

Fig.S1. FT-IR spectra of compound 3

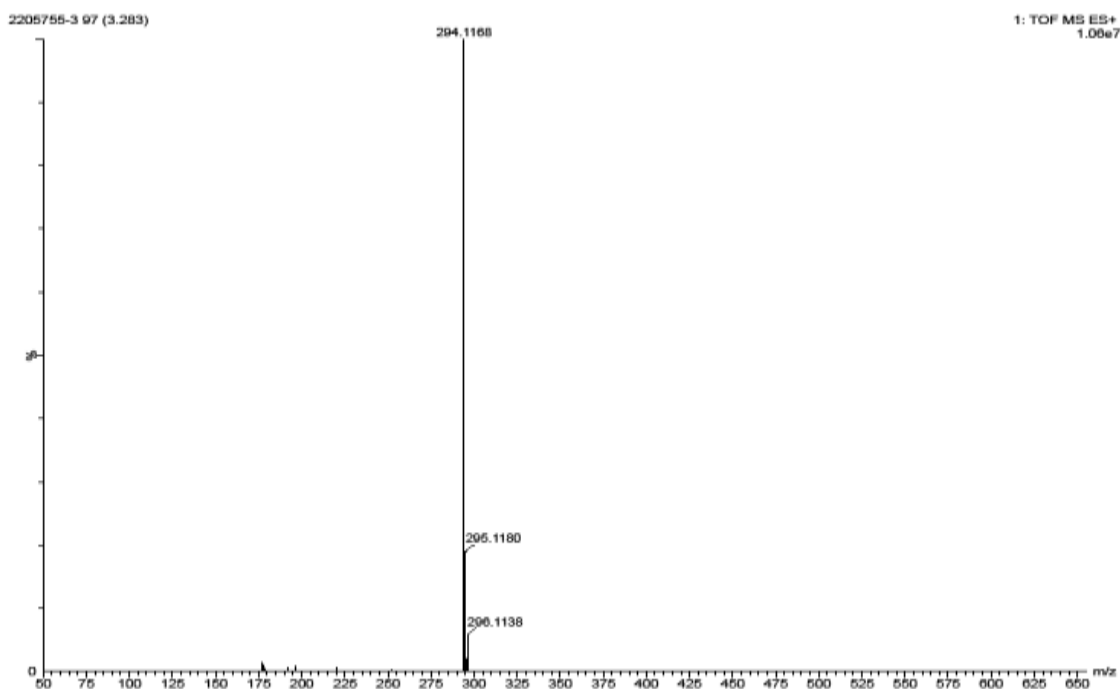
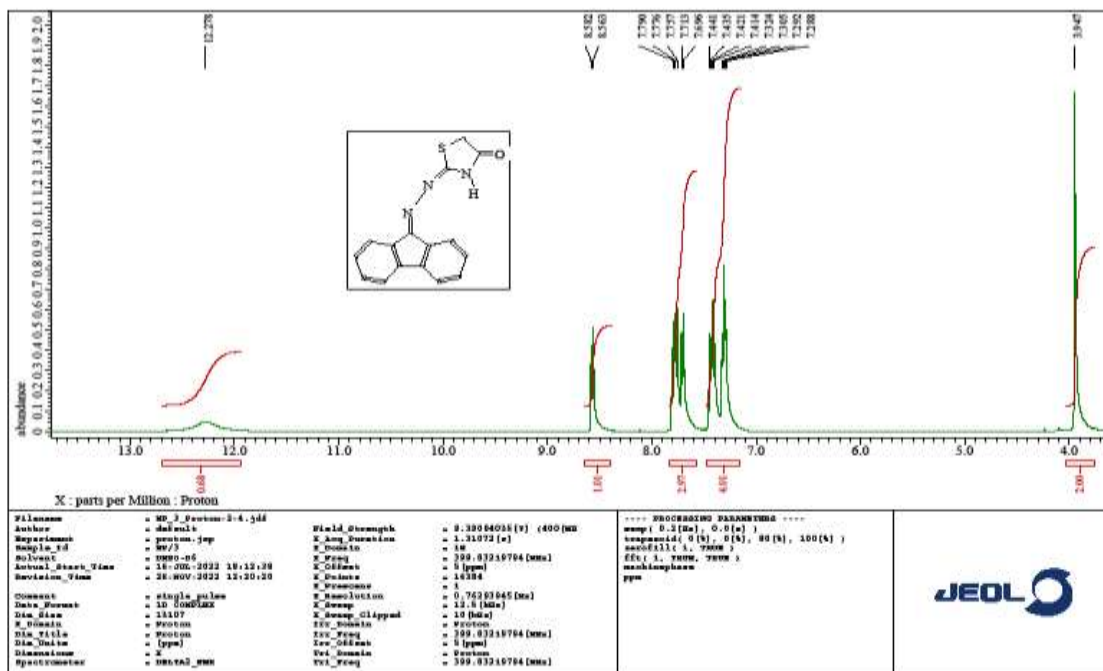
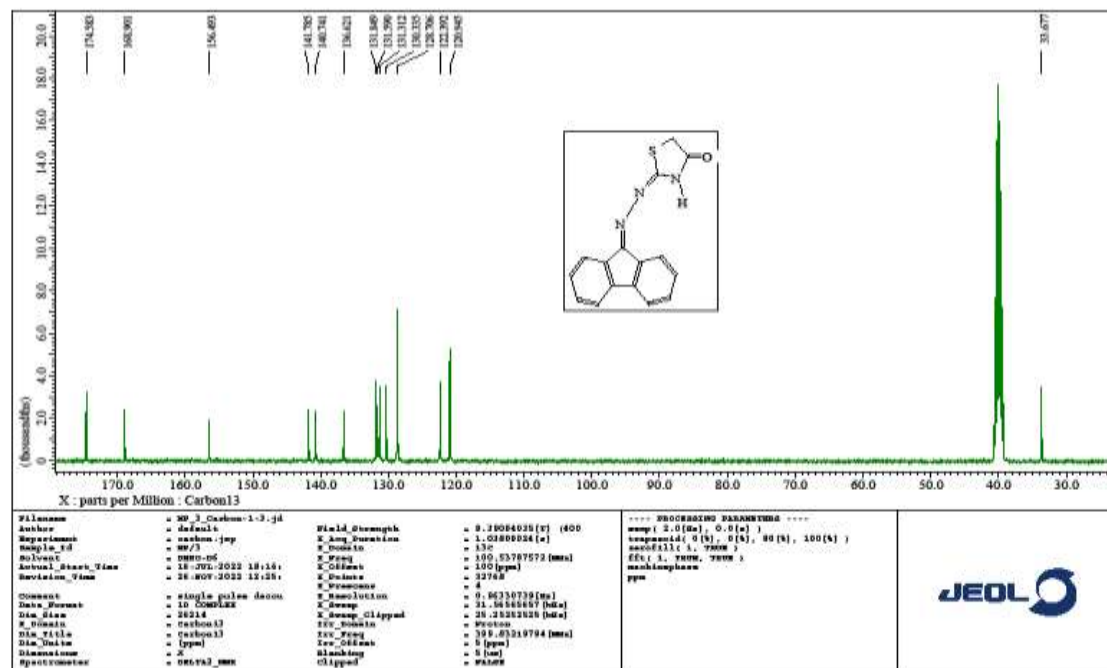


Fig.S2. Mass spectra of compound 3



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Fig.S3. ¹H spectra of compound 3



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Fig.S4. ¹³C spectra of compound 3

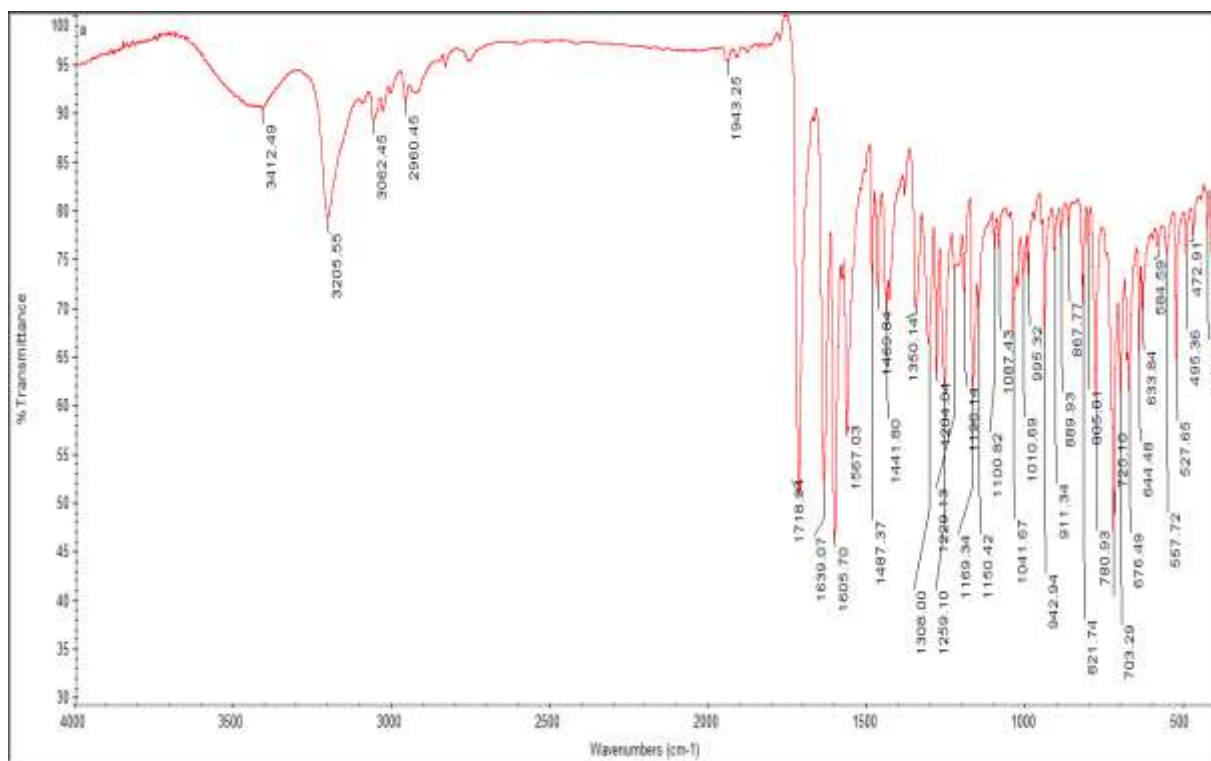


Fig.S5. FT-IR spectra of compound 5a

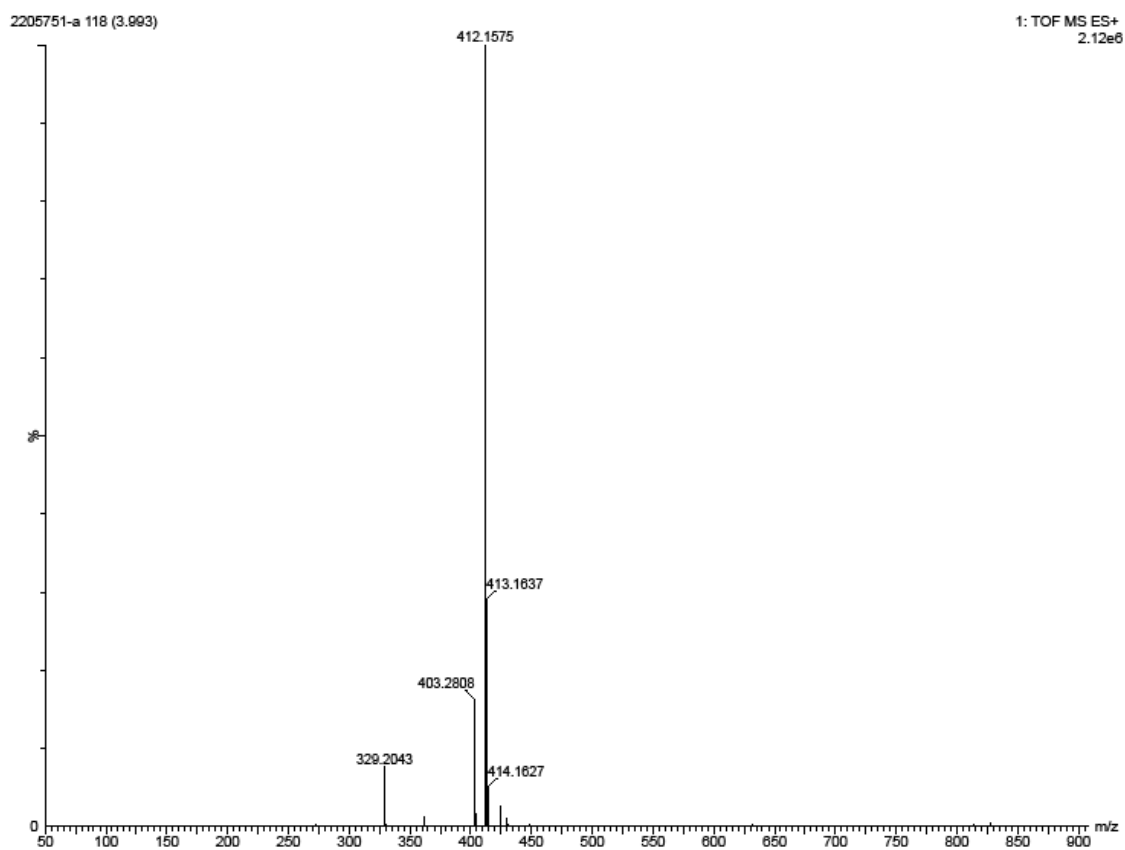
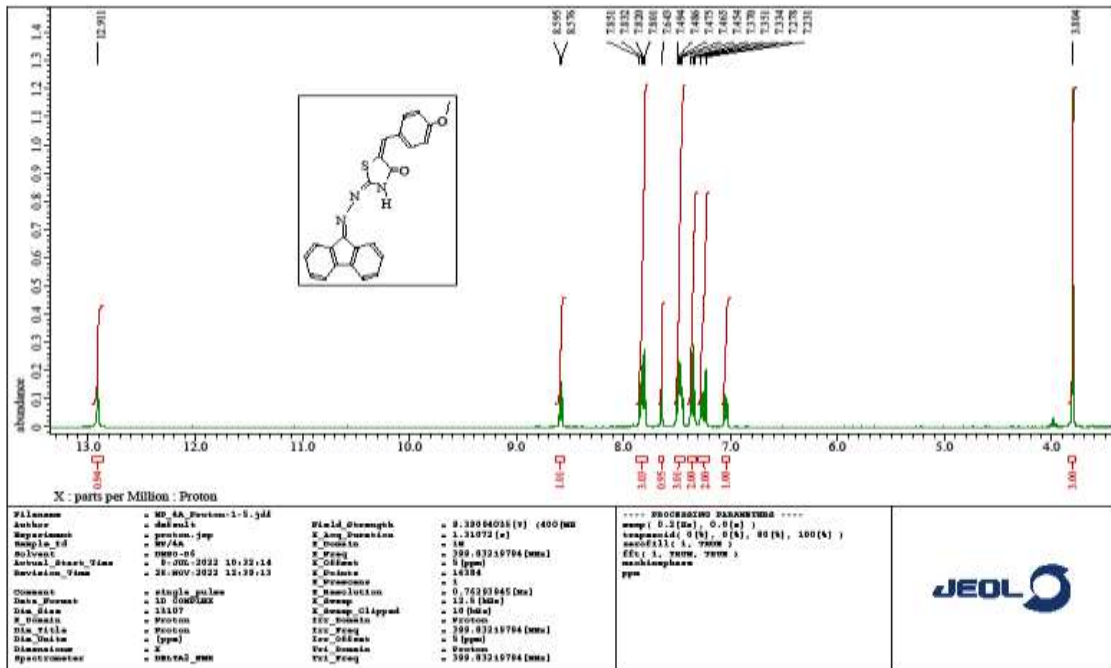
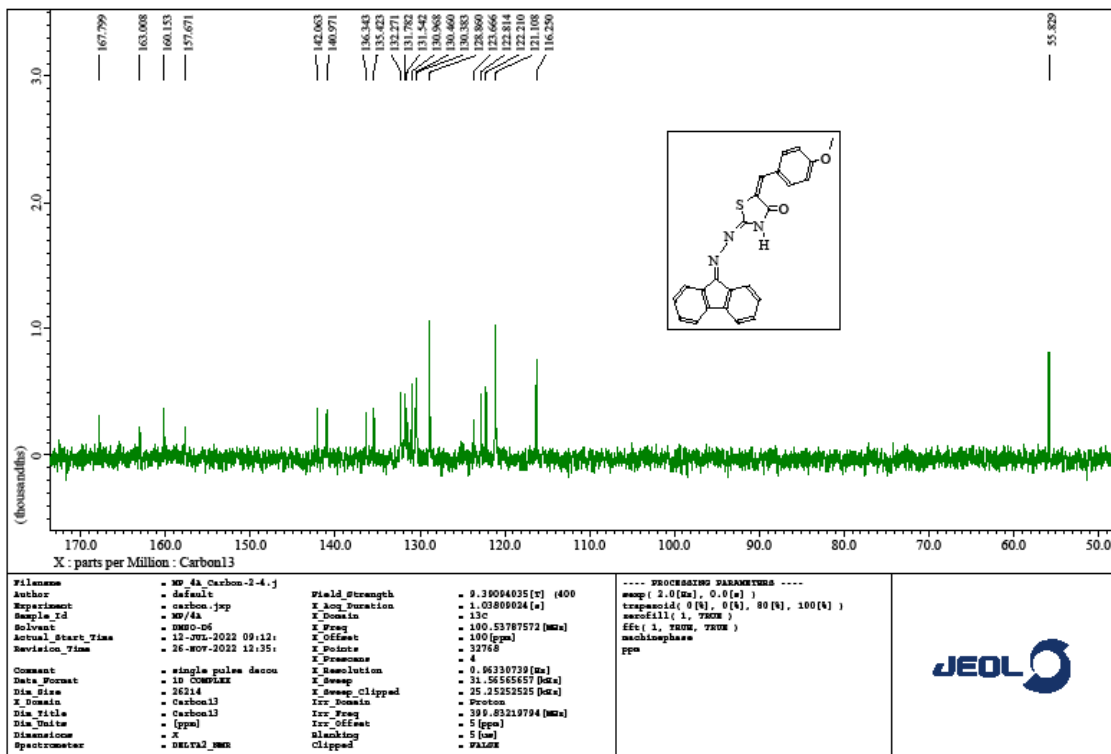


Fig.S6. Mass spectra of compound 5a



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Fig.S7. ^1H spectra of compound 5a



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Fig.S8. ^{13}C spectra of compound 5a

