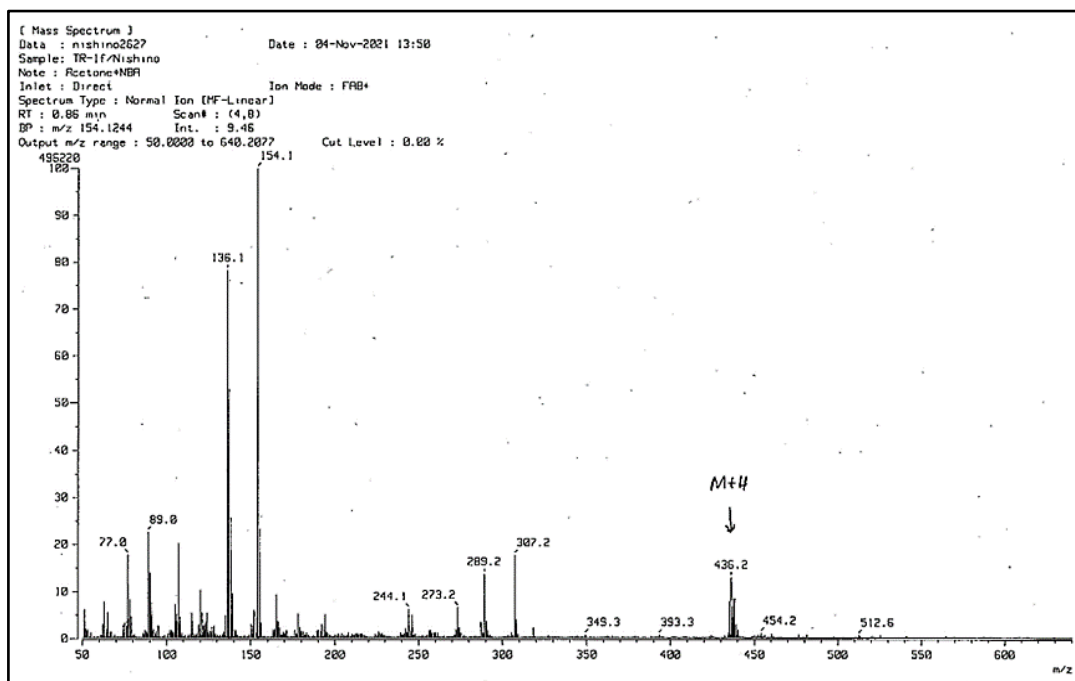


Fig. S41. ^1H NMR spectrum of **2l**.



[Elemental Composition]
 Date : 04-Nov-2021 14:41 Page: 1
 Data : nishino2631
 Sample: TR-1f/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.50 min Scan# : (5,9)
 Elements : C 100/0, H 100/0, N 4/2, Cl 3/1, S 2/0
 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
435.0366	95.6	-16.4 / -7.1	26.5	C 28 H 8 N 4 Cl
		-20.6 / -9.0	21.5	C 27 H 13 N 2 Cl 2
		+8.3 / +3.6	22.0	C 26 H 11 N 3 Cl 2
		+0.6 / +0.2	18.0	C 23 H 15 N 3 Cl 2 S
		-7.2 / -3.1	14.0	C 20 H 19 N 3 Cl 2 S 2
		+21.7 / +9.5	14.5	C 19 H 17 N 4 Cl 2 S 2
		+17.5 / +7.6	9.5	C 18 H 22 N 2 Cl 3 S 2
436.0420	100.0	-22.0 / -9.6	26.0	C 28 H 9 N 4 Cl
		+2.7 / +1.2	21.5	C 26 H 12 N 3 Cl 2
		-5.1 / -2.2	17.5	C 23 H 16 N 3 Cl 2 S
		+19.6 / +8.5	13.0	C 21 H 19 N 2 Cl 3 S
		-12.8 / -5.6	13.5	C 20 H 20 N 3 Cl 2 S 2
		+16.0 / +7.0	14.0	C 19 H 18 N 4 Cl 2 S 2
		+11.8 / +5.2	9.0	C 18 H 23 N 2 Cl 3 S 2

Fig. S42. HRMS spectrum of 2l

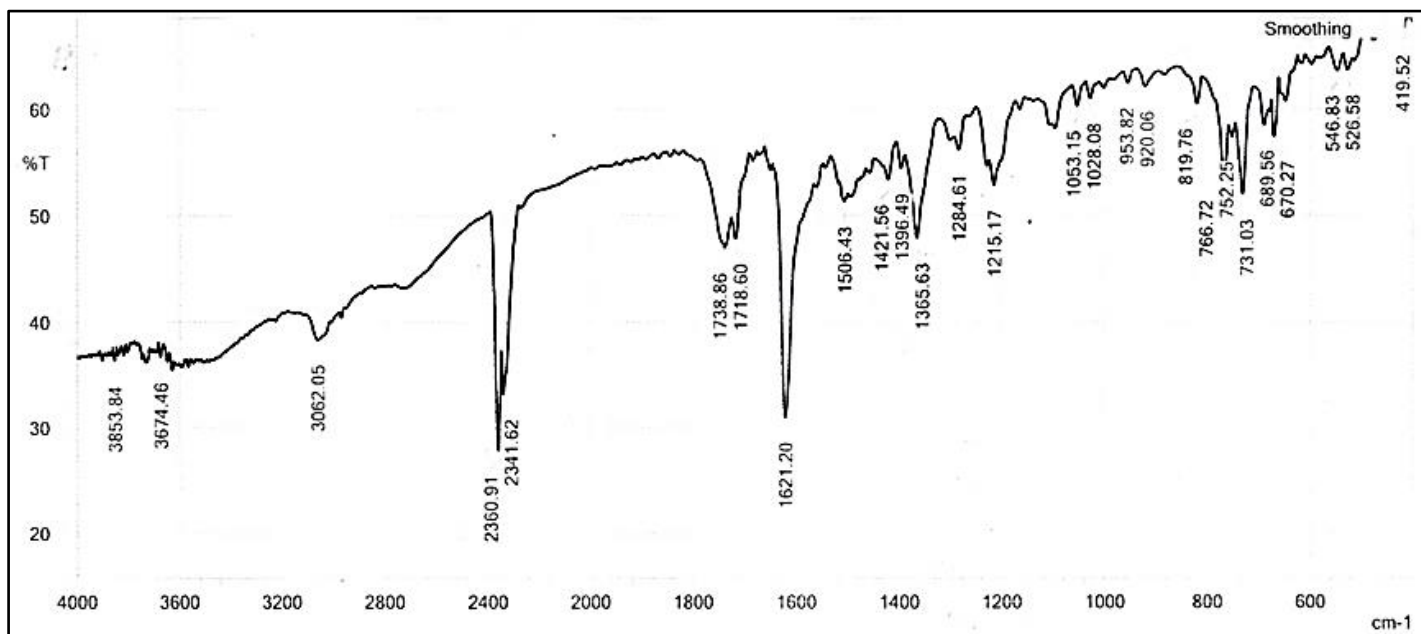


Fig. S43. IR spectrum of 2m.

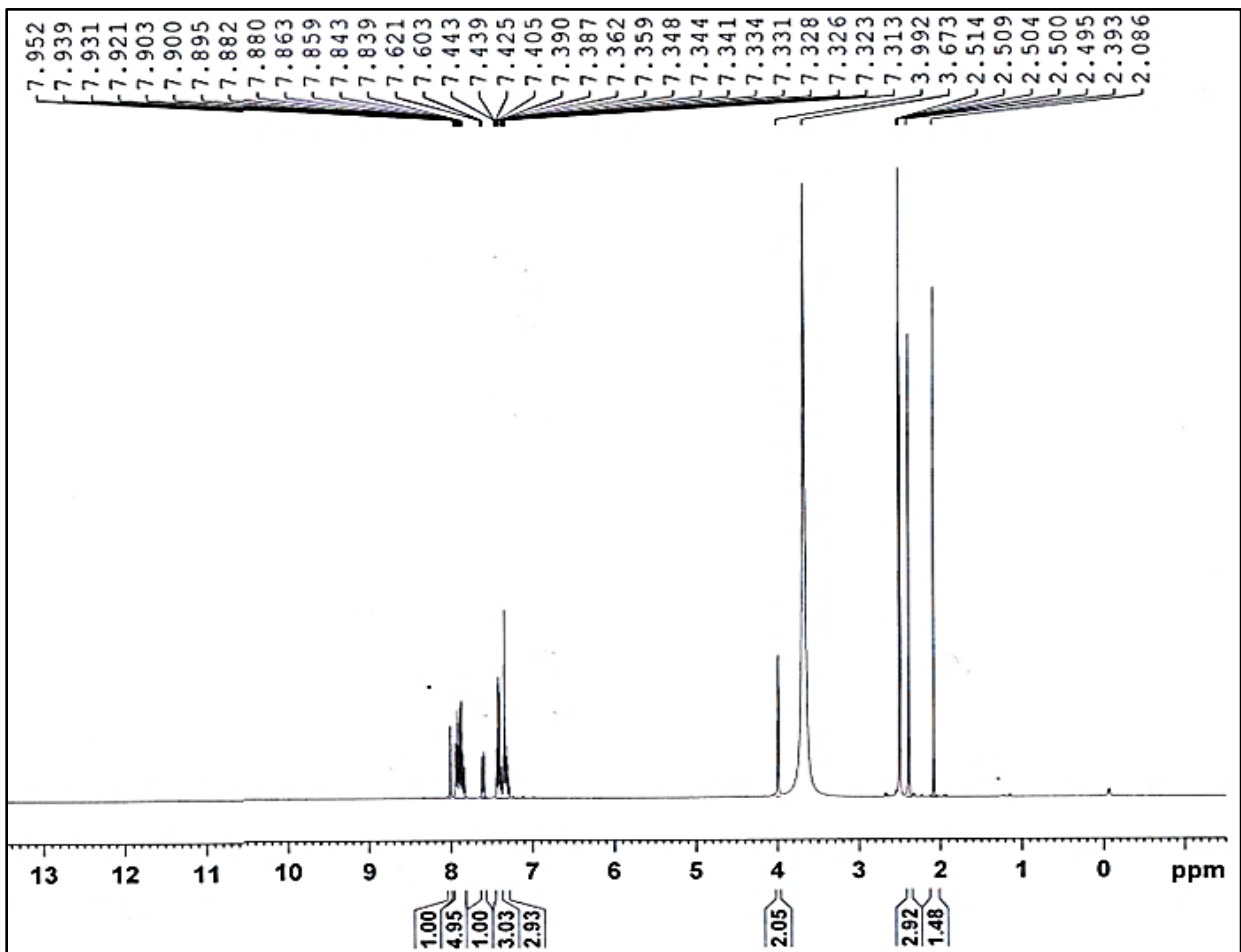
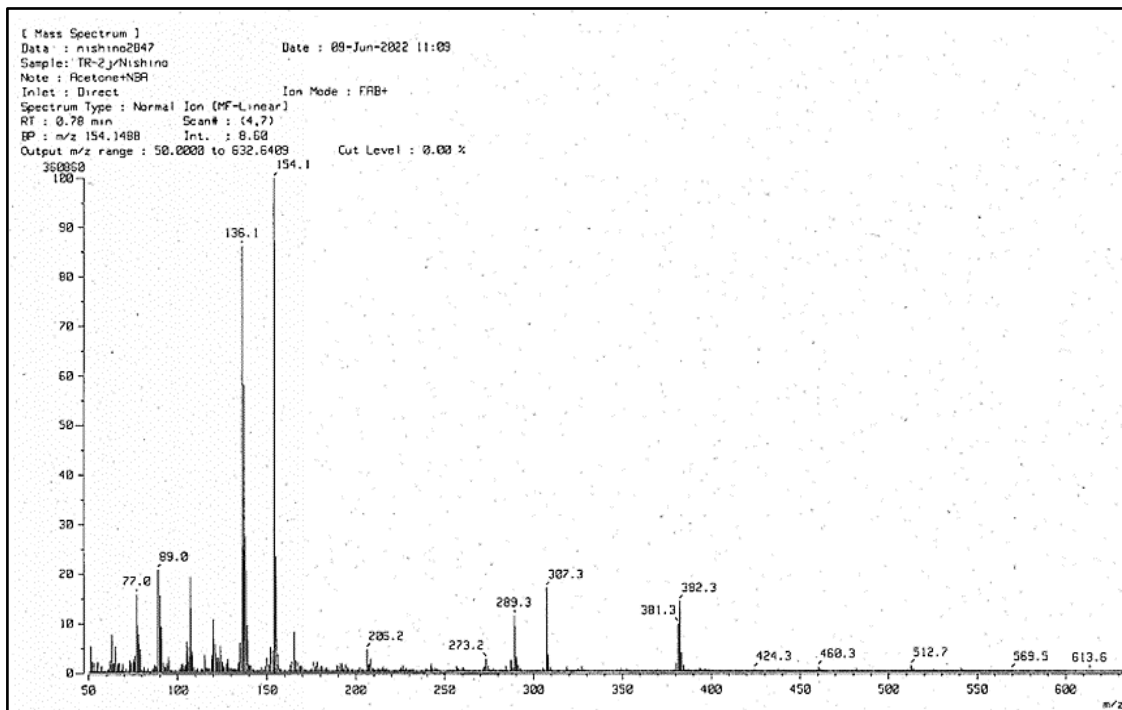


