Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

An Efficient Desulfitative C-C Cross Coupling of Fused aryl Thiazolidine-2-thione with Boronic Acids and Boronic Acid Pinacol esters: Formation of Fused aryl Thiazoles

Kandasamy Rajaguru[a] Arumugam Mariappan,[a] Ramachandran Manjusri,[a] Shanmugam Muthusubramanian,[a]* and Nattamai Bhuvanesh[b]

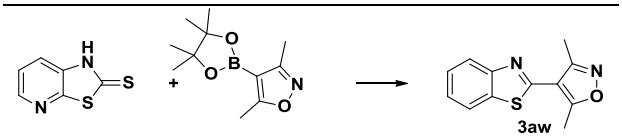
[a]*Department of Organic Chemistry, School of Chemistry, Madurai Kamaraj University, Madurai - 625 021, India*

[b]*X-ray Diffraction Laboratory, Department of Chemistry, Texas A & M University, College Station, Texas 77842, USA.*

E-mail: muthumanian2001@yahoo.com

Table of contents **Page No**

Table S1. Desulfitative coupling experimented with water[a]



Entry	Dioxane : Water (mL)	Time (h)
1	4.9 : 0.1	18
2	4.8 : 0.2	18
3	4.5 : 0.5	18
4	4.0 : 1.0	18
5	4.0 : 1.0	24[b]