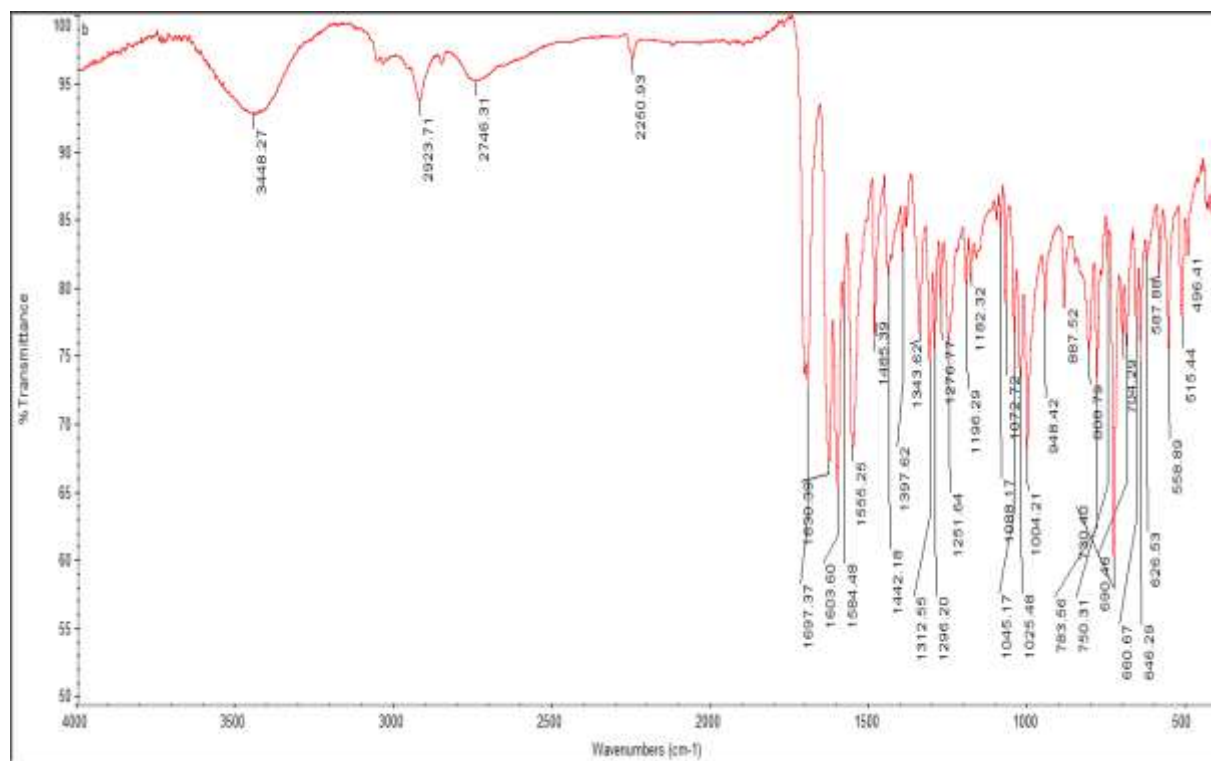


Fig.S9. FT-IR spectra of compound 5b

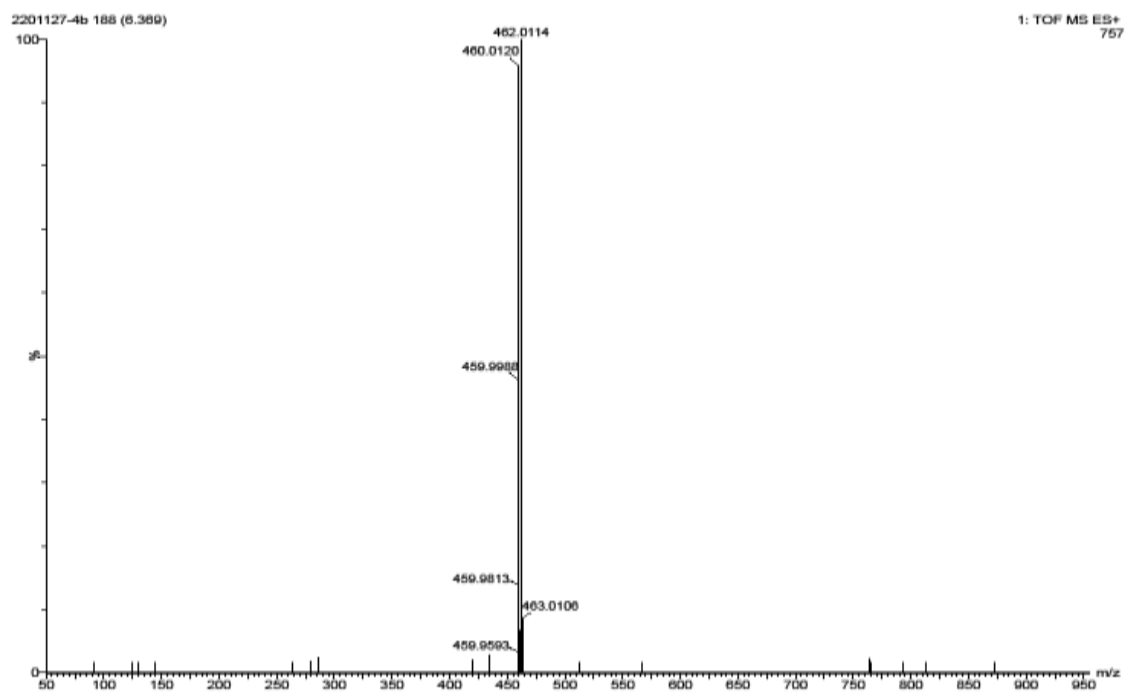


Fig.S10. Mass spectra of compound 5b

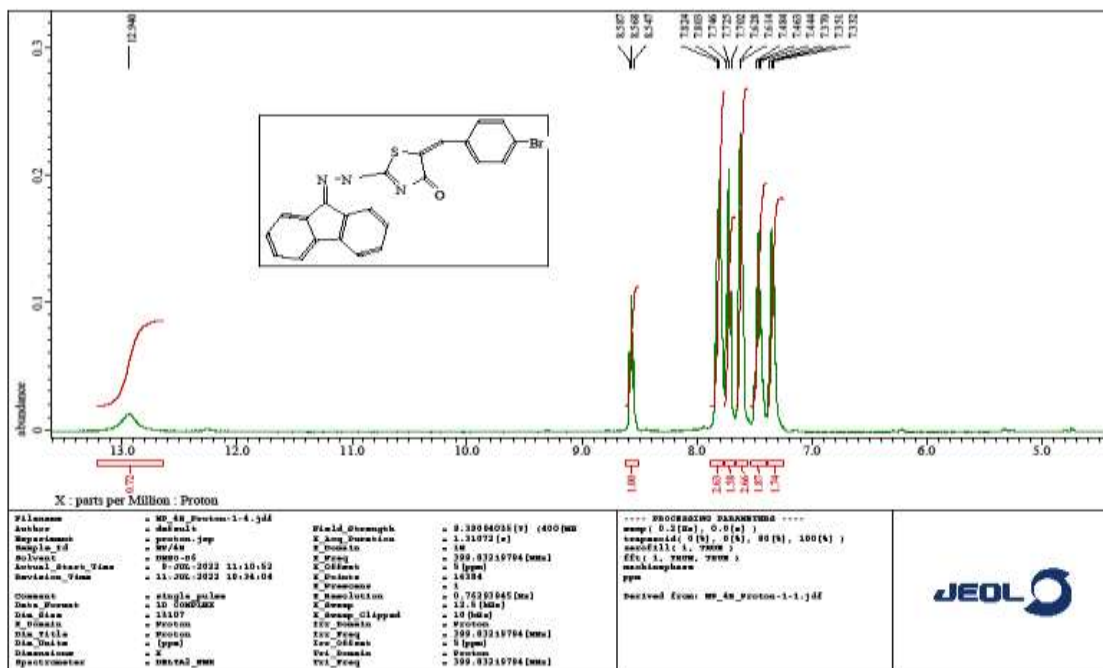


Fig.S11. ^1H spectra of compound 5b

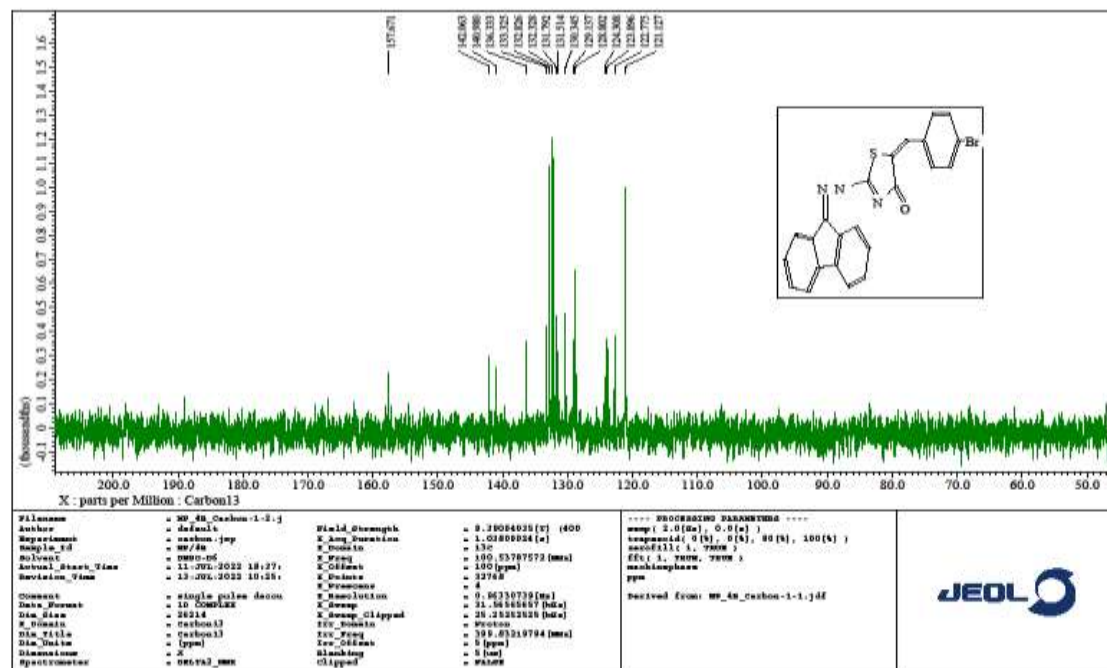


Fig.S12. ^{13}C spectra of compound 5b

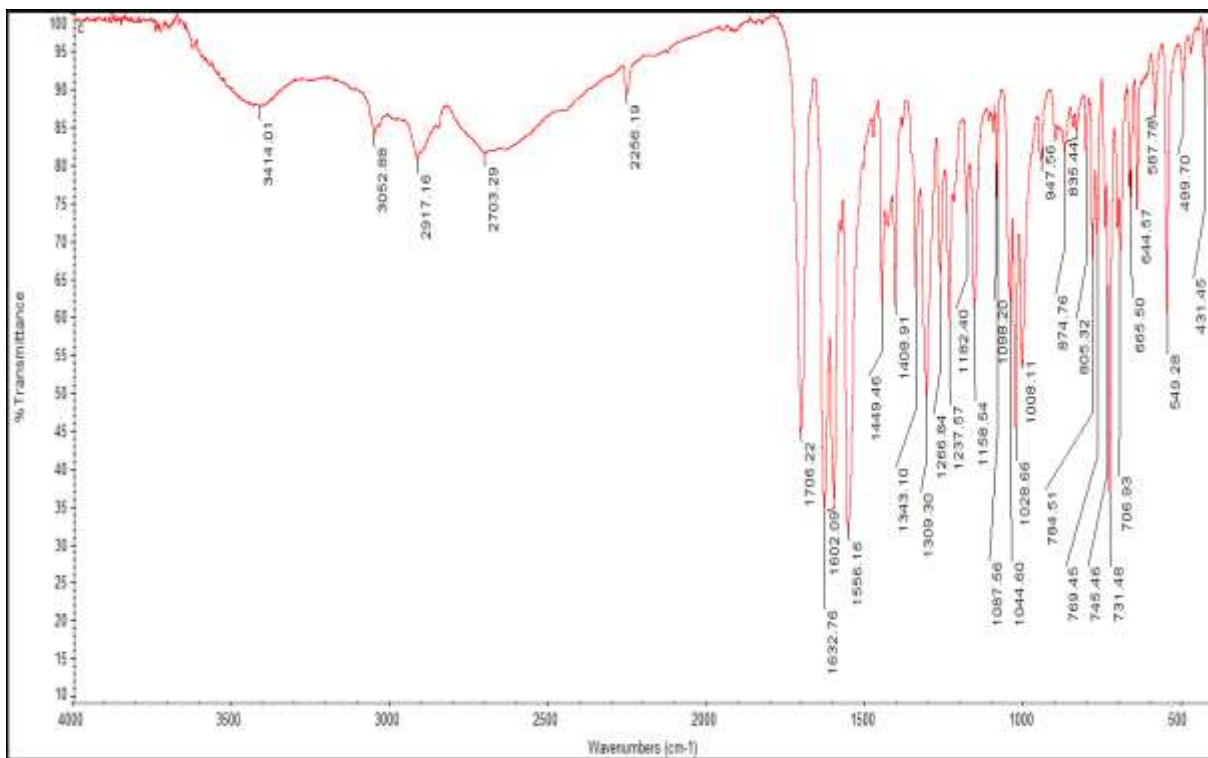


Fig.S13. FT-IR spectra of compound 5c

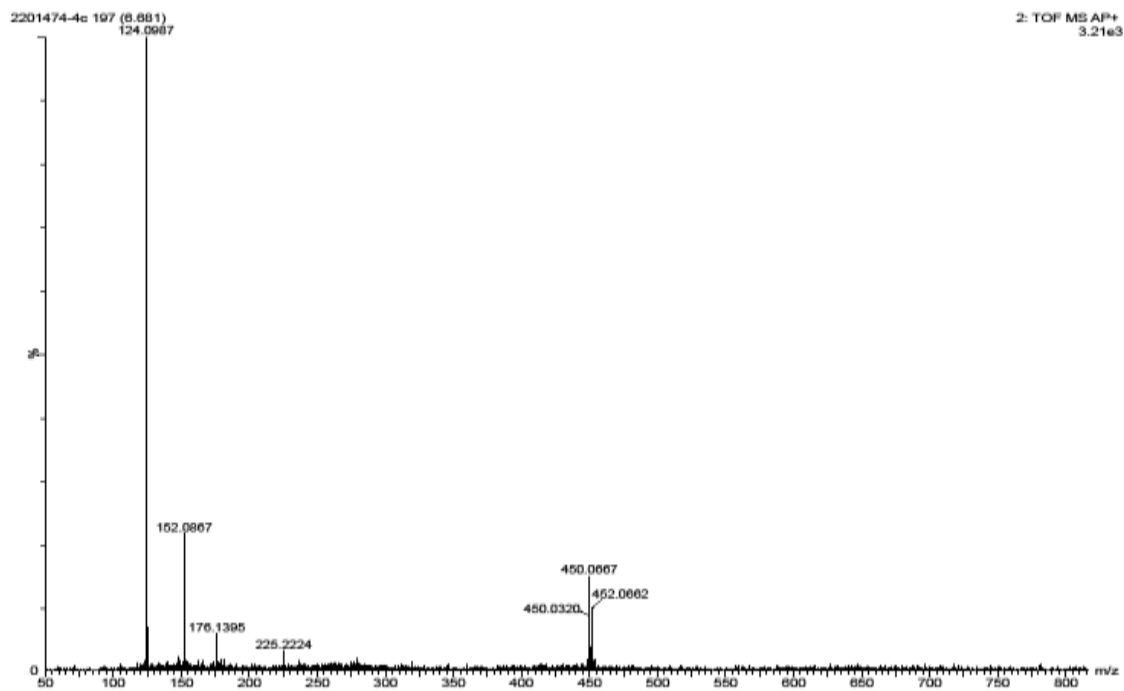
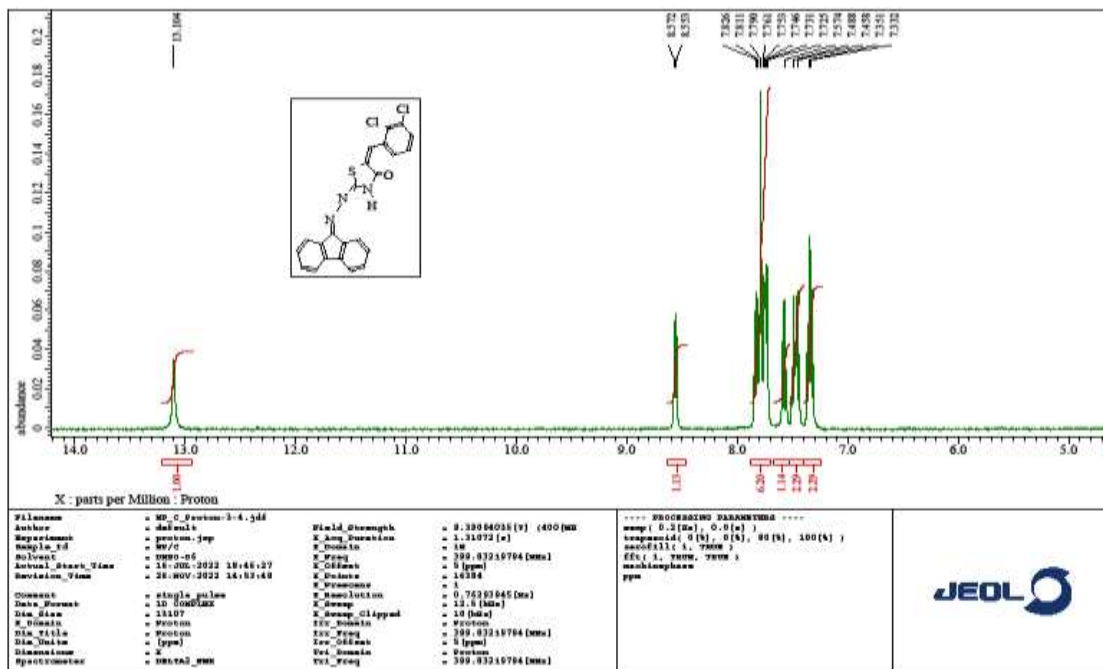
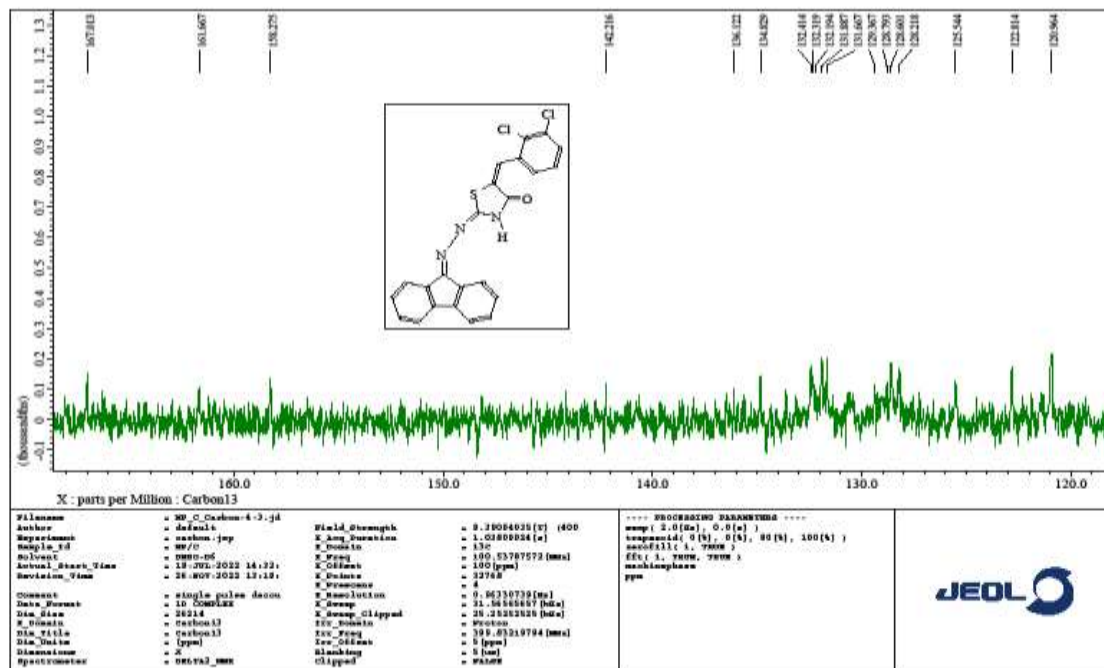


Fig.S14. Mass spectra of compound 5c



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Fig.S15. ¹H spectra of compound 5C



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Fig.S16. ¹³C spectra of compound 5C

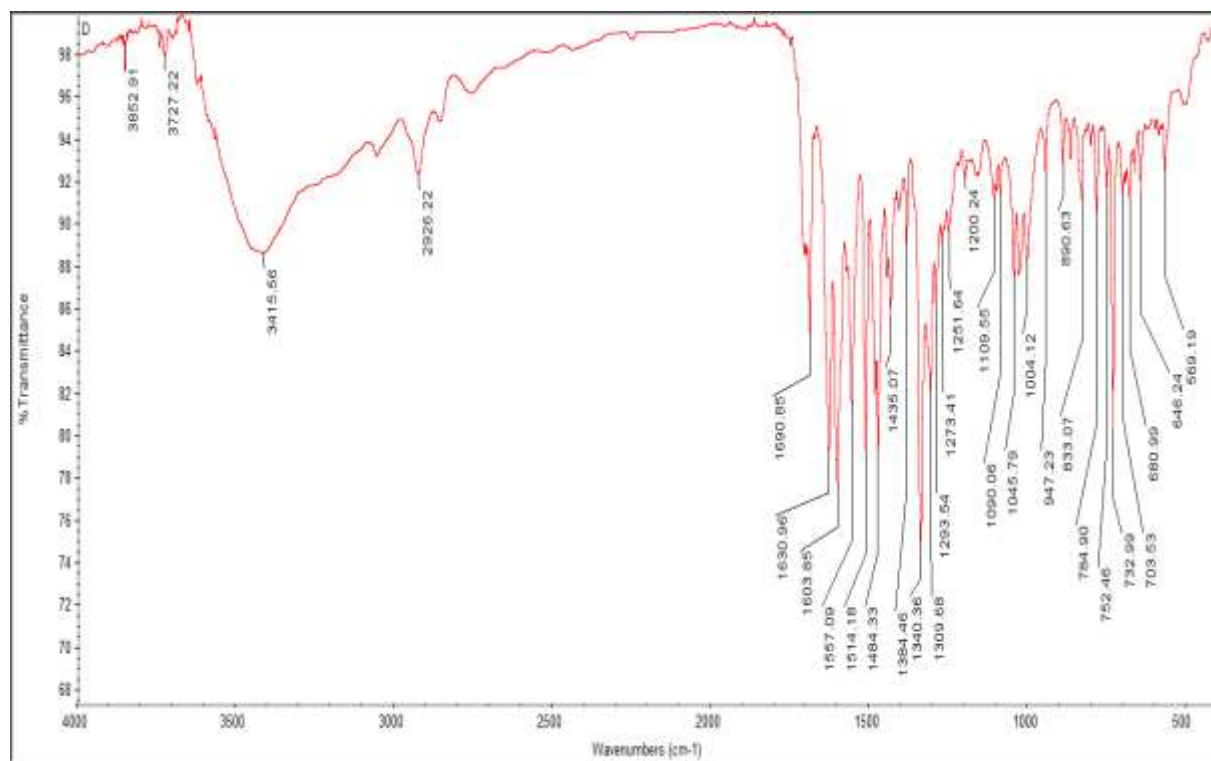


Fig.S17. FT-IR spectra of compound 5d

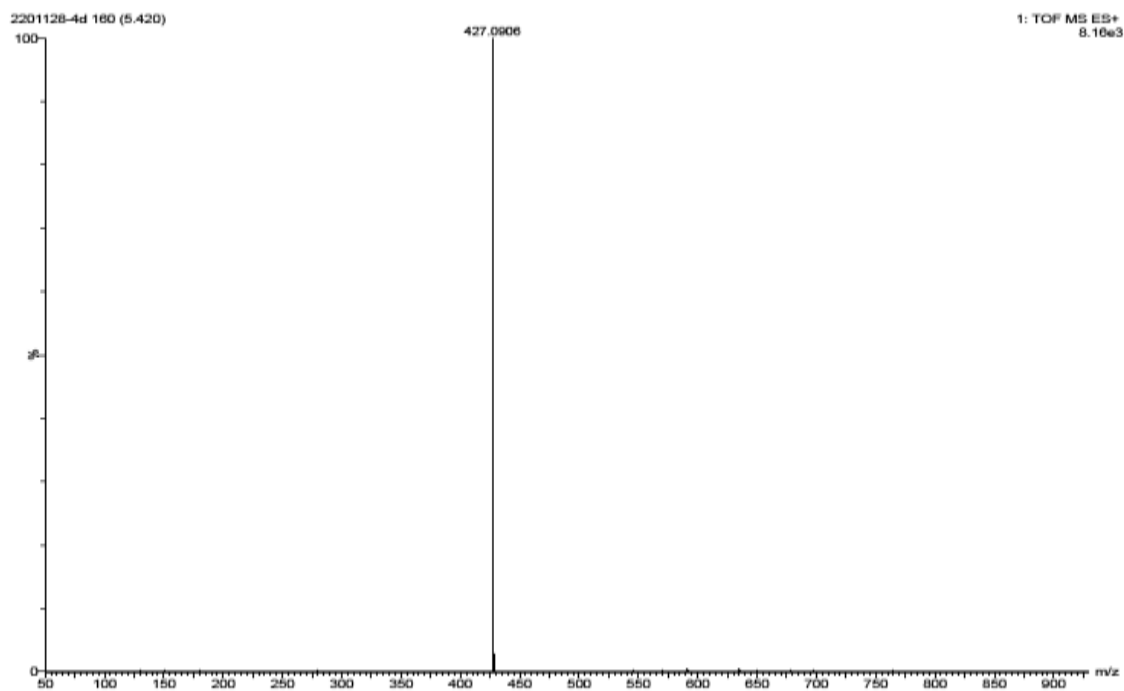
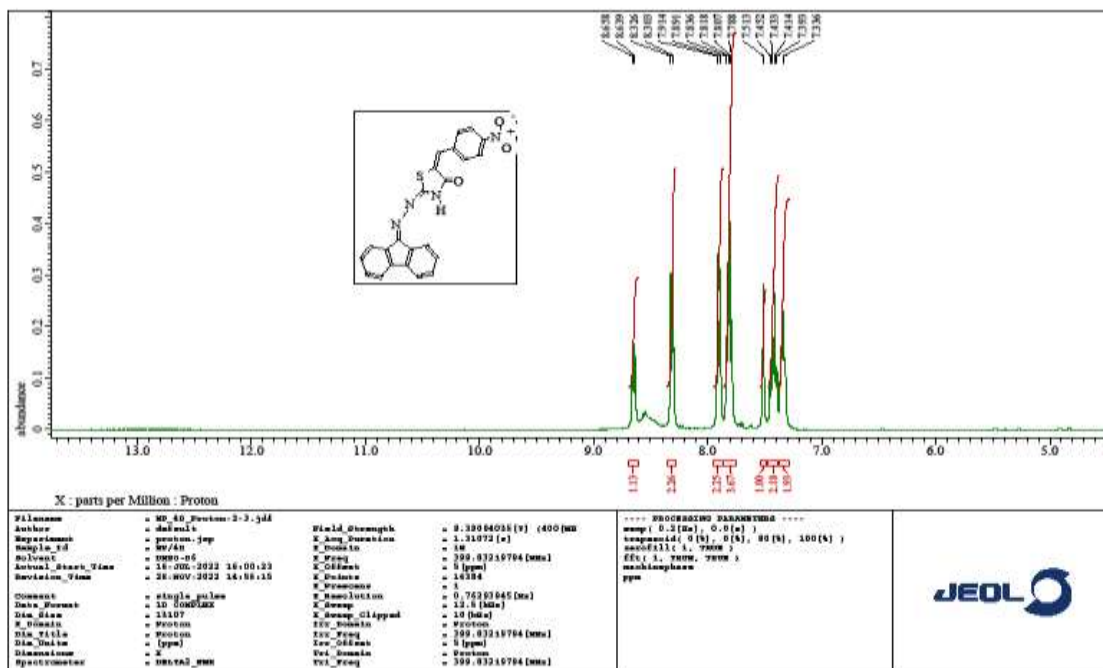
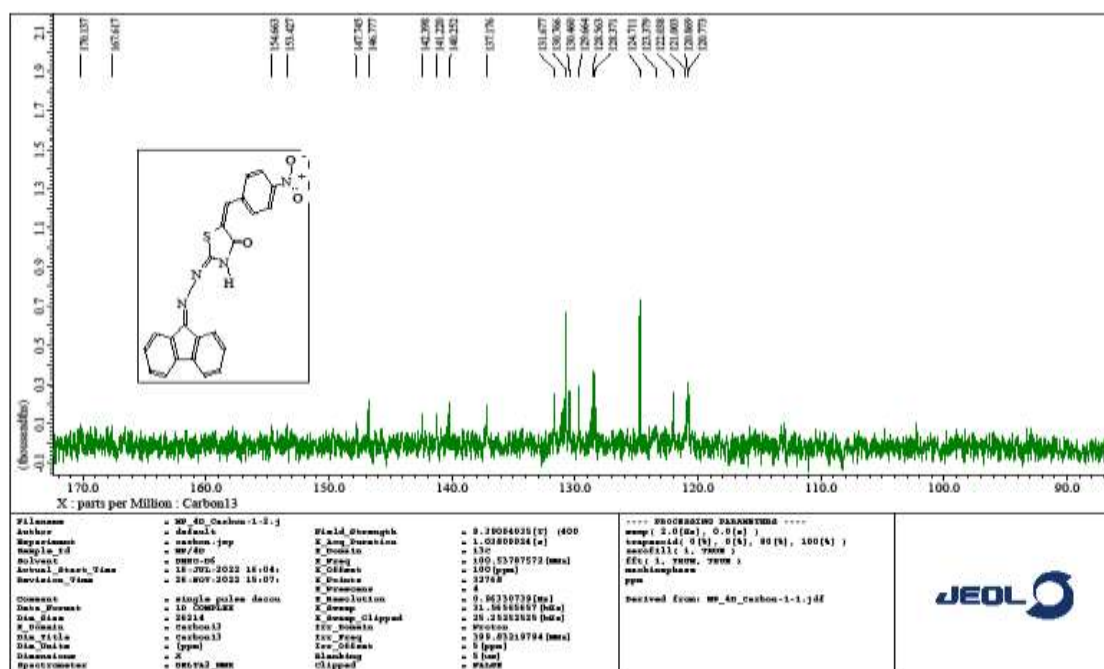