Fig. S44. ^1H NMR spectrum of **2m**.



[Elemental Composition]
 Date : 09-Jun-2022 11:18 Page: 1
 Data : nishino2848
 Sample: TR-2j/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.38 min Scan# : (5,8)
 Elements : C 100/0, H 100/0, N 4/2, S 2/0
 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
381.1304	75.4	-23.1 / -8.8	21.5	C 28 H 17 N 2
		+9.9 / +3.8	22.0	C 27 H 15 N 3
		+1.1 / +0.4	18.0	C 24 H 19 N 3 S
		-7.8 / -3.0	14.0	C 21 H 23 N 3 S 2
		+25.2 / +9.6	14.5	C 20 H 21 N 4 S 2

Fig. S45. HRMS spectrum of **2m**.

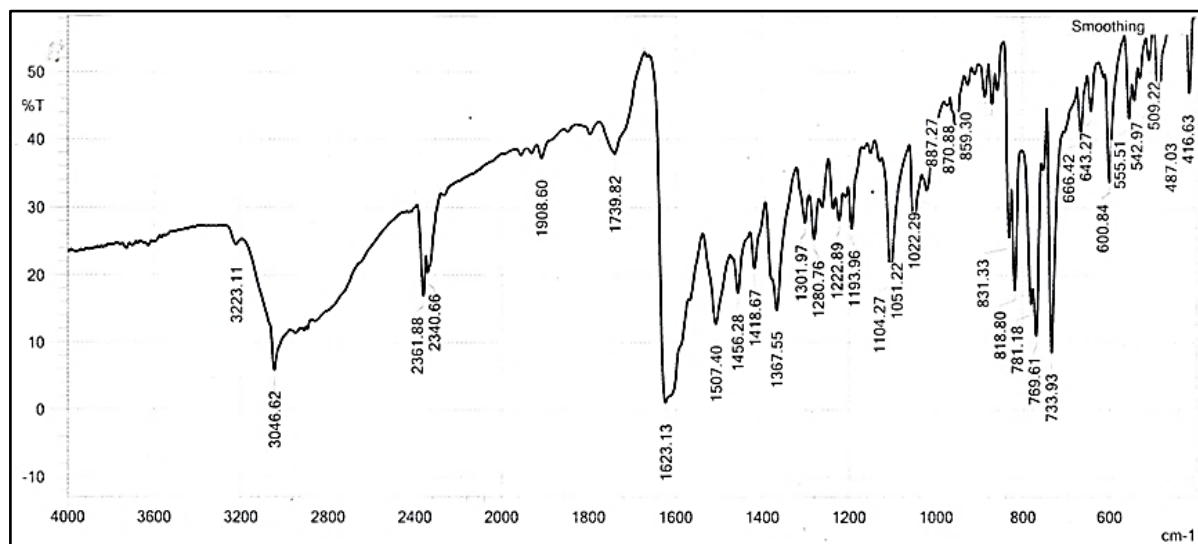


Fig. S46. IR spectrum of 2n.

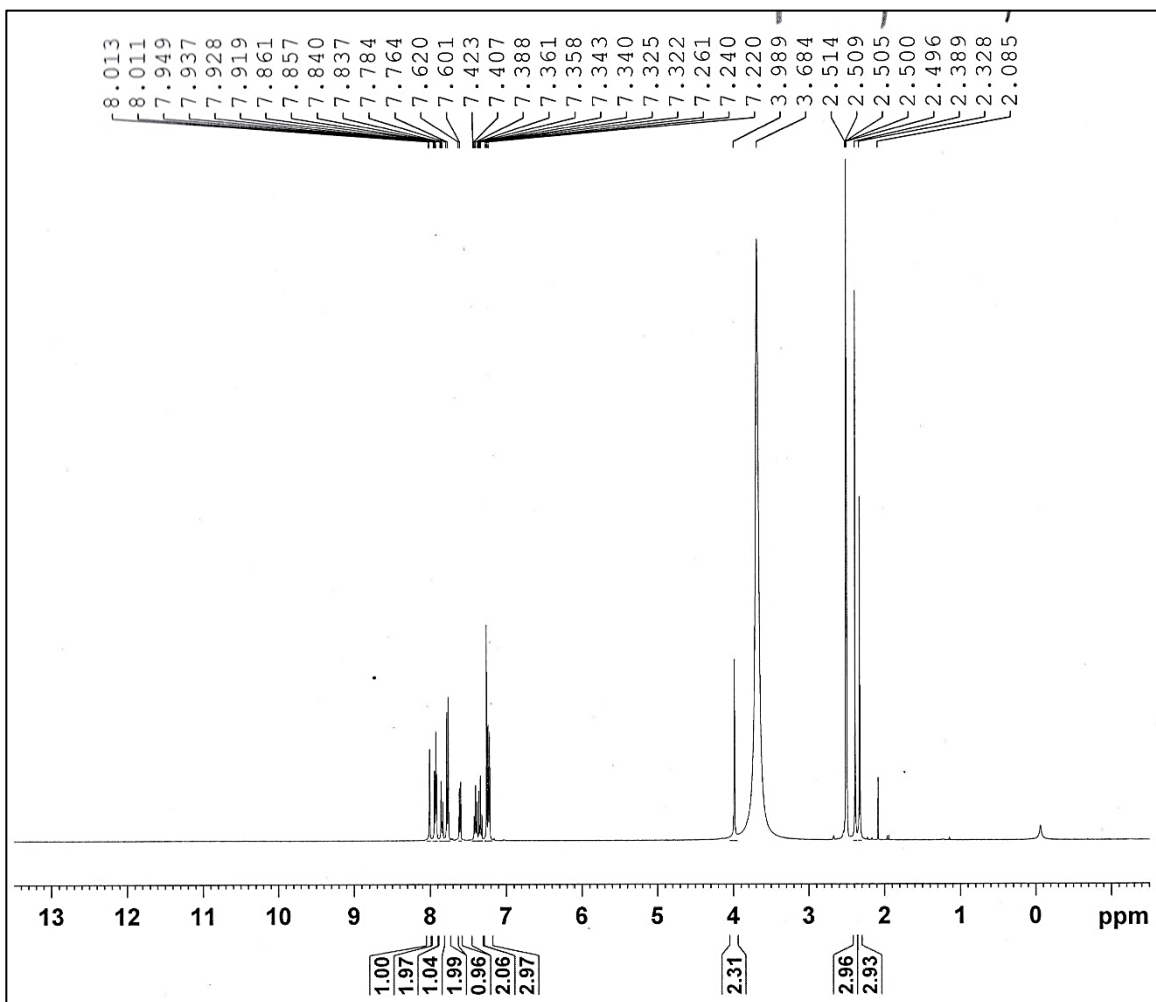
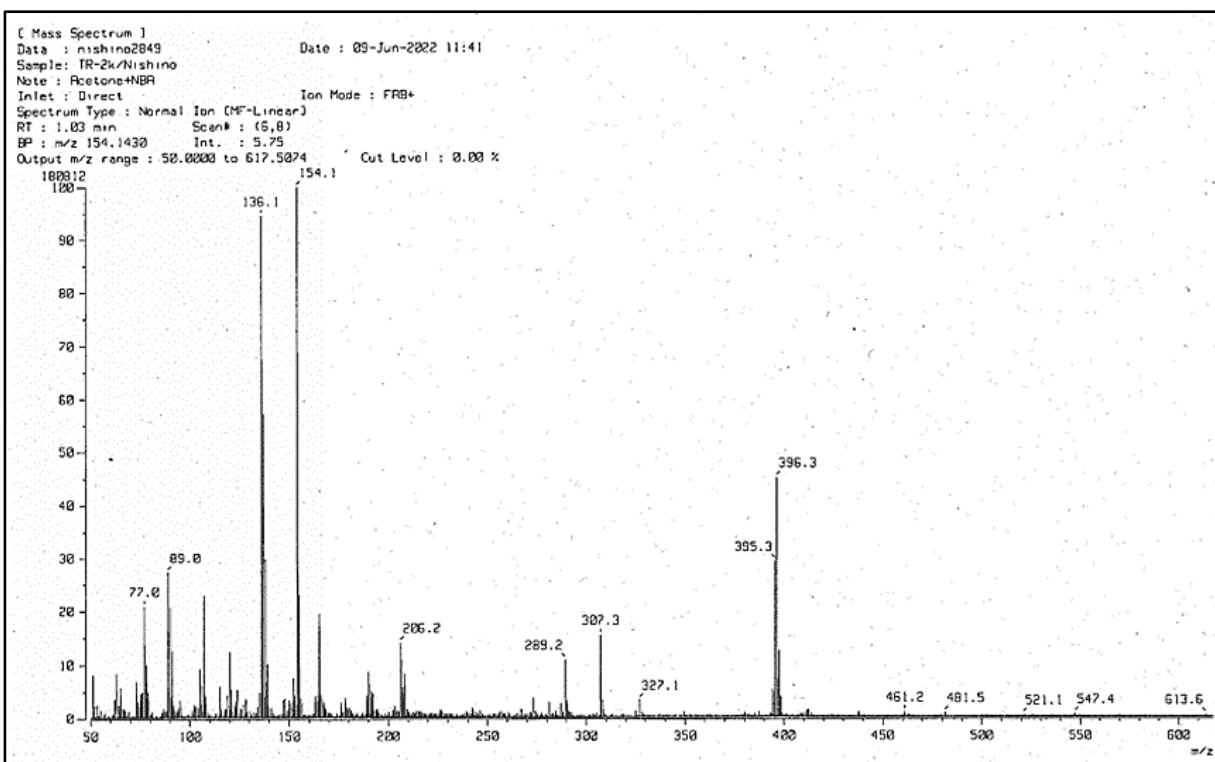


Fig. S47. ^1H NMR spectrum of **2n**.