[a] Under optimized condition [b] Reaction performed without CuTC

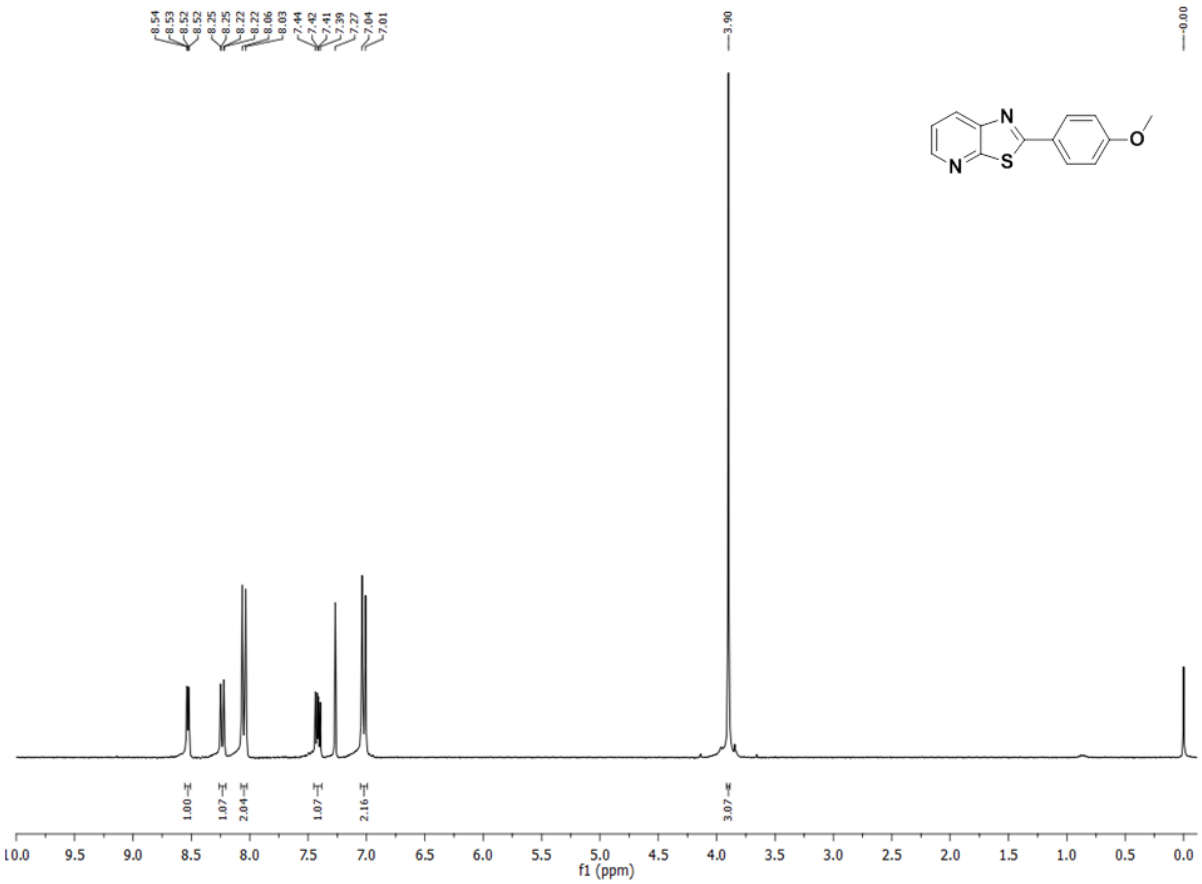


Figure 1. ^{1}H NMR Spectrum of compound **3aa**

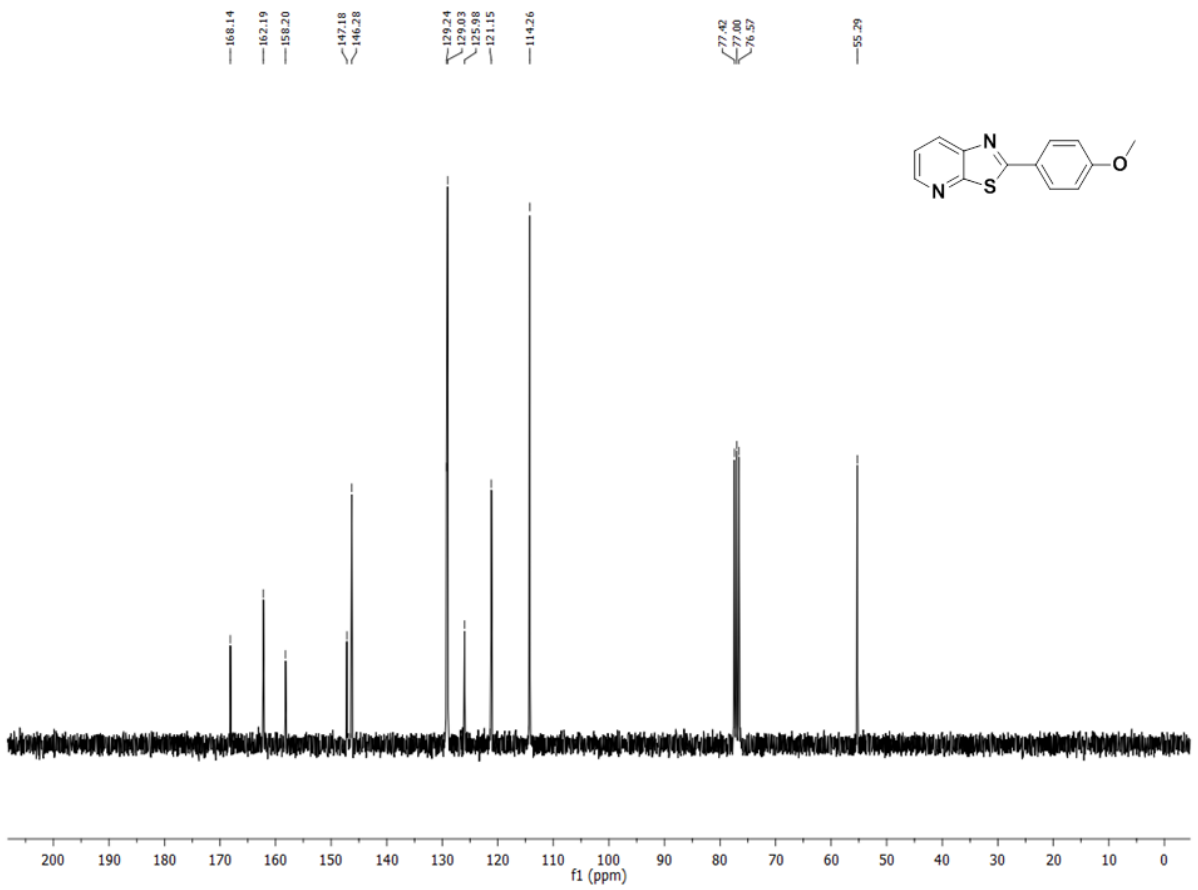


Figure 2. ^{13}C Spectrum of compound **3aa**

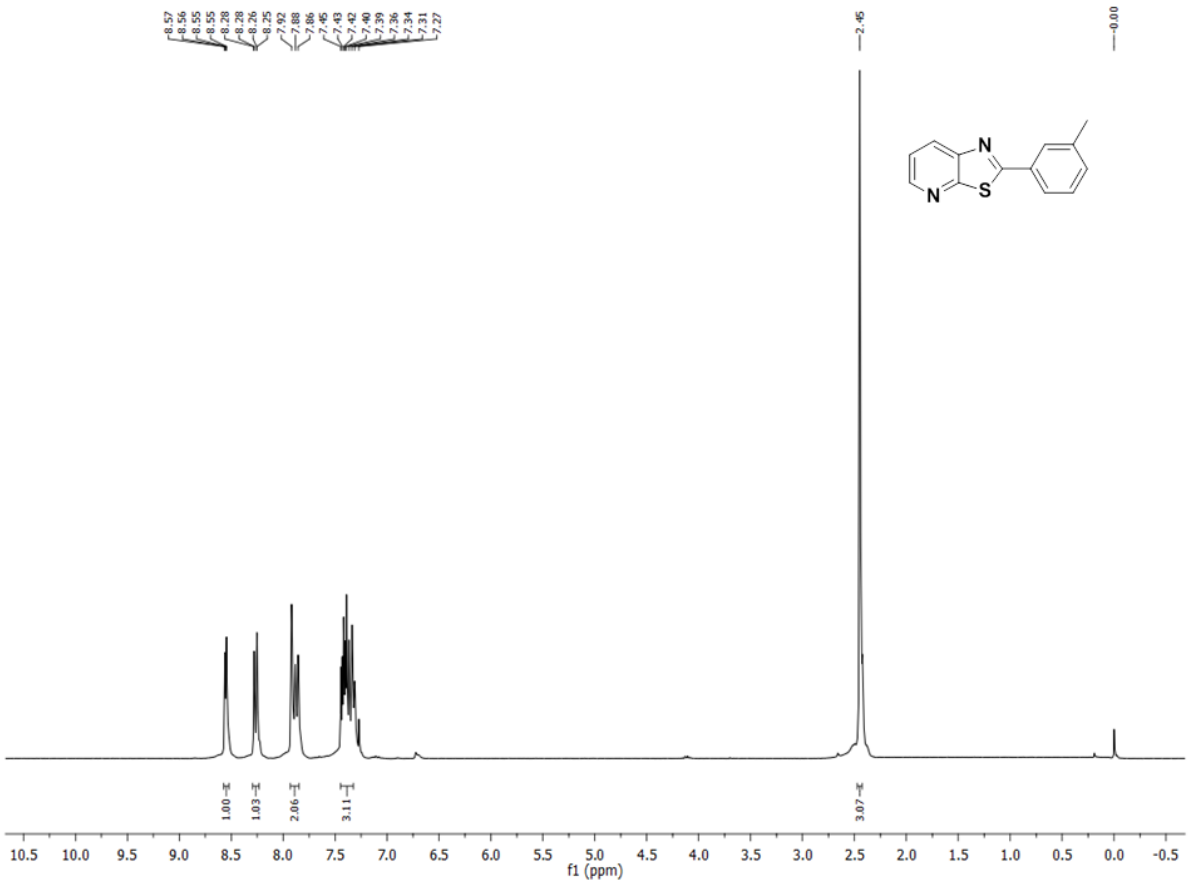


Figure 3. ^{1}H NMR Spectrum of compound **3ab**

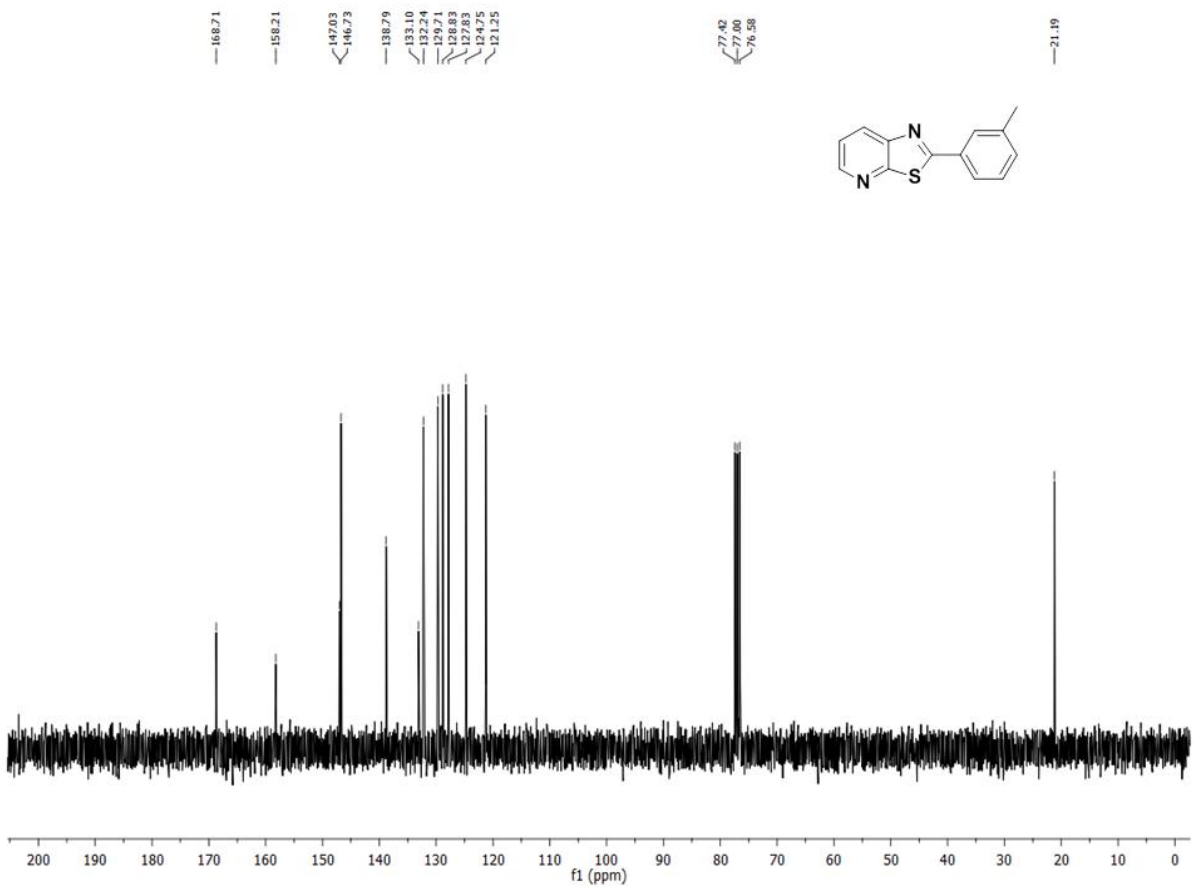


Figure 4. ^{13}C Spectrum of compound **3ab**

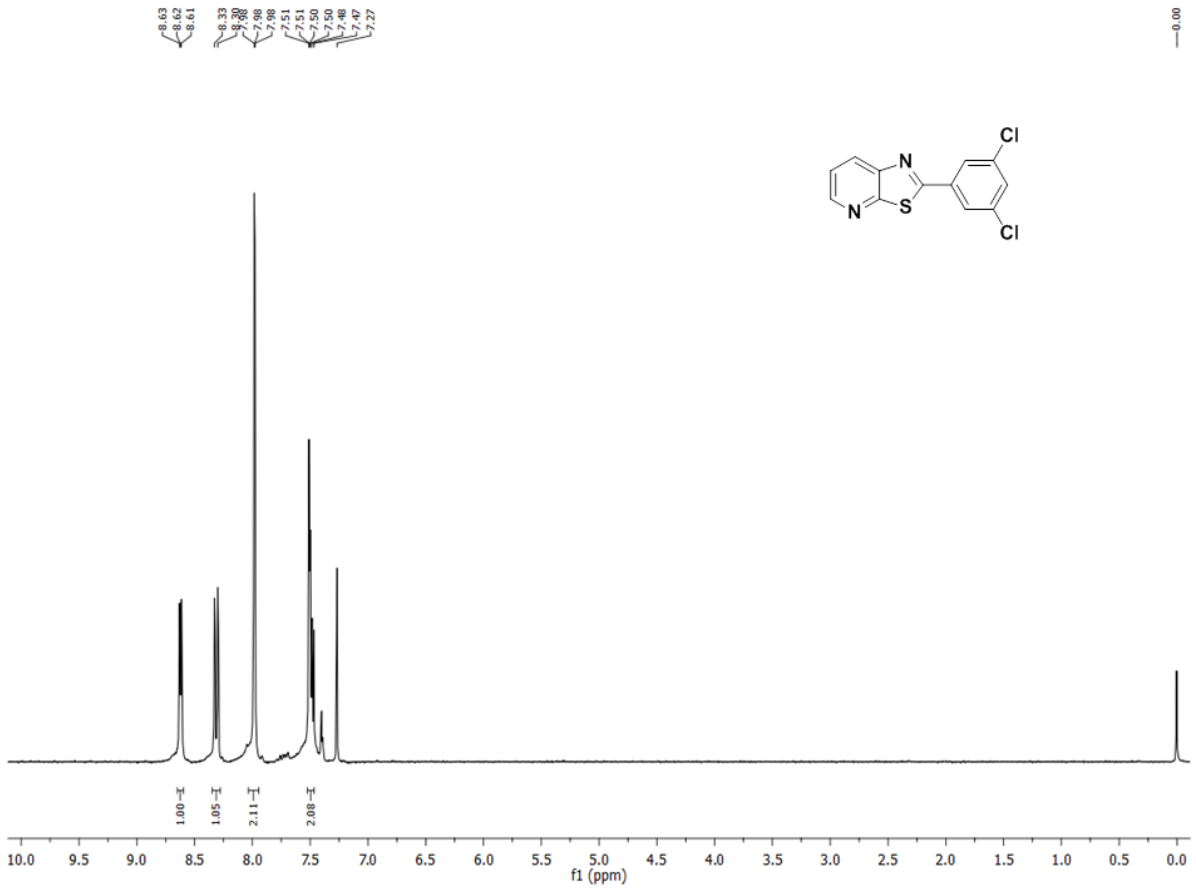


Figure 5. ^{1}H NMR Spectrum of compound **3ac**

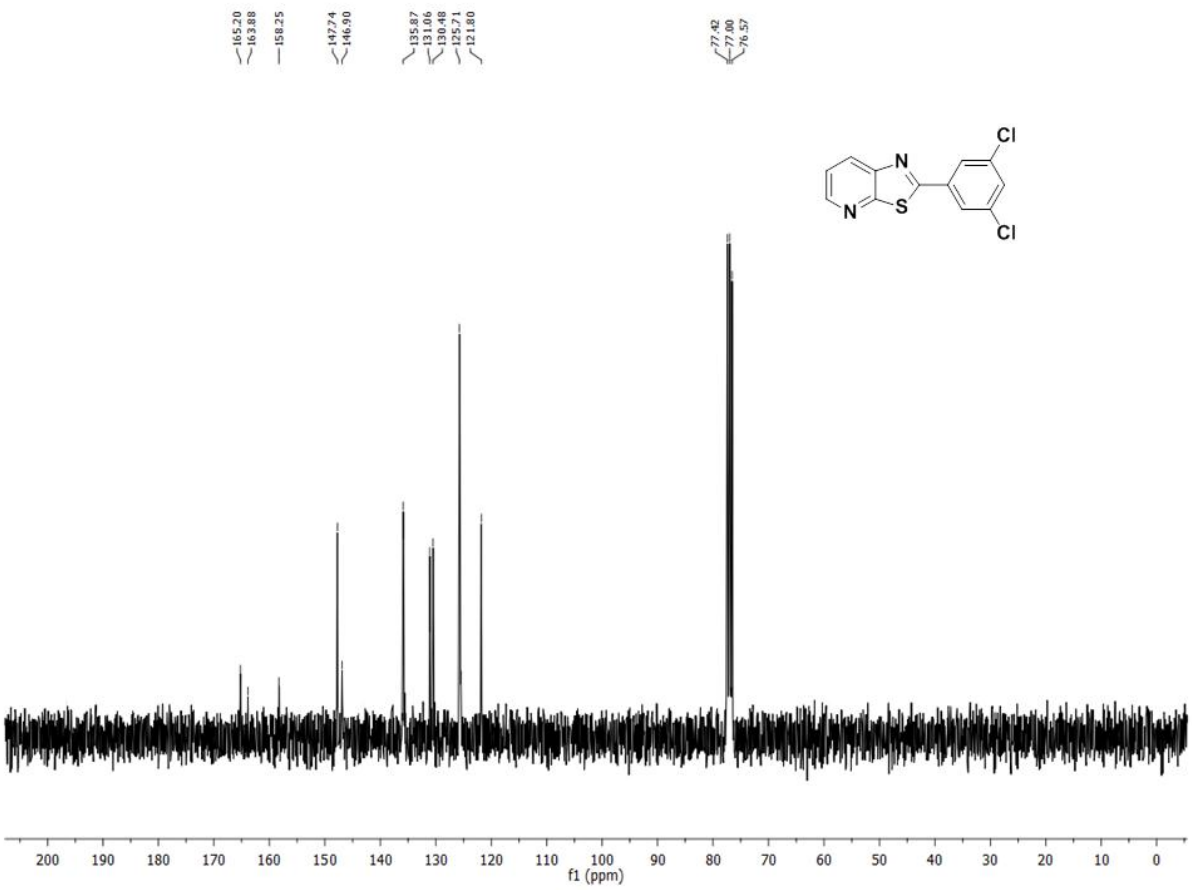


Figure 6. ^{13}C Spectrum of compound **3ac**