Fig.S18. Mass spectra of compound 5d



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Fig.S19. ¹H spectra of compound 5d



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Fig.S20. ¹³C spectra of compound 5d

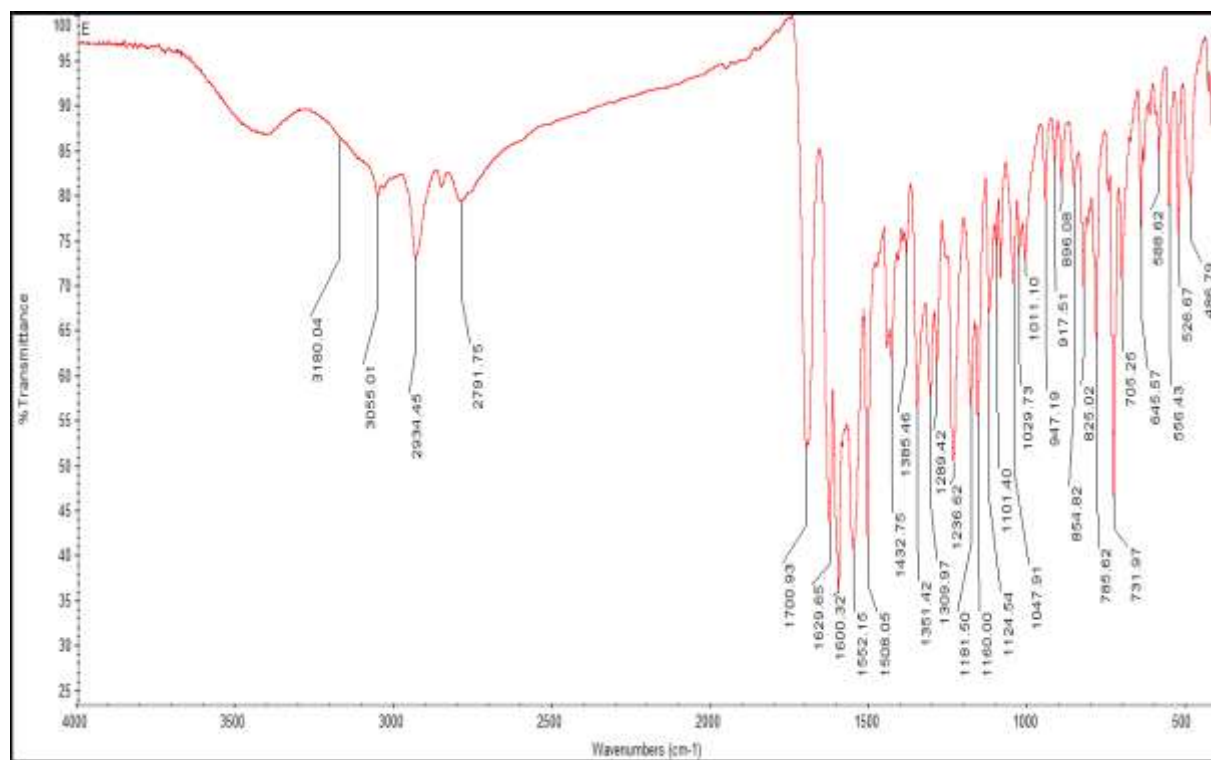


Fig.S21. FT-IR spectra of compound 5e

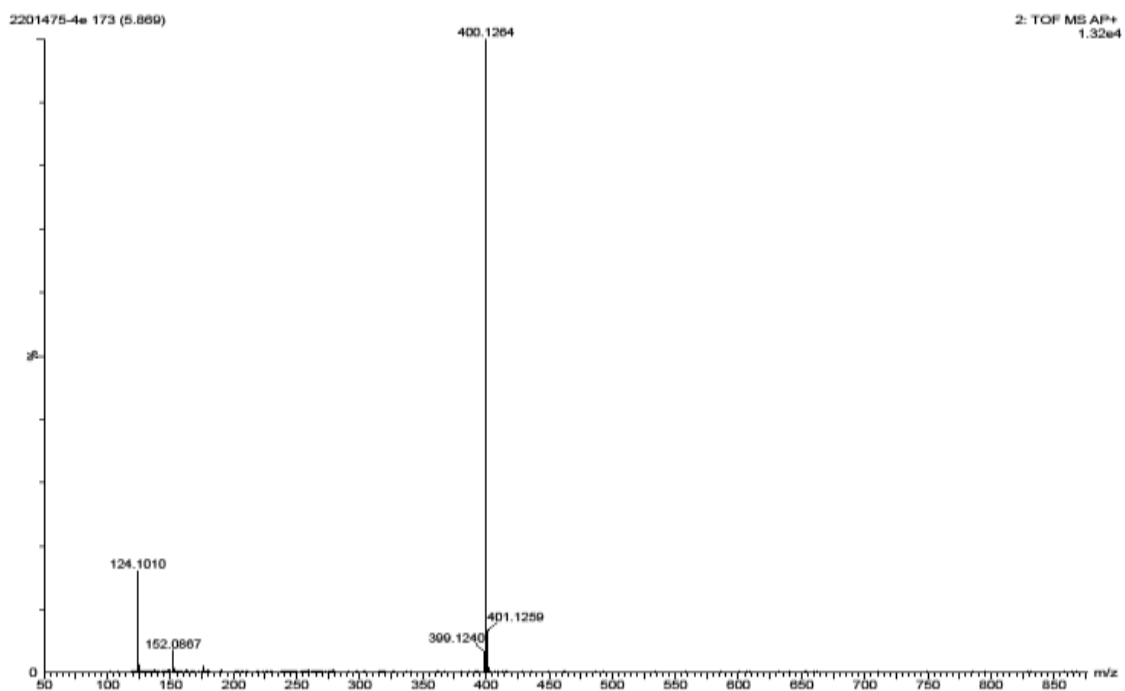
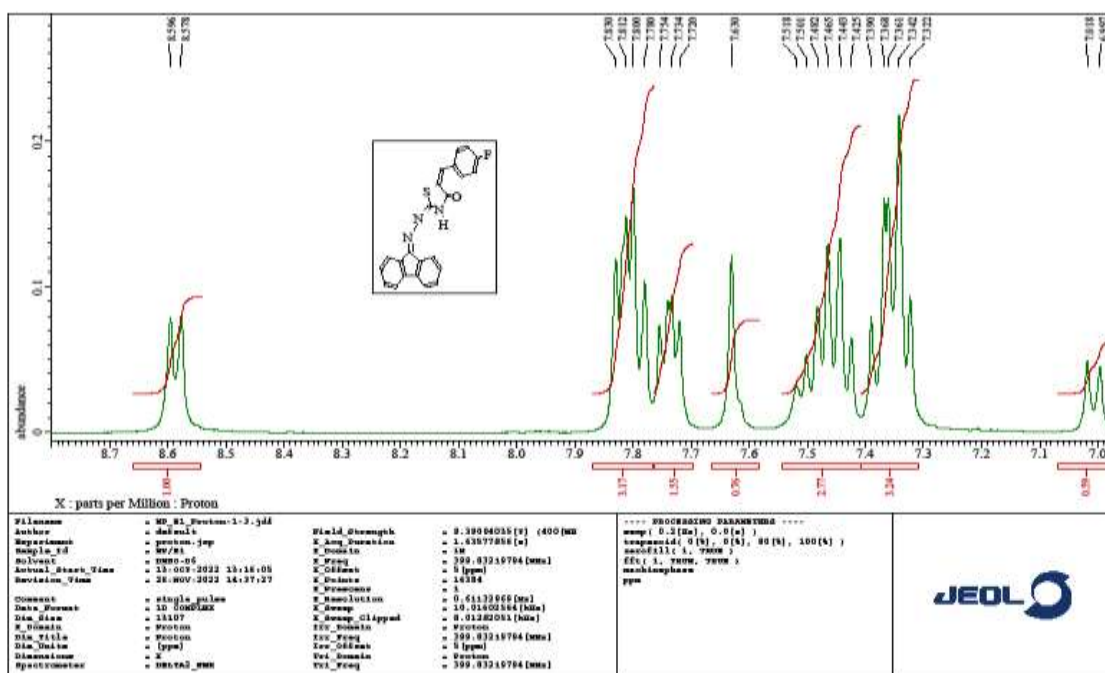
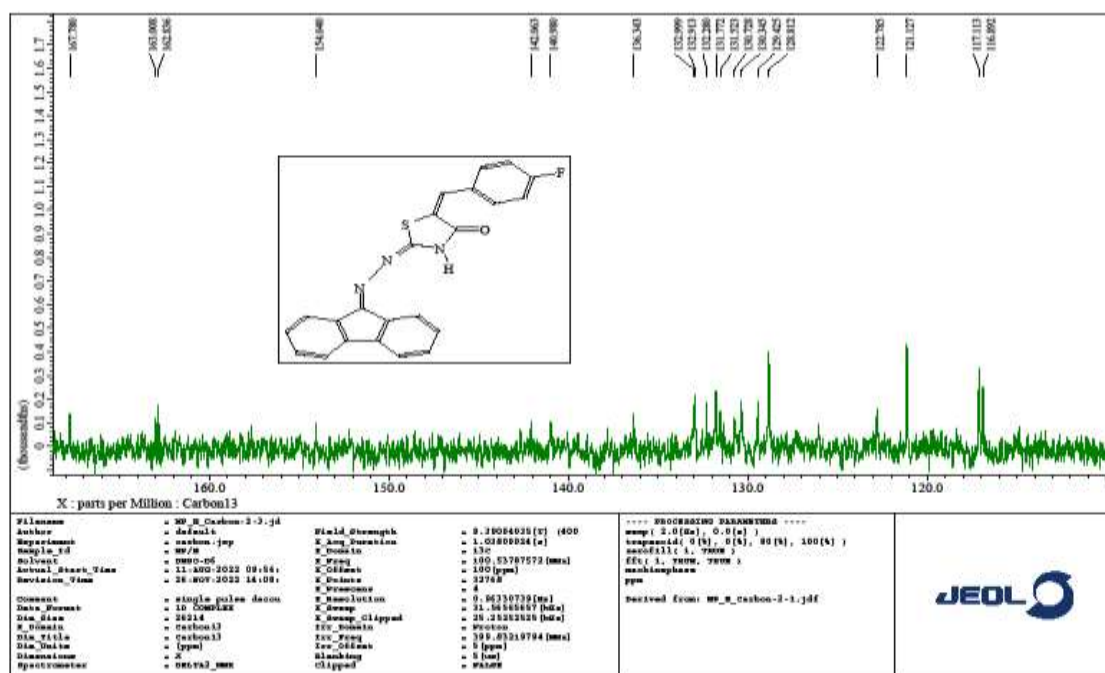


Fig.S22. Mass spectra of compound 5e



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Fig.S23. ¹H spectra of compound 5e



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Fig.S24. ¹³C spectra of compound 5e

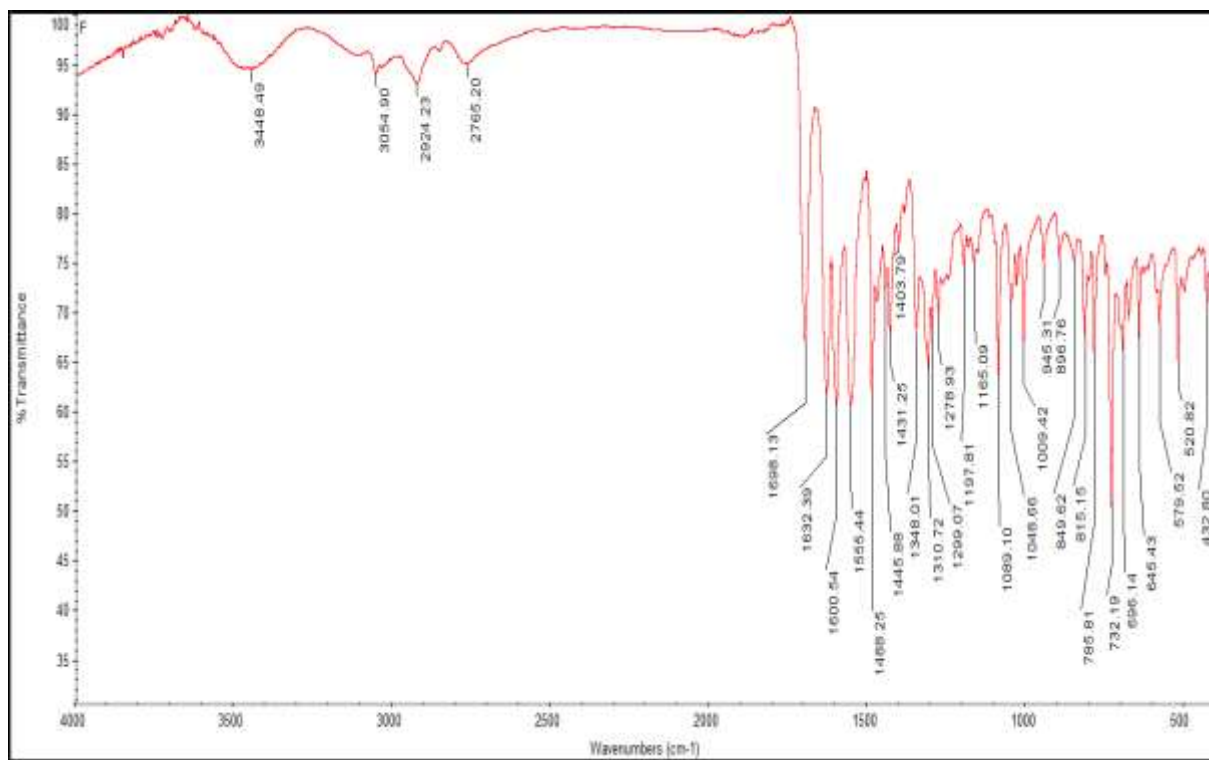


Fig.S25. FT-IR spectra of compound 5f

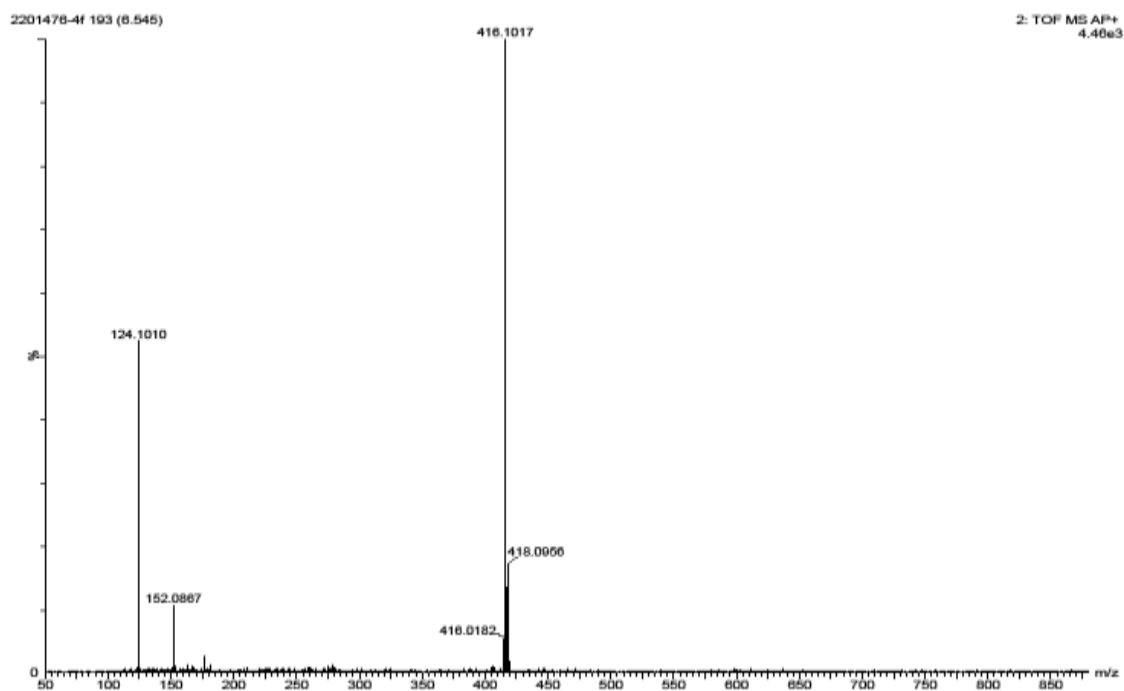
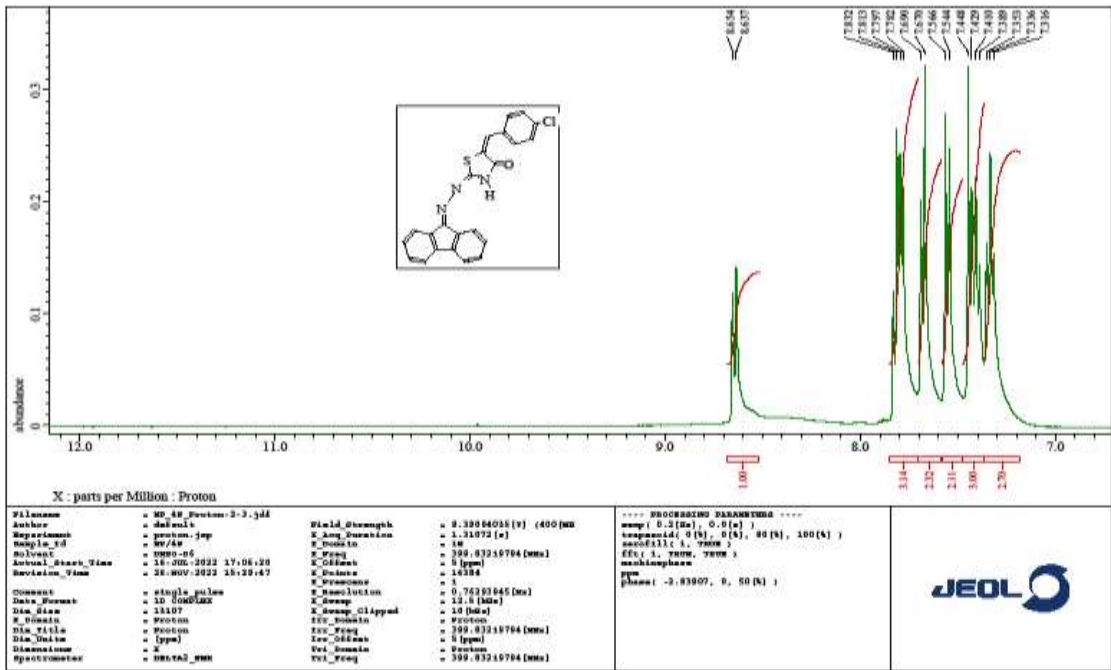
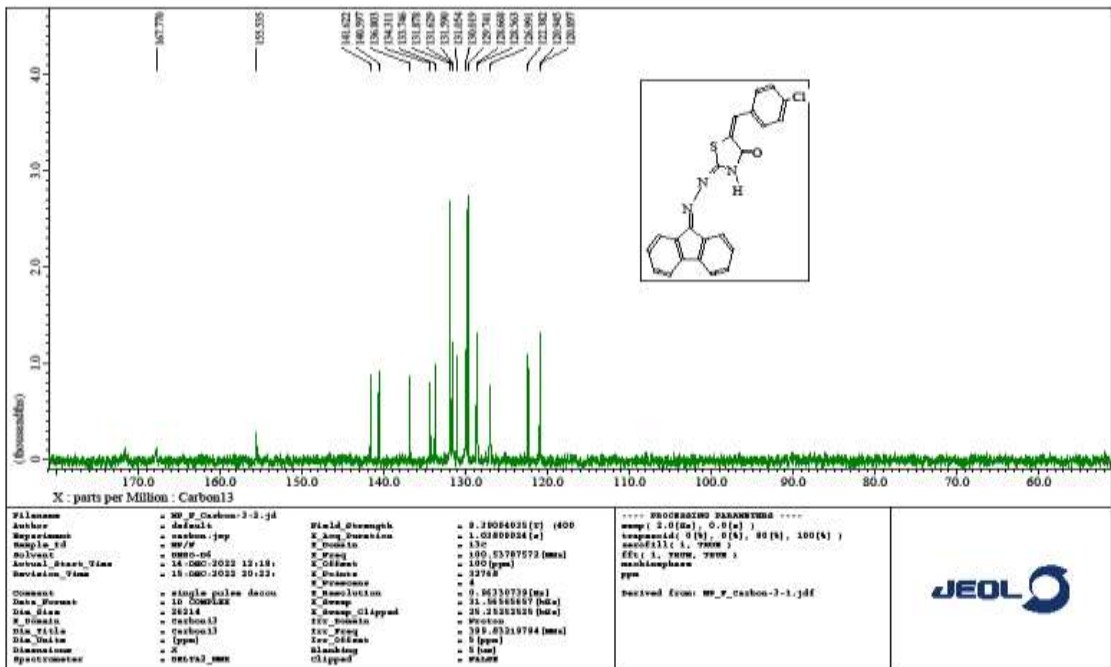


Fig.S26. Mass spectra of compound 5f



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Fig.S27: ¹H spectra of compound 5f



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Fig.S28: ¹³C spectra of compound 5f