[Elemental Composition]
 Date : 09-Jun-2022 11:49 Page: 1
 Data : nishino2850
 Sample: TR-2k/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.25 min Scan#: (4,8)
 Elements : C 100/0, H 100/0, N 4/2, S 2/0
 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
396.1518	100.0	+4.3 / +1.7	21.5	C 28 H 18 N 3
		-4.2 / -1.7	17.5	C 25 H 22 N 3 S
		-12.7 / -5.0	13.5	C 22 H 26 N 3 S 2
		+19.1 / +7.6	14.0	C 21 H 24 N 4 S 2

Fig. S48. HRMS spectrum of 2n.

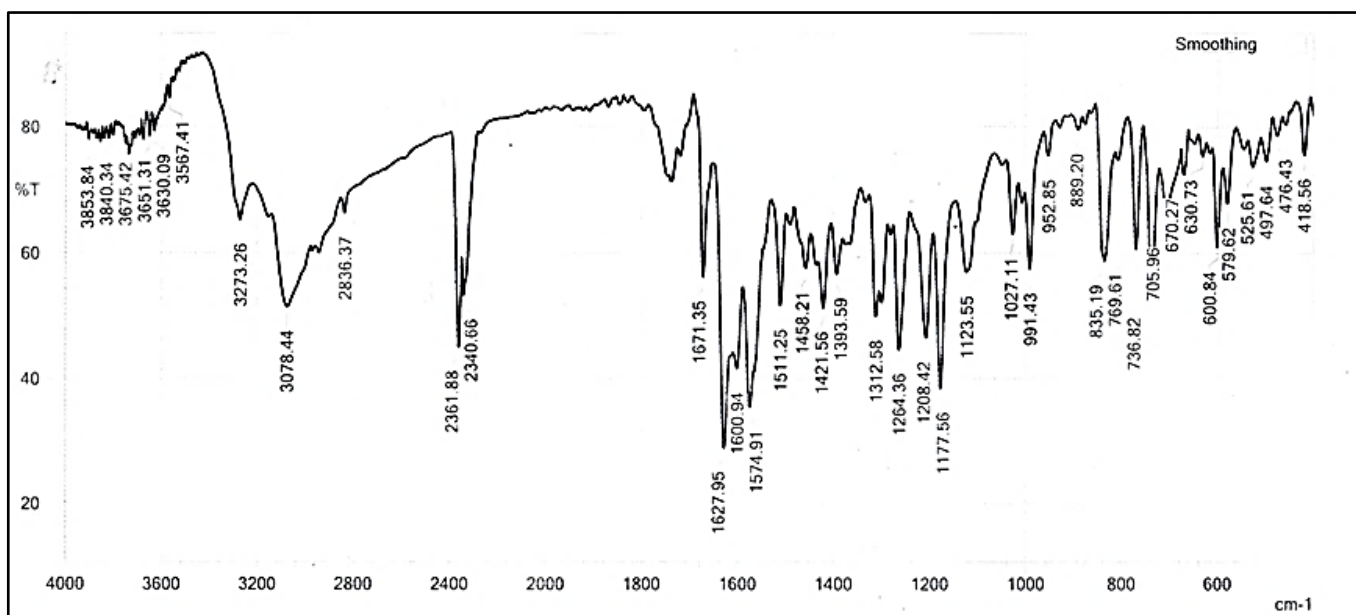


Fig. S49. IR spectrum of 20.

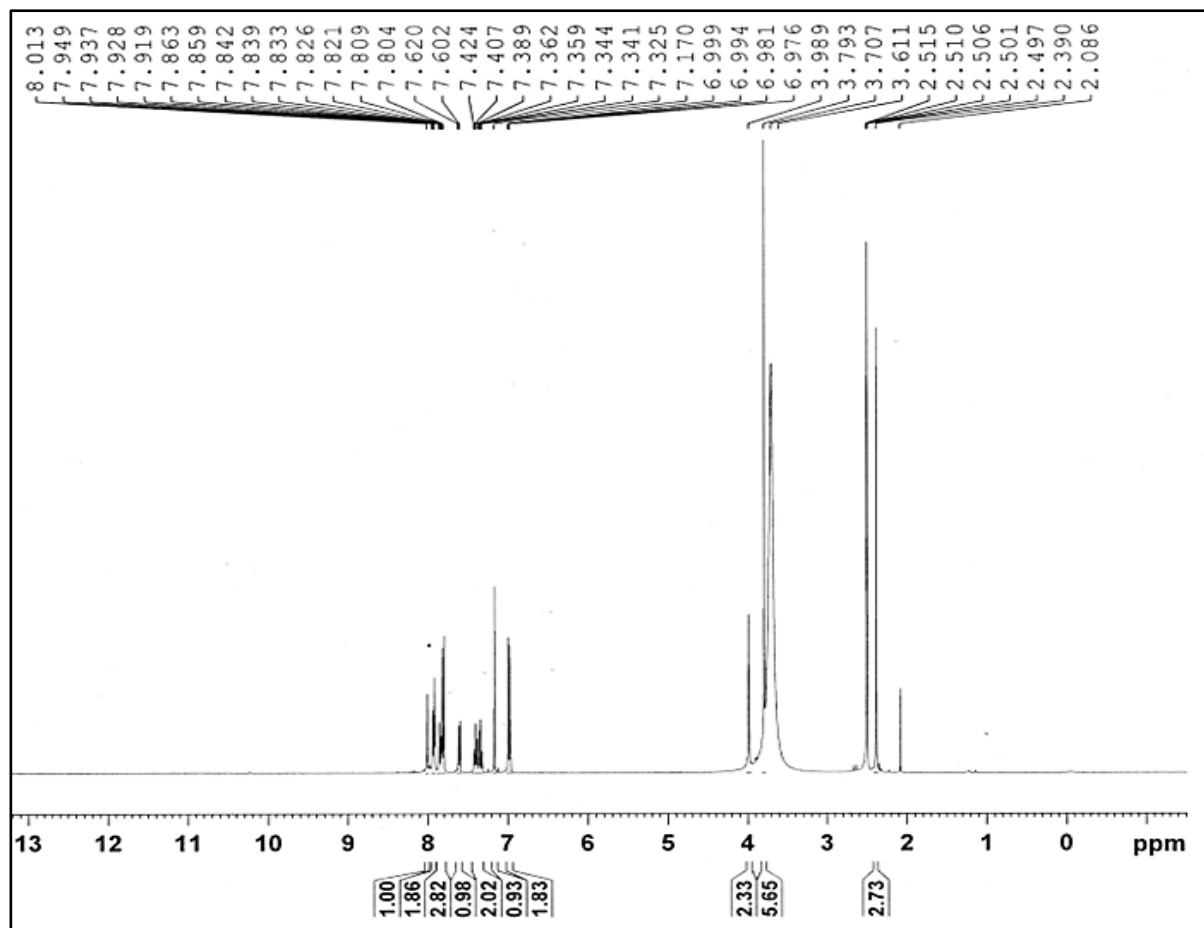
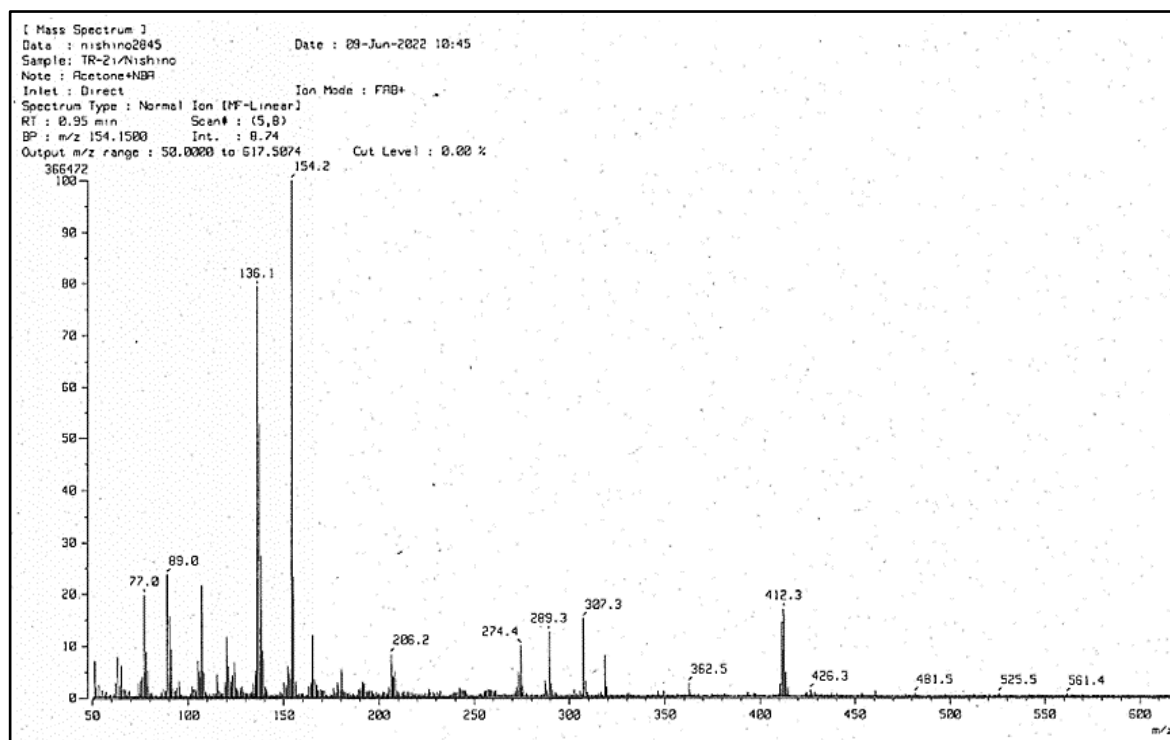


Fig. S50. ^1H NMR spectrum of **2o**.



[Elemental Composition]
 Date : 09-Jun-2022 10:53 Page: 1
 Data : nishino2846
 Sample: TR-2i/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.38 min Scan#: (5,8)
 Elements : C 100/0, H 100/0, O 2/0, N 4/2, S 2/0
 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
412.1470	85.2	+5.0 / +2.0	21.5	C 28 H 18 O N 3
		-3.2 / -1.3	17.5	C 25 H 22 O N 3 S
		-11.4 / -4.7	13.5	C 22 H 26 O N 3 S 2
		+19.1 / +7.9	14.0	C 21 H 24 O N 4 S 2

Fig. S51. HRMS spectrum of 2o.

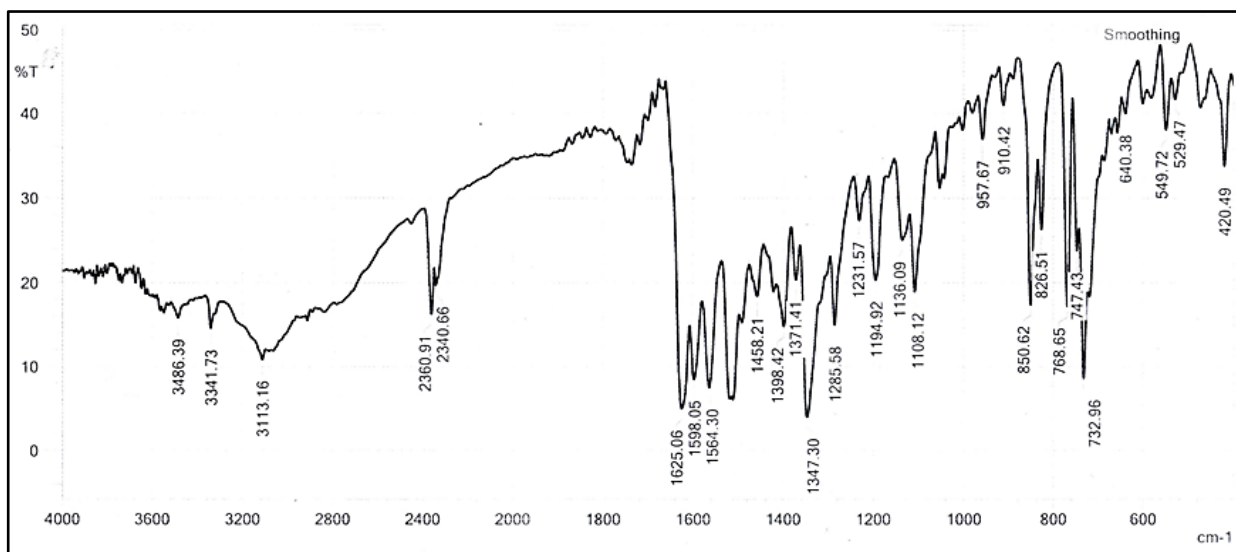


Fig. S52. IR spectrum of **2p**.