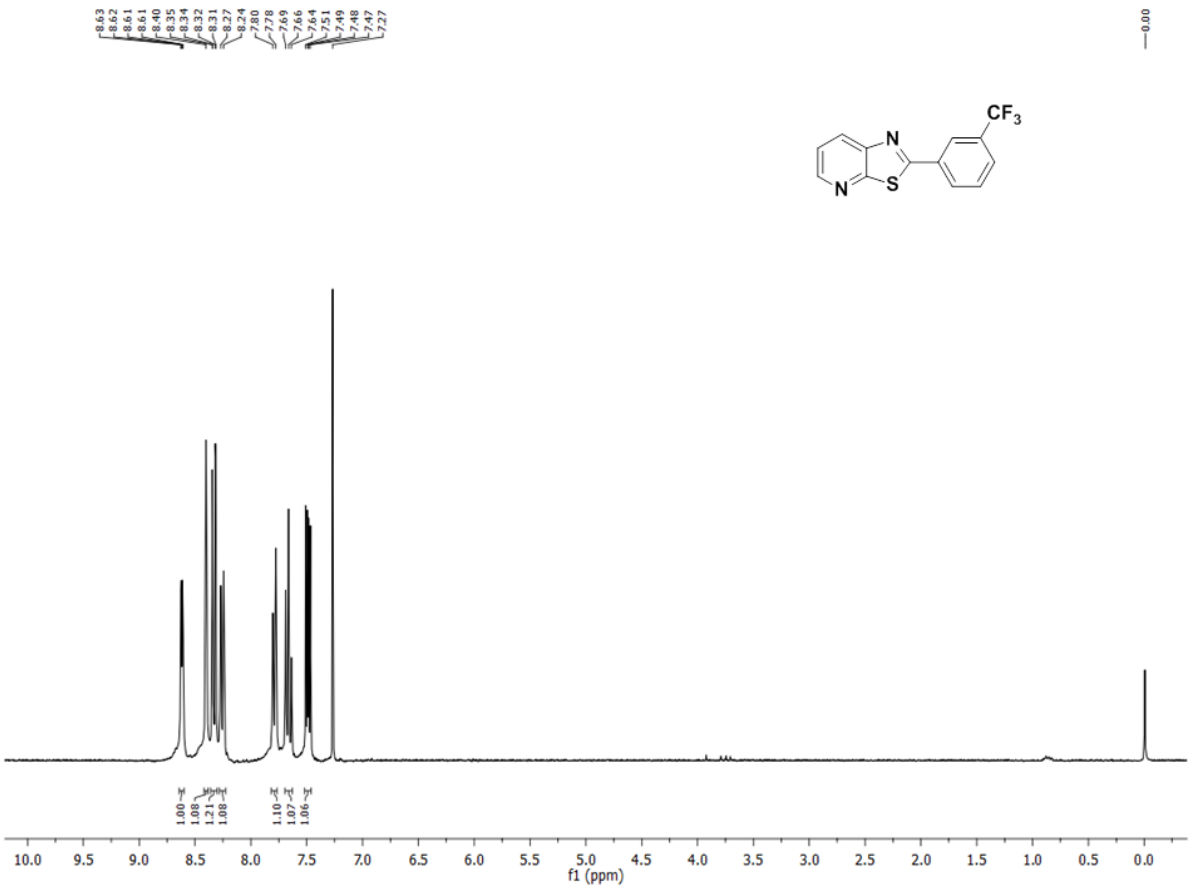


Figure 7. ^{1}H NMR Spectrum of compound **3ad**

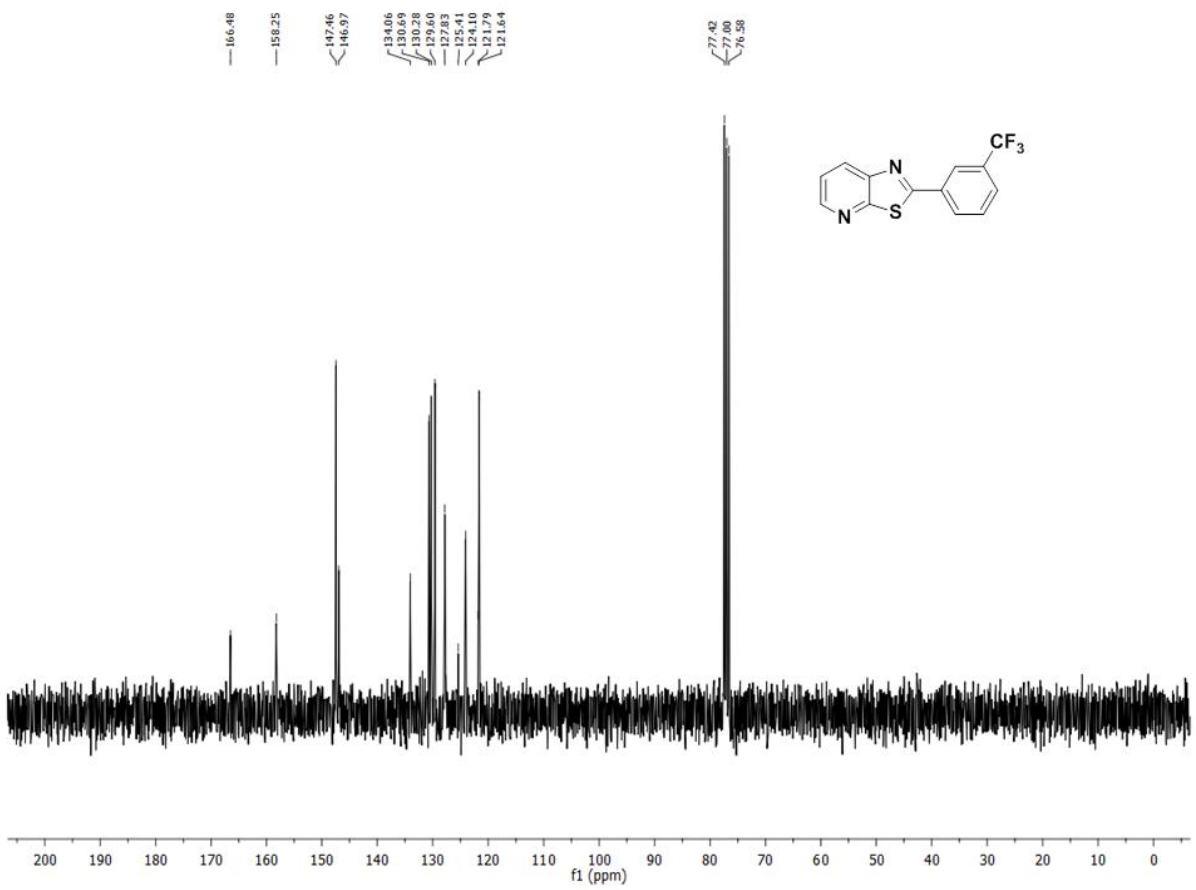


Figure 8. ^{13}C Spectrum of compound **3ad**

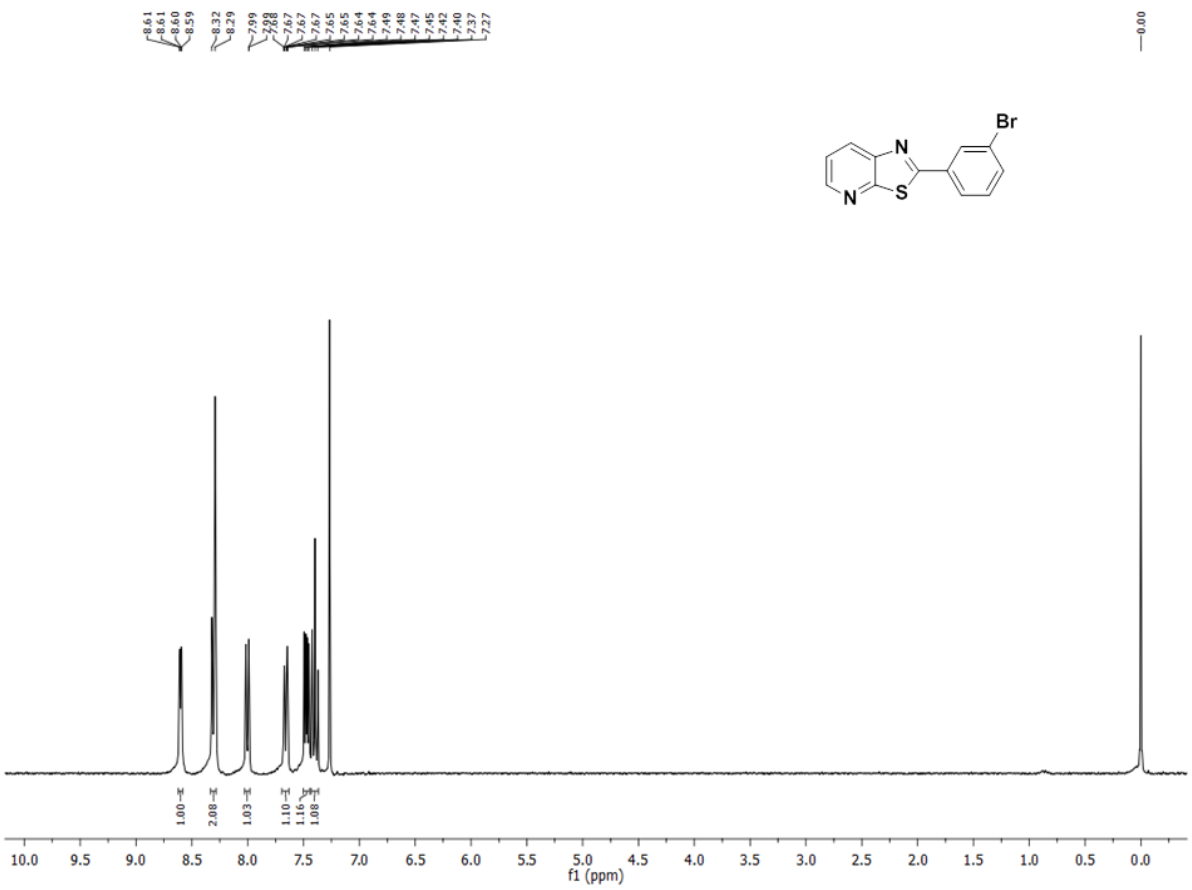


Figure 9. ^{1}H NMR Spectrum of compound **3ae**

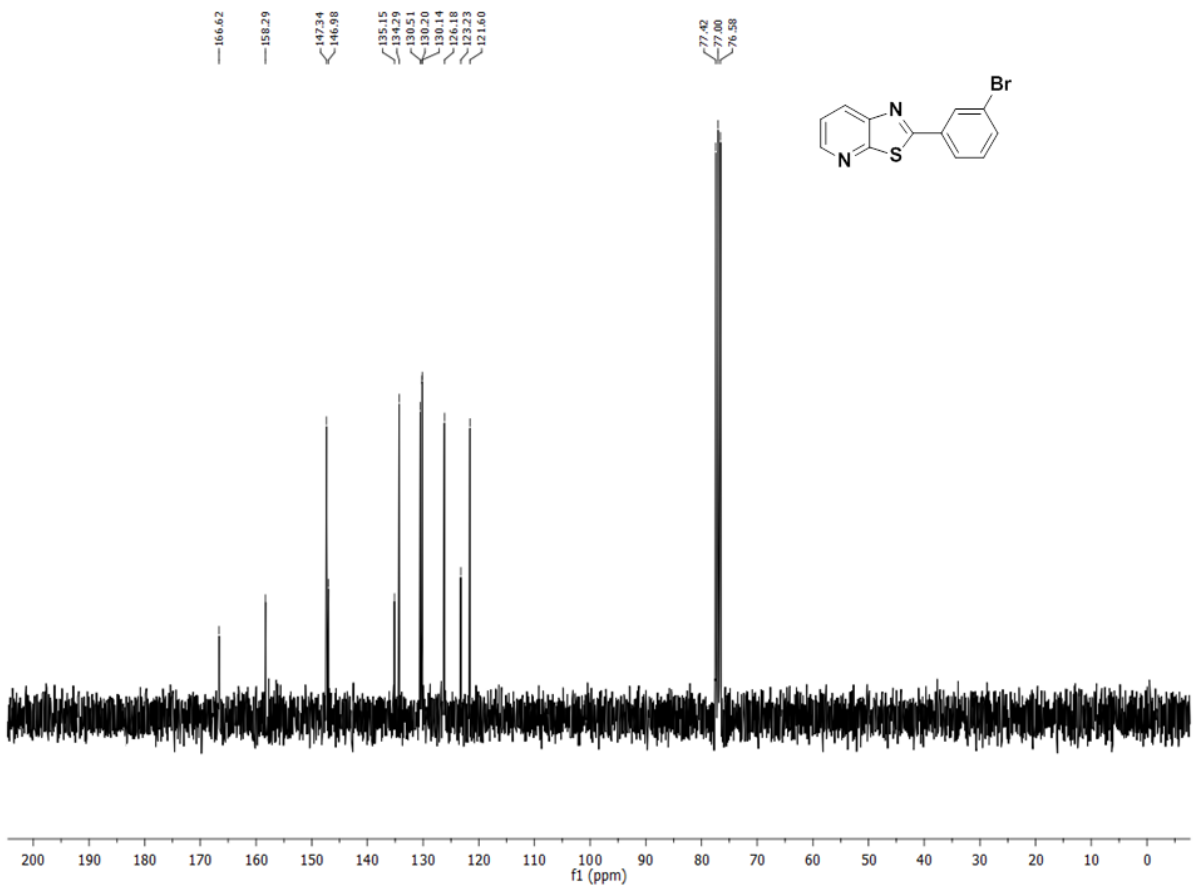


Figure 10. ^{13}C Spectrum of compound **3ae**

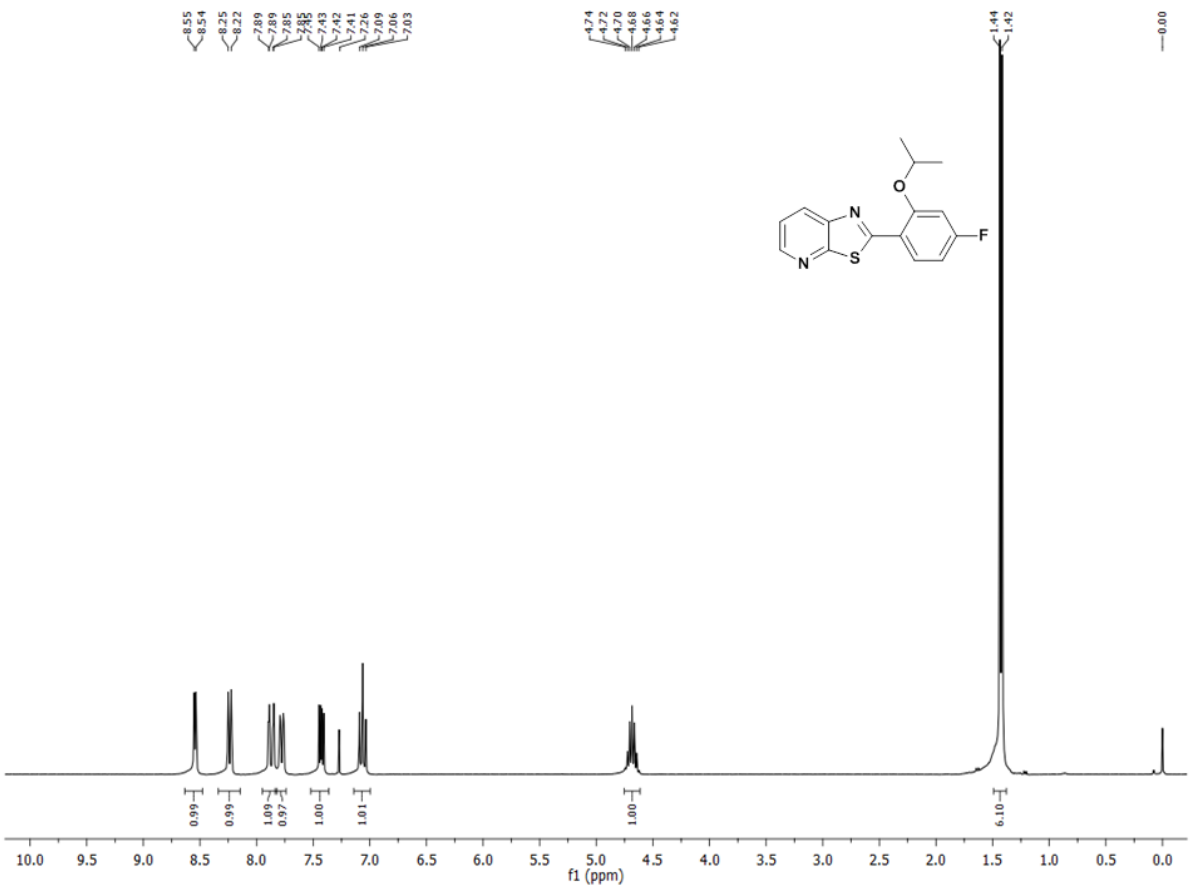


Figure 11. ^{1}H NMR Spectrum of compound **3af**

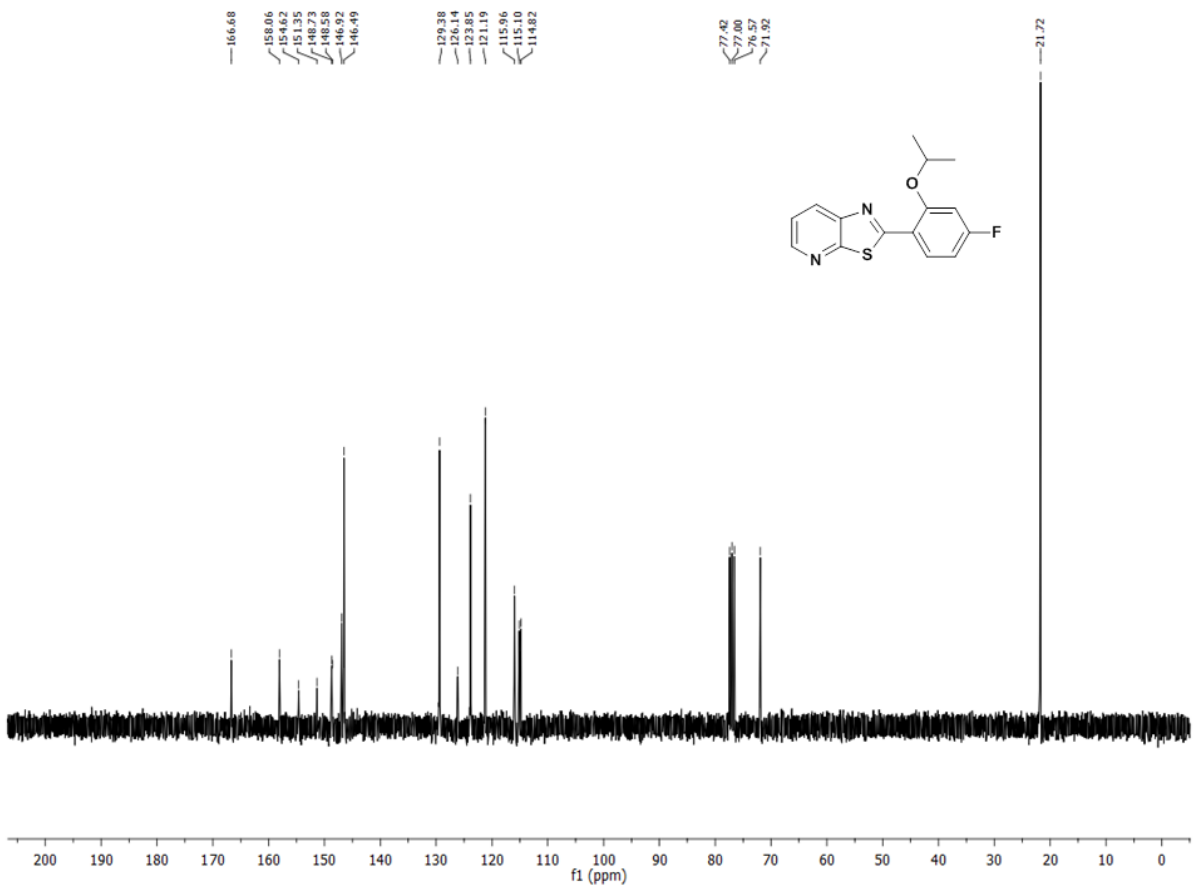


Figure 12. ^{13}C Spectrum of compound **3af**

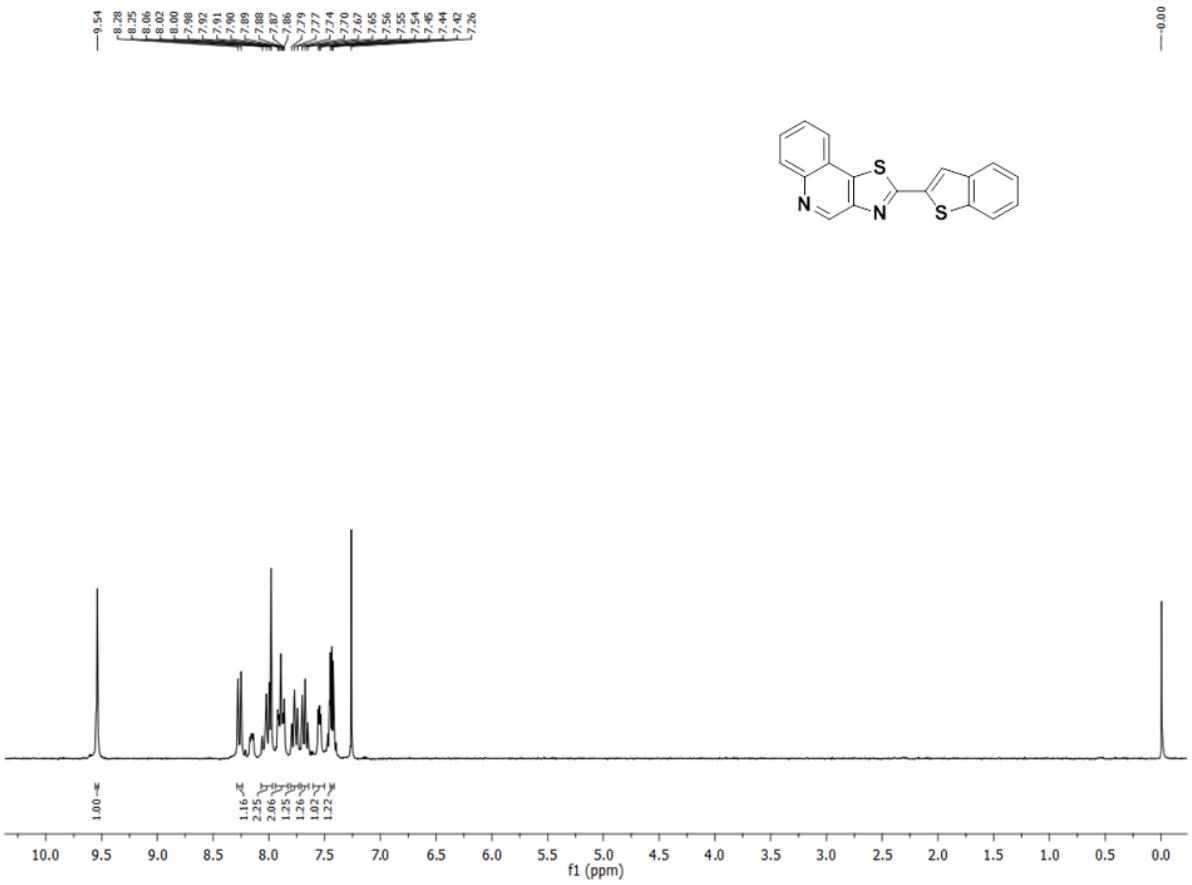


Figure 13. ^{1}H NMR Spectrum of compound **3ag**