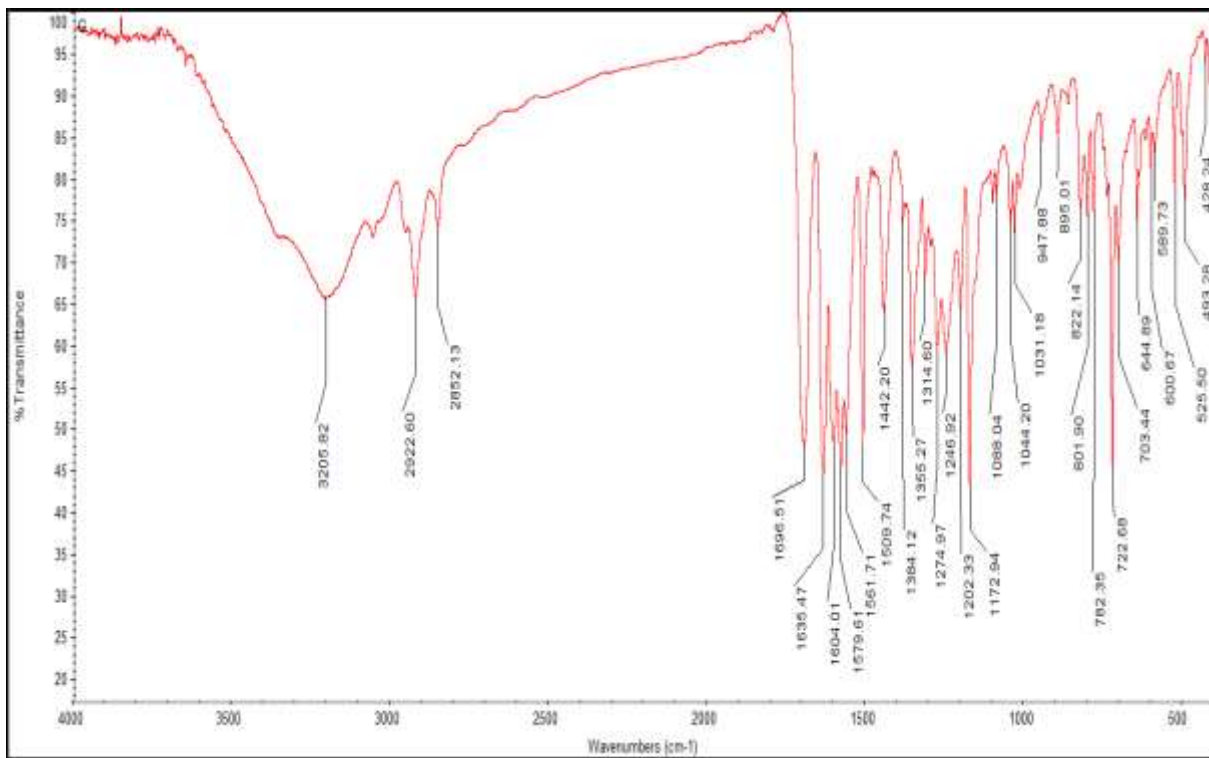


Fig.S29. FT-IR spectra of compound 5g

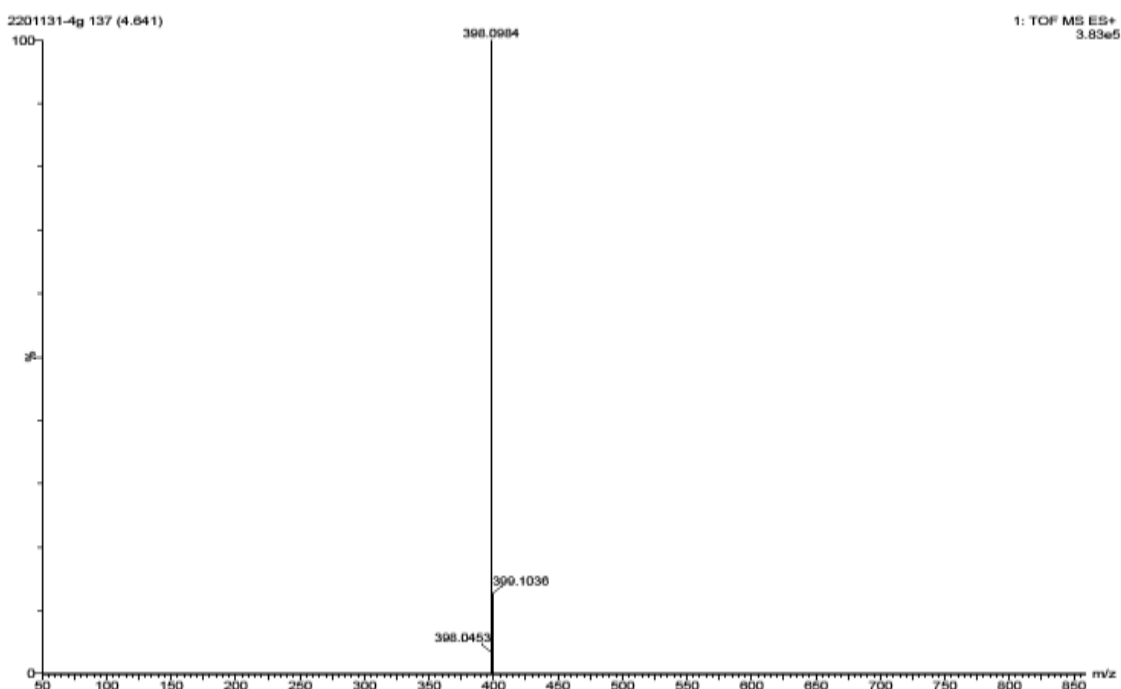
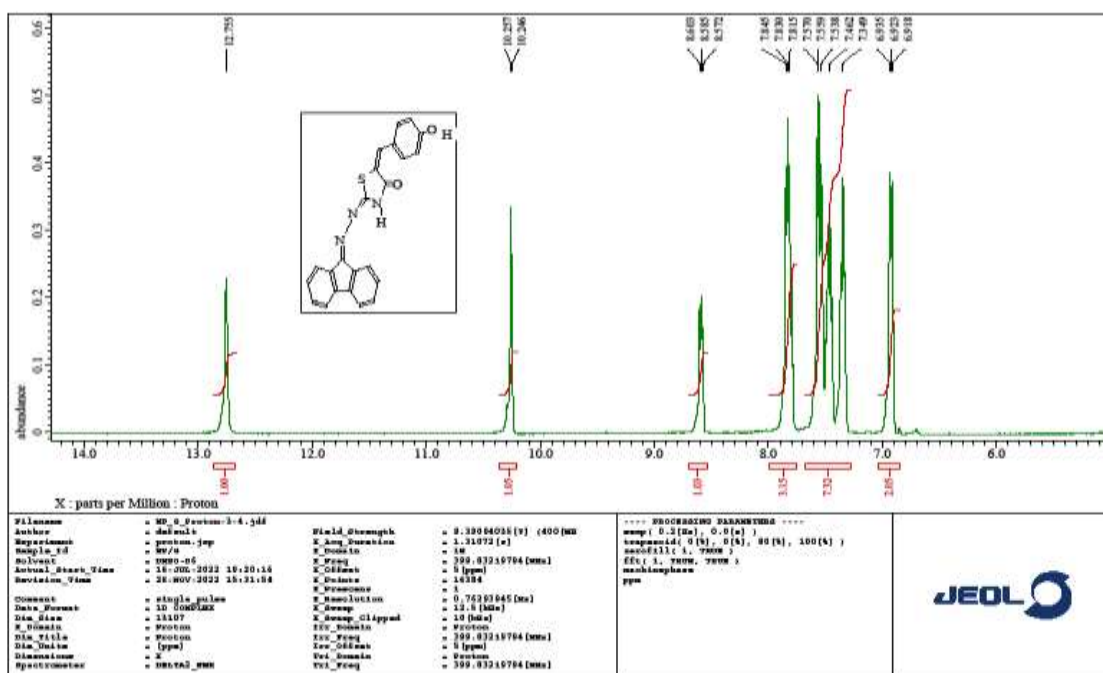
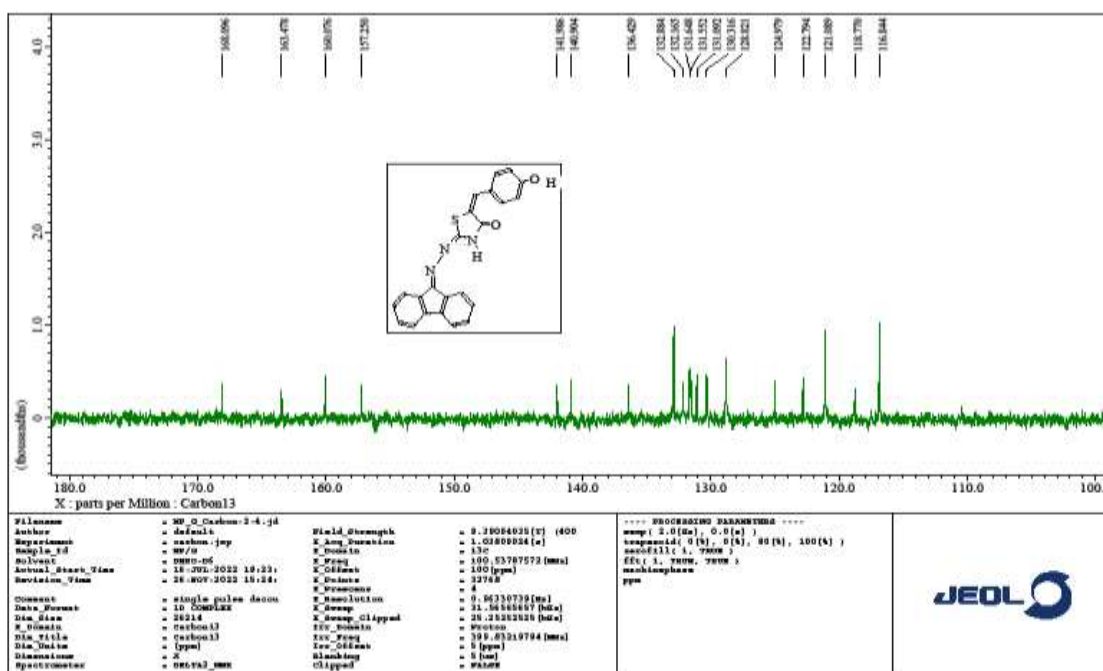


Fig.S30. Mass spectra of compound 5g



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Fig.S31. ^1H spectra of compound 5g



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Fig.S32. ^{13}C spectra of compound 5g

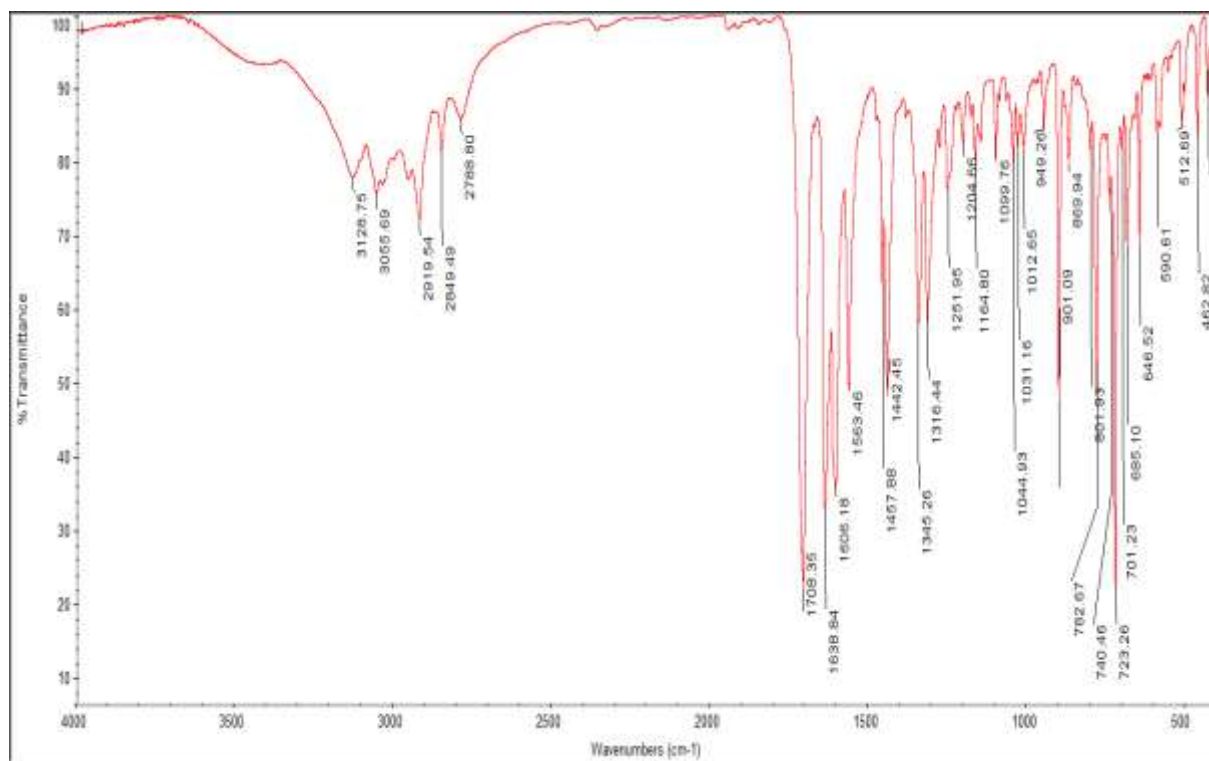


Fig.S33. FT-IR spectra of compound 5i

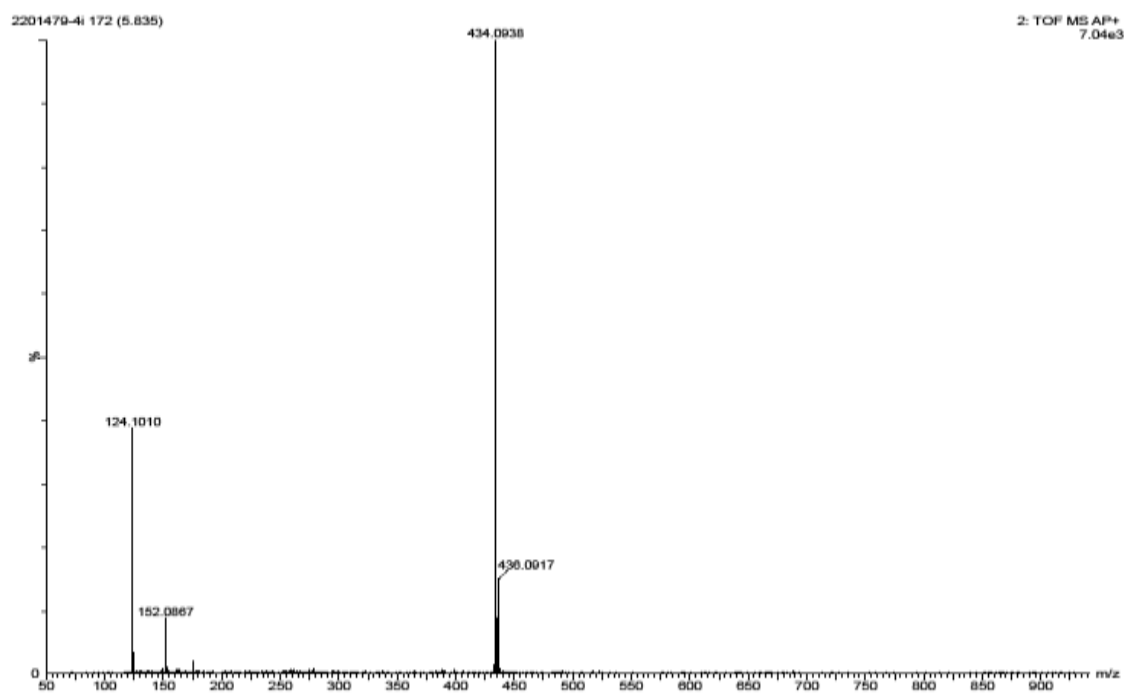
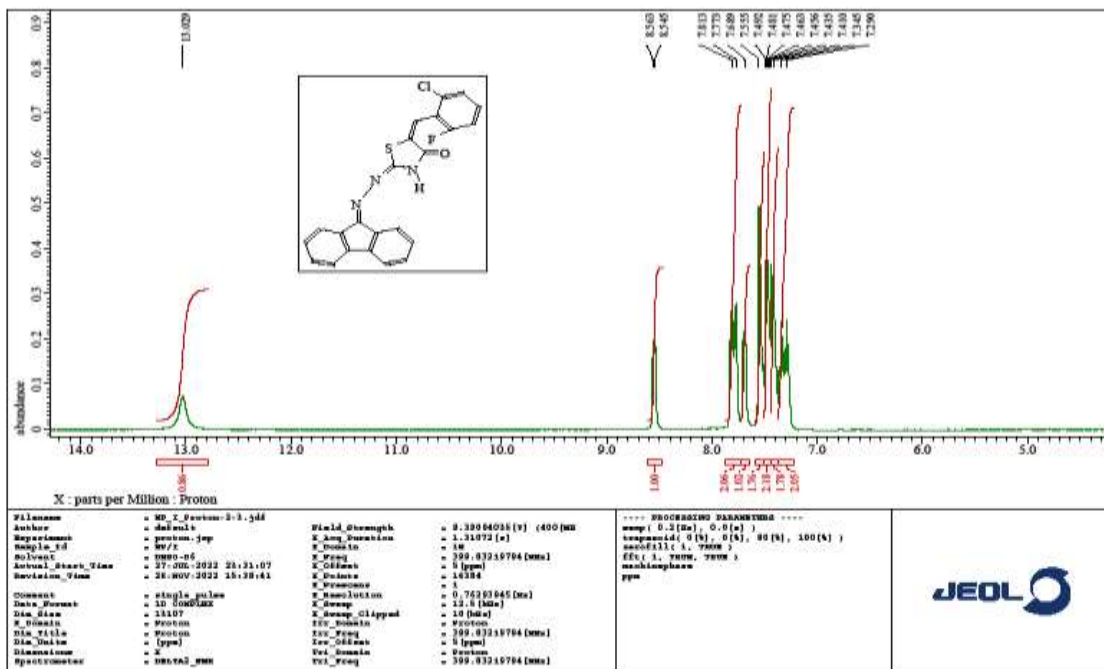
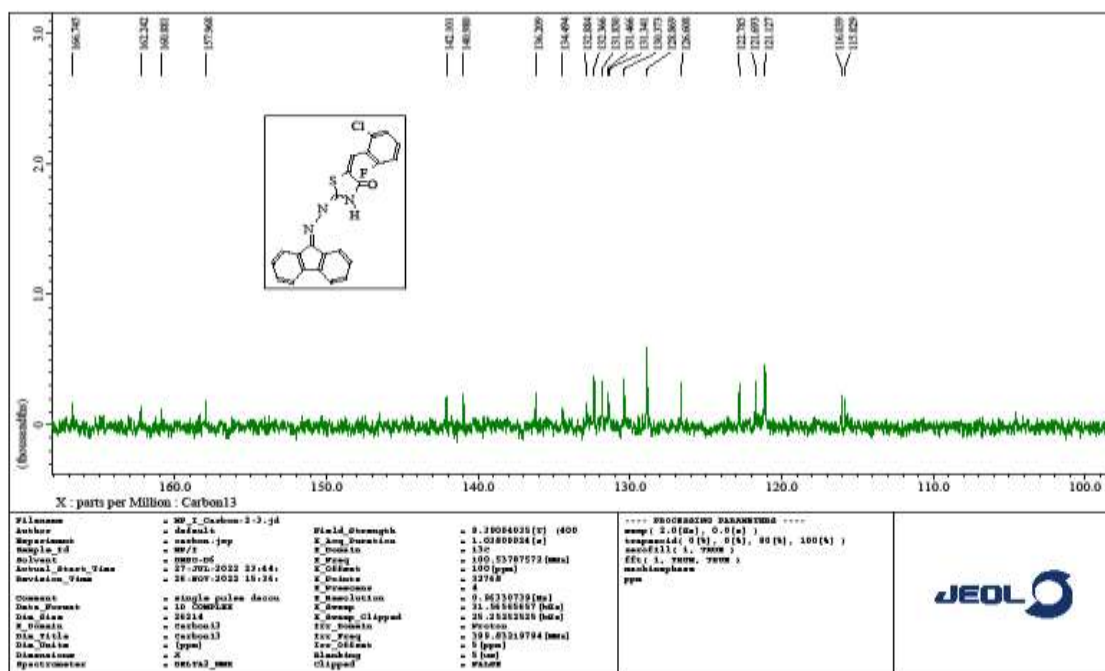


Fig.S34. Mass spectra of compound 5i



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Fig.S35. ^1H spectra of compound 5i



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Fig.S36. ^{13}C spectra of compound 5i