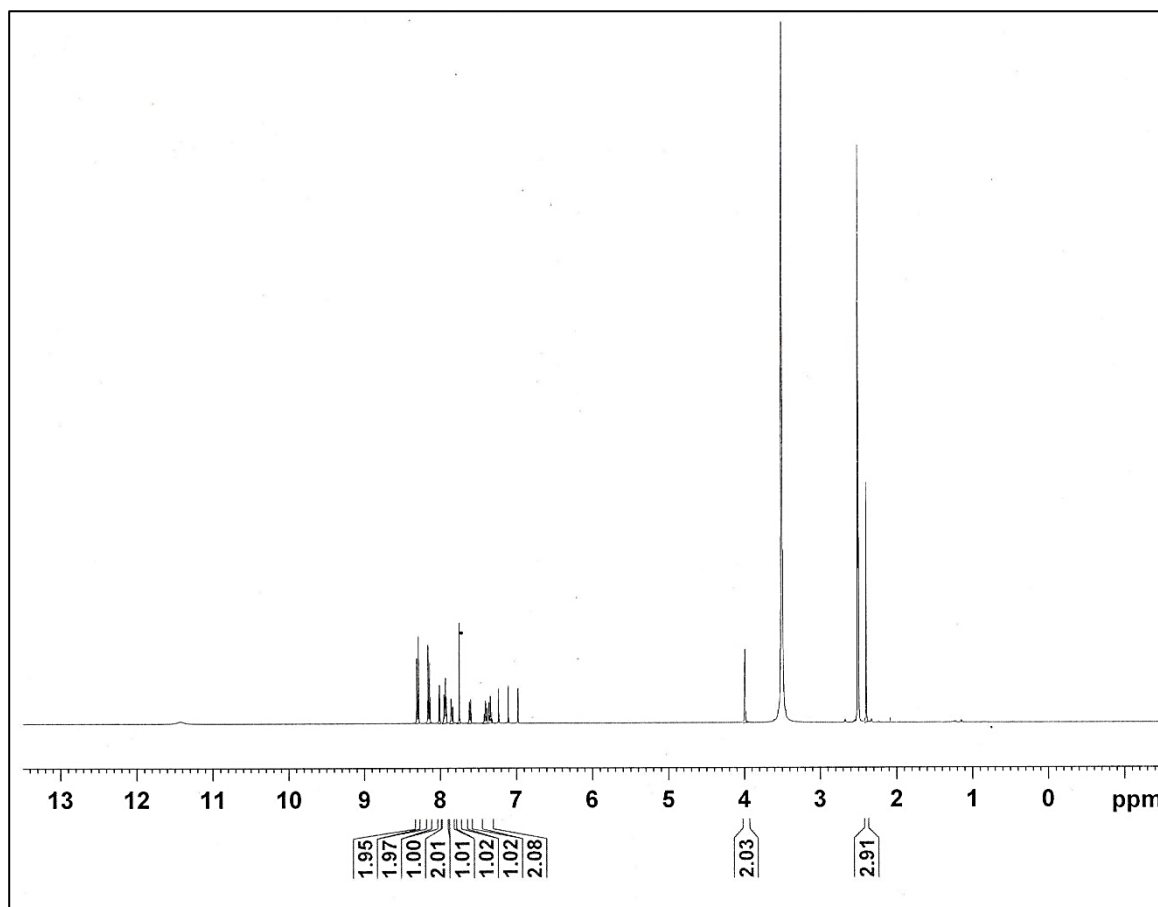
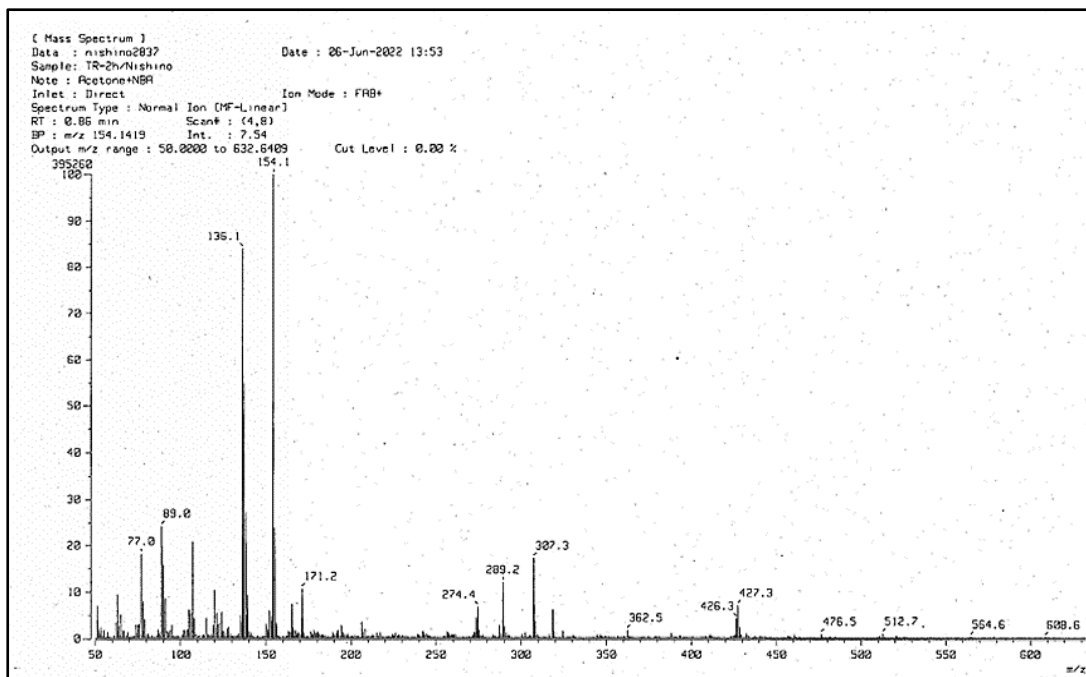


Fig. S53. ^1H NMR spectrum of **2p**.



[Elemental Composition]
 Date : 06-Jun-2022 14:11 Page: 1
 Data : nishino2838
 Sample: TR-2h/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.75 min Scan# : (6,10)
 Elements : C 100/0, H 100/0, O 3/1, N 5/3, S 2/0
 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
427.1233	43.9	-20.5 / -8.8	22.0 C 28 H 17 O 2 N 3
		+8.9 / +3.8	22.5 C 27 H 15 O 2 N 4
		+1.1 / +0.4	18.5 C 24 H 19 O 2 N 4 S
		-6.8 / -2.9	14.5 C 21 H 23 O 2 N 4 S 2
		+22.6 / +9.7	15.0 C 20 H 21 O 2 N 5 S 2

Fig. S54. HRMS spectrum of 2p.

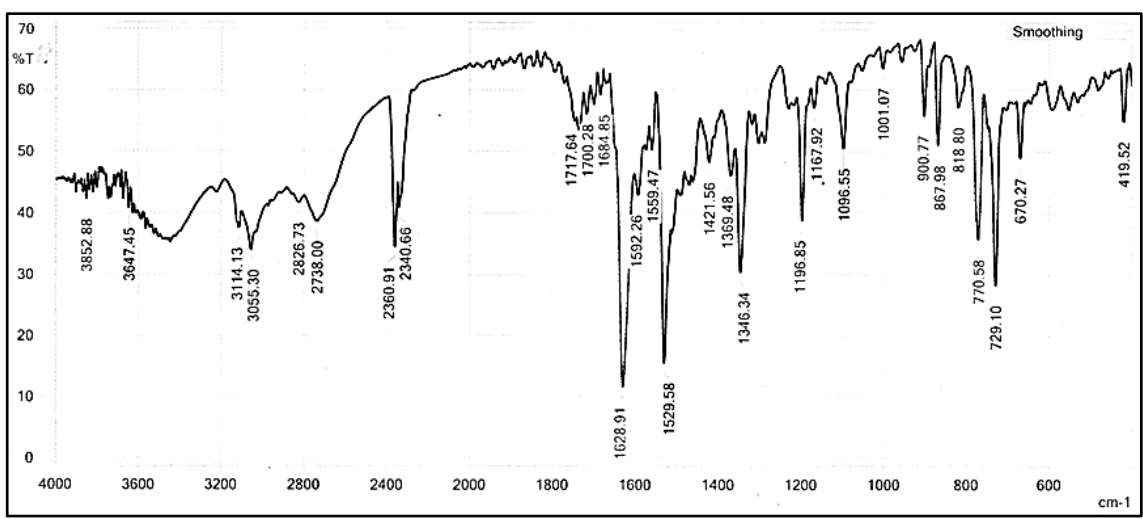


Fig. S55. IR spectrum of 2q.