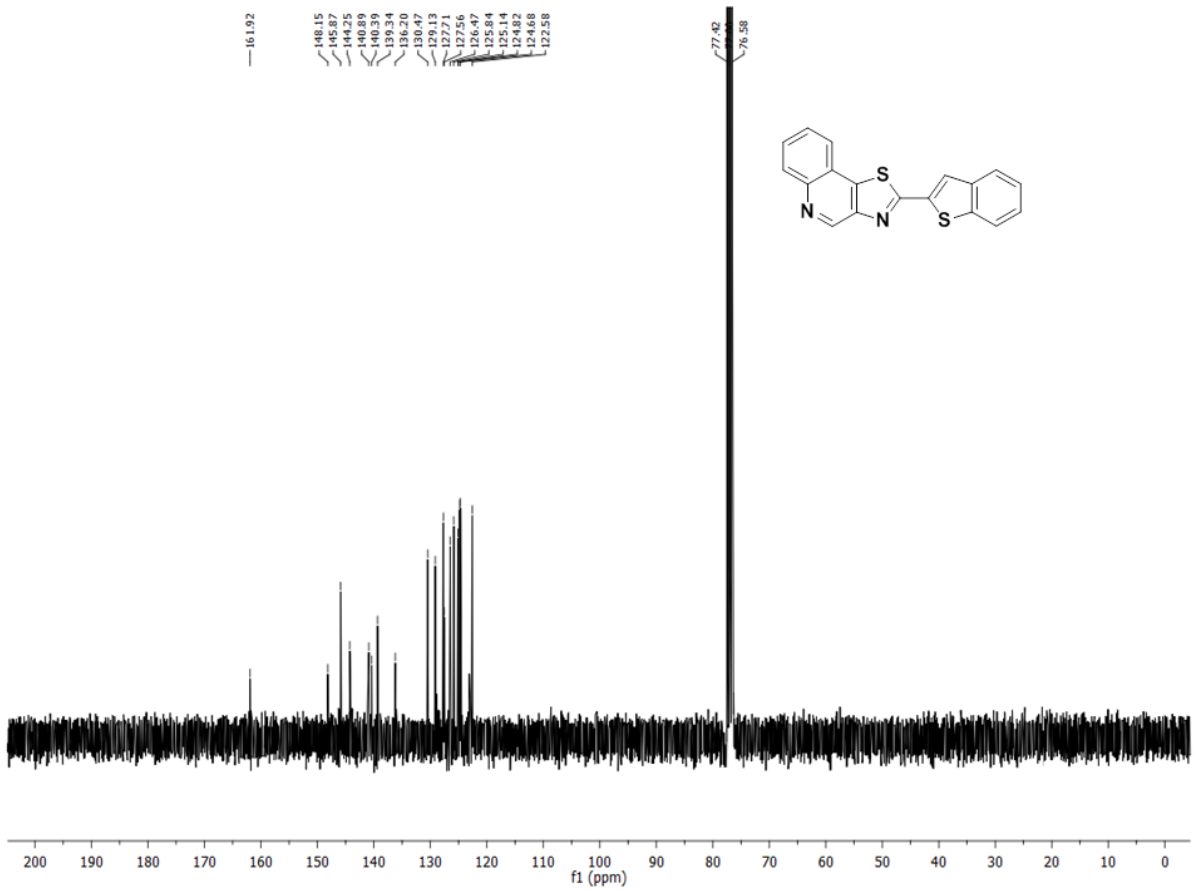


Figure 14. ^{13}C Spectrum of compound **3ag**

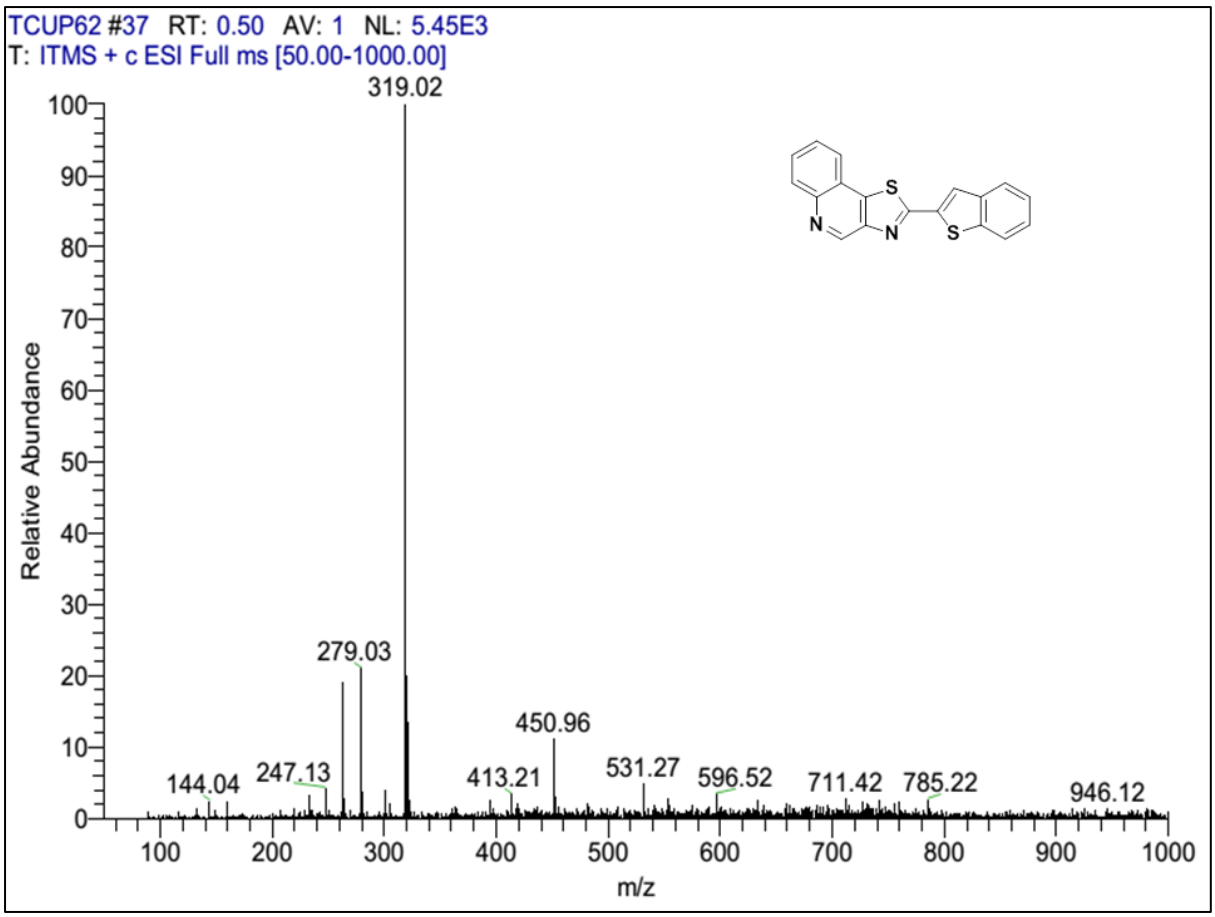


Figure 15. Mass Spectrum of compound **3ag**

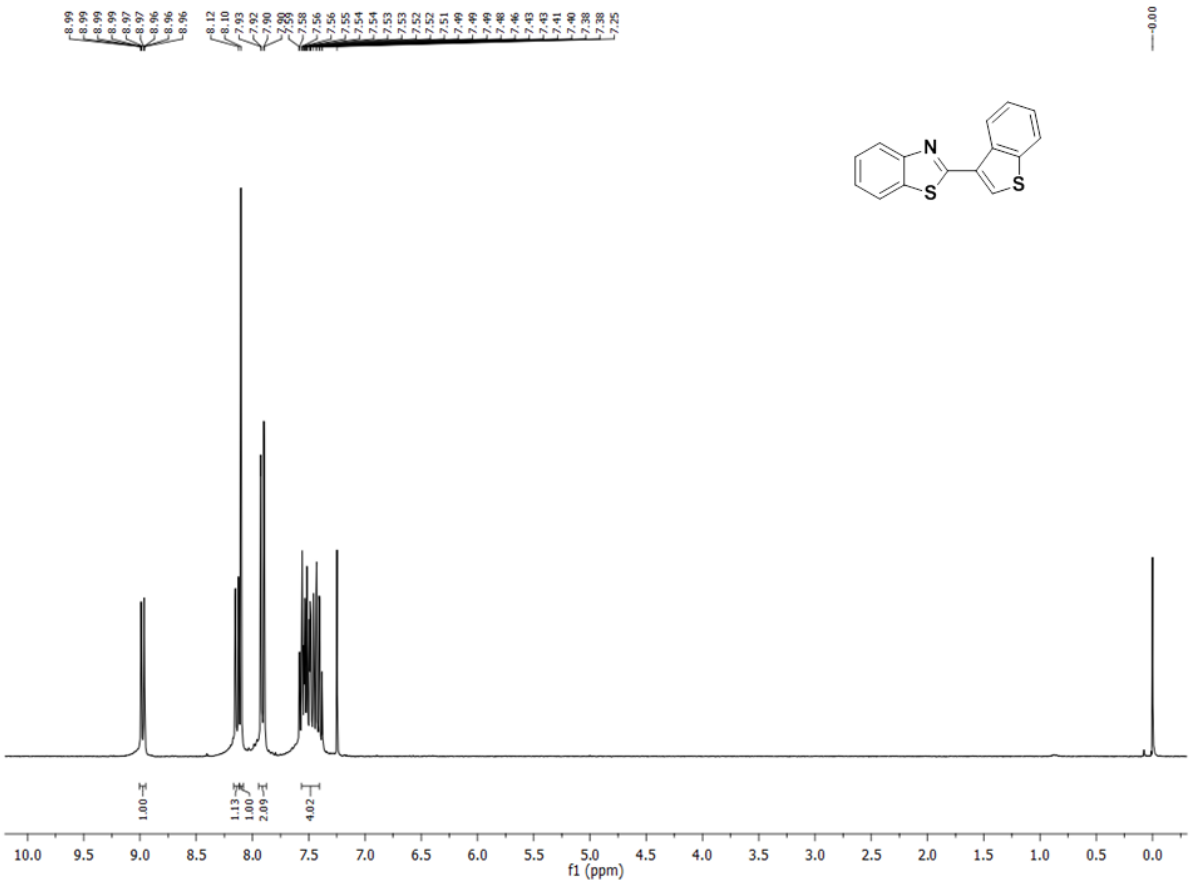


Figure 16. ^{1}H NMR Spectrum of compound **3ah**

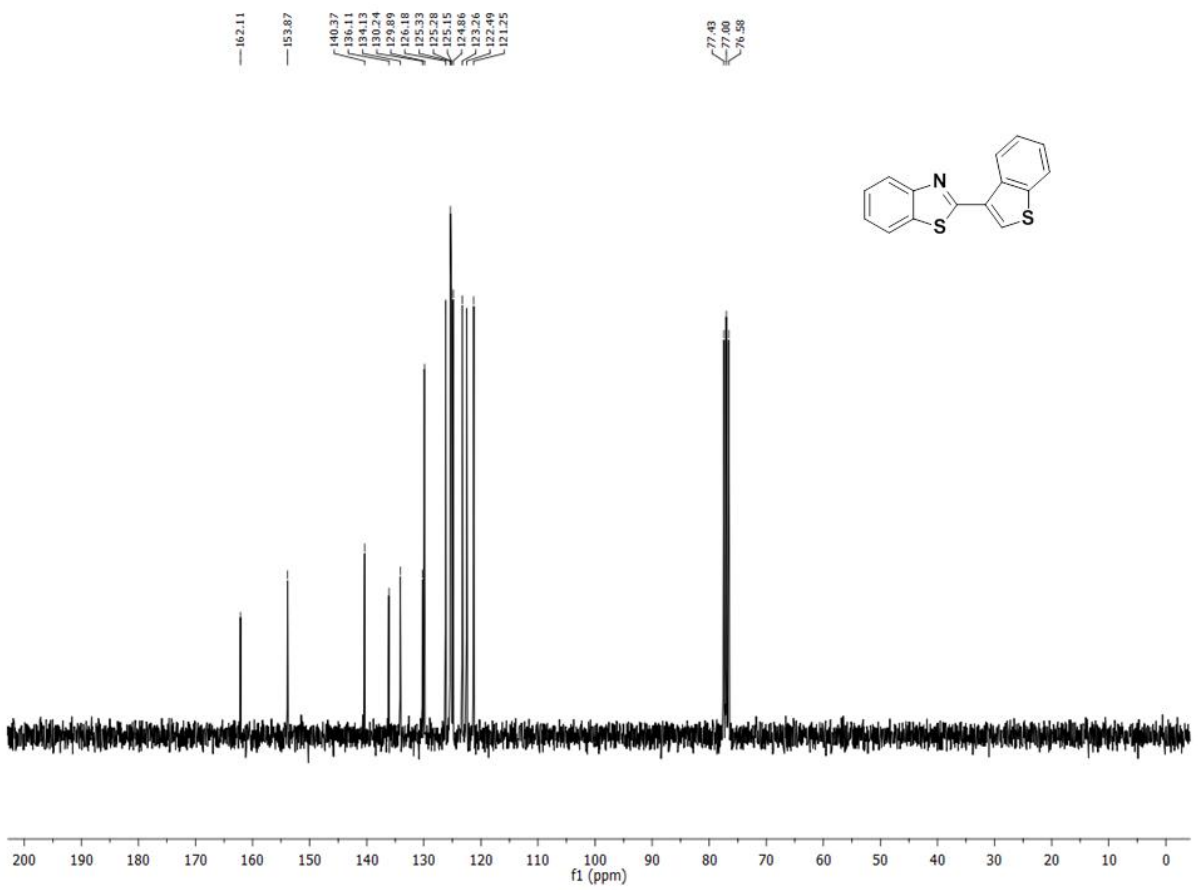


Figure 17. ^{13}C Spectrum of compound **3ah**

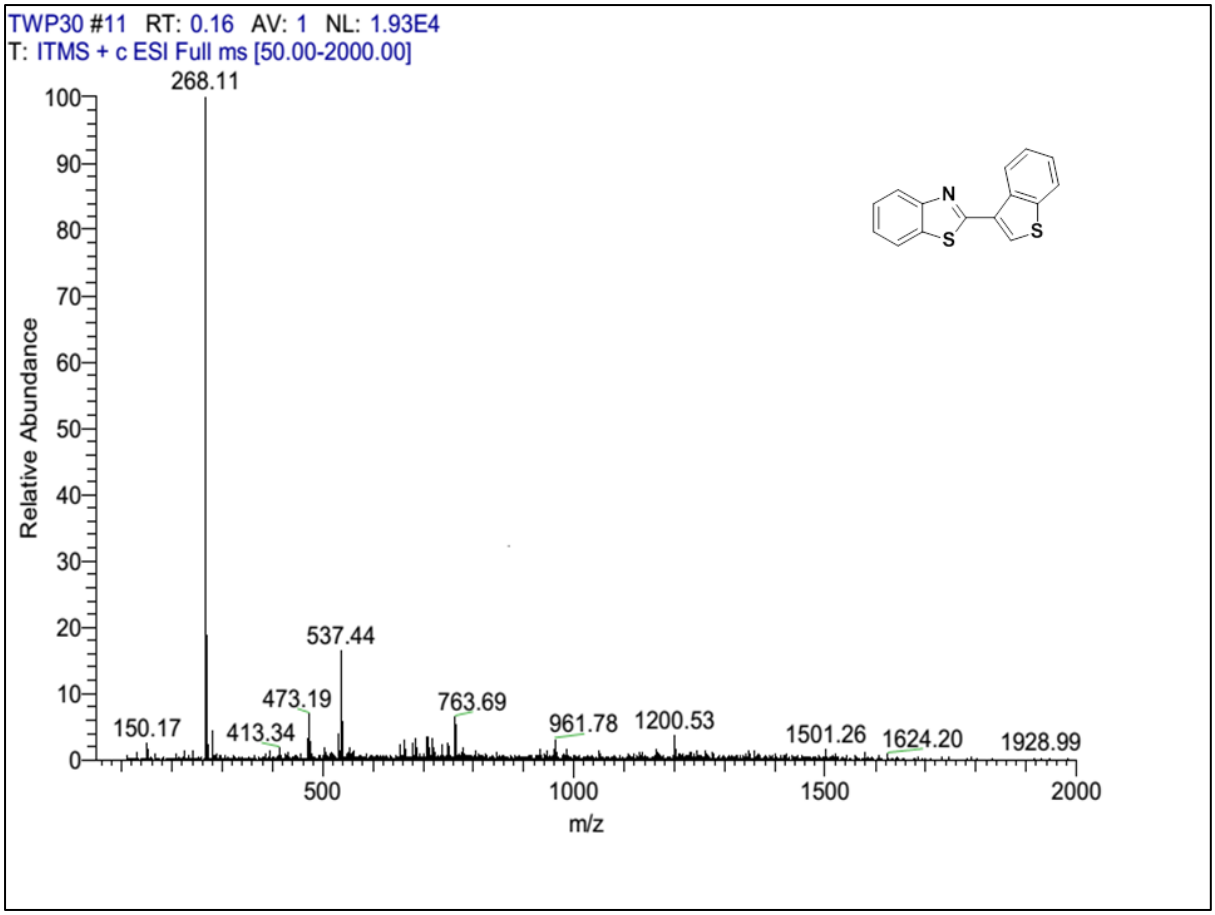


Figure 18. Mass Spectrum of compound **3ah**

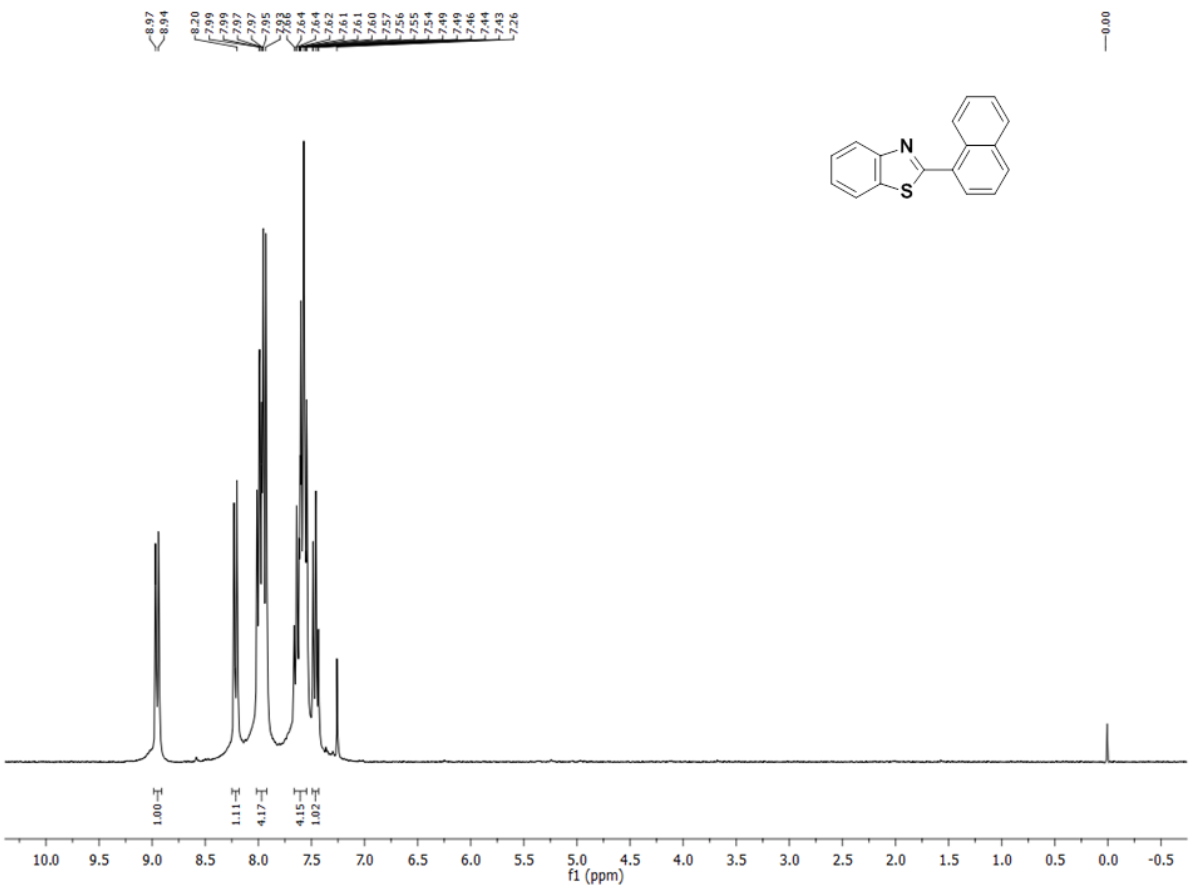


Figure 19. ^{1}H NMR Spectrum of compound **3ai**

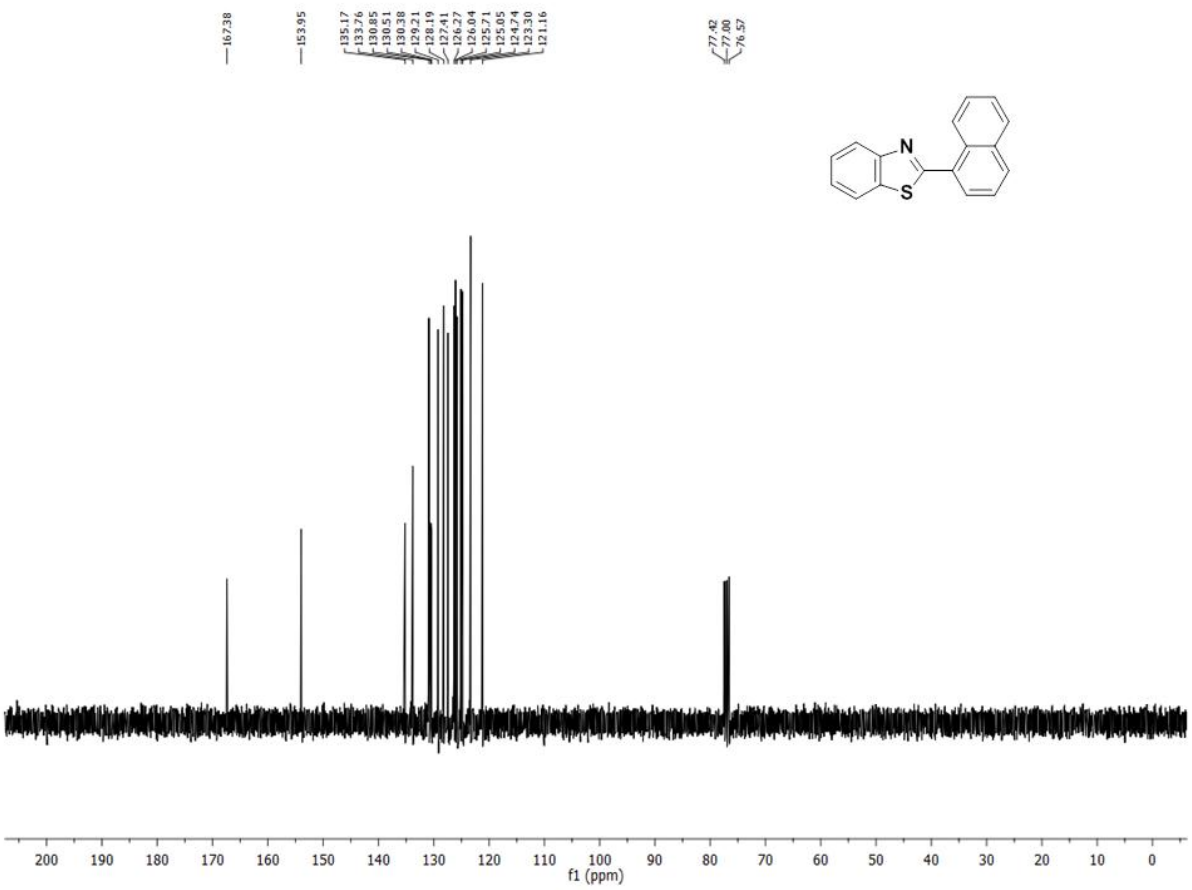


Figure 20. ^{13}C Spectrum of compound **3ai**