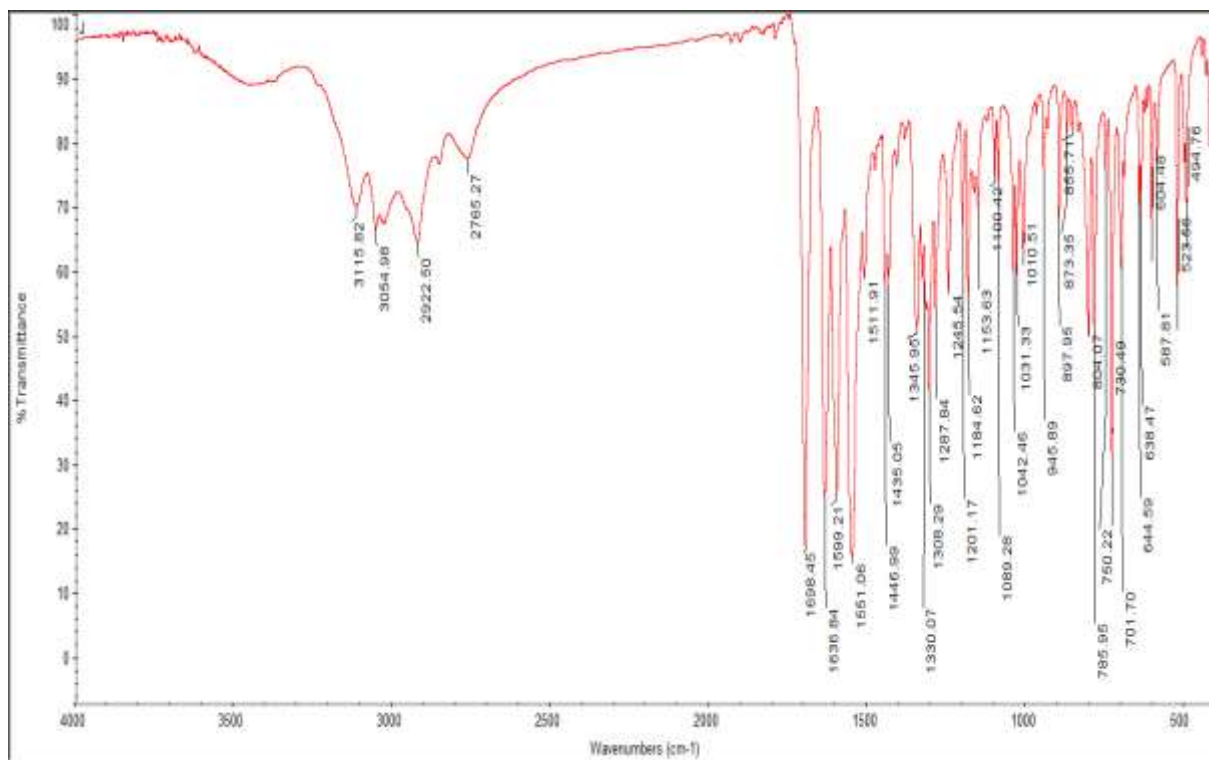


Fig.S37. FT-IR spectra of compound 5j

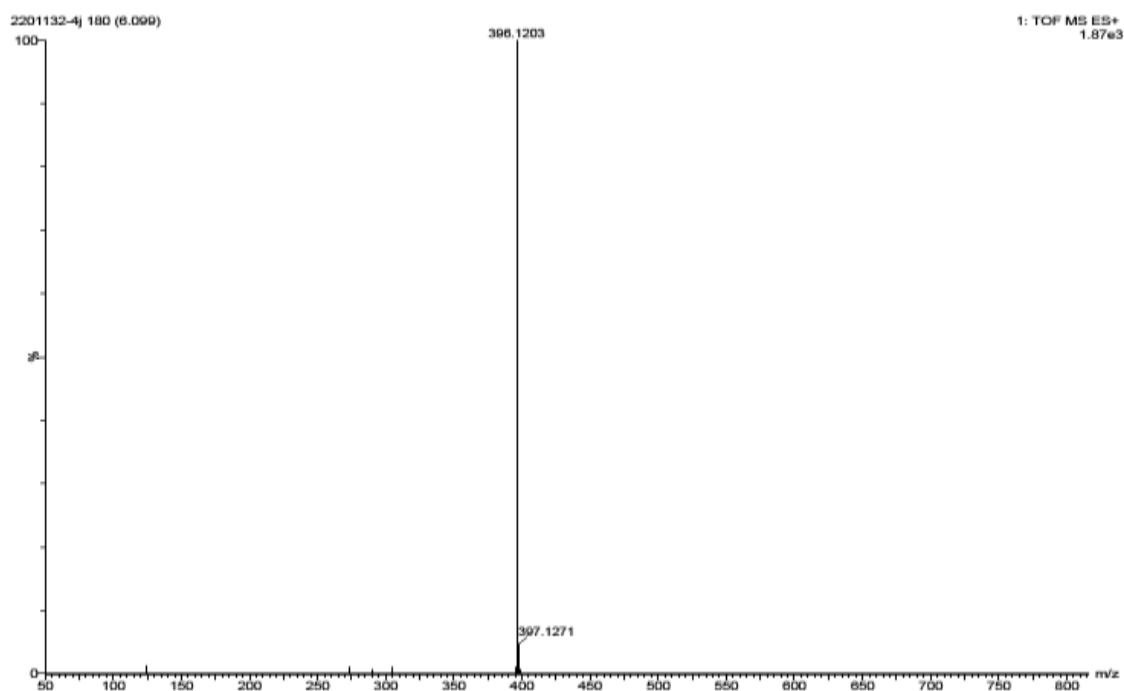
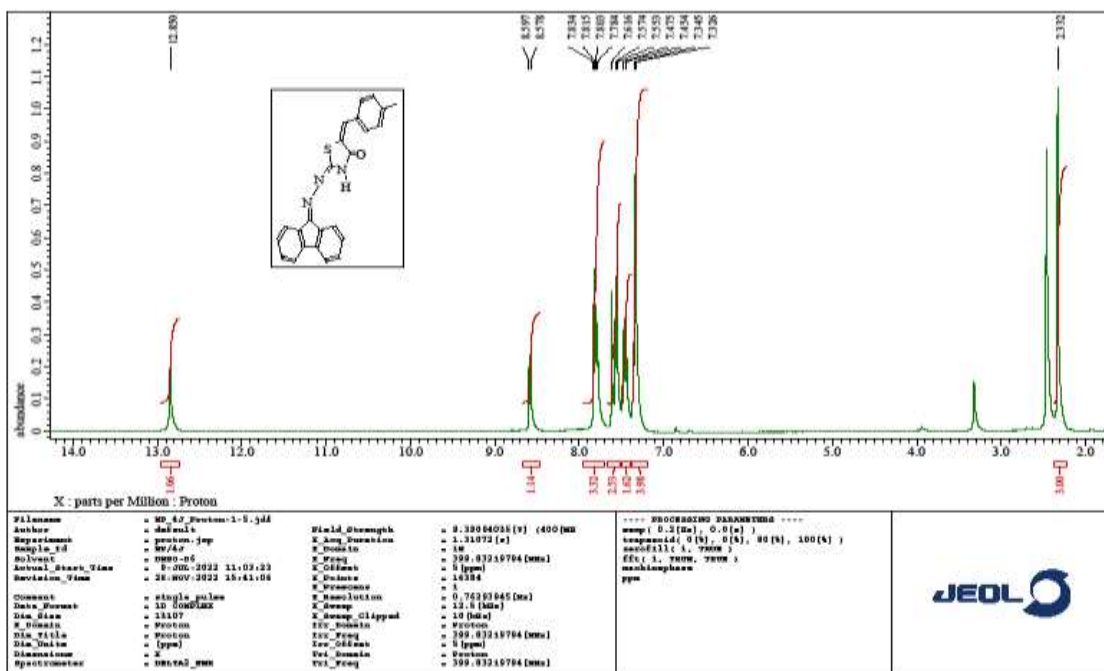
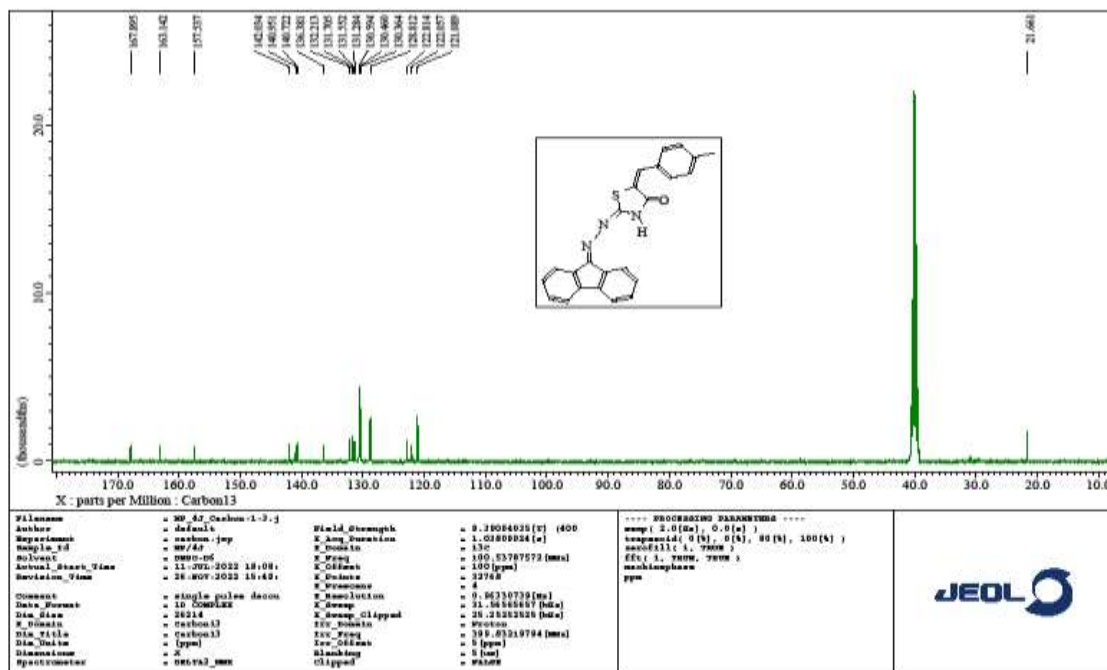


Fig.S38. Mass spectra of compound 5j



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Fig.S39. ^1H spectra of compound 5j



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Fig.S40. ^{13}C spectra of compound 5j

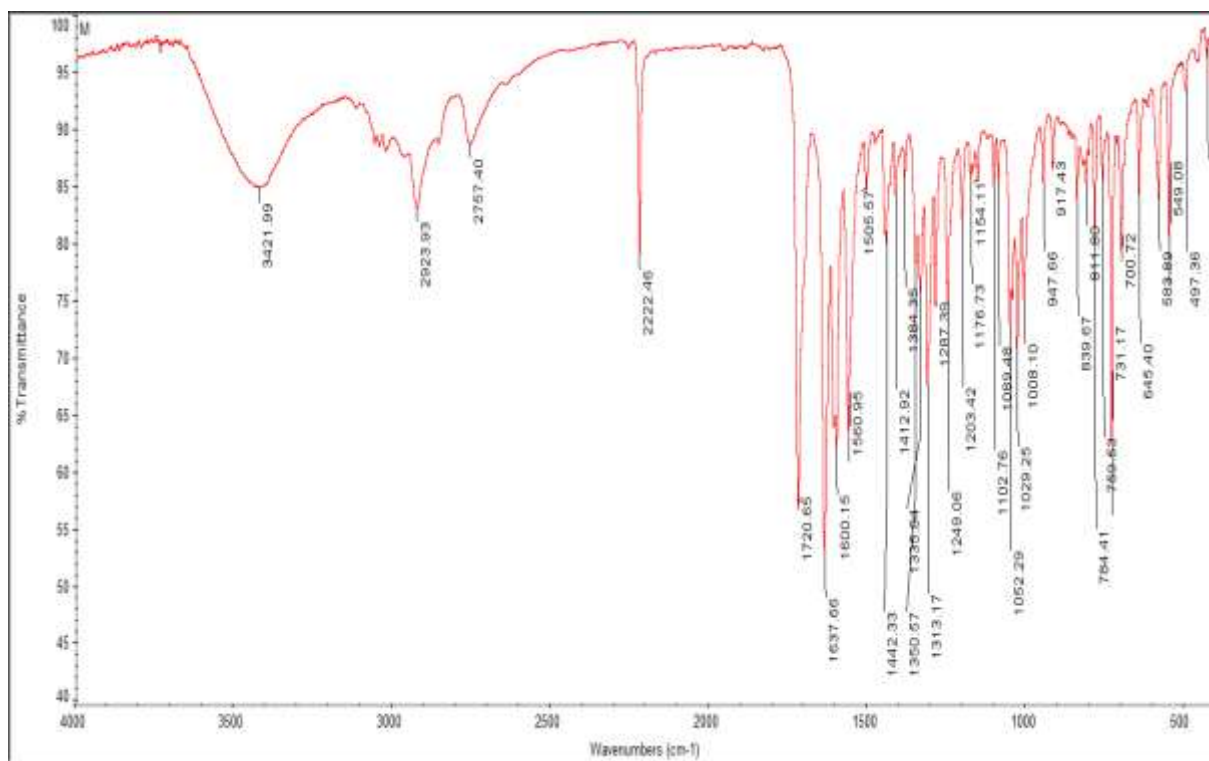


Fig.S41. FT-IR spectra of compound 5k

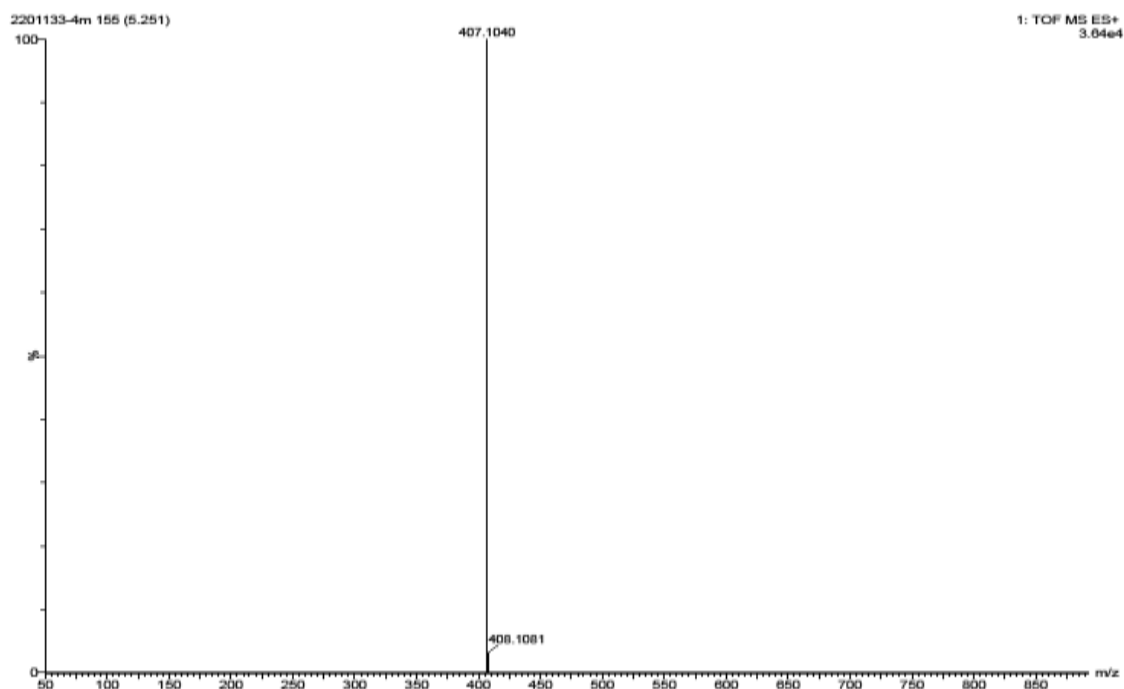
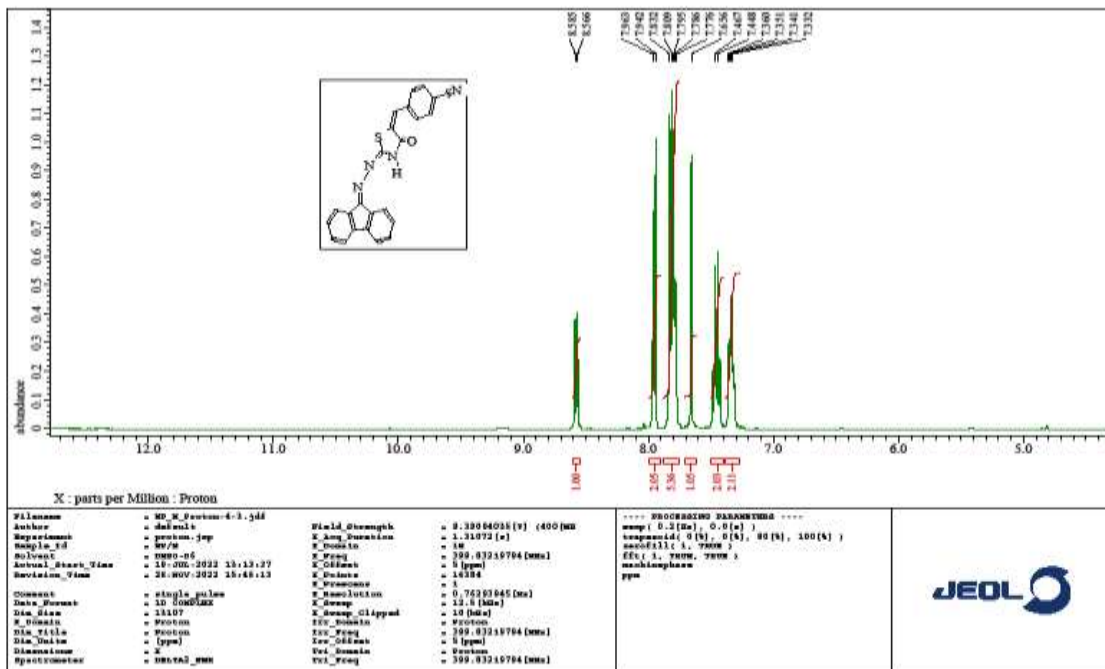
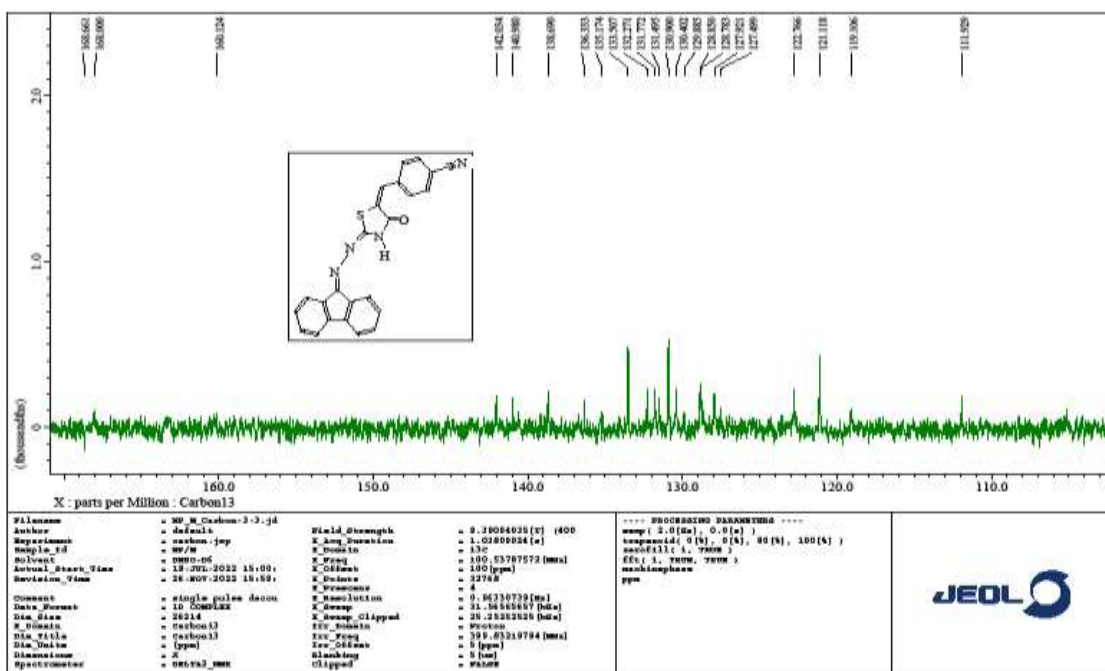


Fig.S42. Mass spectra of compound 5k



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Fig.S43. ^1H spectra of compound 5k



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Fig.S44. ^{13}C spectra of compound 5k