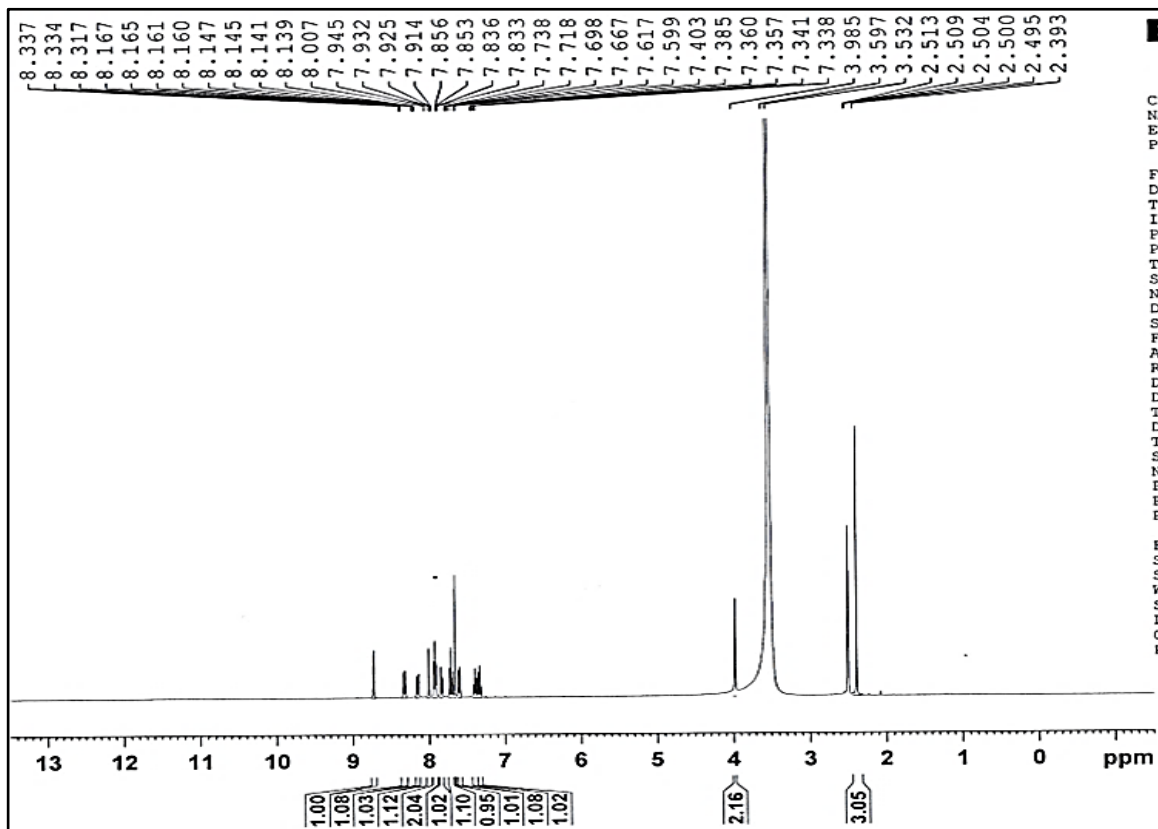
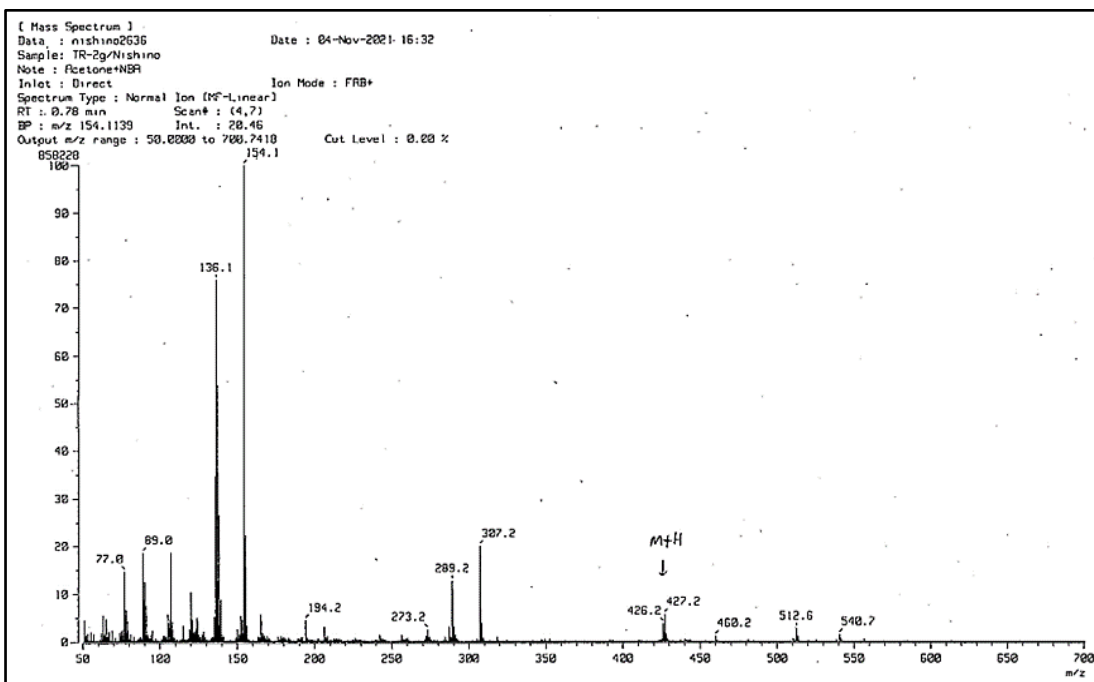


Fig. S56. ^1H NMR spectrum of **2q**.



[Elemental Composition]
 Date : 04-Nov-2021 16:38 Page: 1
 Data : nishino2638
 Sample: TR-2g/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 5.50 min Scan# : (20,26)
 Elements : C 100/0, H 100/0, O 3/1, N 5/3, S 2/0
 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
426.1159	32.4	-19.6 / -8.3	22.5	C 28 H 16 O 2 N 3
		+9.9 / +4.2	23.0	C 27 H 14 O 2 N 4
		+2.0 / +0.9	19.0	C 24 H 18 O 2 N 4 S
		-5.9 / -2.5	15.0	C 21 H 22 O 2 N 4 S 2
427.1223	27.4	-23.0 / -9.8	22.0	C 28 H 17 O 2 N 3
		+6.4 / +2.8	22.5	C 27 H 15 O 2 N 4
		-1.5 / -0.6	18.5	C 24 H 19 O 2 N 4 S
		-9.3 / -4.0	14.5	C 21 H 23 O 2 N 4 S 2
		+20.1 / +8.6	15.0	C 20 H 21 O 2 N 5 S 2

Fig. S57. IR spectrum of 2q.

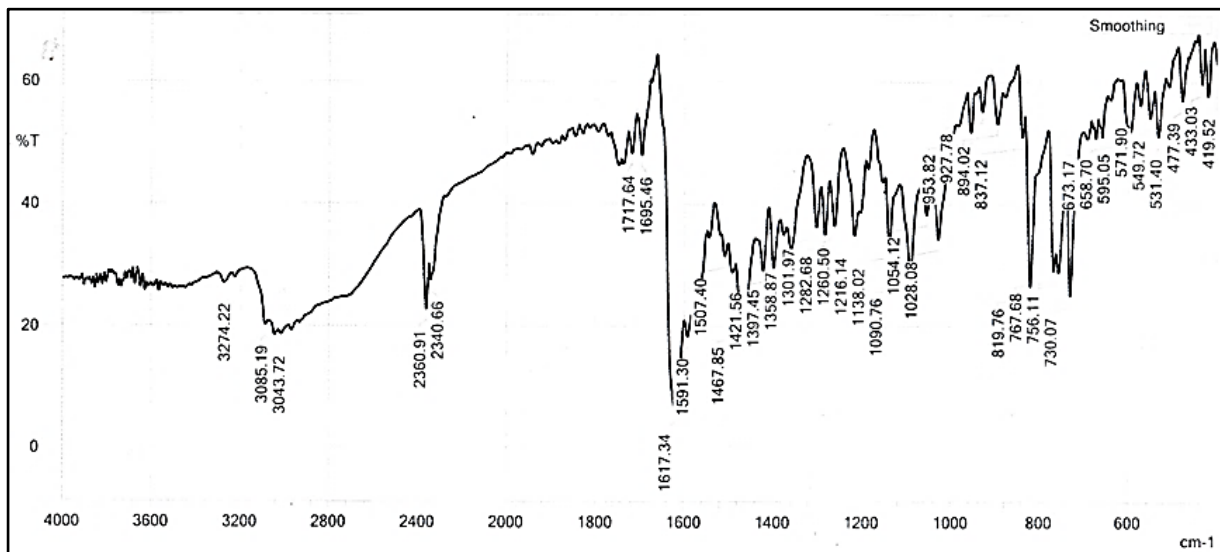


Fig. S58. IR spectrum of **2r**.

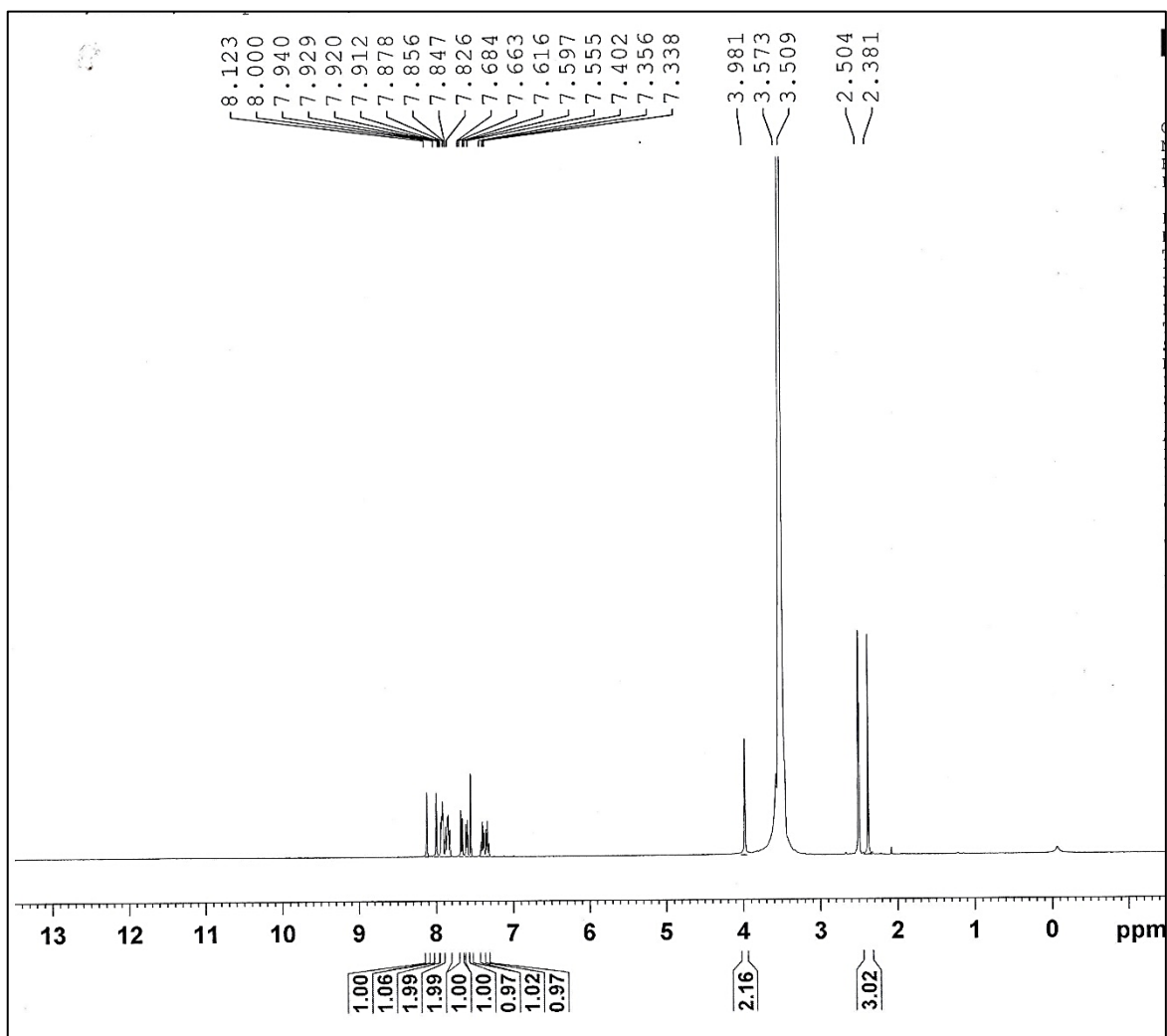
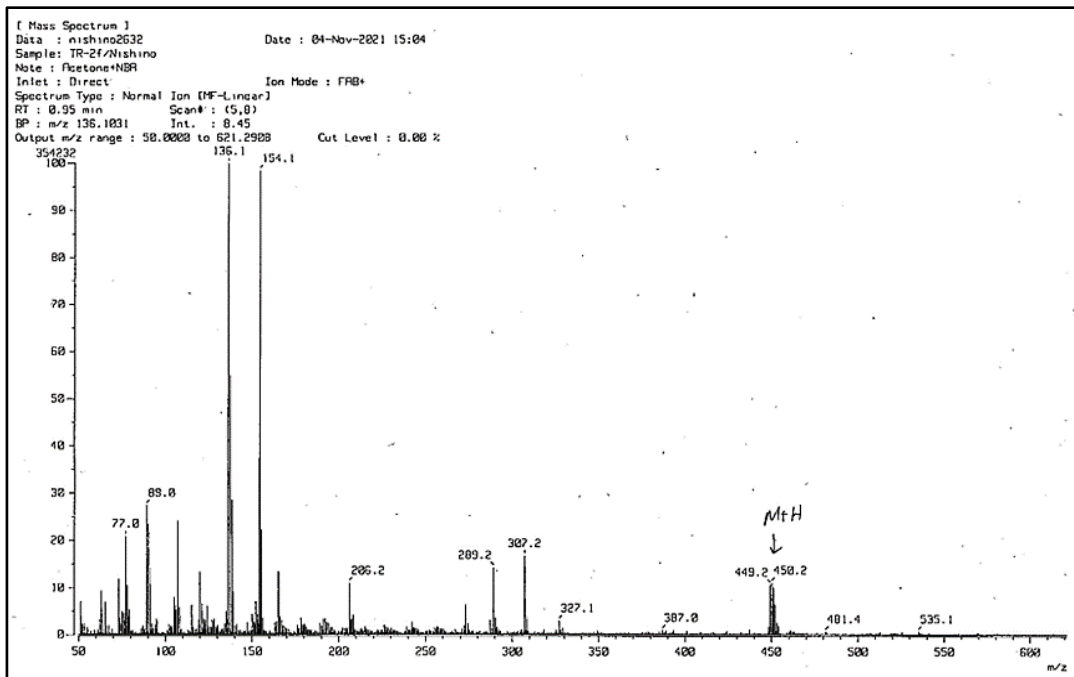