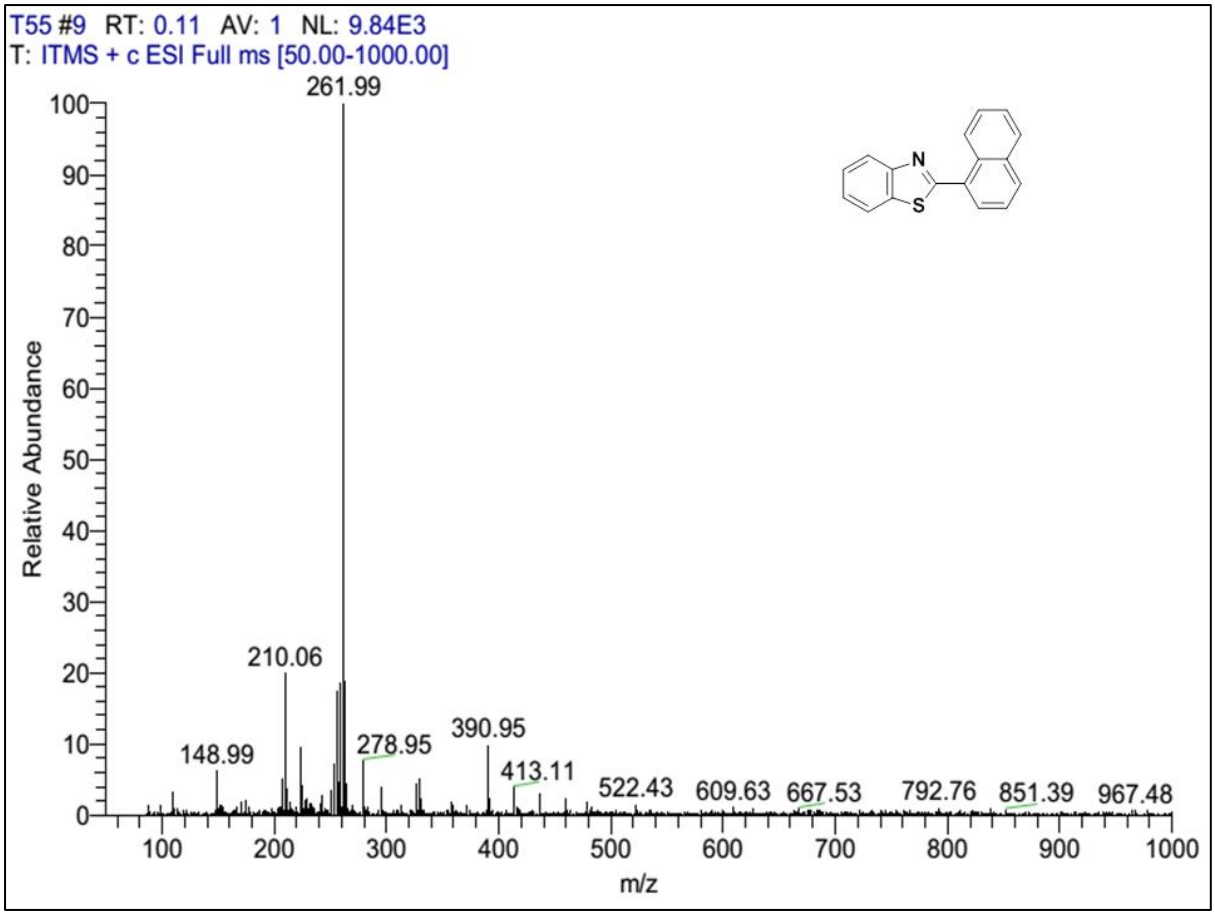


Figure 21. Mass Spectrum of compound **3ai**

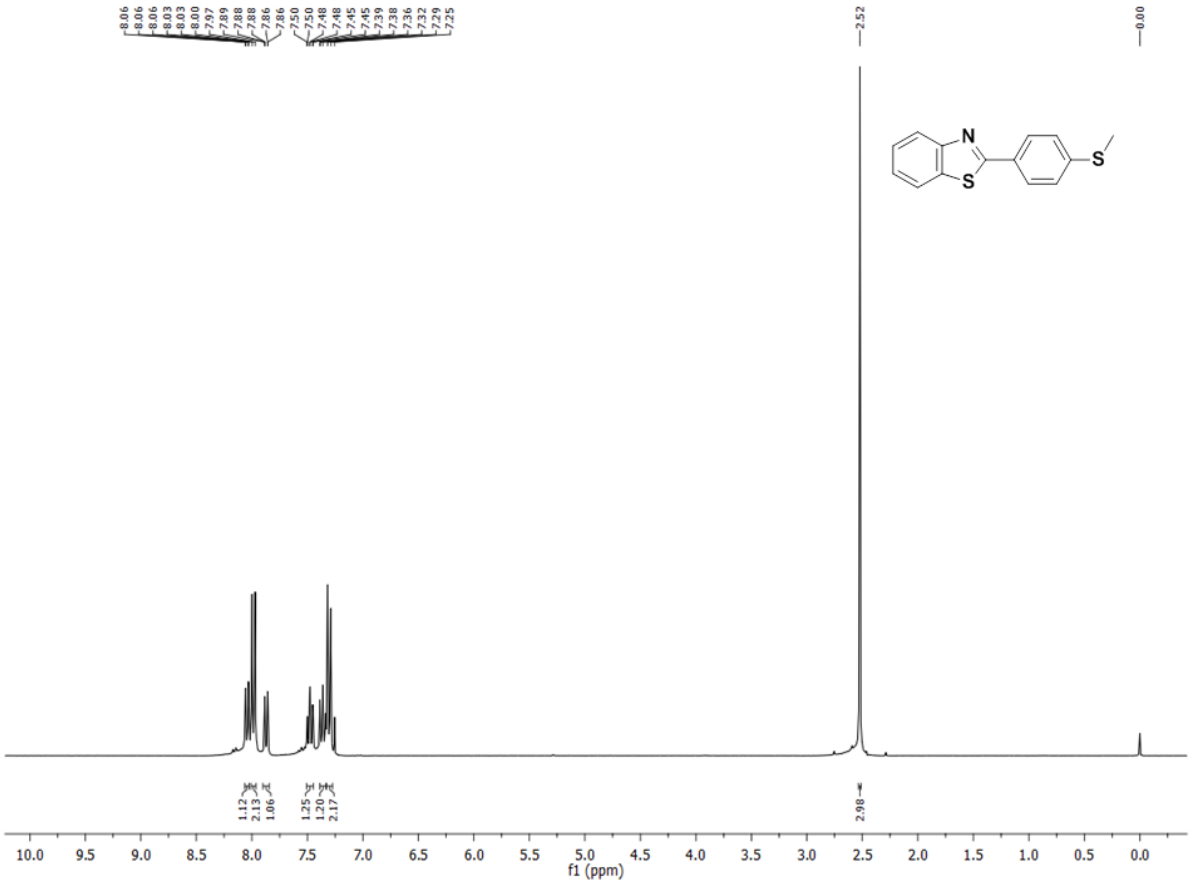


Figure 22. ^{1}H NMR Spectrum of compound **3aj**

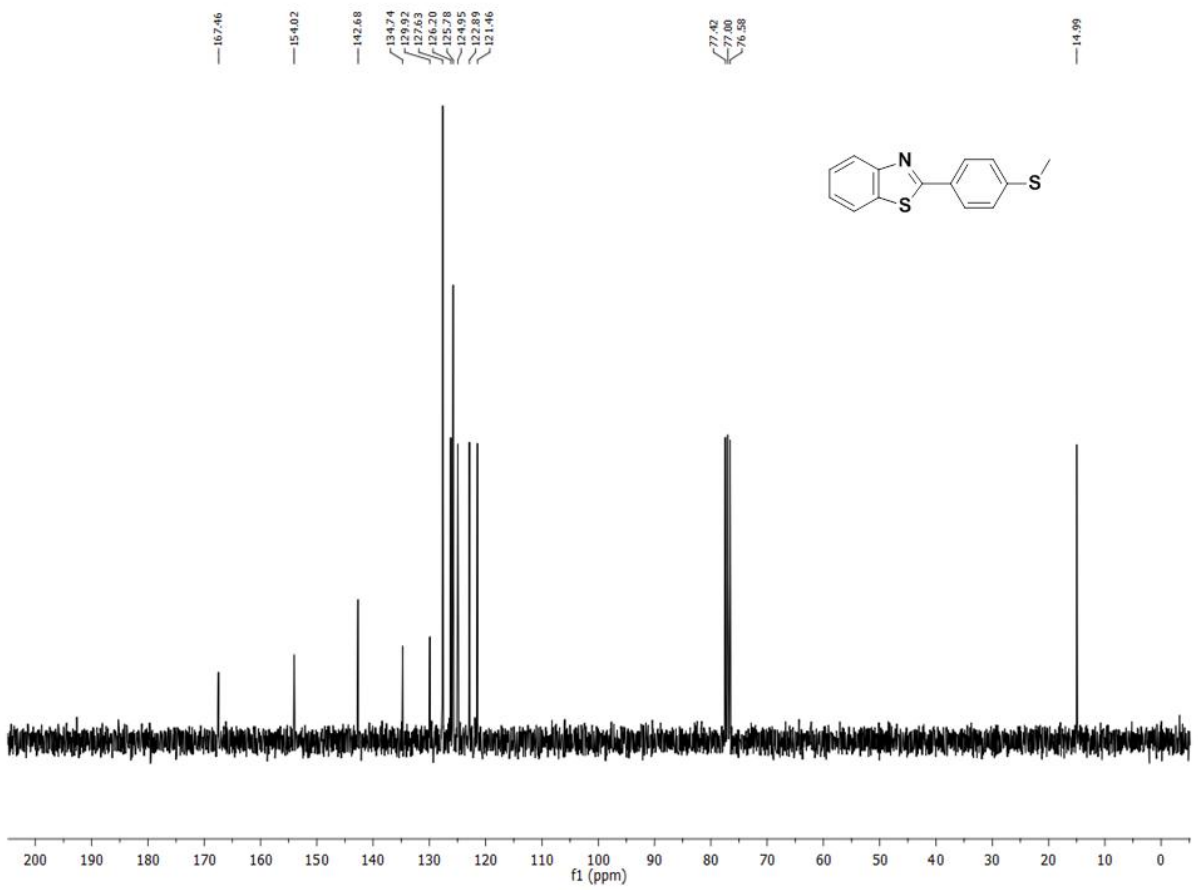


Figure 23. ^{13}C Spectrum of compound **3aj**

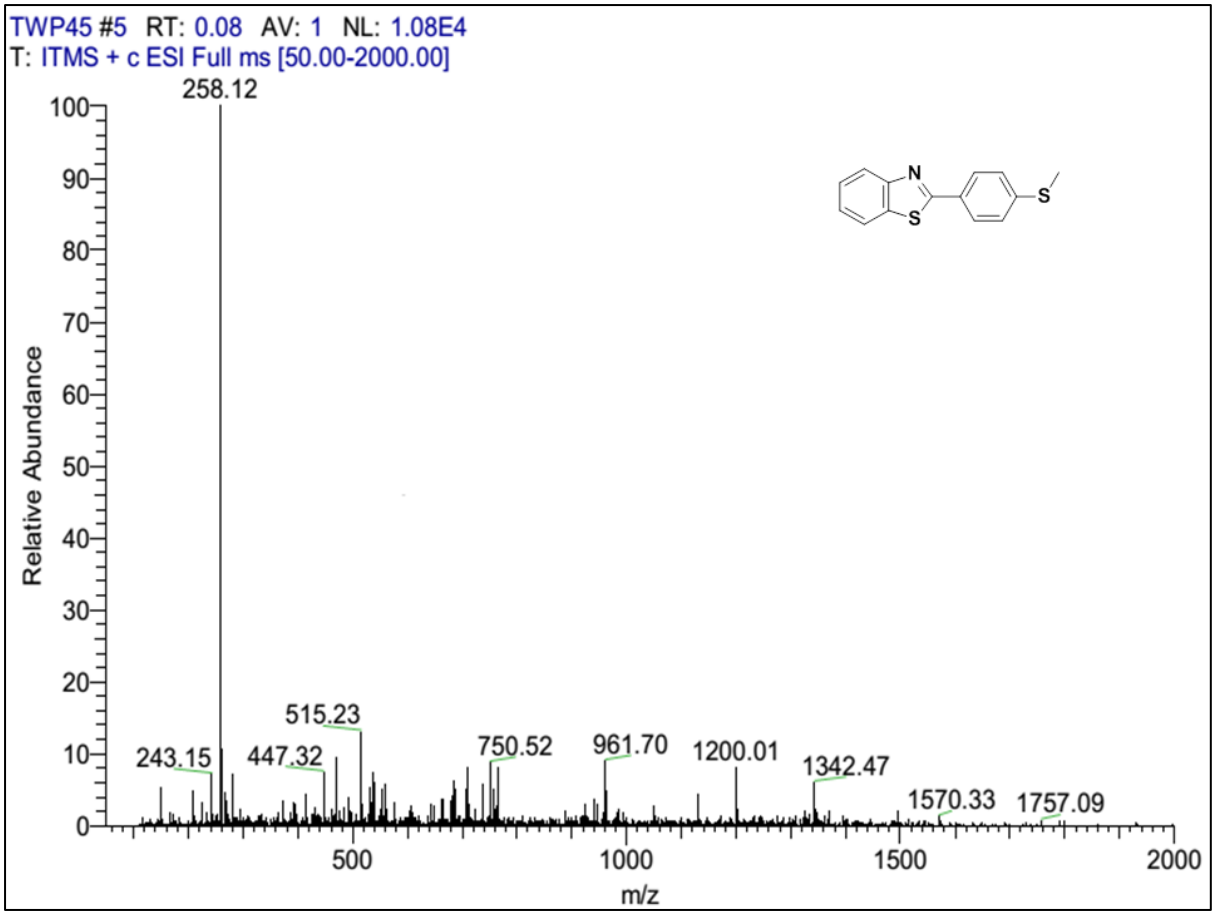


Figure 24. Mass Spectrum of compound **3aj**

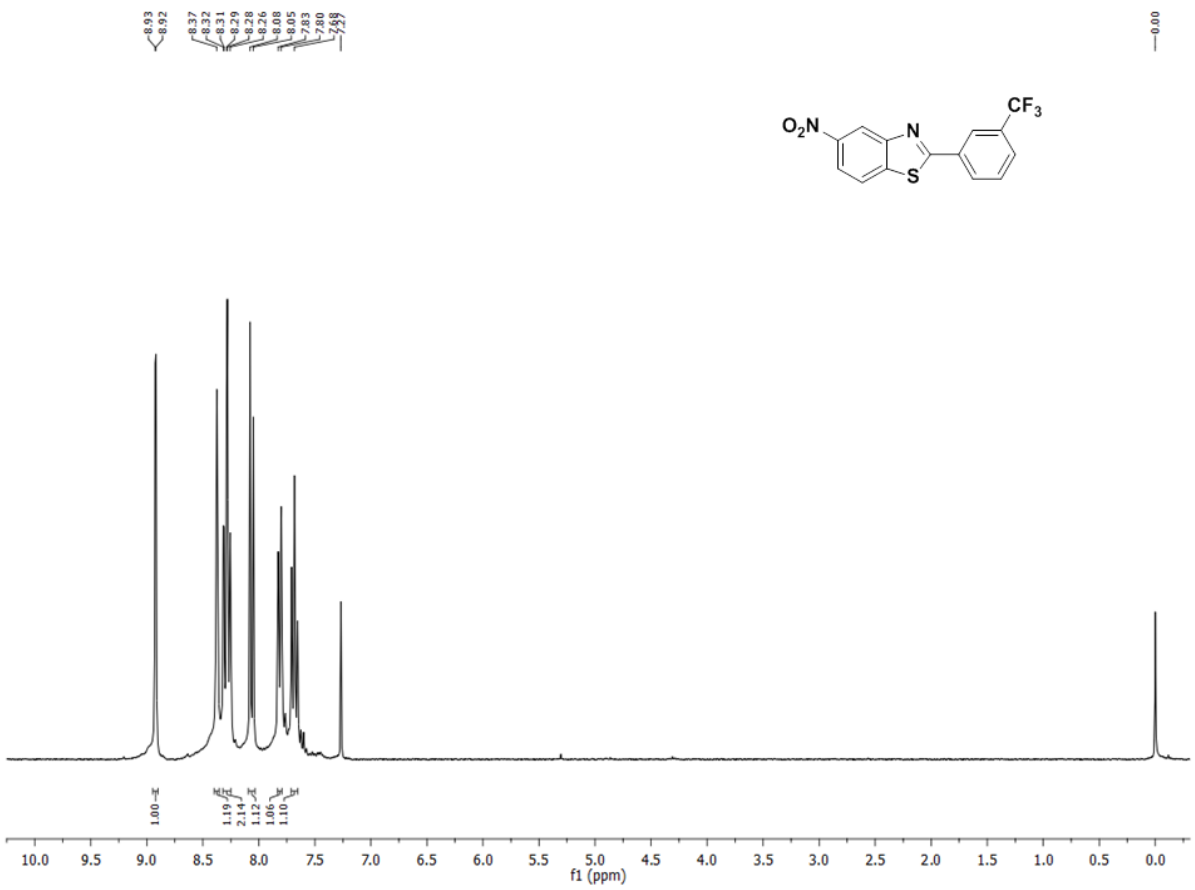


Figure 25. ^{1}H NMR Spectrum of compound **3ak**

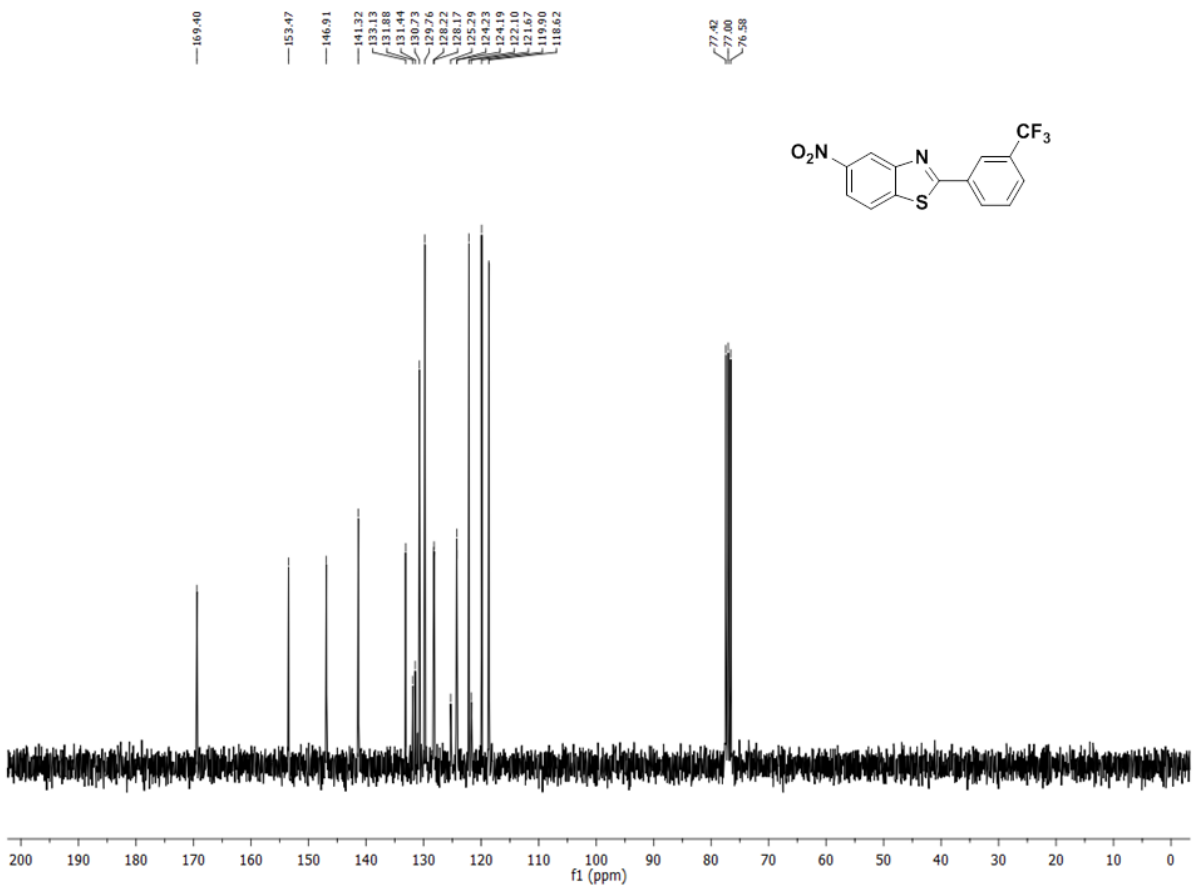


Figure 26. ^{13}C Spectrum of compound **3ak**

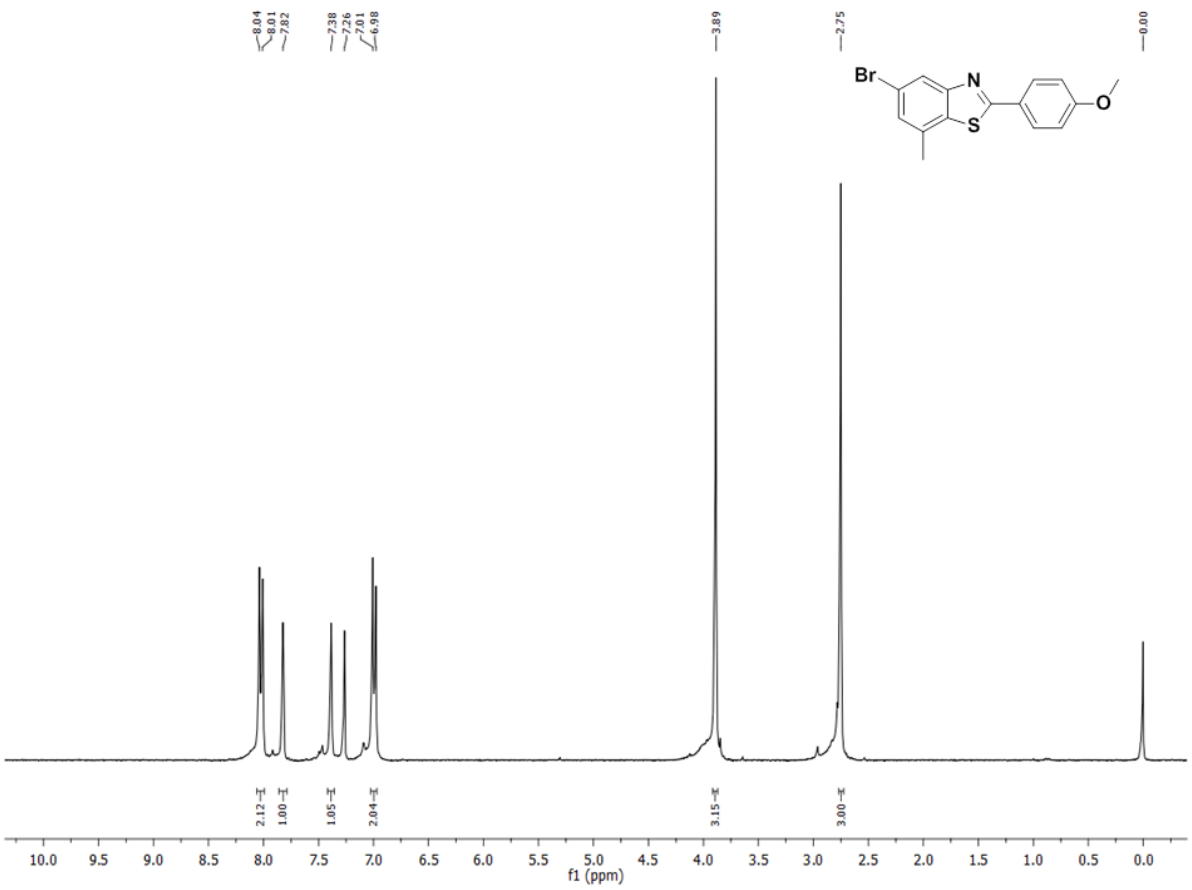