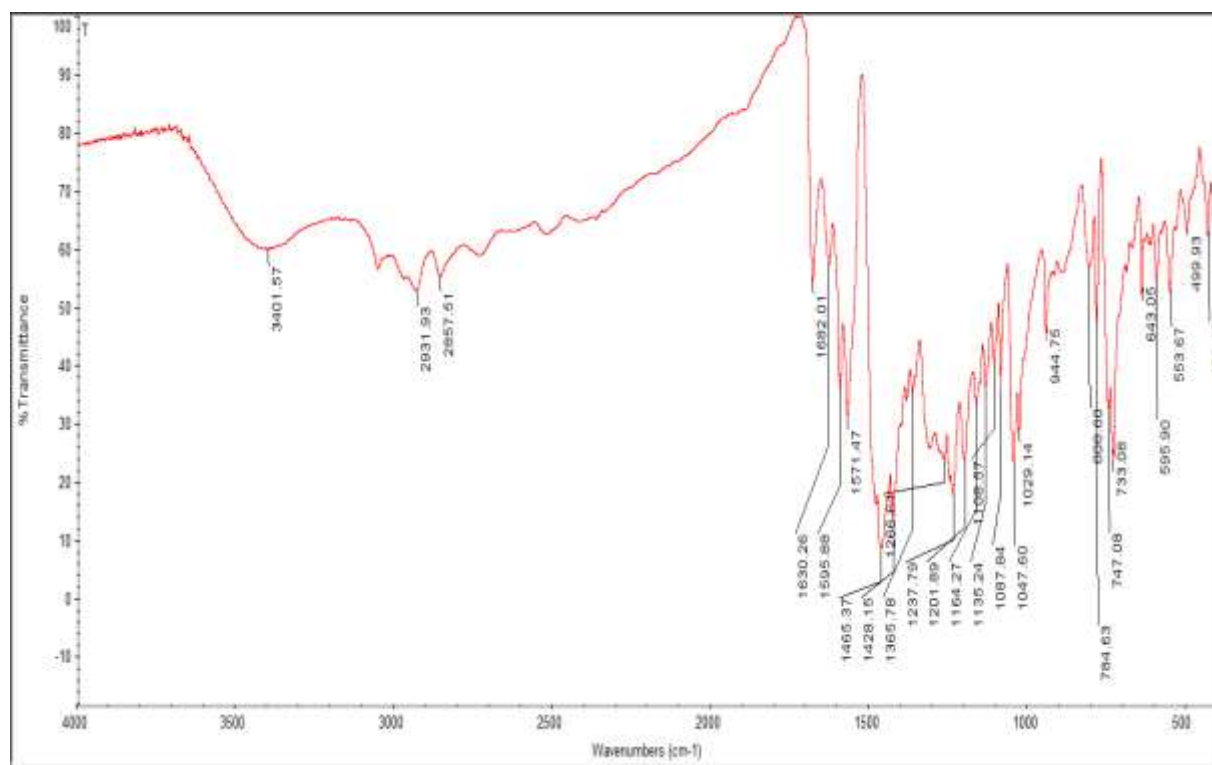


Fig.S45. FT-IR spectra of compound 5I

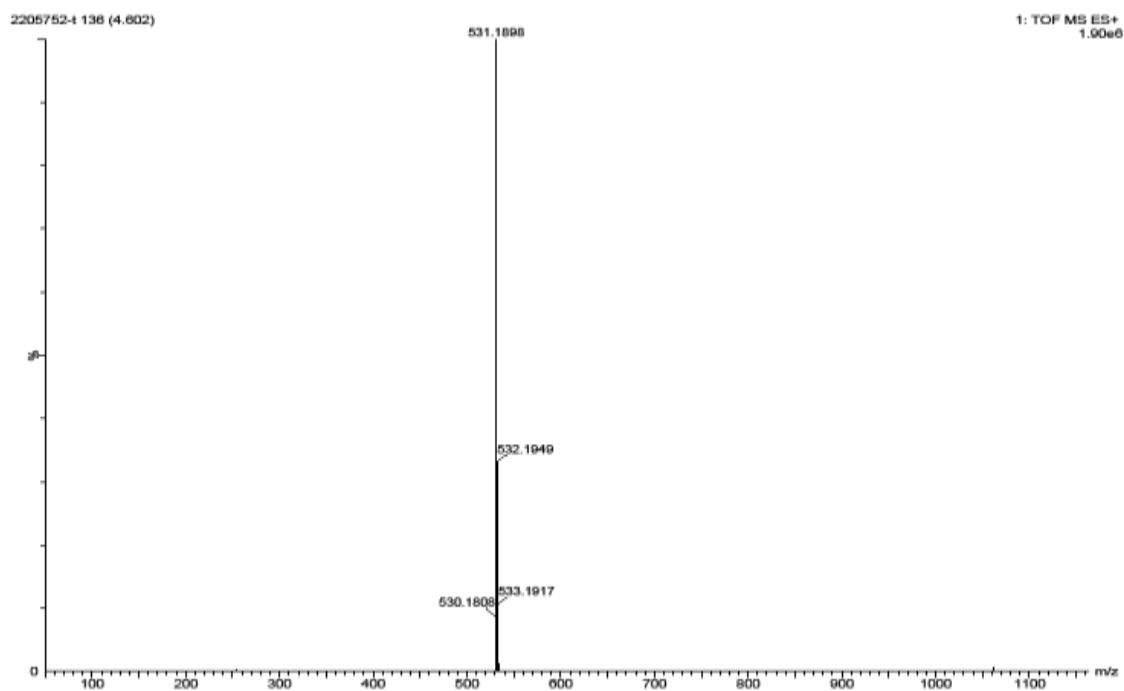


Fig.S46. Mass spectra of compound 5I

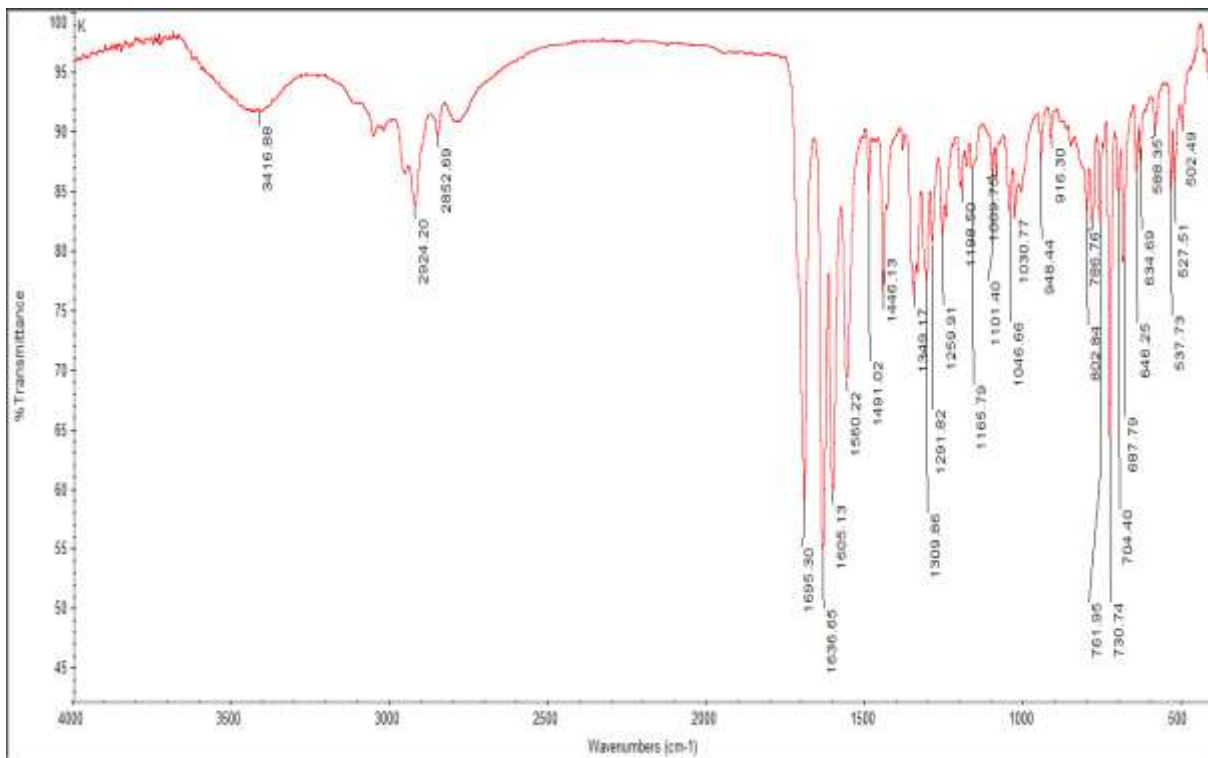


Fig.S49. FT-IR spectra of compound 5m

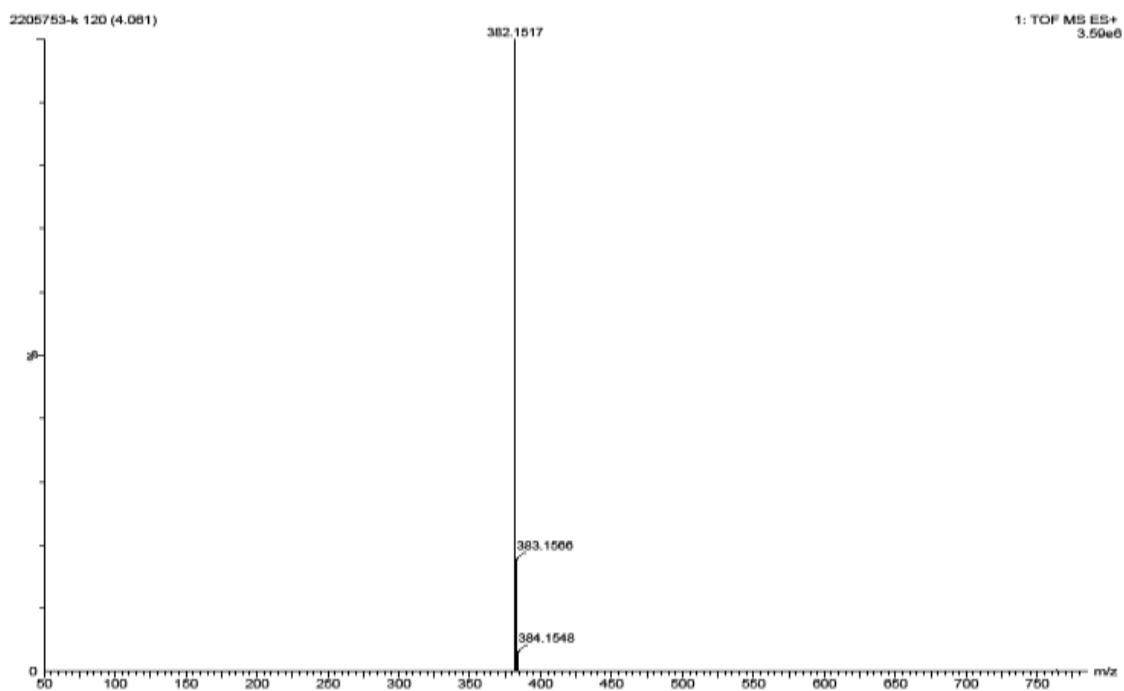
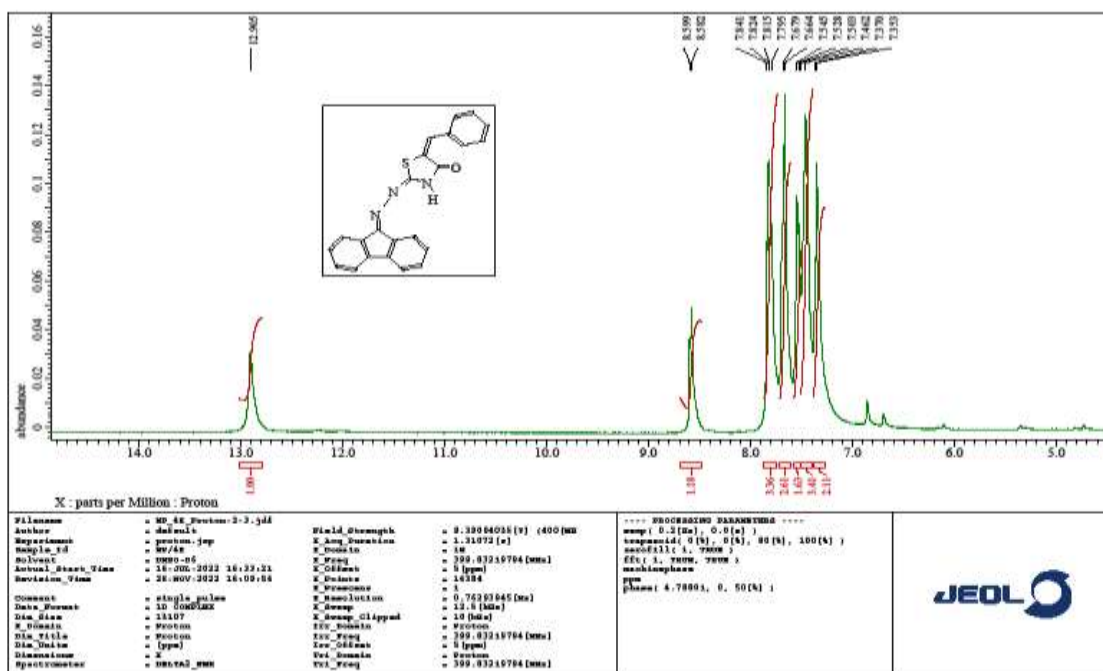
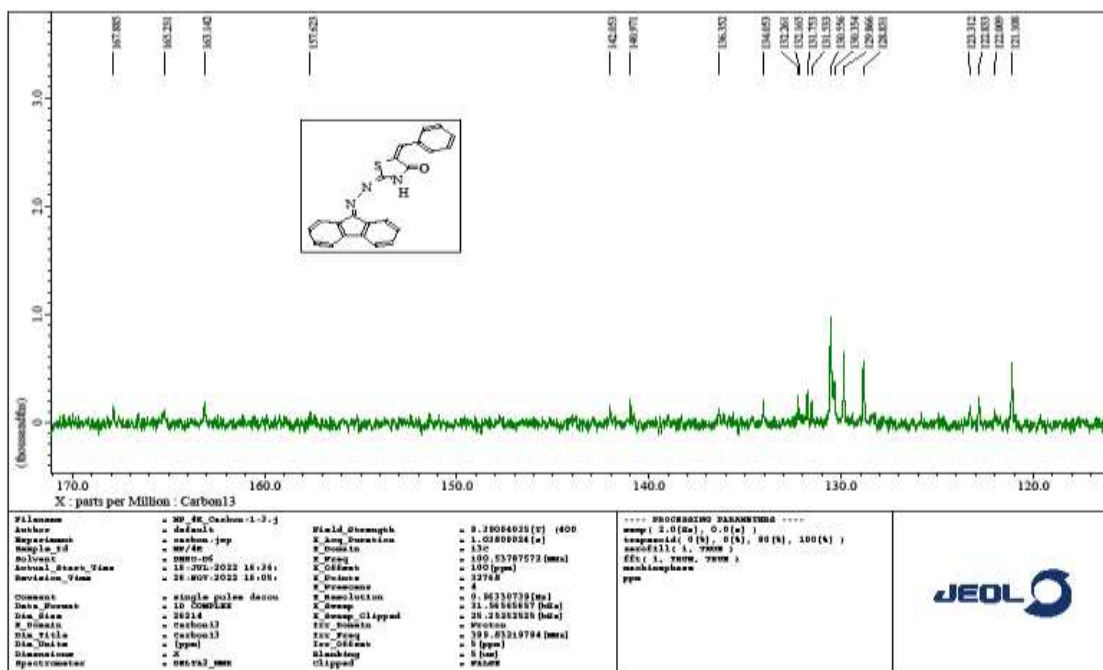


Fig.S50. Mass spectra of compound 5m



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Fig.S51. ¹H spectra of compound 5m



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Fig.S52. ¹³C spectra of compound 5m

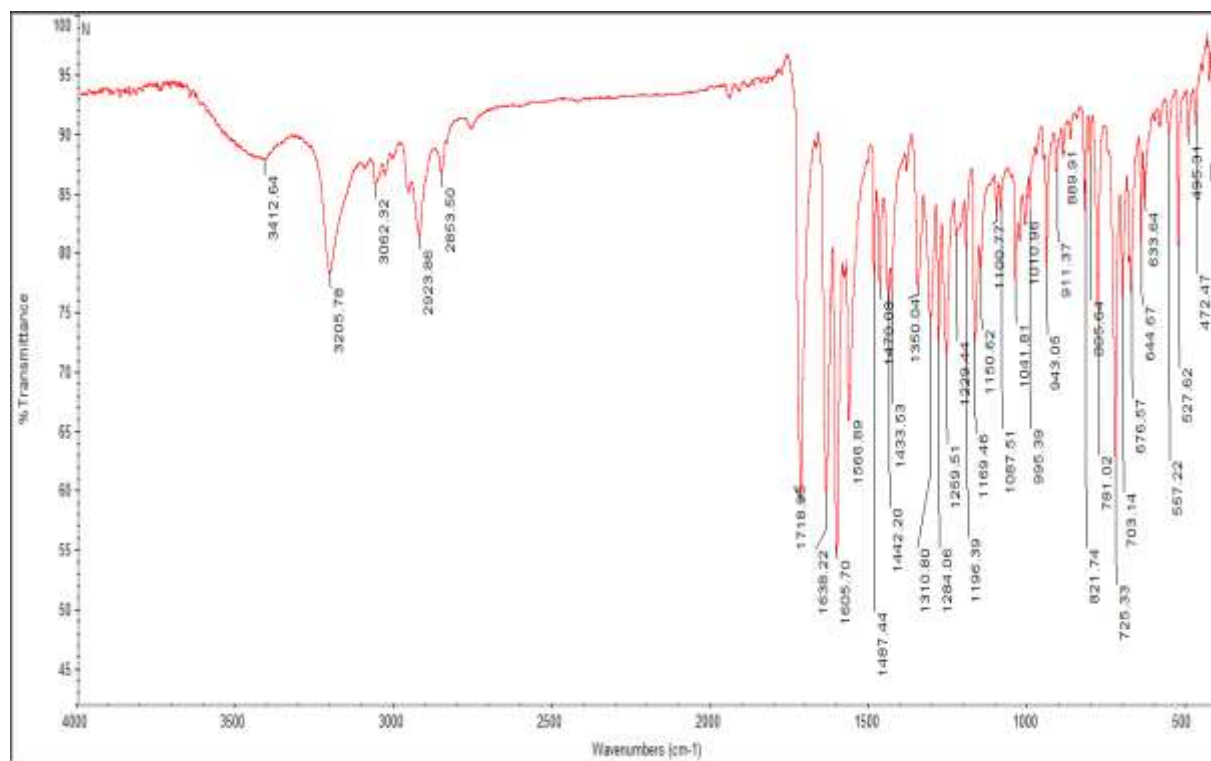


Fig.S53. FT-IR spectra of compound 5n

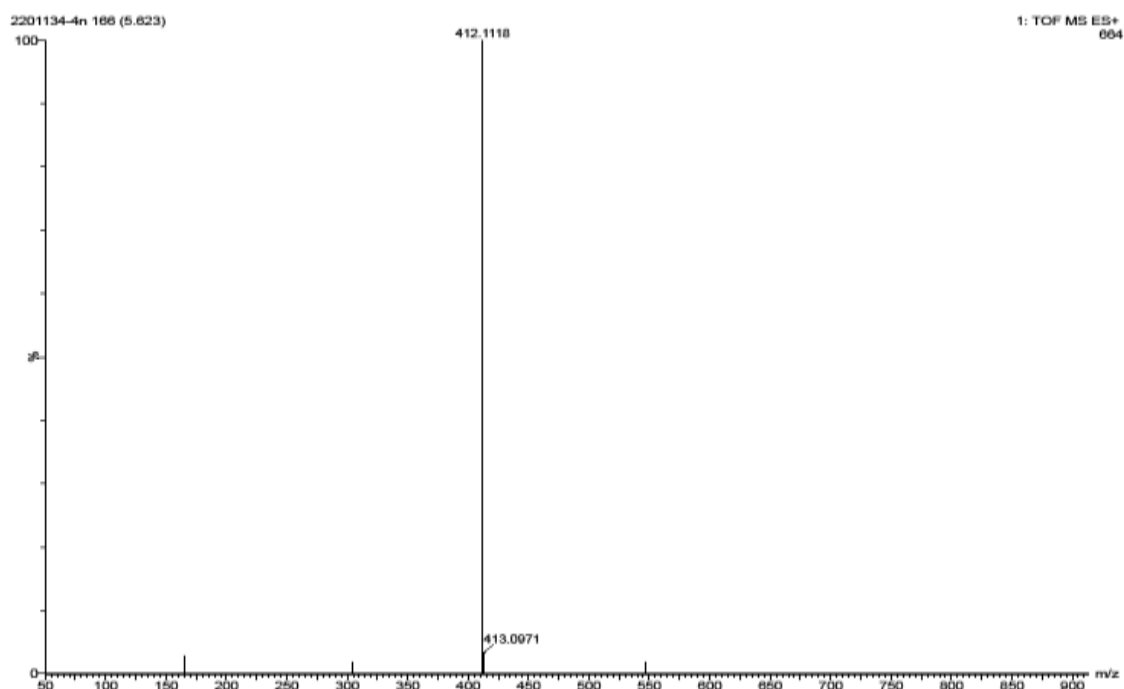
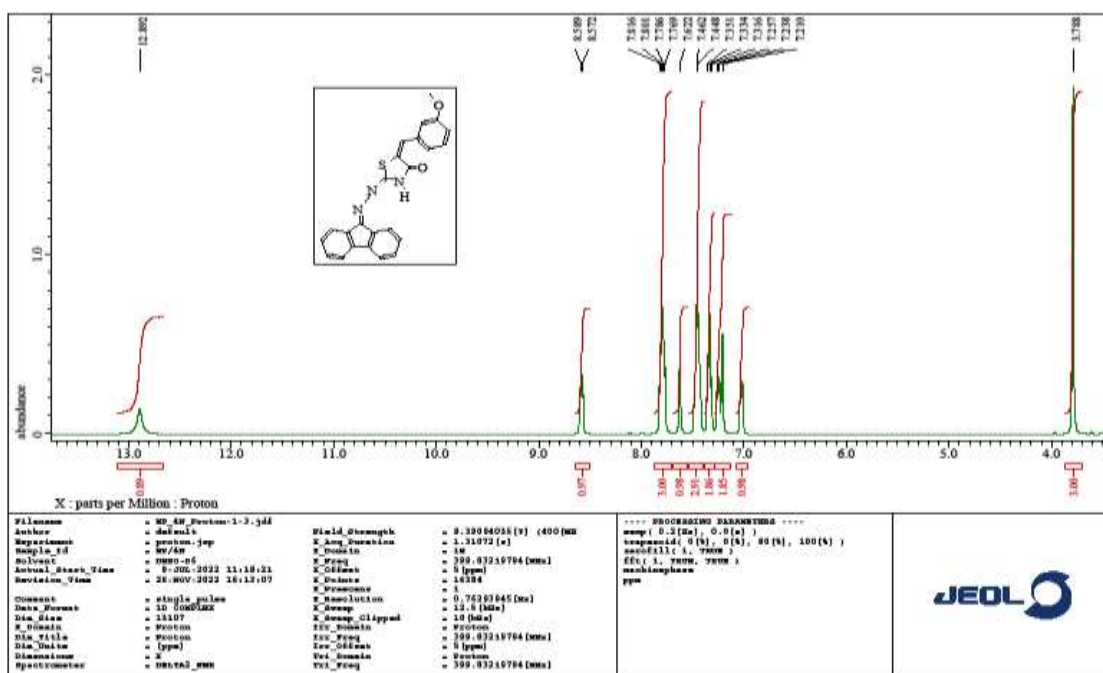
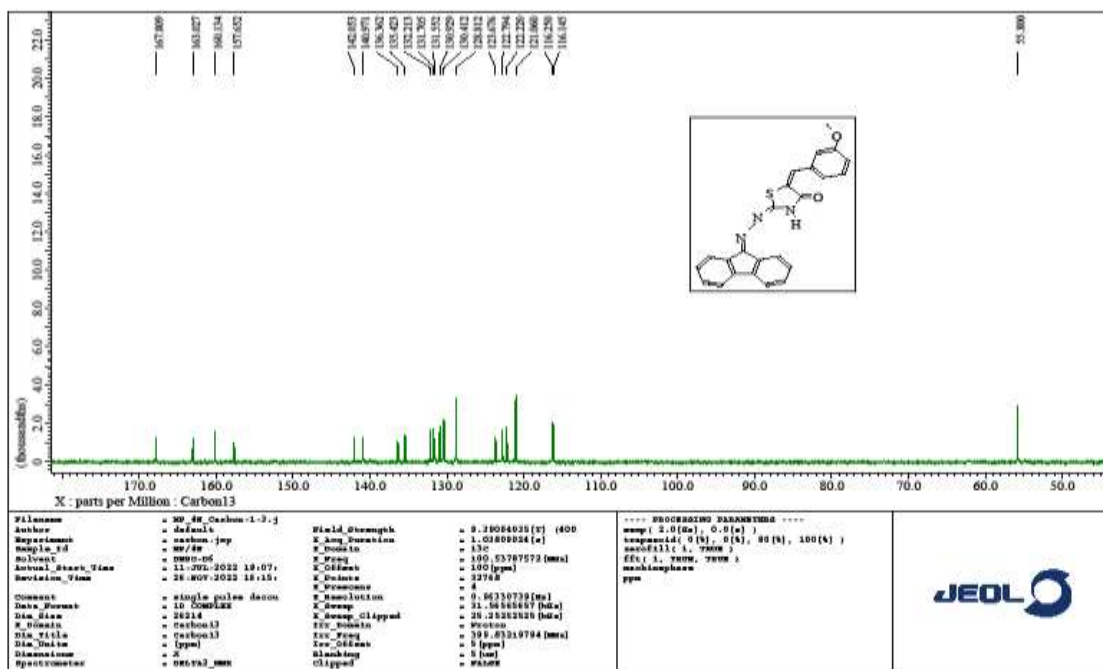


Fig.S54. Mass spectra of compound 5n



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Fig.S55. ¹H spectra of compound 5n



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Fig.S56. ¹³C spectra of compound 5n