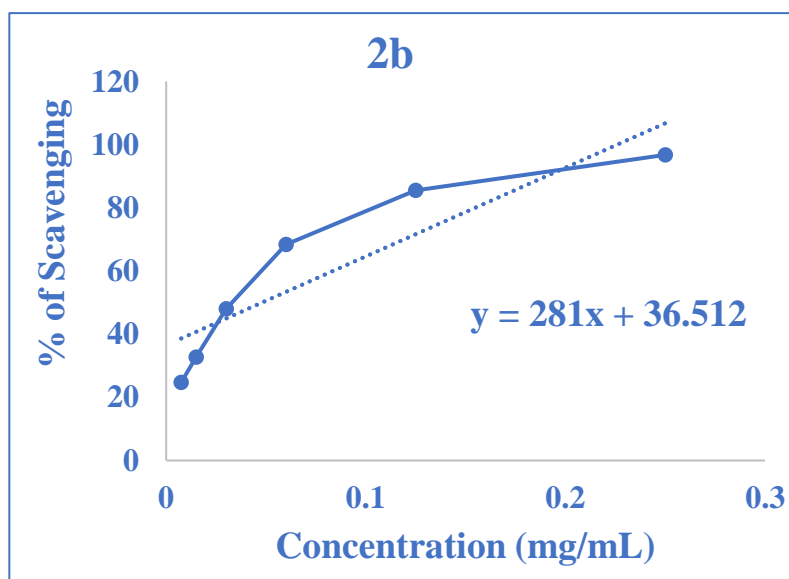
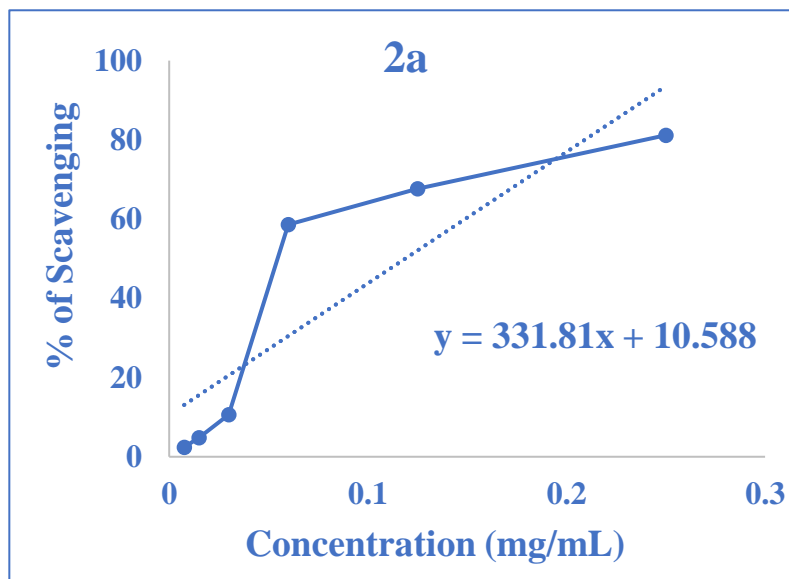
Fig. S59. ¹H NMR spectrum of 2r.

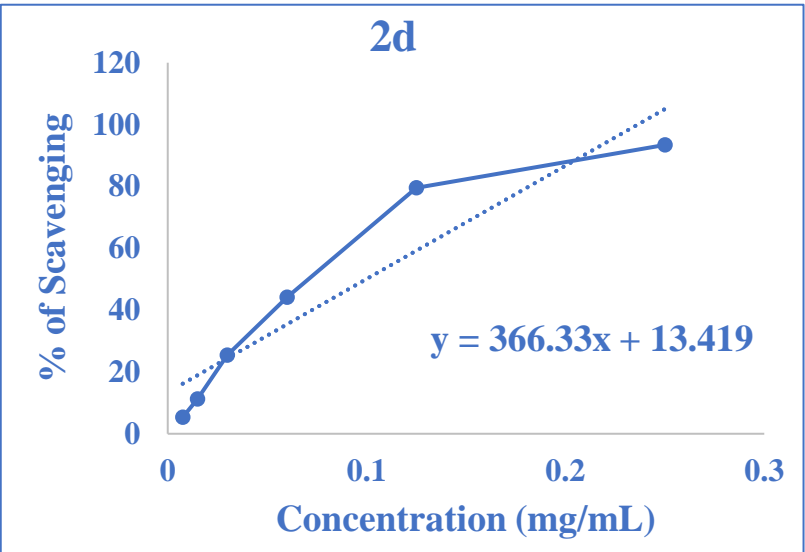
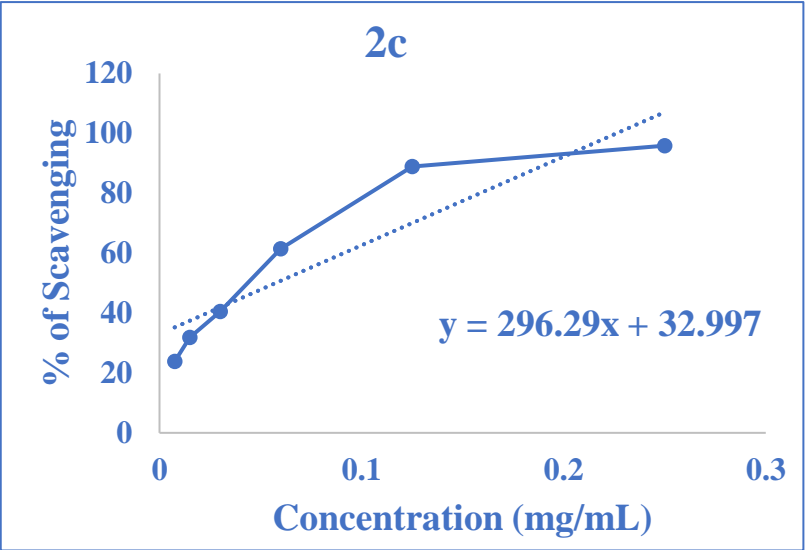


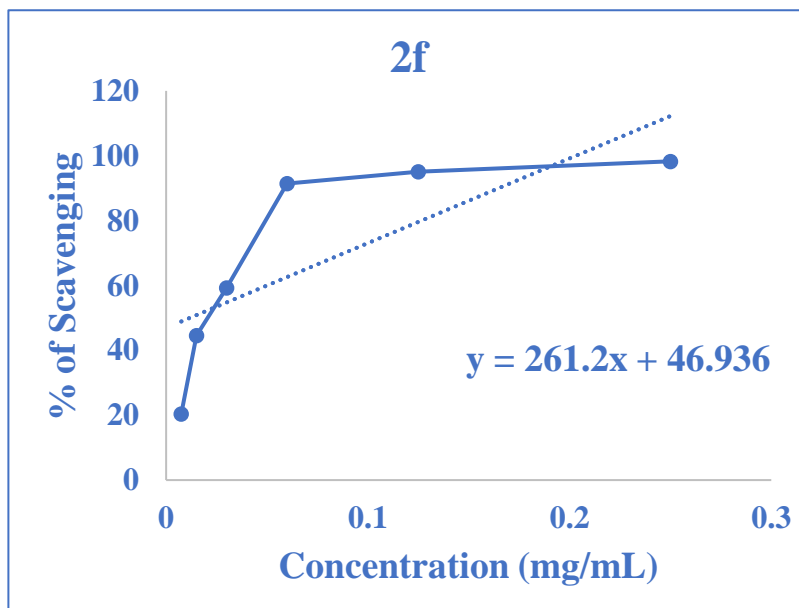
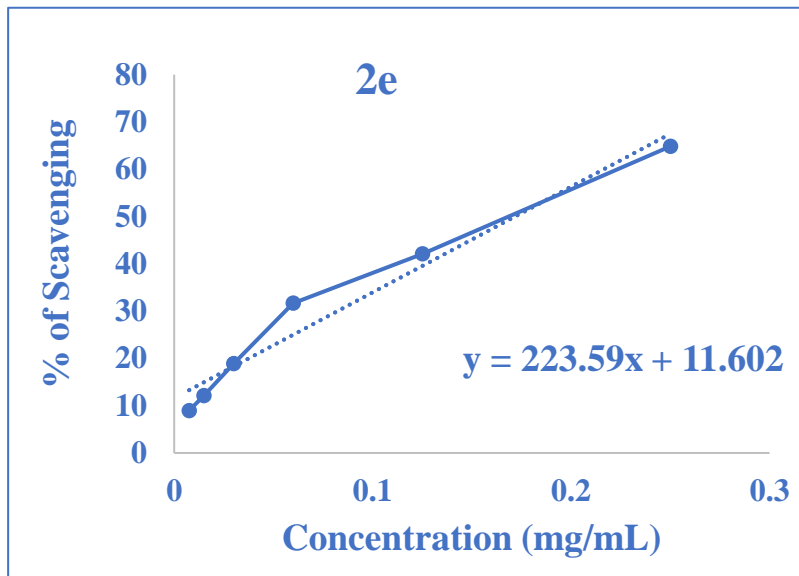
[Elemental Composition]
 Date : 04-Nov-2021 16:17 Page: 1
 Data : nishino2635
 Sample: TR-2f/Nishino
 Note : Acetone+NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.63 min Scan# : (5,10)
 Elements : C 100/0, H 100/0, N 4/2, Cl 3/1, S 2/0
 Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
 Unsaturation (U.S.) : -0.5 - 50.0