Figure 27. ^{1}H NMR Spectrum of compound **3al**

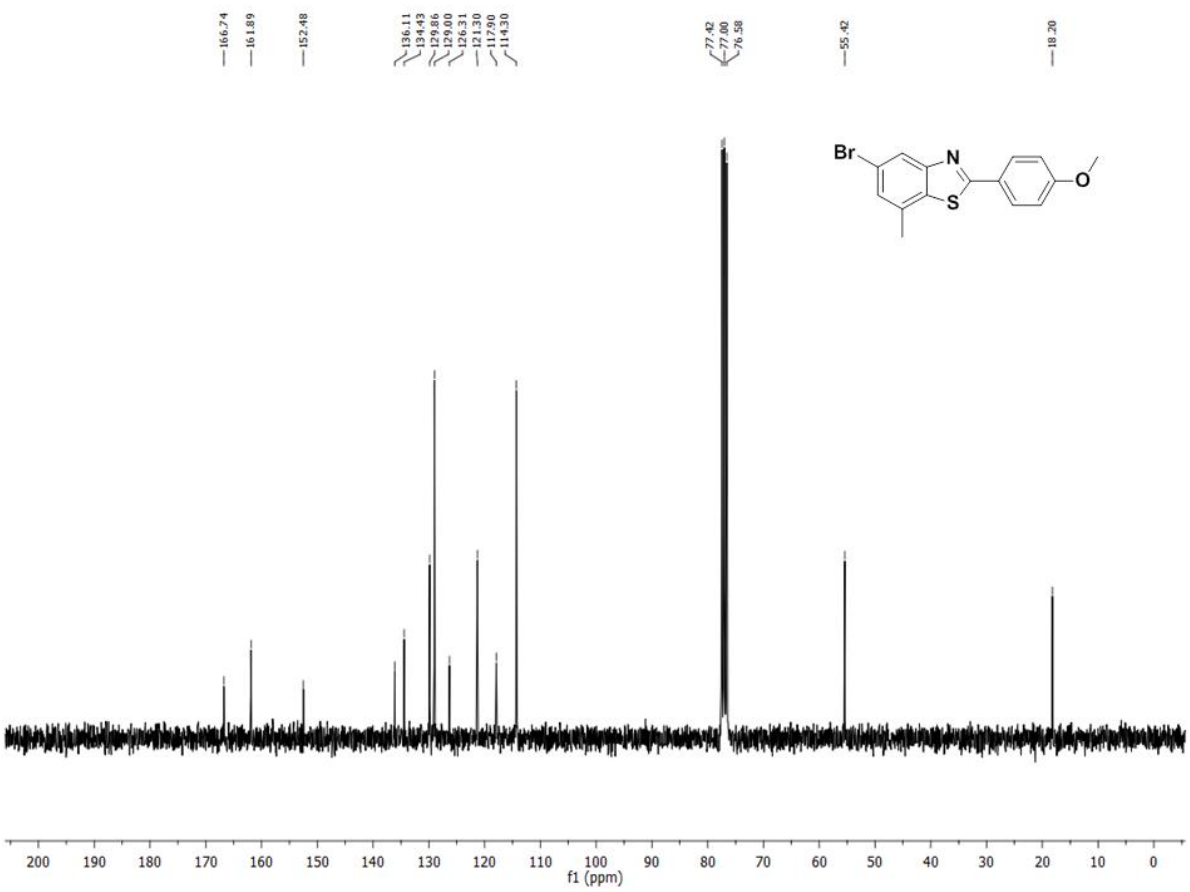


Figure 28. ^{13}C Spectrum of compound **3al**

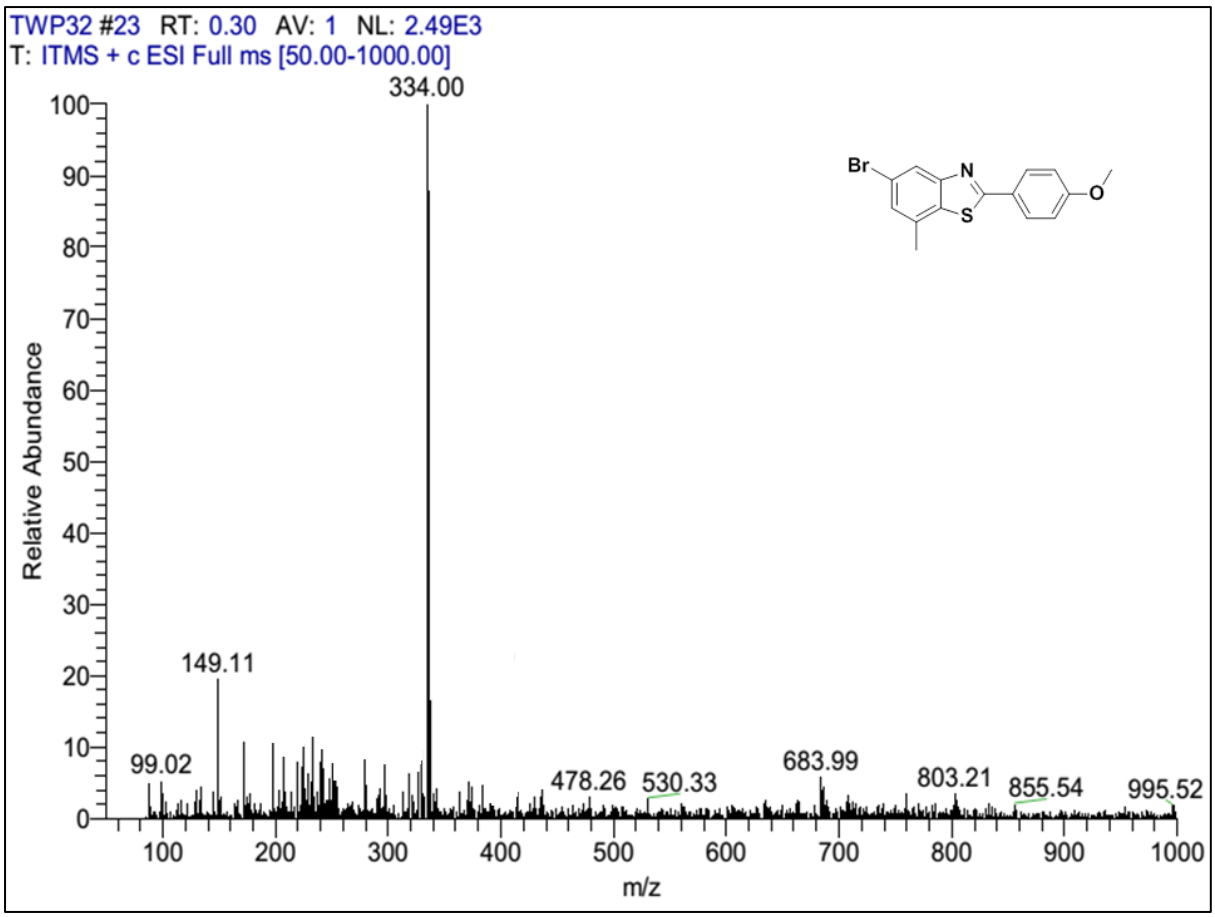


Figure 29. Mass Spectrum of compound **3al**

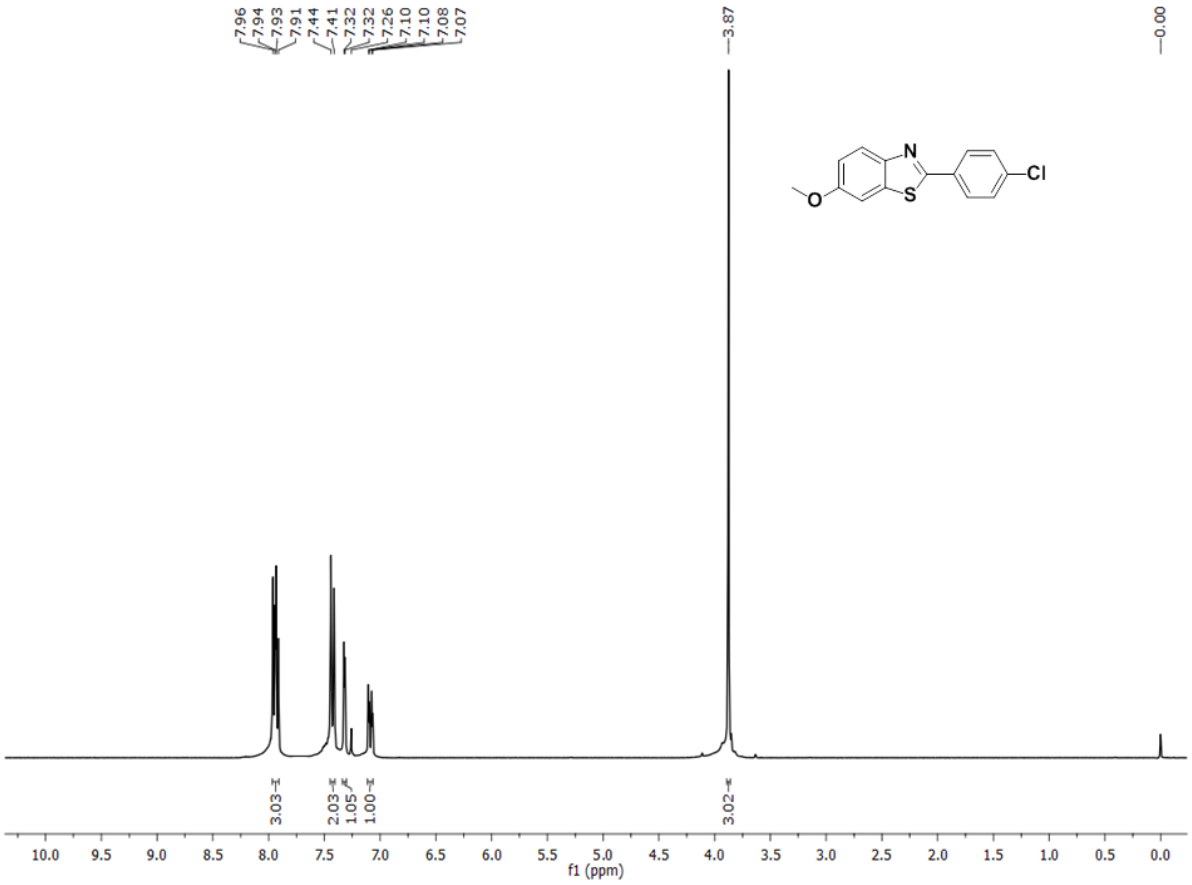


Figure 30. ^{1}H NMR Spectrum of compound **3am**

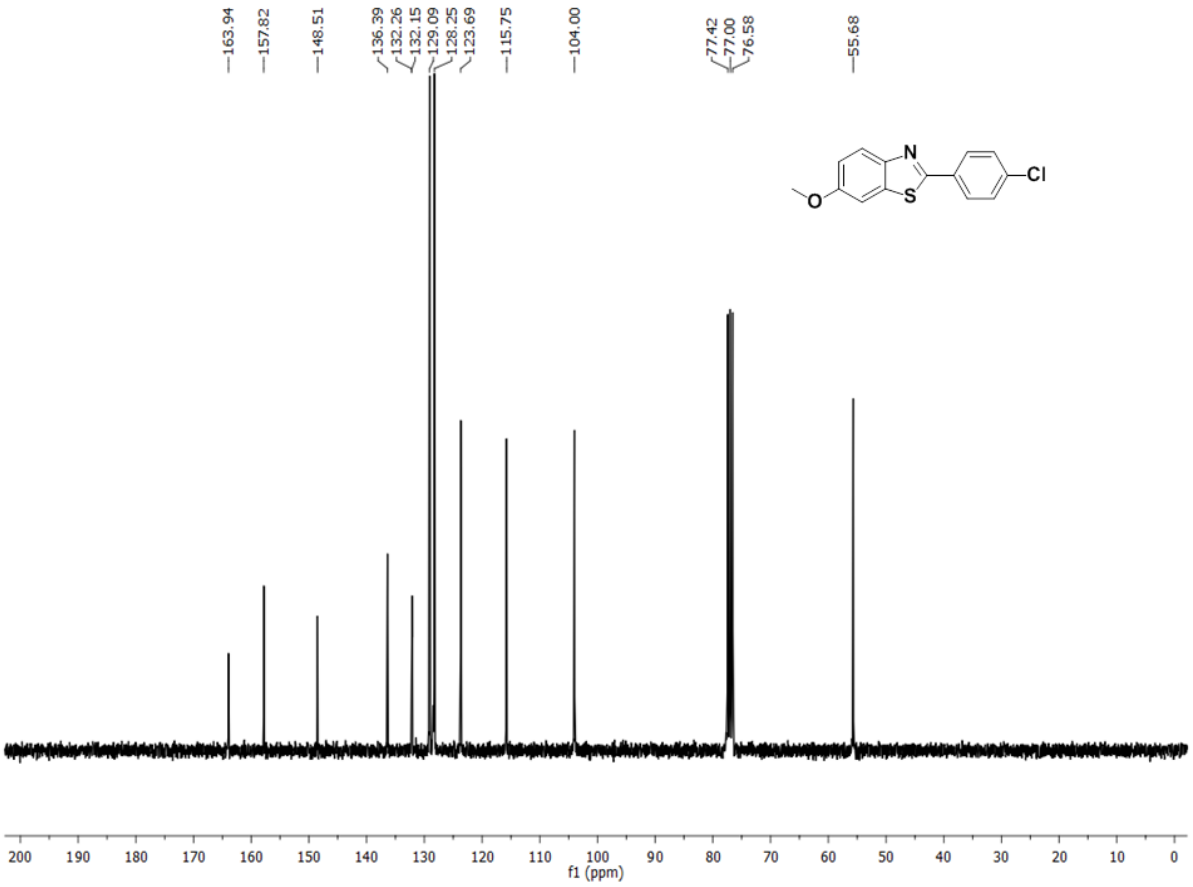


Figure 31. ^{13}C NMR Spectrum of compound **3am**

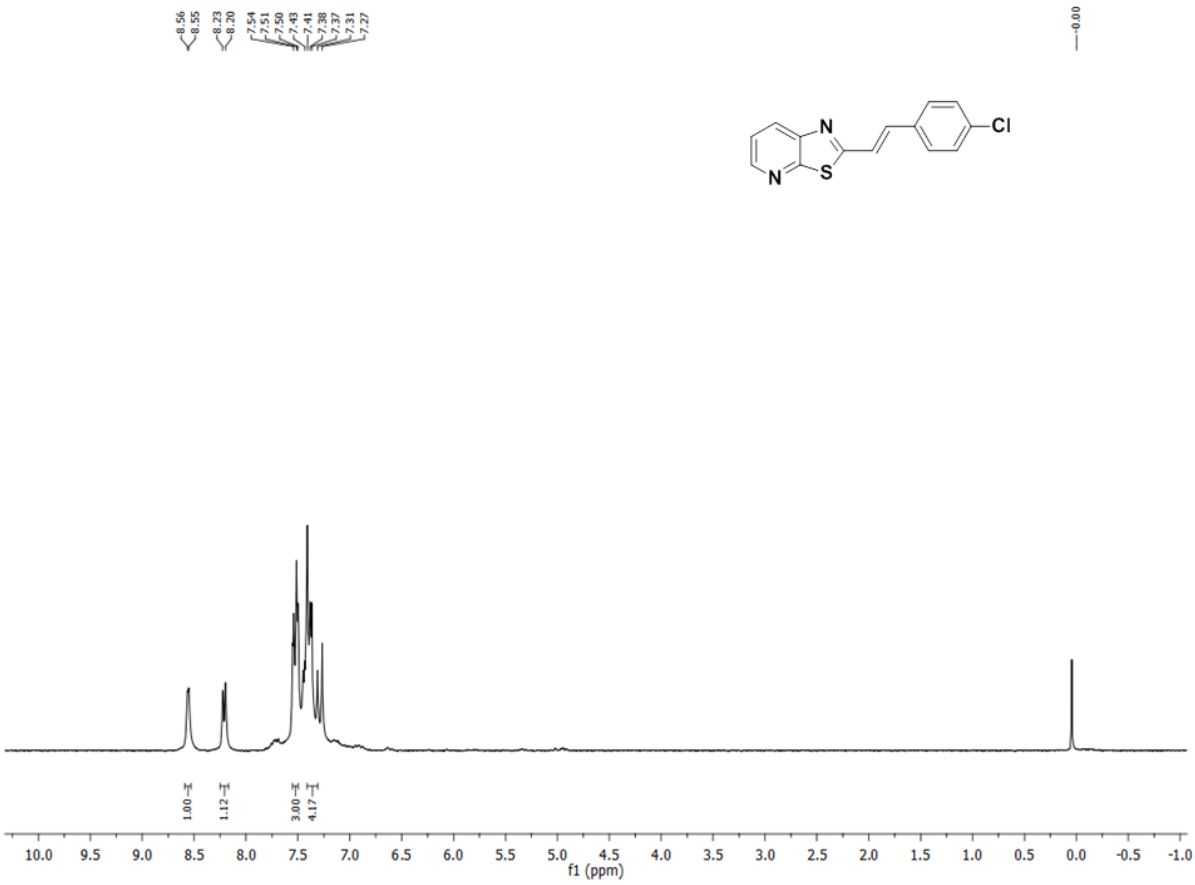


Figure 32. ^{1}H NMR Spectrum of compound **3an**

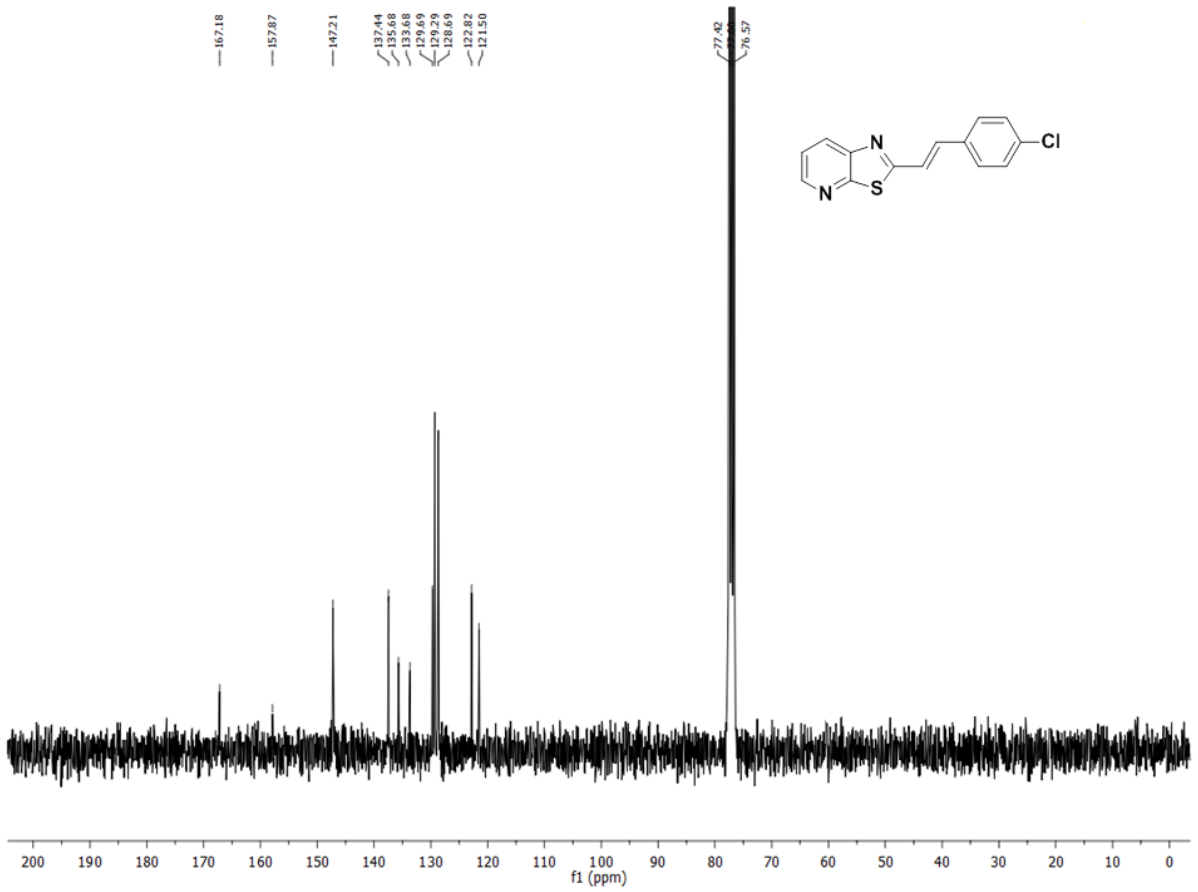


Figure 33. ^{13}C Spectrum of compound **3an**

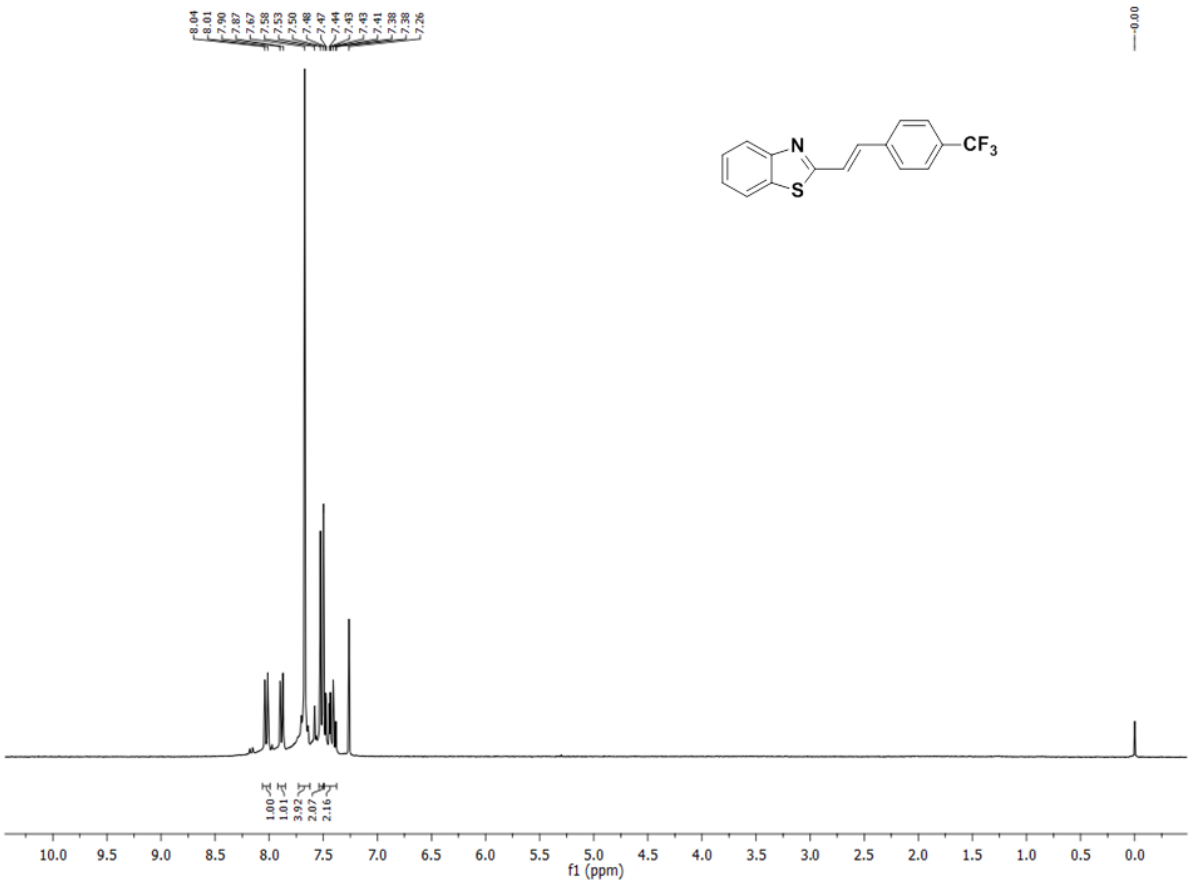