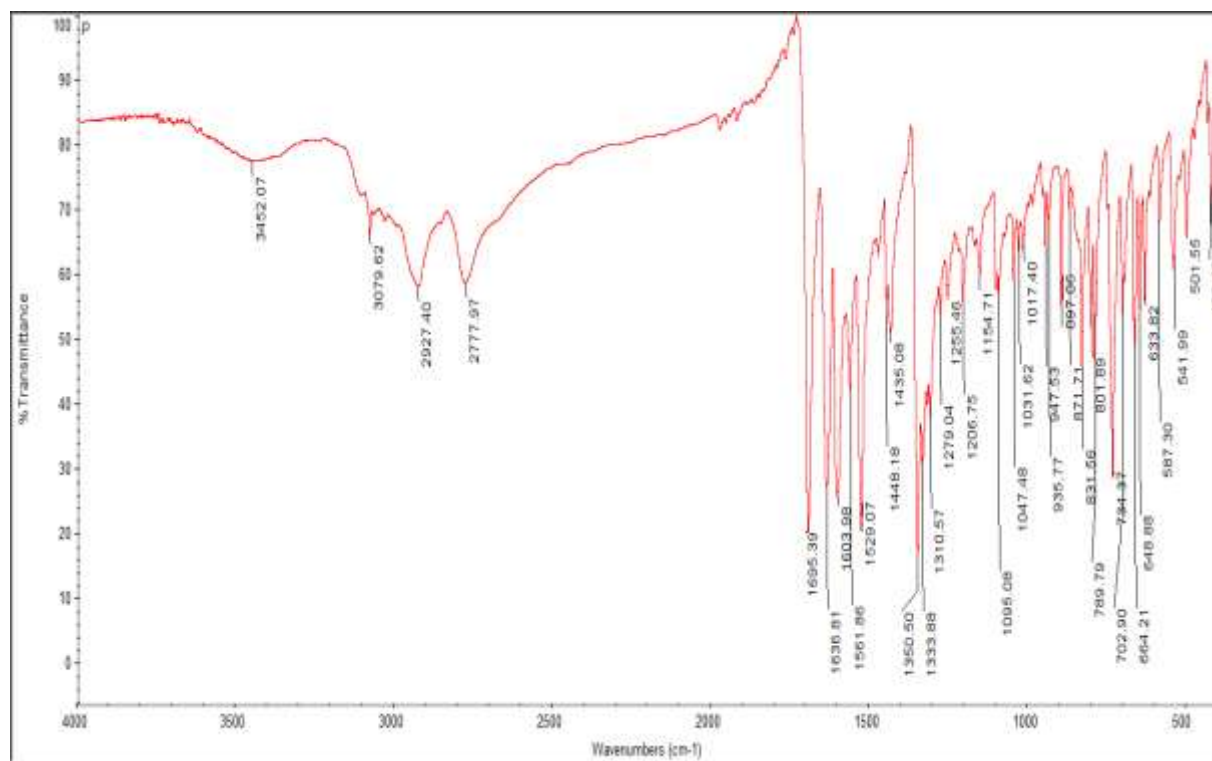


Fig.S57. FT-IR spectra of compound 5p

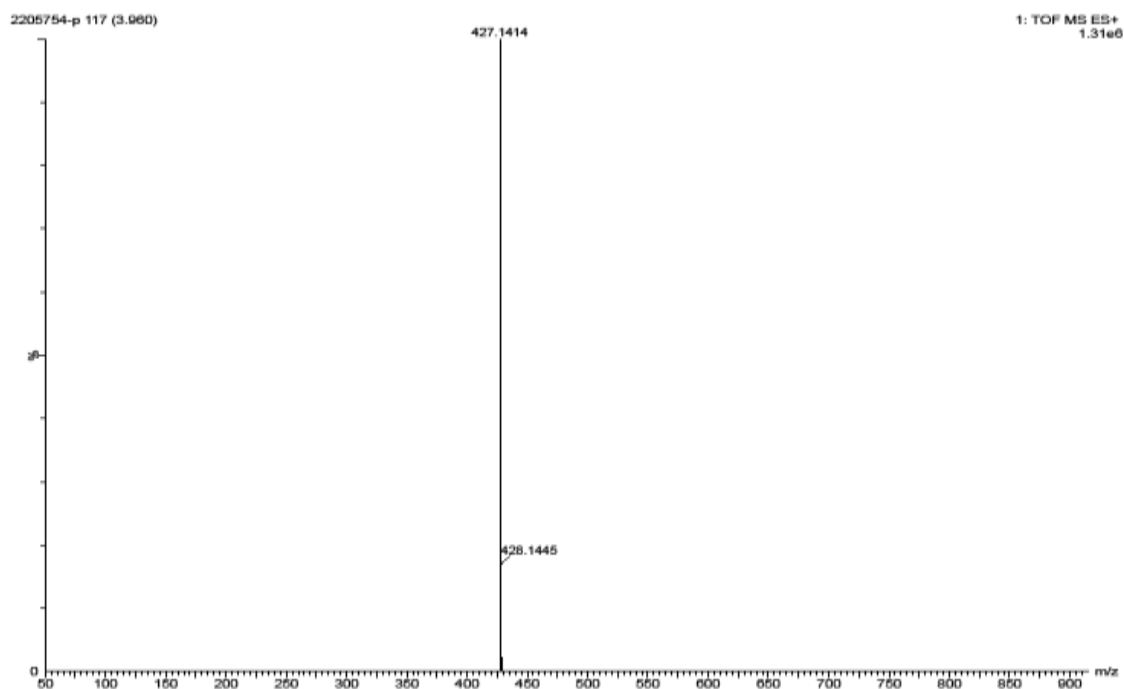


Fig.S58. Mass spectra of compound 5p

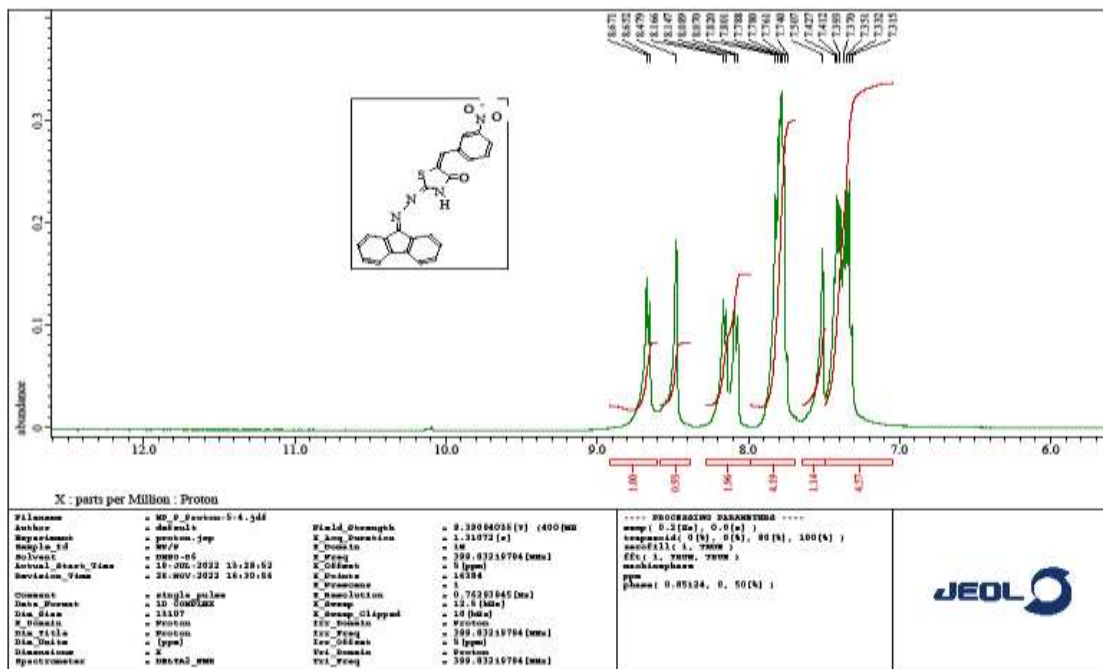


Fig.S59. ¹H spectra of compound 5p

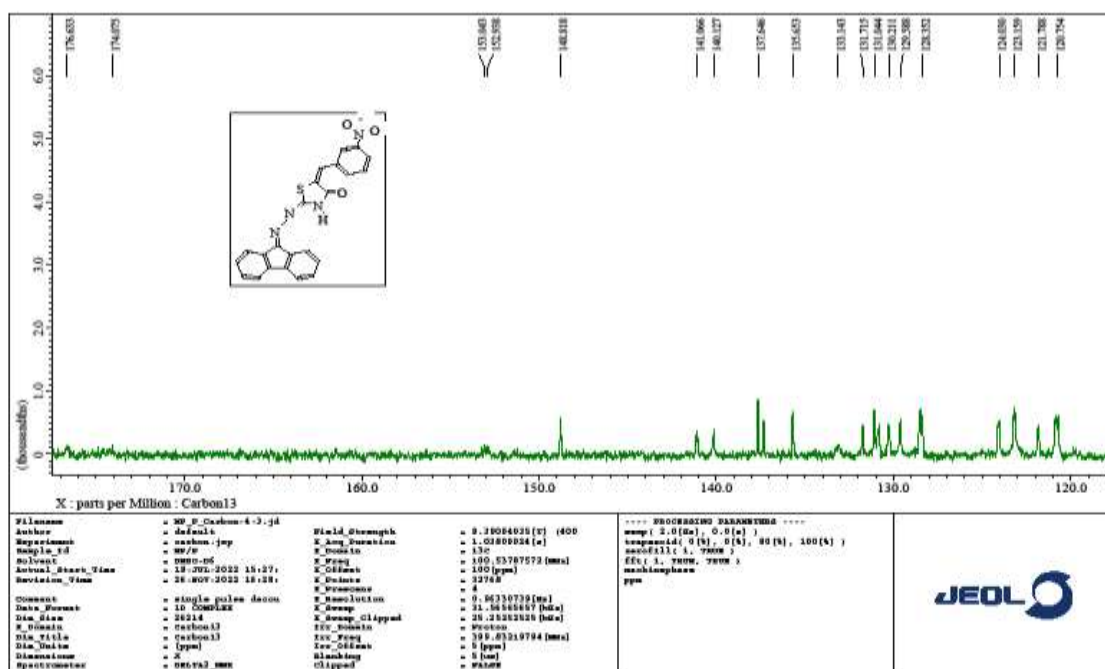


Fig.S60. ¹³C spectra of compound 5p

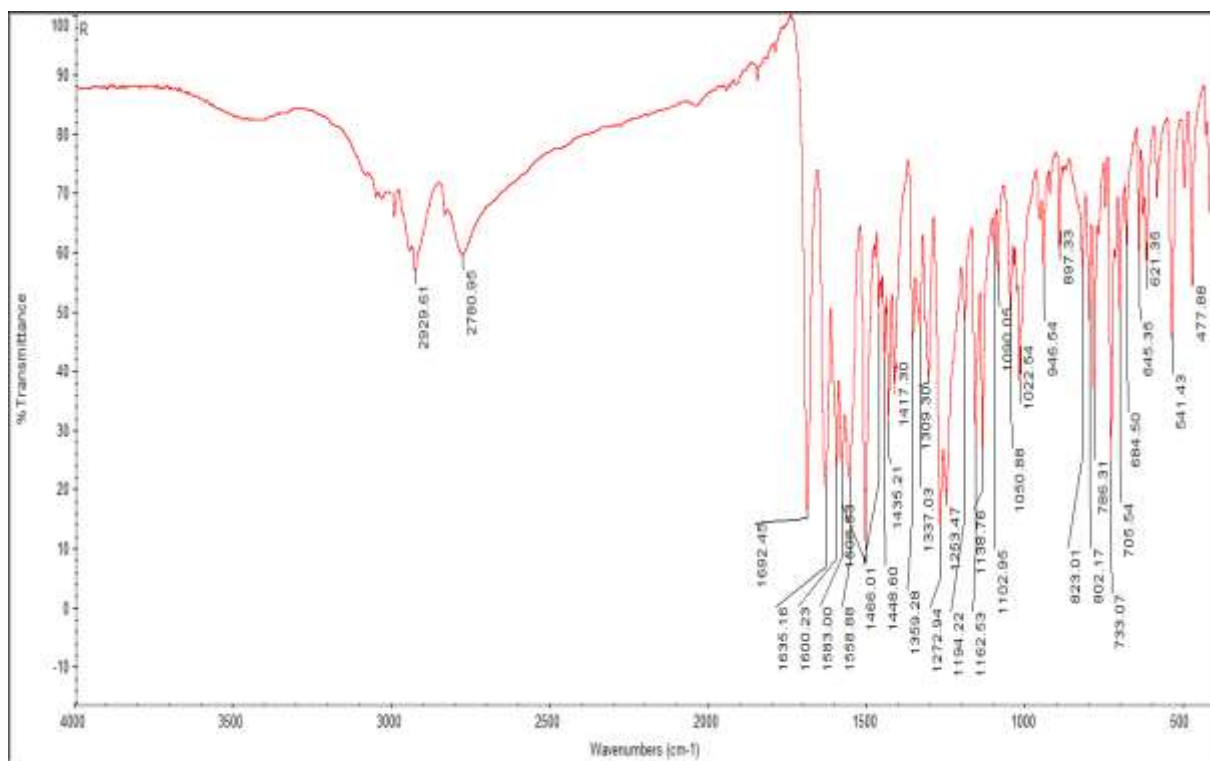


Fig.S61. FT-IR spectra of compound 5r

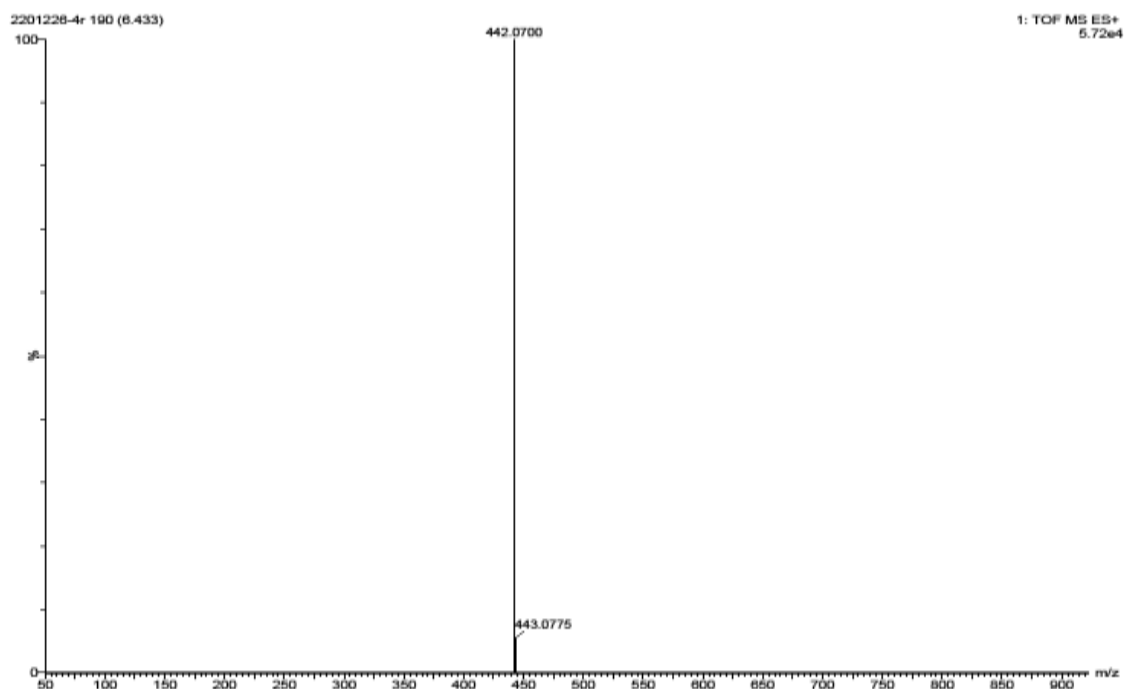
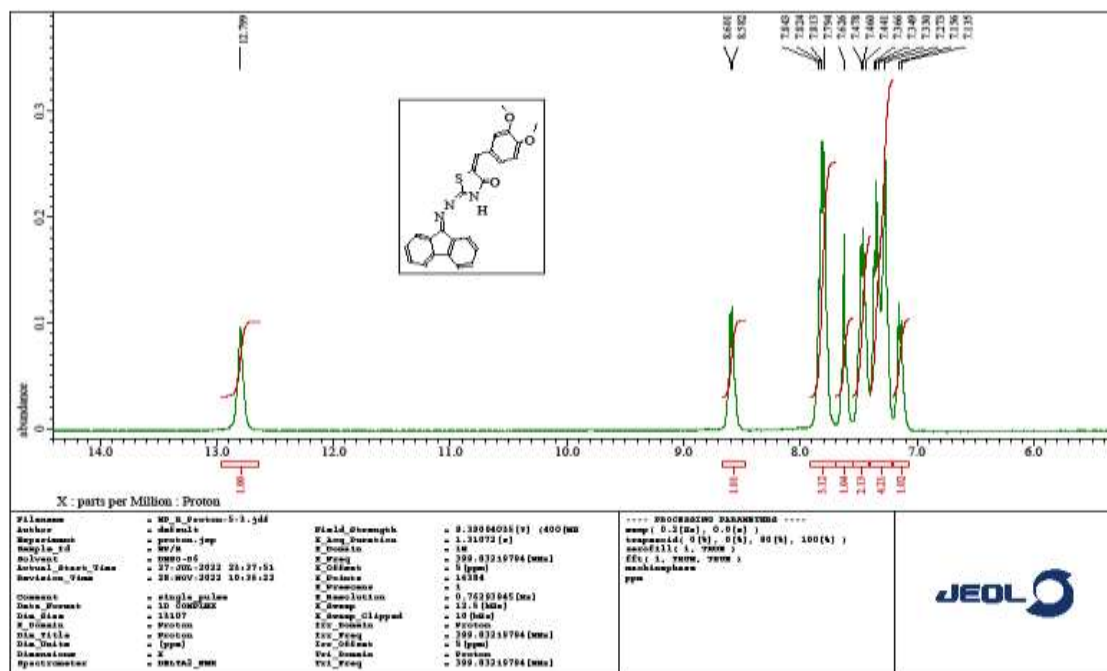
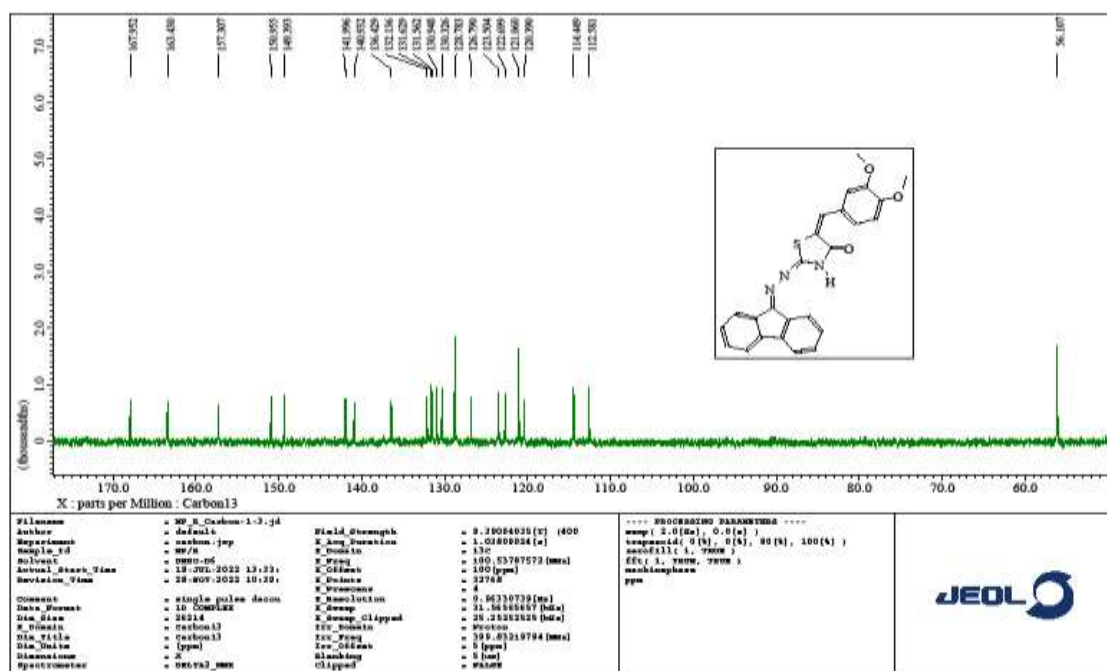


Fig.S62. Mass spectra of compound 5r



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Fig.S63. ^1H spectra of compound 5r



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Fig.S64. ^{13}C spectra of compound 5r