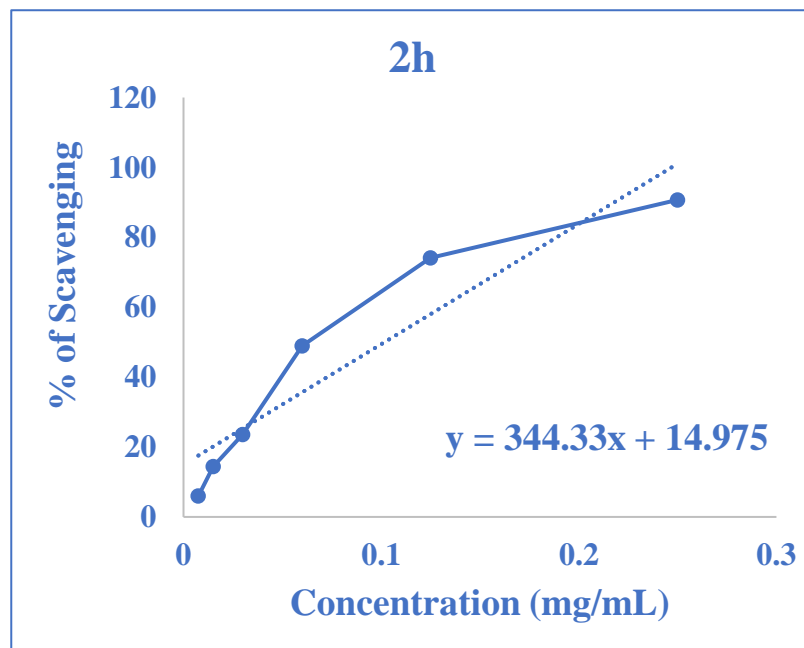
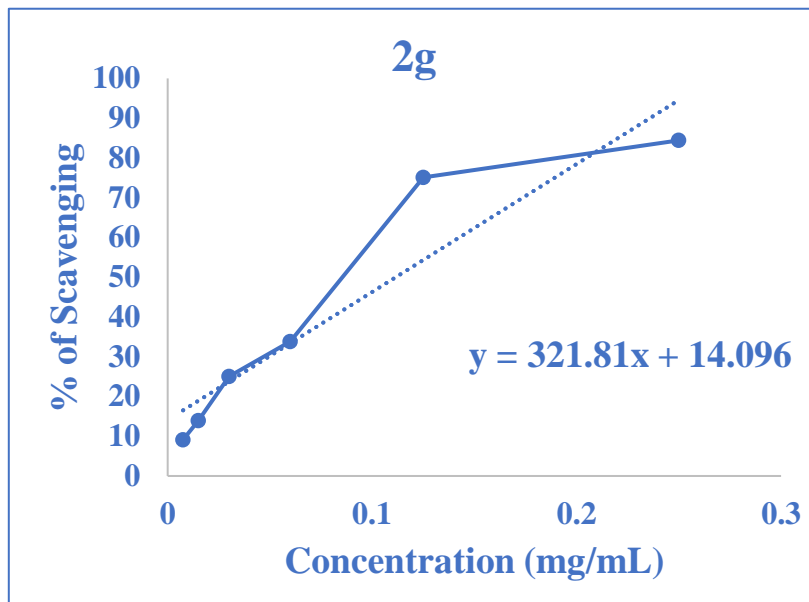
Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
449.0556	100.0	-8.4 / -3.8	26.5	C 29 H 10 N 4 Cl
		-12.5 / -5.6	21.5	C 28 H 15 N 2 Cl 2
		+15.5 / +7.0	22.0	C 27 H 13 N 3 Cl 2
		-15.9 / -7.1	22.5	C 26 H 14 N 4 Cl S
		-20.0 / -9.0	17.5	C 25 H 19 N 2 Cl 2 S
		+8.0 / +3.6	18.0	C 24 H 17 N 3 Cl 2 S
450.0599	83.6	+0.5 / +0.2	14.0	C 21 H 21 N 3 Cl 2 S 2
		-16.2 / -7.3	26.0	C 29 H 11 N 4 Cl
		-20.3 / -9.1	21.0	C 28 H 16 N 2 Cl 2
		+7.7 / +3.5	21.5	C 27 H 14 N 3 Cl 2
		+0.2 / +0.1	17.5	C 24 H 18 N 3 Cl 2 S
		-7.3 / -3.3	13.5	C 21 H 22 N 3 Cl 2 S 2
		+20.6 / +9.3	14.0	C 20 H 20 N 4 Cl 2 S 2
+16.6 / +7.5	9.0	C 19 H 25 N 2 Cl 3 S 2		

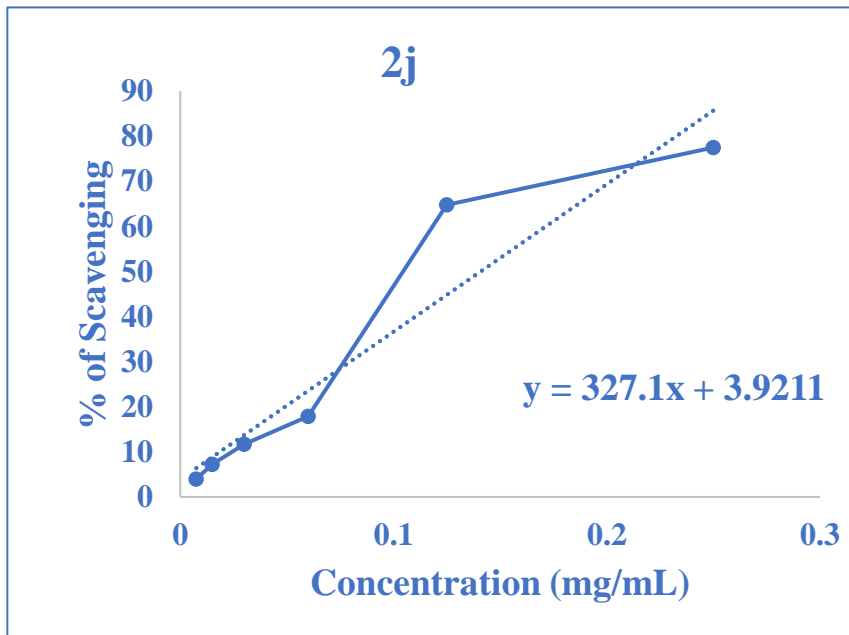
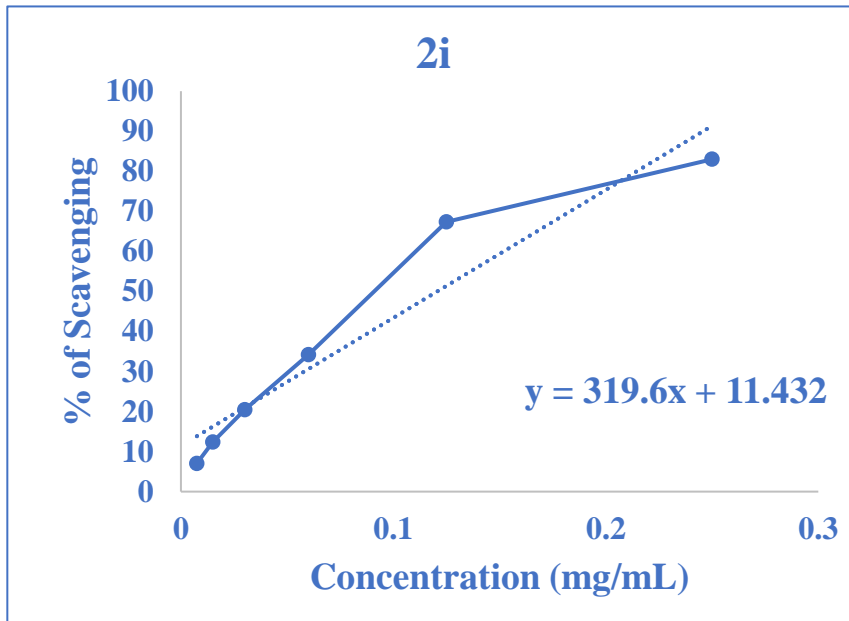
Fig. S60. HRMS spectrum of 2r.

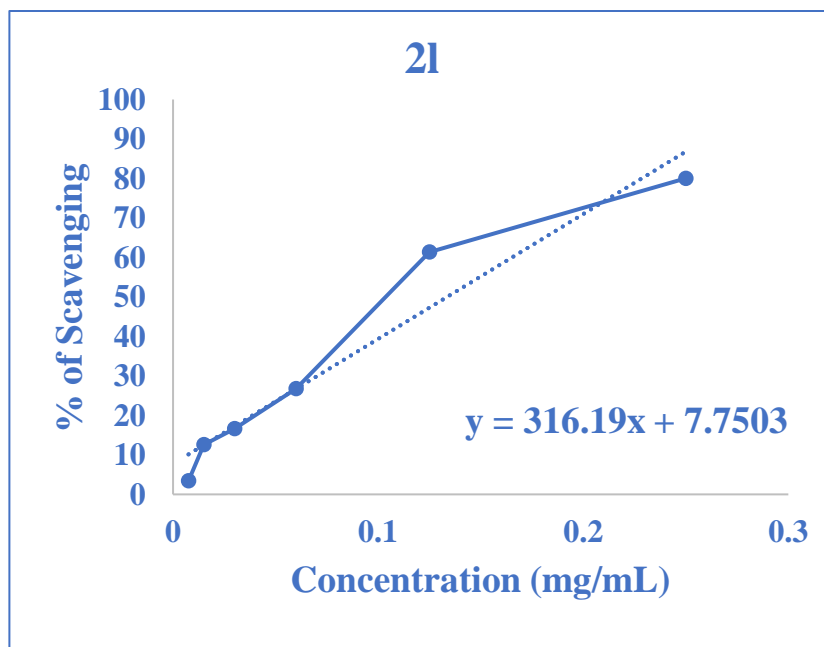
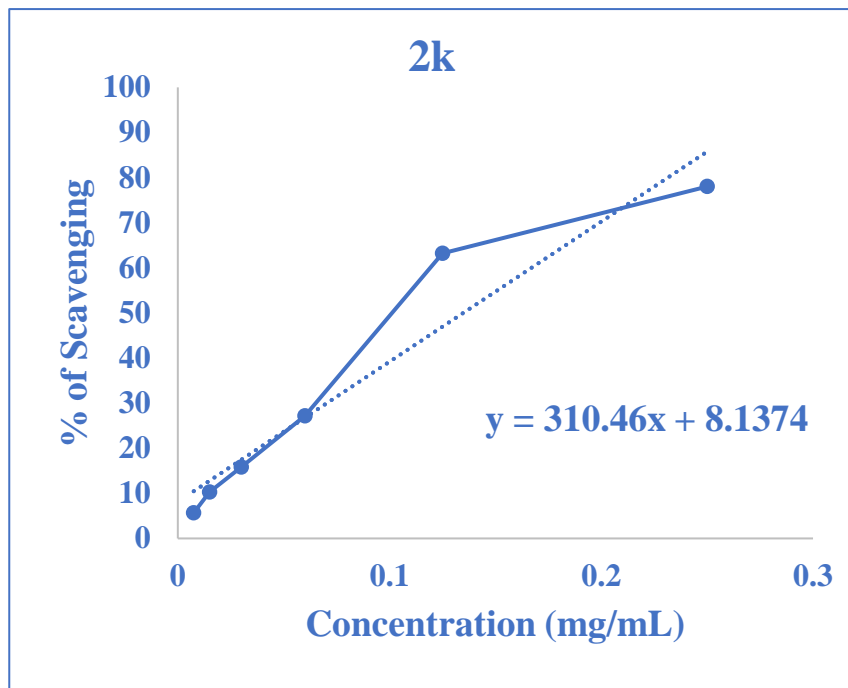