Figure 34. ^{1}H NMR Spectrum of compound **3ao**

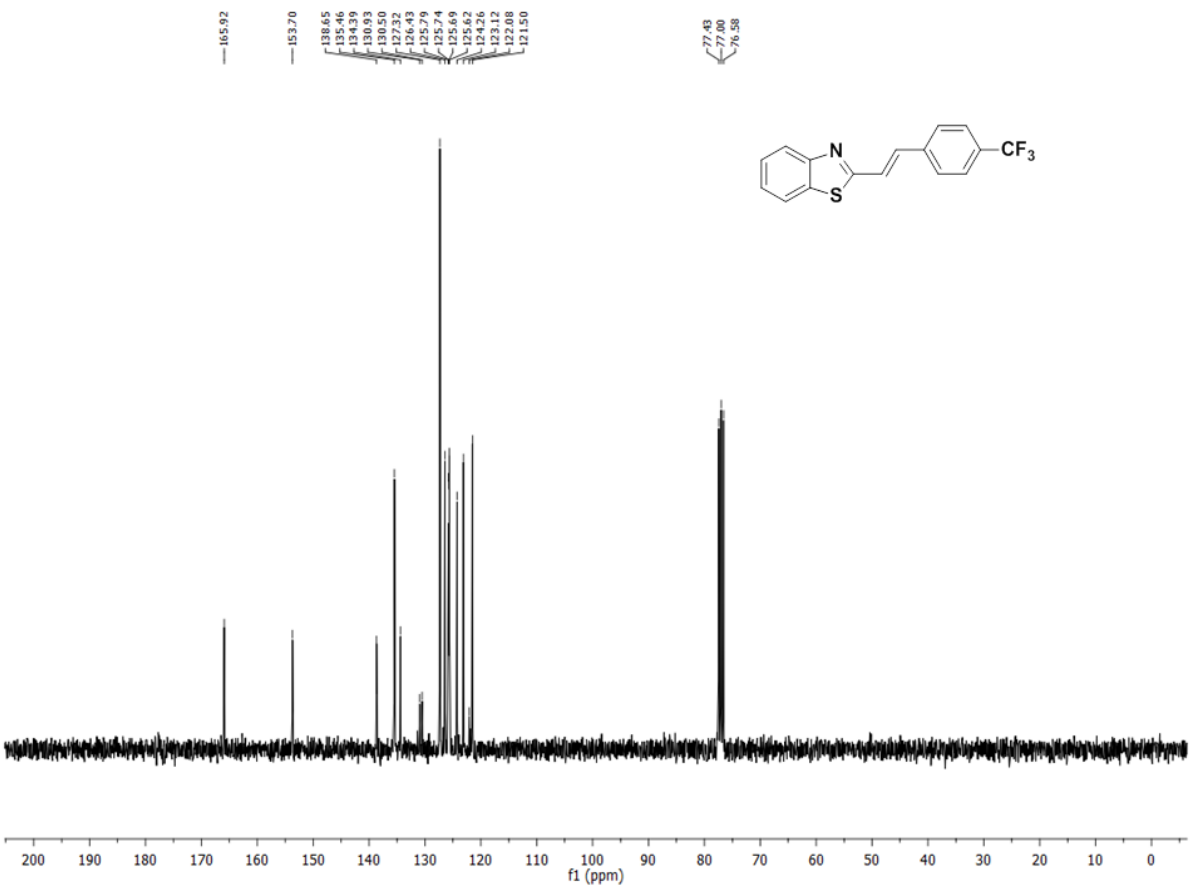


Figure 35. ^{13}C Spectrum of compound **3ao**

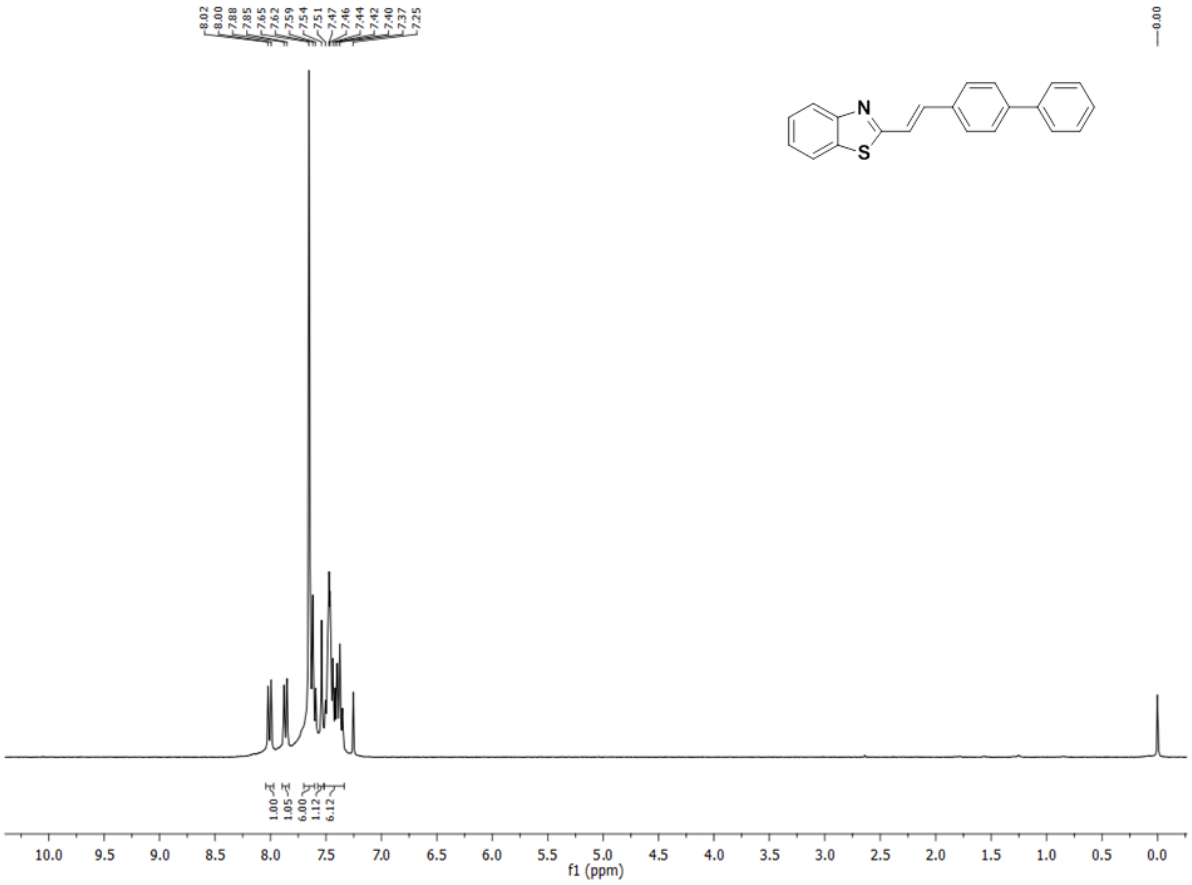


Figure 36. ^{1}H NMR Spectrum of compound **3ap**

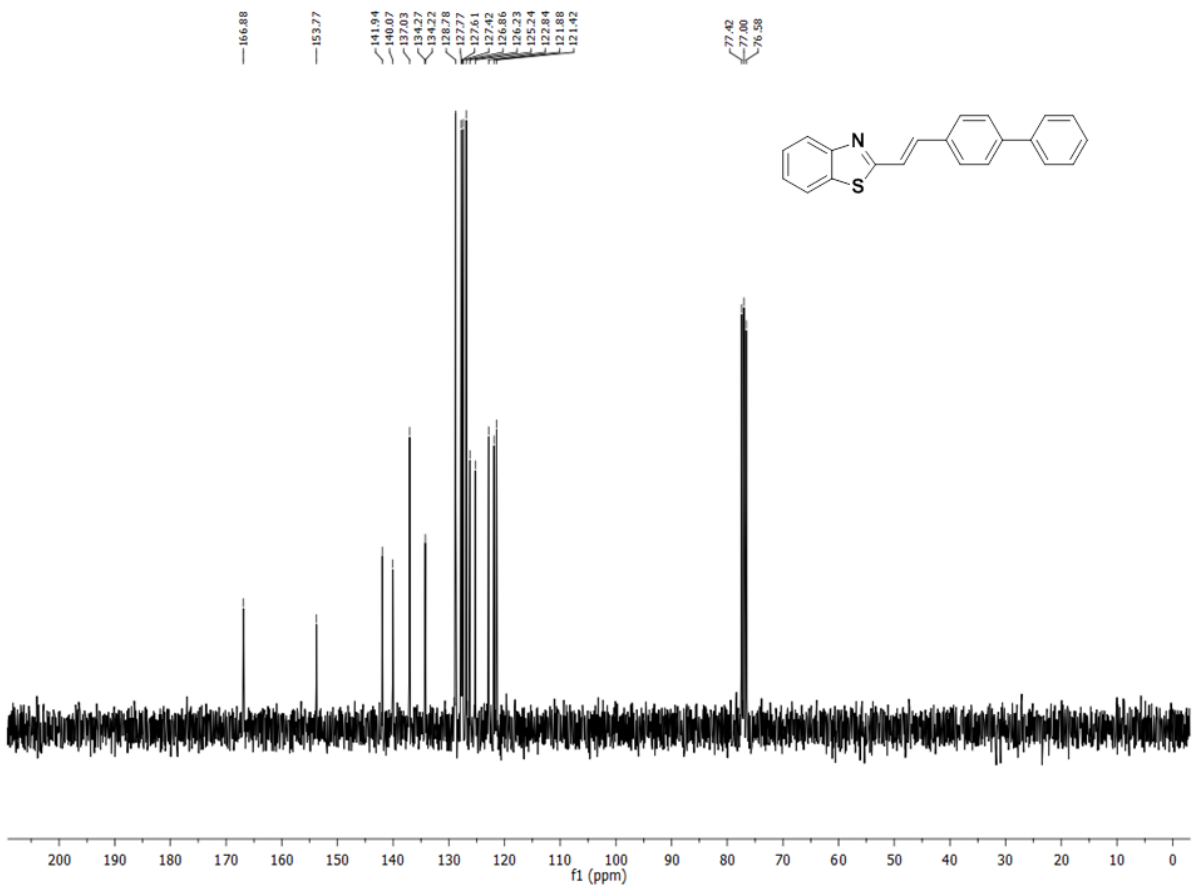


Figure 37. ^{13}C Spectrum of compound **3ap**

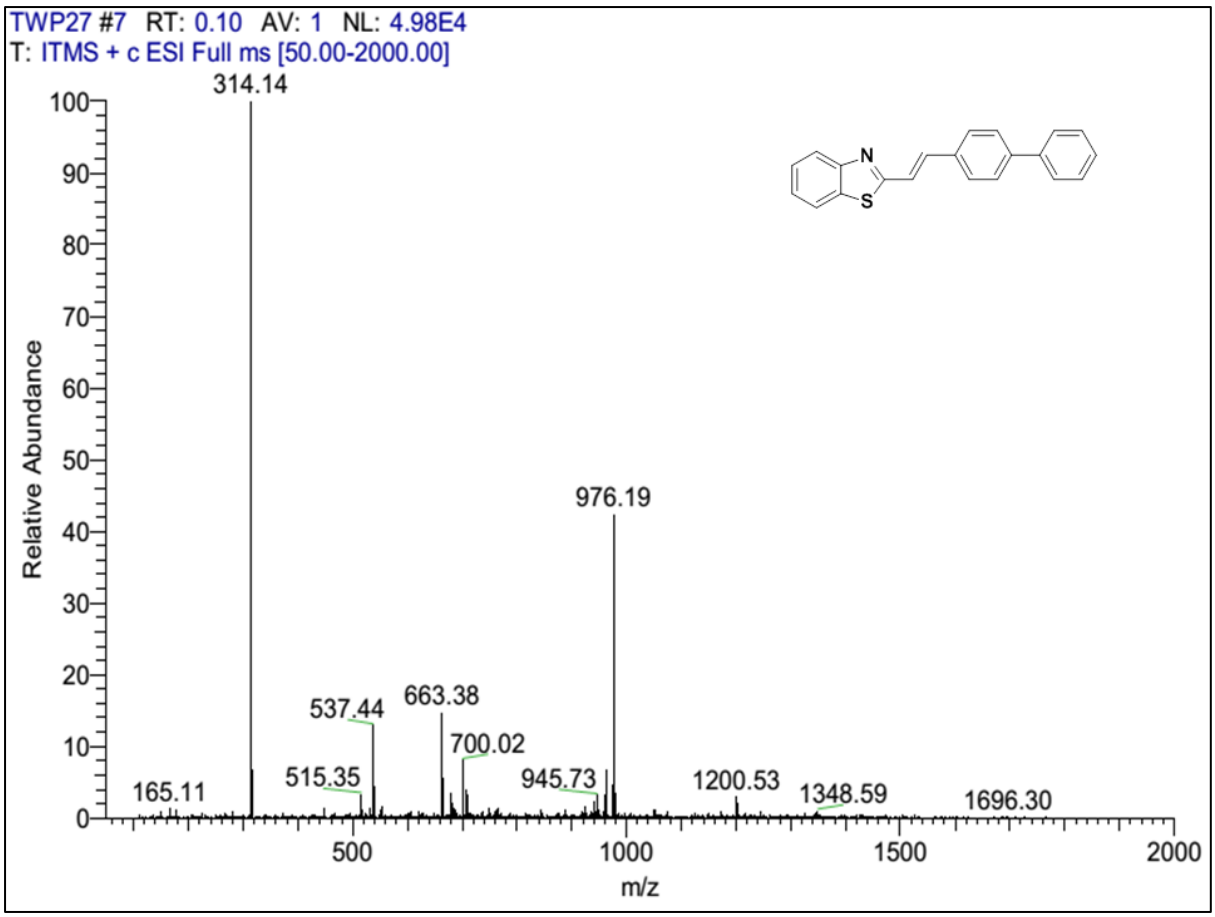


Figure 38. Mass Spectrum of compound **3ap**

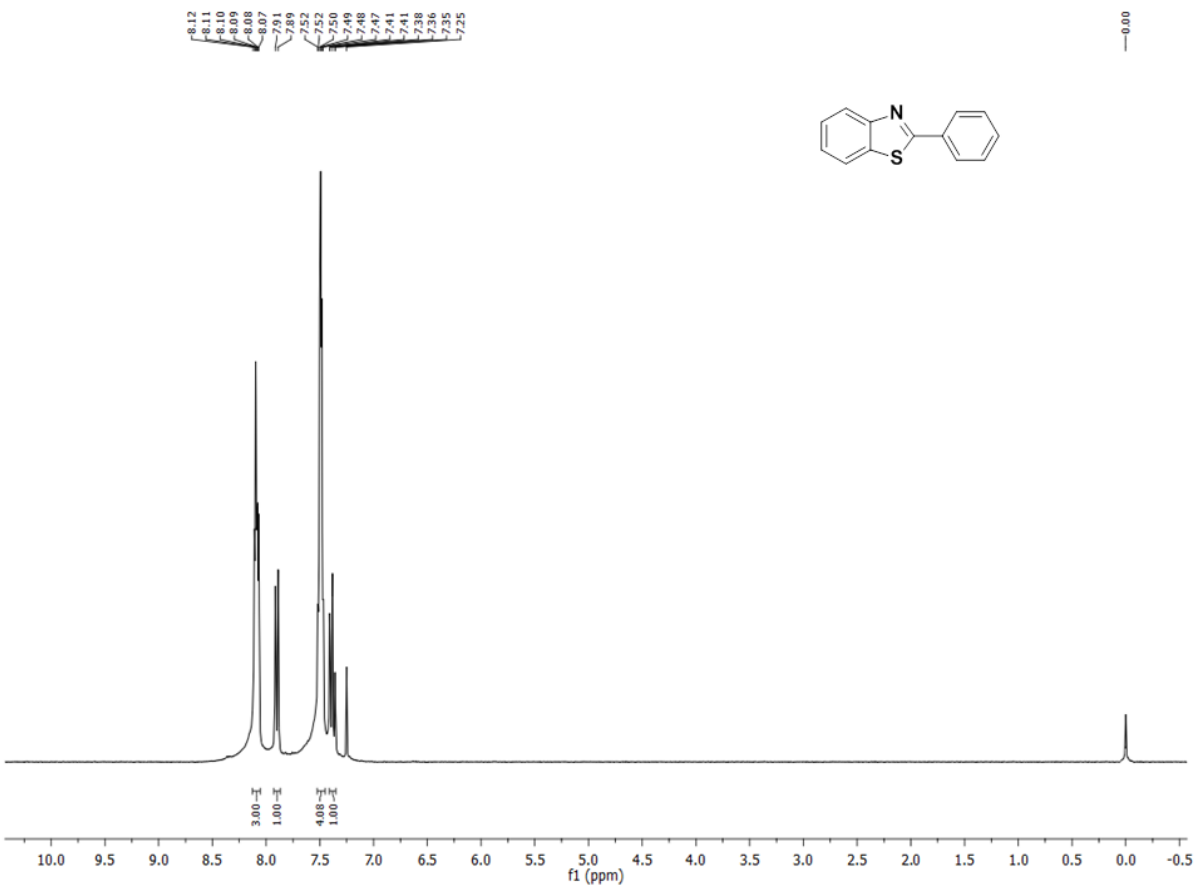


Figure 39. ^{1}H NMR Spectrum of compound **3aq**

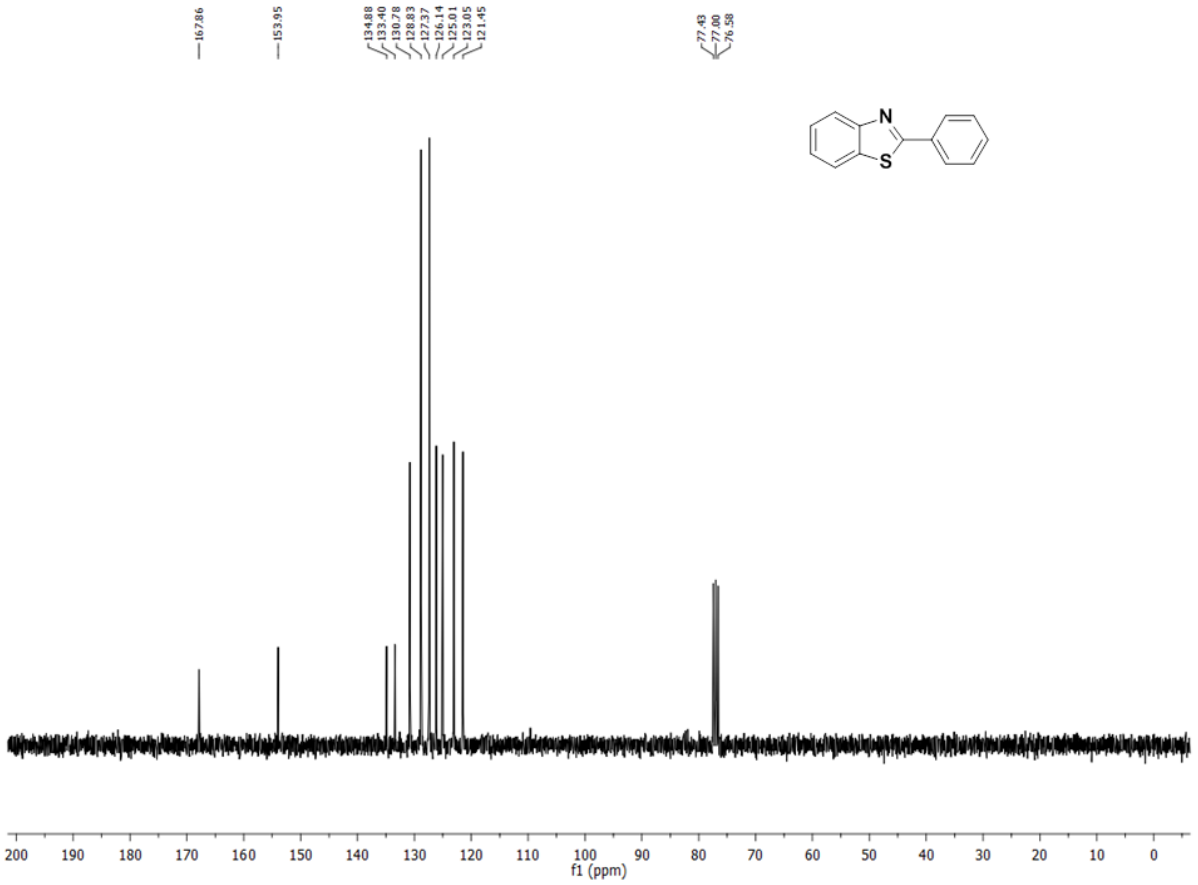


Figure 40. ^{13}C Spectrum of compound **3aq**