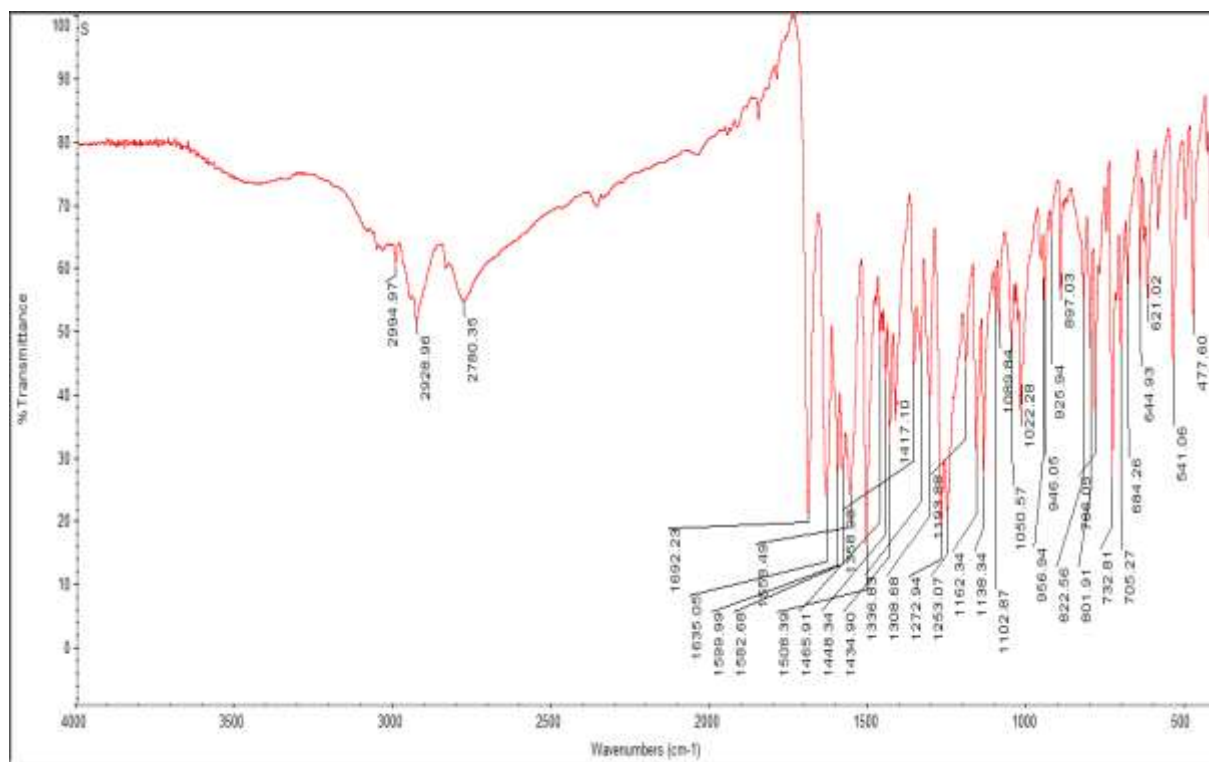


Fig.S65. FT-IR spectra of compound 5s

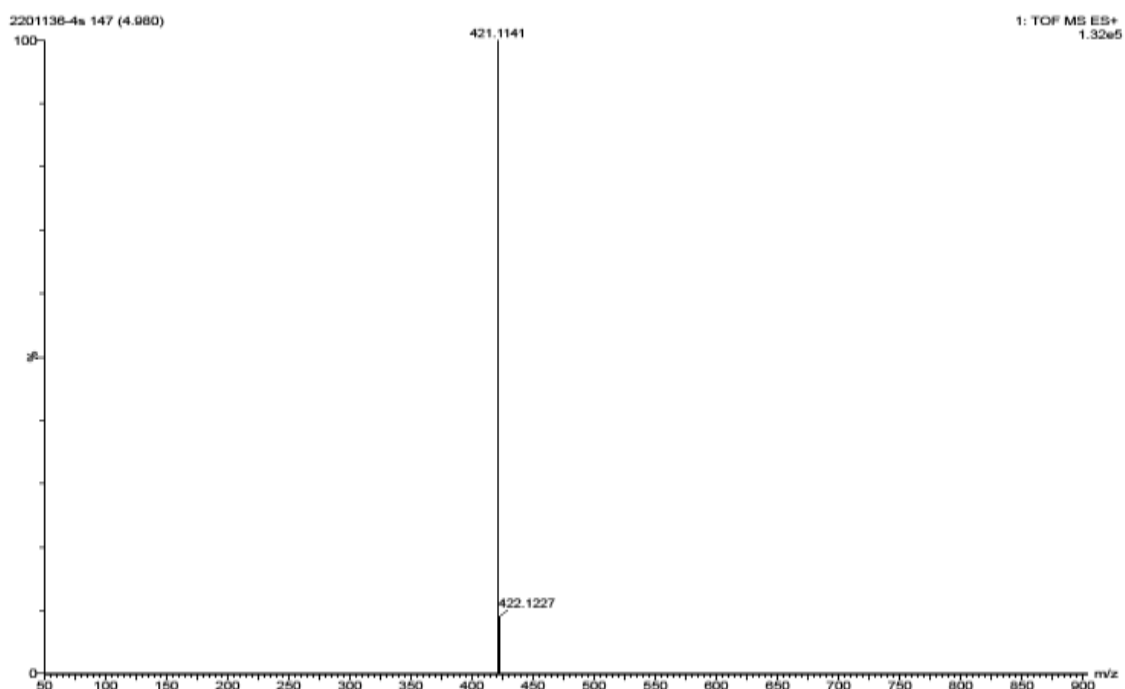
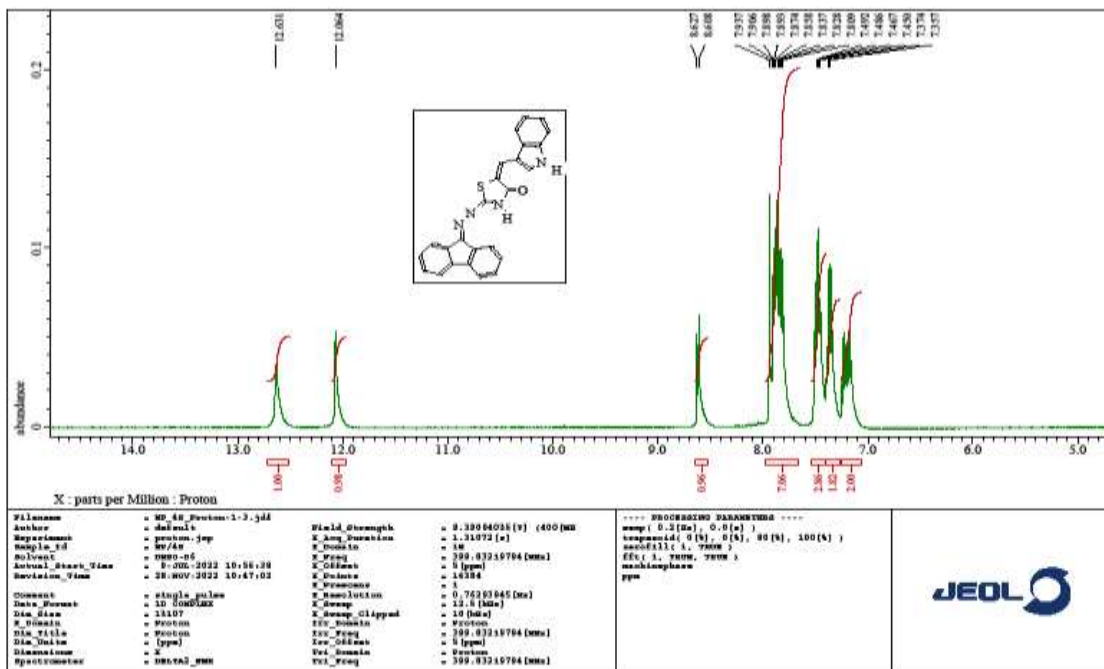
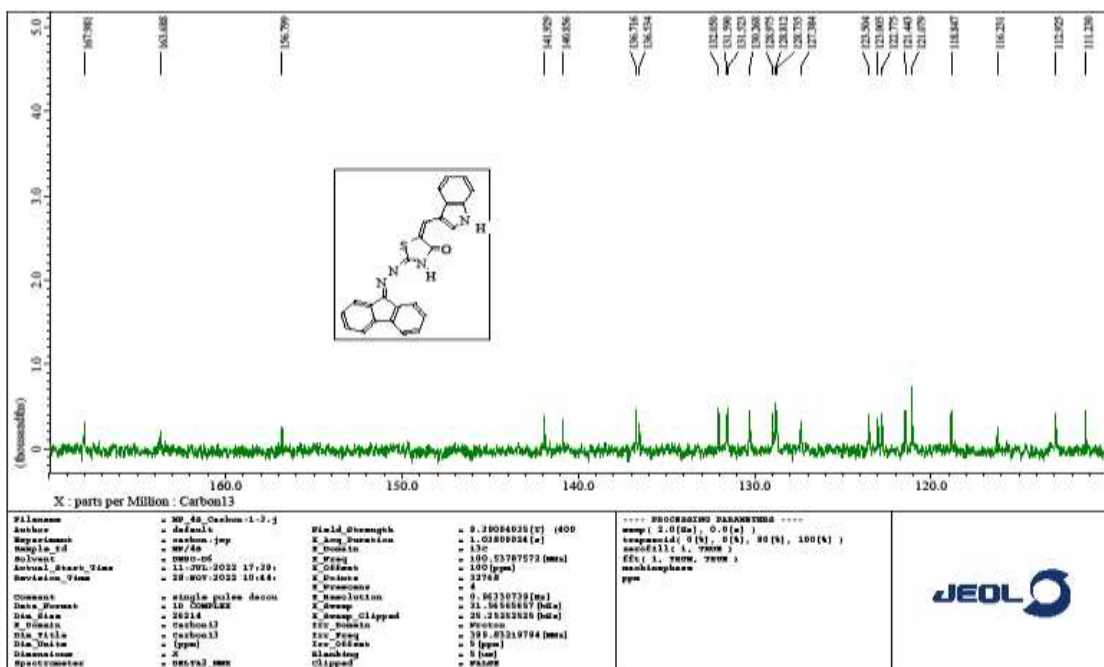


Fig.S66. Mass spectra of compound 5s



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Fig.S67. ^1H spectra of compound 5s



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Fig.S68. ^{13}C spectra of compound 5s

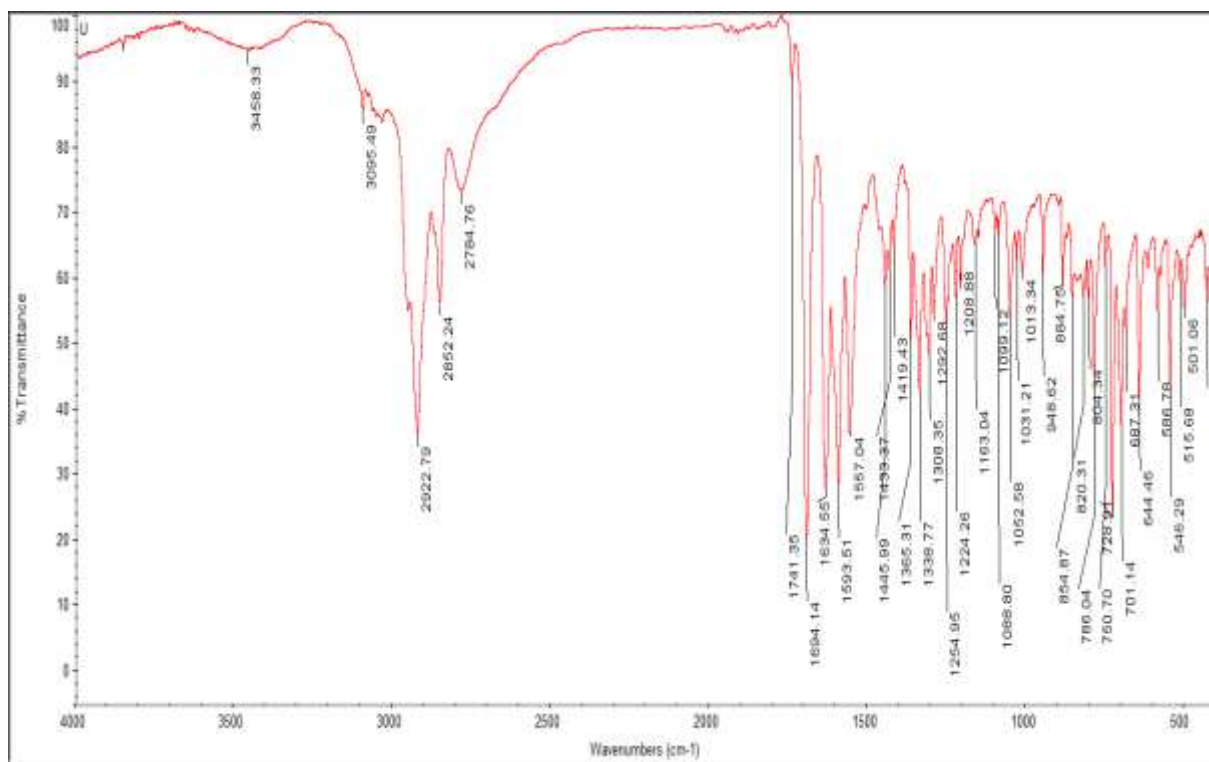


Fig.S69. FT-IR spectra of compound 5u

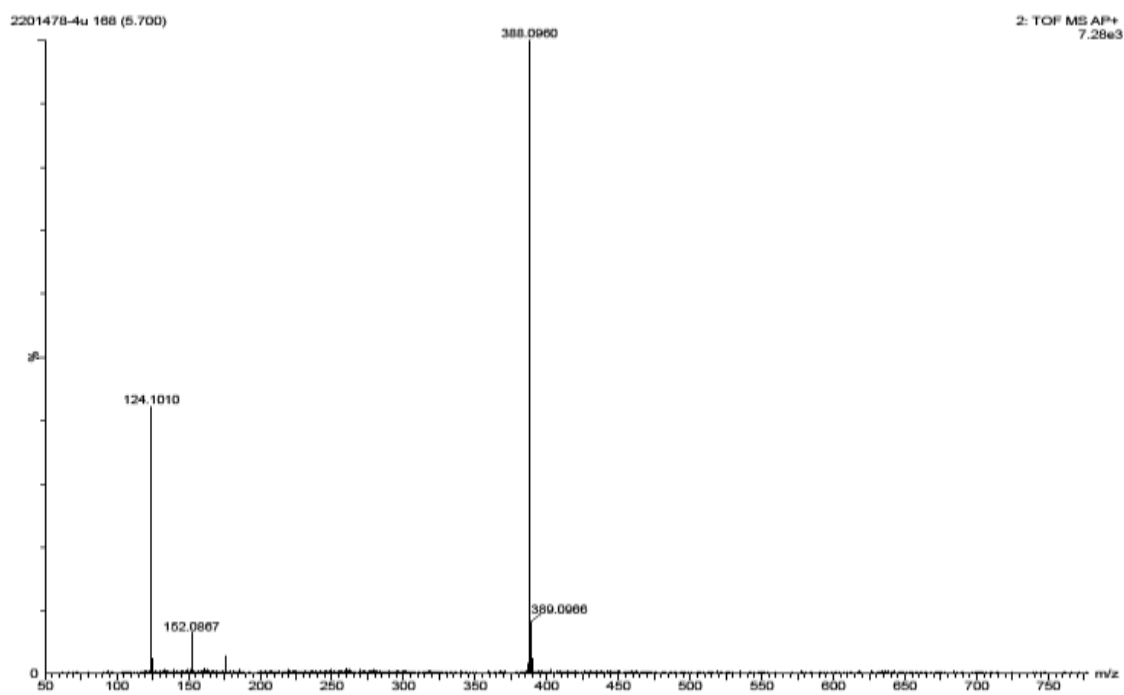
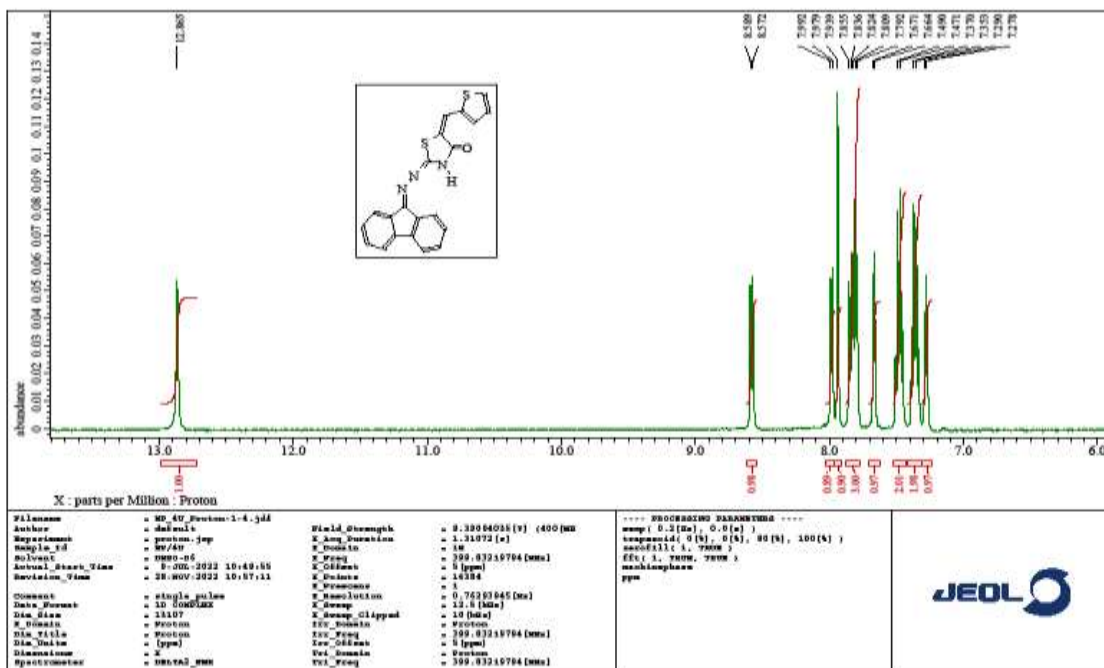
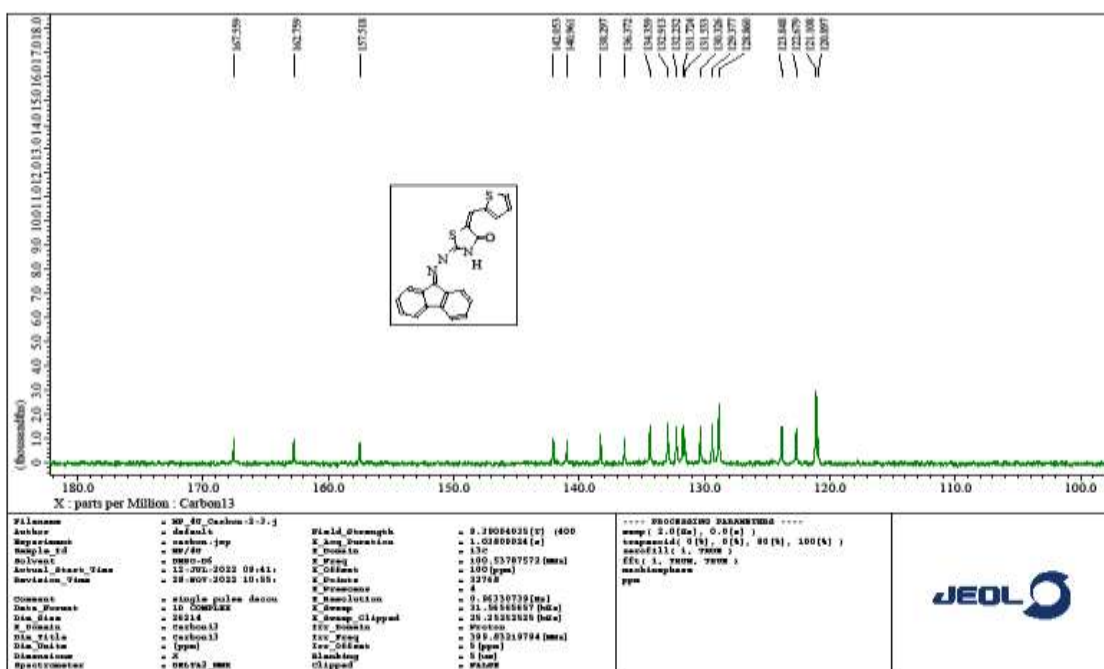


Fig.S70. Mass spectra of compound 5u



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Fig.S71. ¹H spectra of compound 5u



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Fig.S72. ¹³C spectra of compound 5u

Table S1. Selected geometric parameters (Å, °) (bond lengths, bond angles and torsion angles) for compound 5s

S1—C16	1.752 (2)	C1—C2	1.481 (3)
S1—C14	1.748 (2)	C13—C12	1.376 (3)
O1—C15	1.229 (2)	C13—C8	1.398 (3)
N2—N1	1.396 (3)	C12—C11	1.386 (3)
N2—C14	1.286 (3)	C11—C10	1.384 (4)
N1—C1	1.288 (3)	C10—C9	1.374 (4)
N3—C14	1.367 (3)	C9—C8	1.384 (3)
N3—C15	1.366 (3)	C8—C7	1.467 (3)
C22—C21	1.391 (3)	C7—C2	1.405 (3)
C22—C23	1.366 (3)	C7—C6	1.383 (3)
C21—C20	1.377 (3)	C2—C3	1.381 (3)
C20—C19	1.392 (3)	C3—C4	1.386 (3)
C19—C18	1.445 (3)	C4—C5	1.381 (4)
C19—C24	1.405 (3)	C5—C6	1.380 (4)
C18—C17	1.436 (3)	C25—N4	1.352 (3)
C18—C25	1.381 (3)	N4—C24	1.373 (3)
C17—C16	1.344 (3)	C24—C23	1.382 (3)
C16—C15	1.471 (3)	O2—C27	1.389 (3)
C1—C13	1.474 (3)	C26—C27	1.419 (4)
C14—S1—C16	90.89 (10)	C10—C11—C12	120.8 (3)
C14—N2—N1	109.15 (18)	C9—C10—C11	121.1 (3)
C1—N1—N2	115.26 (19)	C10—C9—C8	118.6 (3)
C15—N3—C14	116.82 (18)	C13—C8—C7	108.3 (2)
C23—C22—C21	121.6 (2)	C9—C8—C13	120.3 (2)
C20—C21—C22	121.0 (2)	C9—C8—C7	131.4 (2)
C21—C20—C19	118.9 (2)	C2—C7—C8	108.9 (2)
C20—C19—C18	134.7 (2)	C6—C7—C8	130.5 (2)
C20—C19—C24	118.5 (2)	C6—C7—C2	120.5 (2)
C24—C19—C18	106.78 (19)	C7—C2—C1	107.84 (19)
C17—C18—C19	125.4 (2)	C3—C2—C1	132.2 (2)
C25—C18—C19	105.94 (19)	C3—C2—C7	119.9 (2)
C25—C18—C17	128.6 (2)	C2—C3—C4	119.2 (2)
C16—C17—C18	128.8 (2)	C5—C4—C3	120.5 (2)

C17—C16—S1	126.67 (17)	C6—C5—C4	121.1 (2)
C17—C16—C15	122.7 (2)	C5—C6—C7	118.8 (2)
C15—C16—S1	110.64 (15)	O1—C15—N3	123.01 (19)
N2—C14—S1	125.88 (17)	O1—C15—C16	126.9 (2)
N2—C14—N3	122.6 (2)	N3—C15—C16	110.10 (18)
N3—C14—S1	111.50 (15)	N4—C25—C18	109.9 (2)
N1—C1—C13	121.1 (2)	C25—N4—C24	109.87 (19)
N1—C1—C2	132.7 (2)	N4—C24—C19	107.53 (19)
C13—C1—C2	106.10 (19)	N4—C24—C23	129.7 (2)
C12—C13—C1	130.4 (2)	C23—C24—C19	122.7 (2)
C12—C13—C8	120.9 (2)	C22—C23—C24	117.2 (2)
C8—C13—C1	108.7 (2)	O2—C27—C26	120.5 (3)
C13—C12—C11	118.3 (2)		
S1—C16—C15—O1	177.5 (2)	C1—C13—C8—C7	-2.2 (3)
S1—C16—C15—N3	-2.6 (2)	C1—C2—C3—C4	177.6 (2)
N2—N1—C1—C13	-179.72 (19)	C13—C1—C2—C7	-3.3 (2)
N2—N1—C1—C2	3.7 (4)	C13—C1—C2—C3	178.4 (3)
N1—N2—C14—S1	1.6 (3)	C13—C12—C11—C10	0.6 (4)
N1—N2—C14—N3	-178.20 (19)	C13—C8—C7—C2	0.1 (3)
N1—C1—C13—C12	5.7 (4)	C13—C8—C7—C6	179.6 (2)
N1—C1—C13—C8	-174.0 (2)	C12—C13—C8—C9	-2.2 (4)
N1—C1—C2—C7	173.7 (2)	C12—C13—C8—C7	178.1 (2)
N1—C1—C2—C3	-4.6 (5)	C12—C11—C10—C9	-1.5 (4)
C22—C21—C20—C19	-0.1 (4)	C11—C10—C9—C8	0.5 (4)
C21—C22—C23—C24	0.0 (4)	C10—C9—C8—C13	1.3 (4)
C21—C20—C19—C18	179.4 (2)	C10—C9—C8—C7	-179.0 (2)
C21—C20—C19—C24	-0.5 (3)	C9—C8—C7—C2	-179.7 (2)
C20—C19—C18—C17	1.8 (4)	C9—C8—C7—C6	-0.2 (5)
C20—C19—C18—C25	179.7 (3)	C8—C13—C12—C11	1.2 (4)
C20—C19—C24—N4	-179.5 (2)	C8—C7—C2—C1	2.1 (3)
C20—C19—C24—C23	0.9 (4)	C8—C7—C2—C3	-179.4 (2)
C19—C18—C17—C16	-179.4 (2)	C8—C7—C6—C5	179.8 (2)
C19—C18—C25—N4	0.0 (3)	C7—C2—C3—C4	-0.5 (4)
C19—C24—C23—C22	-0.6 (4)	C2—C1—C13—C12	-176.9 (2)
C18—C19—C24—N4	0.6 (3)	C2—C1—C13—C8	3.4 (2)
C18—C19—C24—C23	-179.0 (2)	C2—C7—C6—C5	-0.7 (4)

C18—C17—C16—S1	1.4 (4)	C2—C3—C4—C5	-0.3 (4)
C18—C17—C16—C15	-176.5 (2)	C3—C4—C5—C6	0.6 (4)
C18—C25—N4—C24	0.4 (3)	C4—C5—C6—C7	-0.1 (4)
C17—C18—C25—N4	177.9 (2)	C6—C7—C2—C1	-177.5 (2)
C17—C16—C15—O1	-4.3 (4)	C6—C7—C2—C3	1.0 (4)
C17—C16—C15—N3	175.6 (2)	C15—N3—C14—S1	-0.9 (2)
C16—S1—C14—N2	179.6 (2)	C15—N3—C14—N2	178.9 (2)
C16—S1—C14—N3	-0.63 (17)	C25—C18—C17—C16	3.2 (4)
C14—S1—C16—C17	-176.3 (2)	C25—N4—C24—C19	-0.6 (3)
C14—S1—C16—C15	1.82 (17)	C25—N4—C24—C23	179.0 (3)
C14—N2—N1—C1	-173.1 (2)	N4—C24—C23—C22	179.8 (2)
C14—N3—C15—O1	-177.8 (2)	C24—C19—C18—C17	-178.3 (2)
C14—N3—C15—C16	2.2 (3)	C24—C19—C18—C25	-0.4 (3)
C1—C13—C12—C11	-178.5 (2)	C23—C22—C21—C20	0.3 (4)
C1—C13—C8—C9	177.6 (2)		

Fig S73. Angle between the plane of compound **5s**

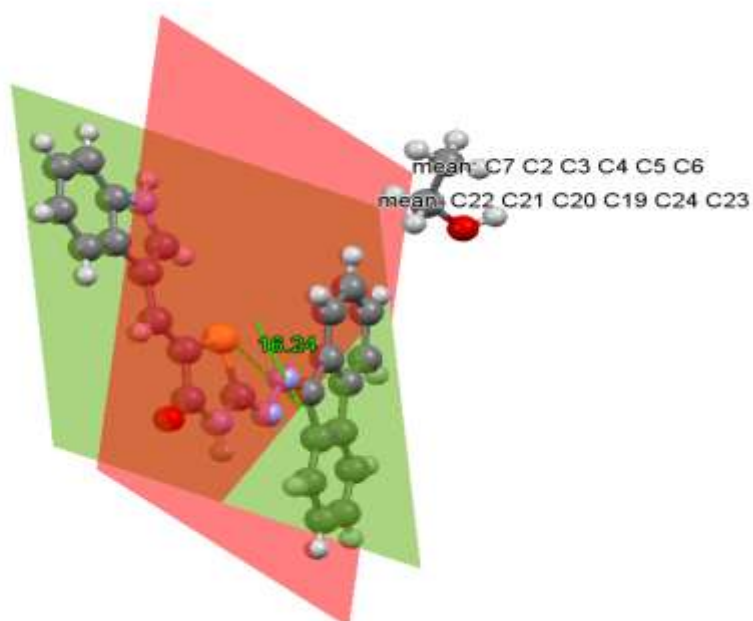


Fig S74. Dihedral angle of compound 5s