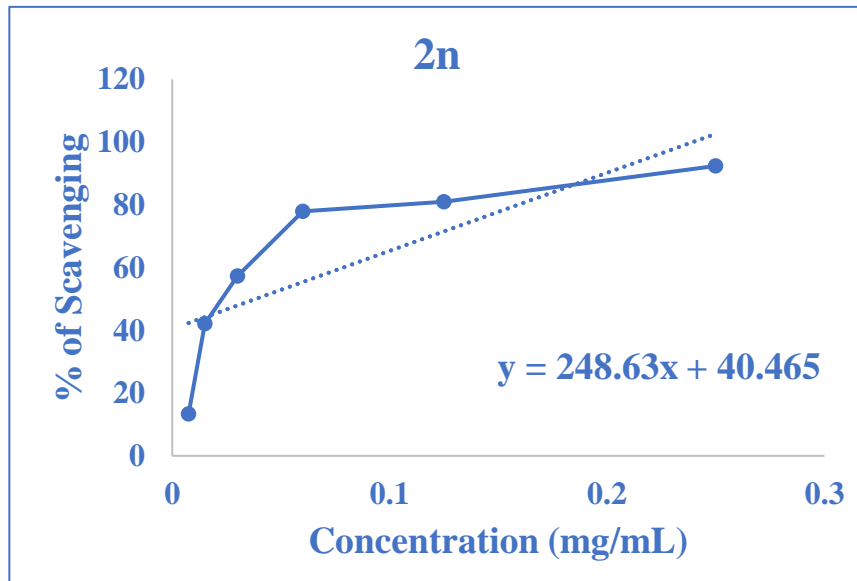
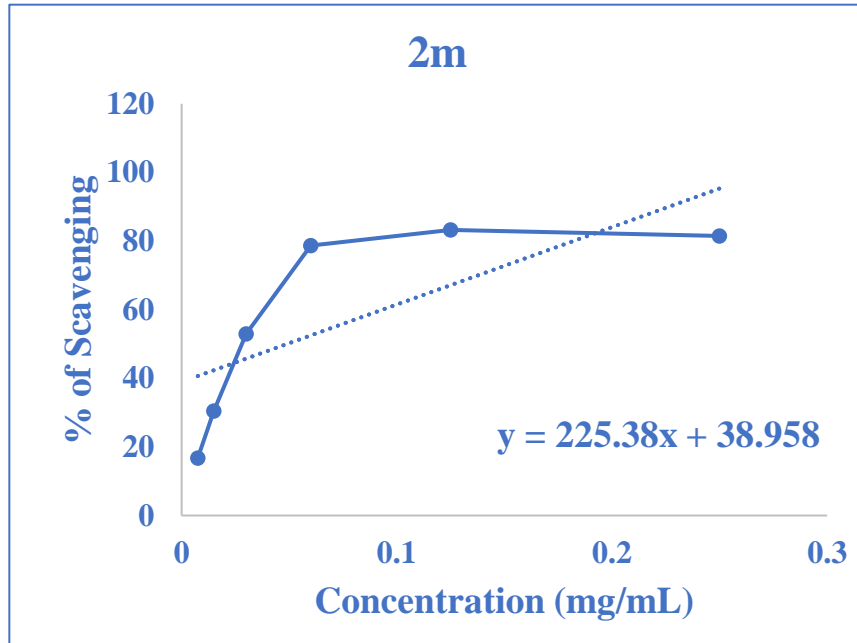


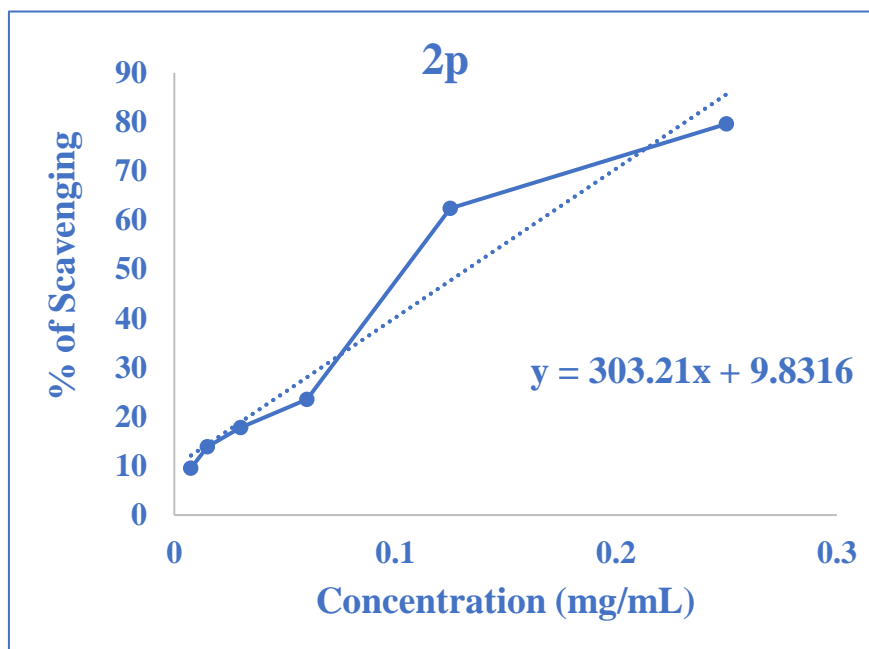
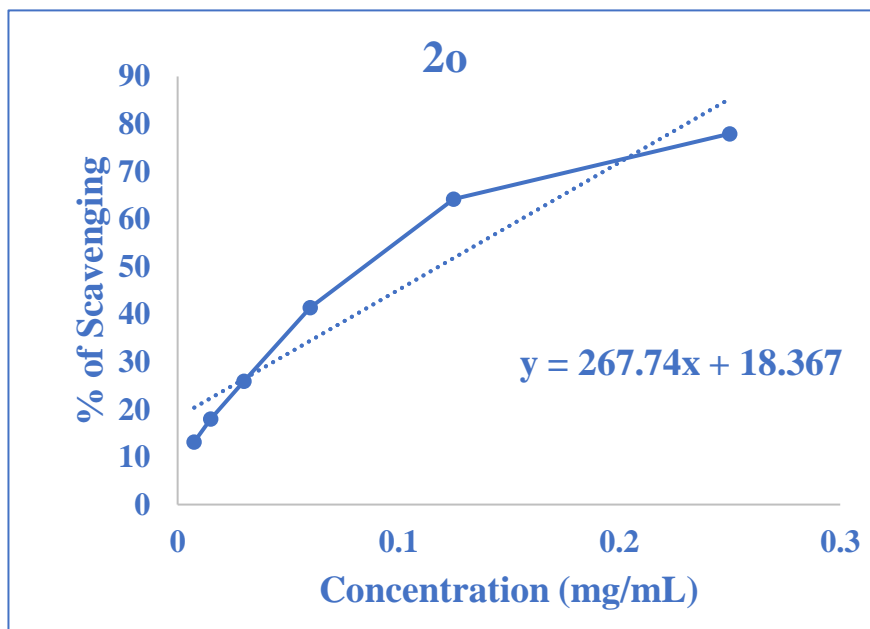


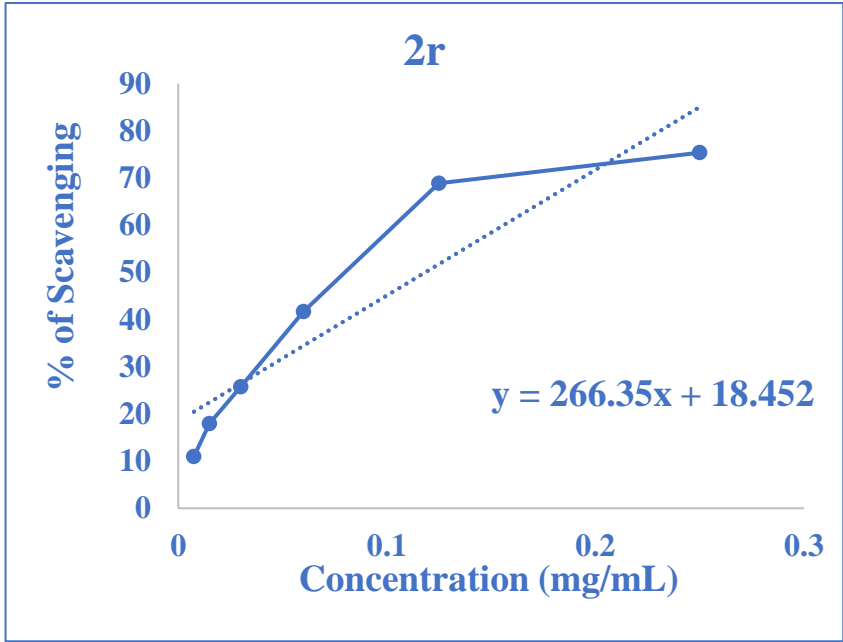
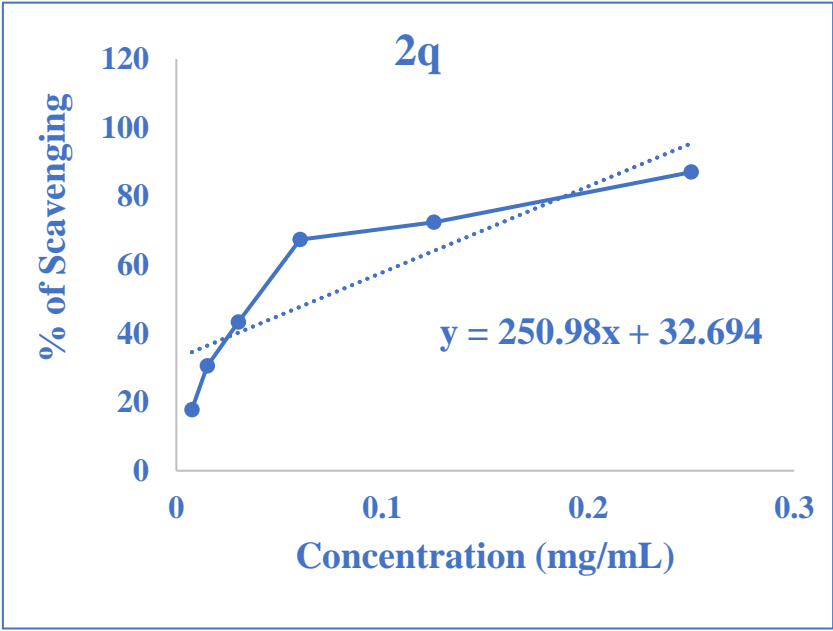












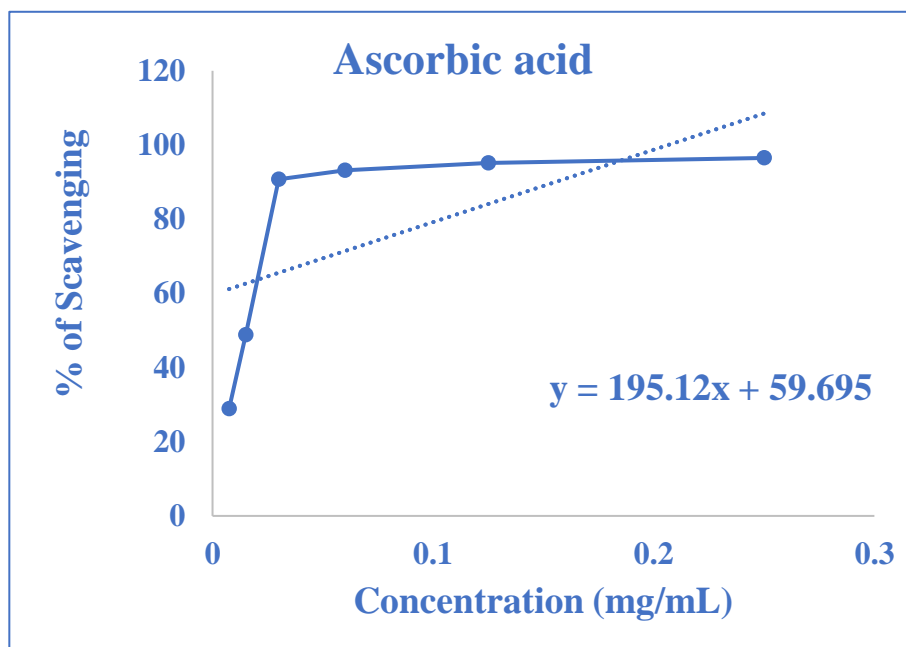


Fig. S61. Concentration-inhibition curves of synthesized compounds **2a-2r** and ascorbic acid.