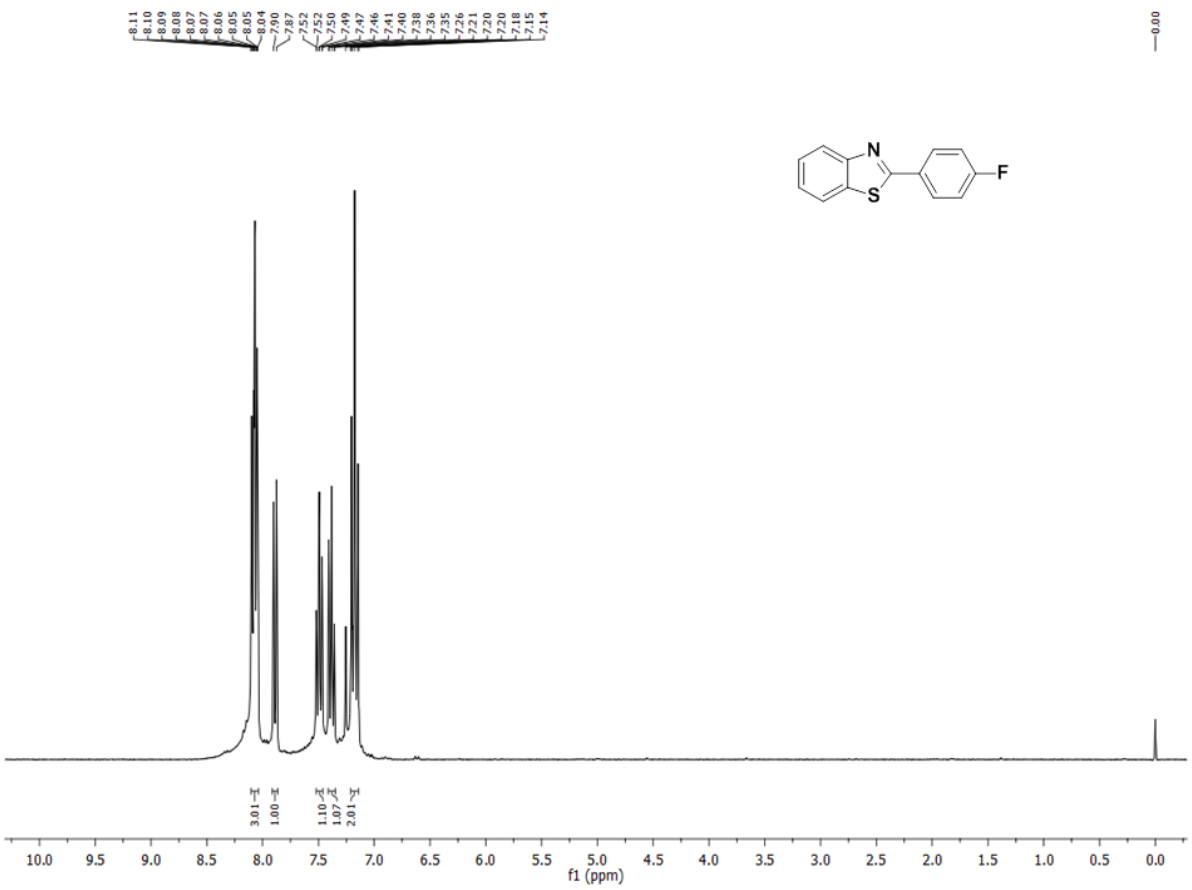


Figure 41. ^{1}H NMR Spectrum of compound **3ar**

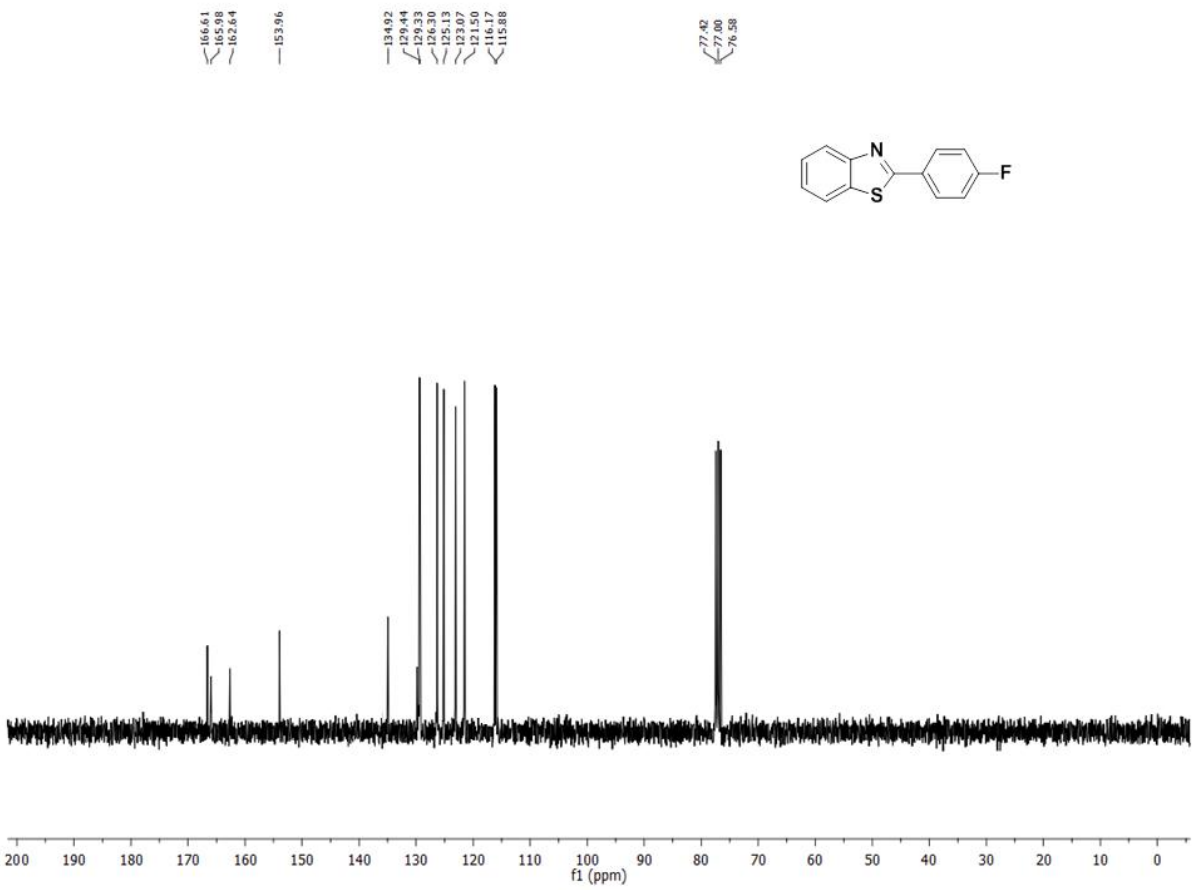


Figure 42. ^{13}C Spectrum of compound **3ar**

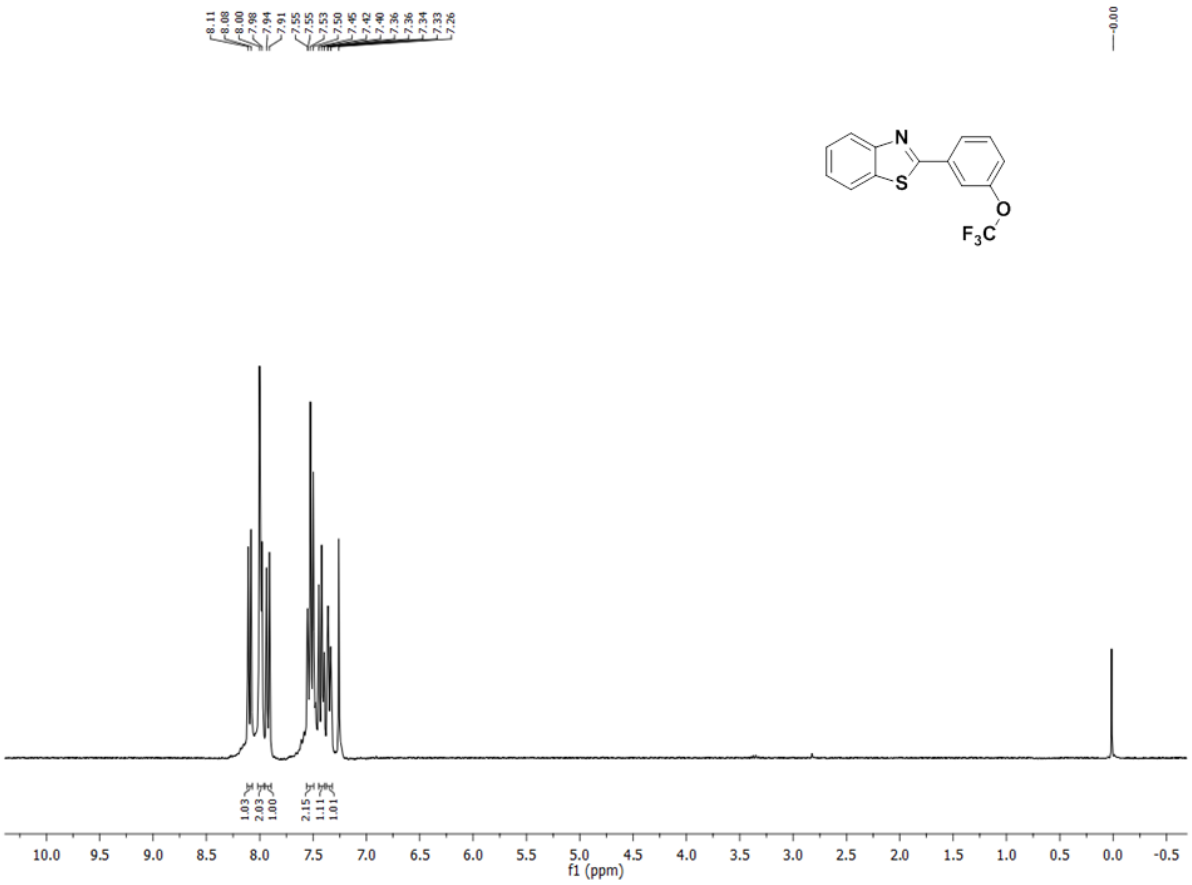


Figure 43. ^{1}H NMR Spectrum of compound **3as**

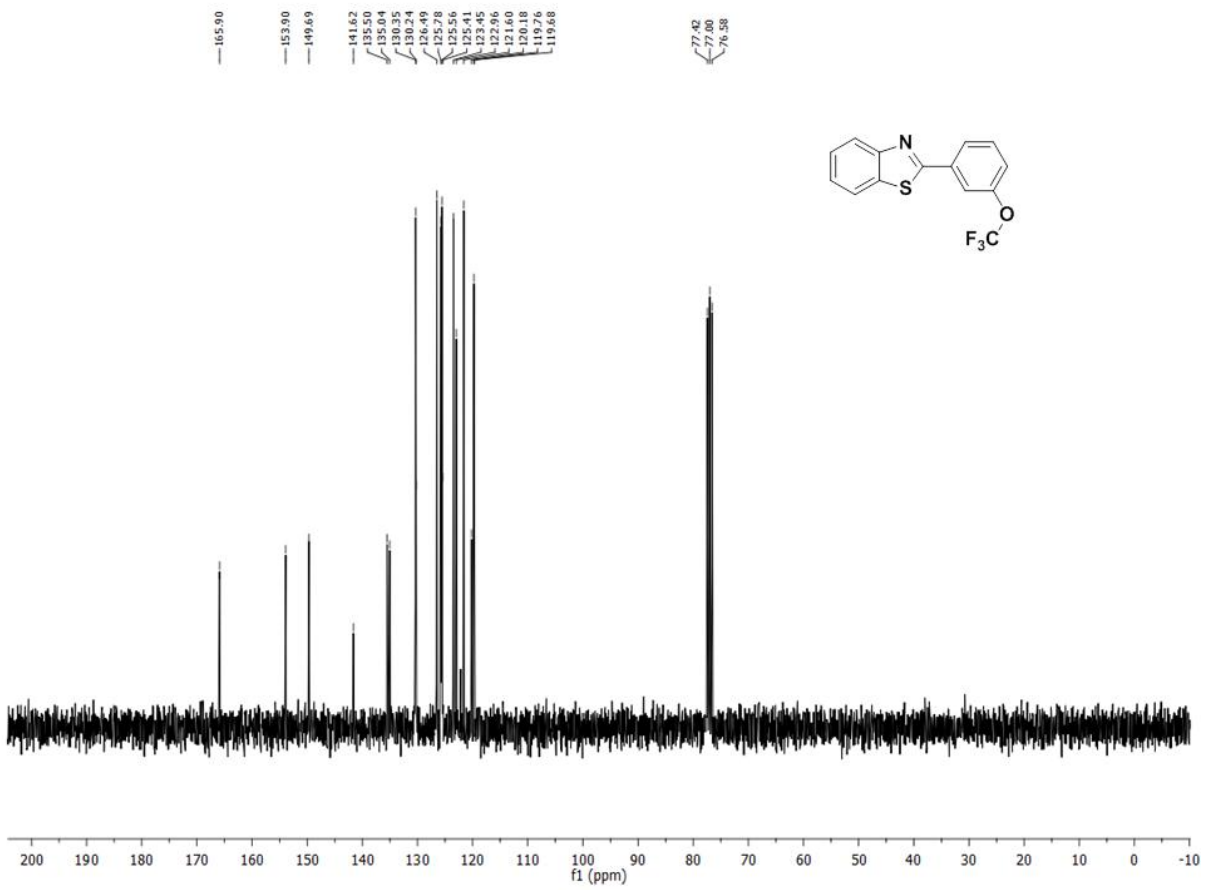


Figure 44. ^{13}C Spectrum of compound **3as**

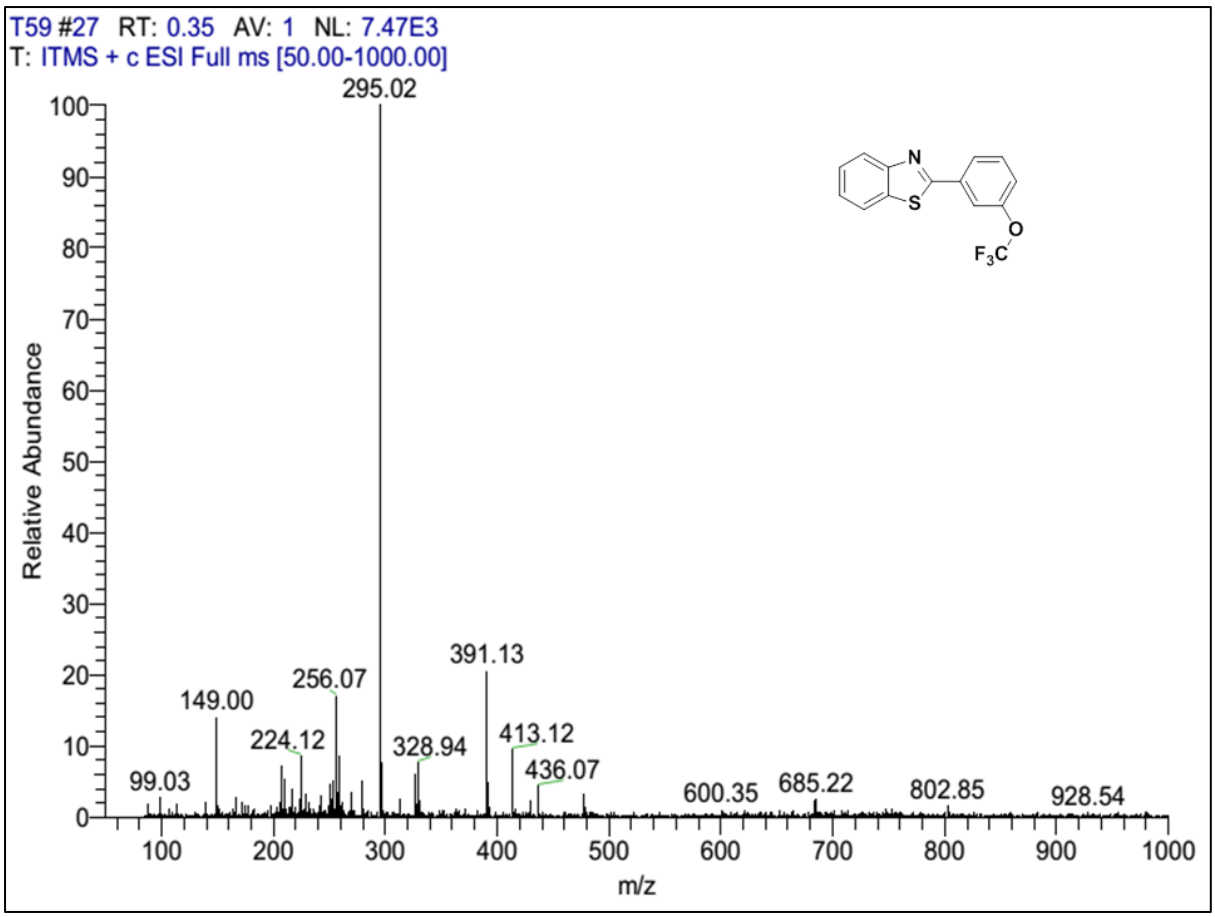


Figure 45. Mass Spectrum of compound **3as**

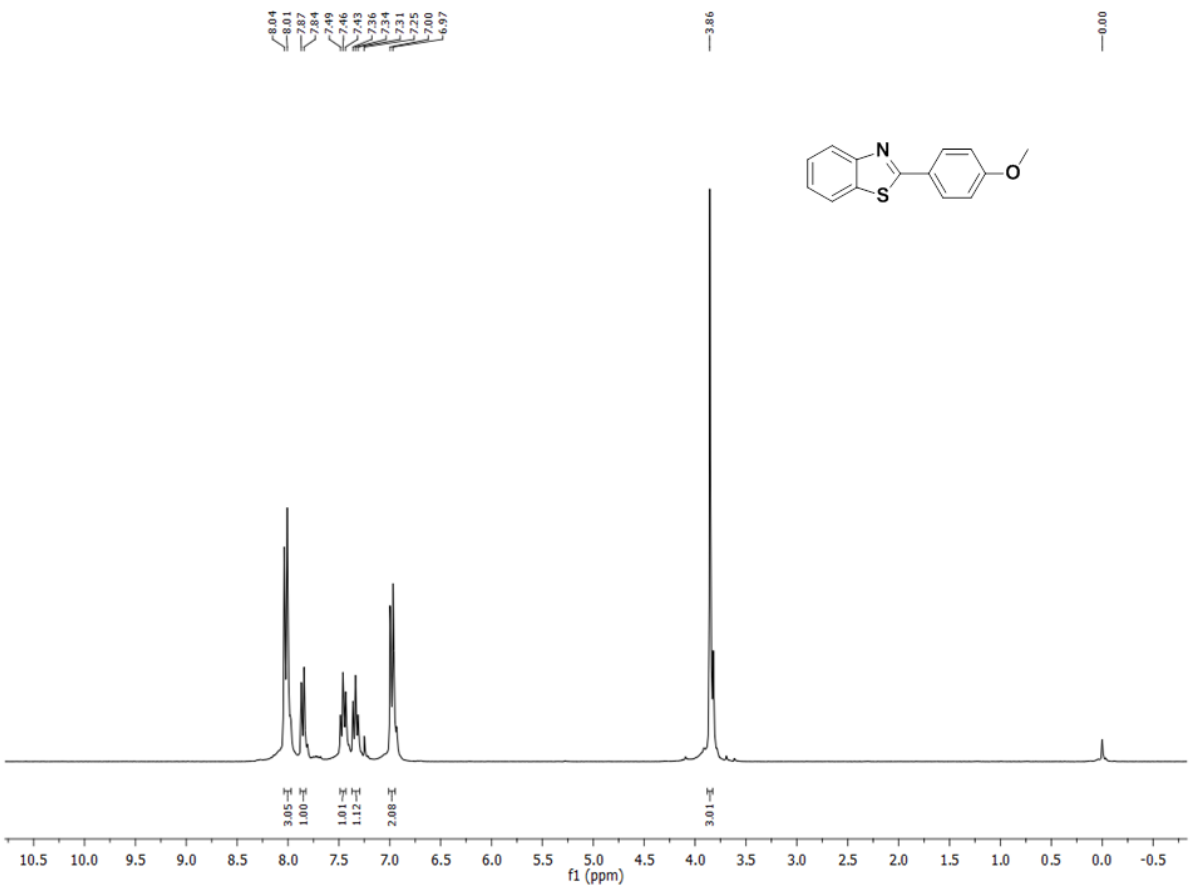


Figure 46. ^{1}H NMR Spectrum of compound **3at**

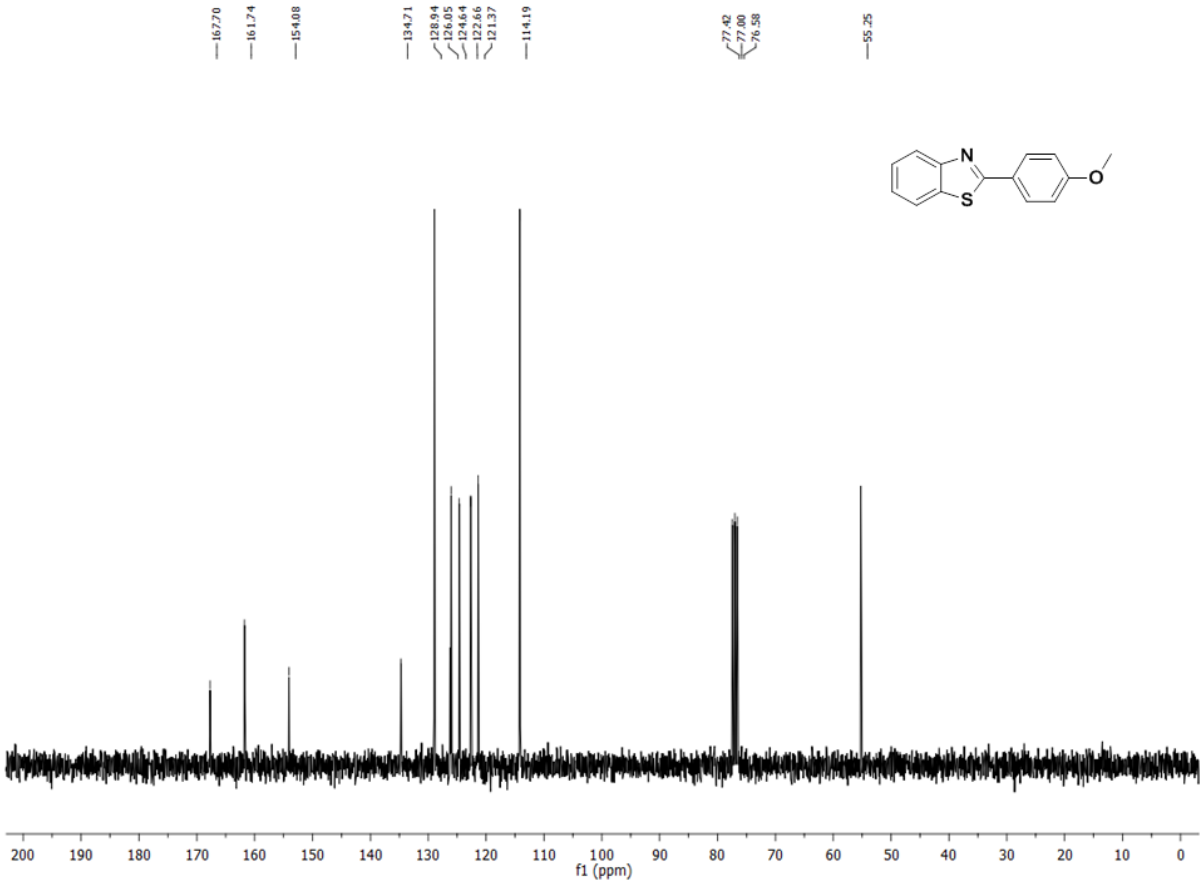


Figure 47. ^{13}C Spectrum of compound **3at**

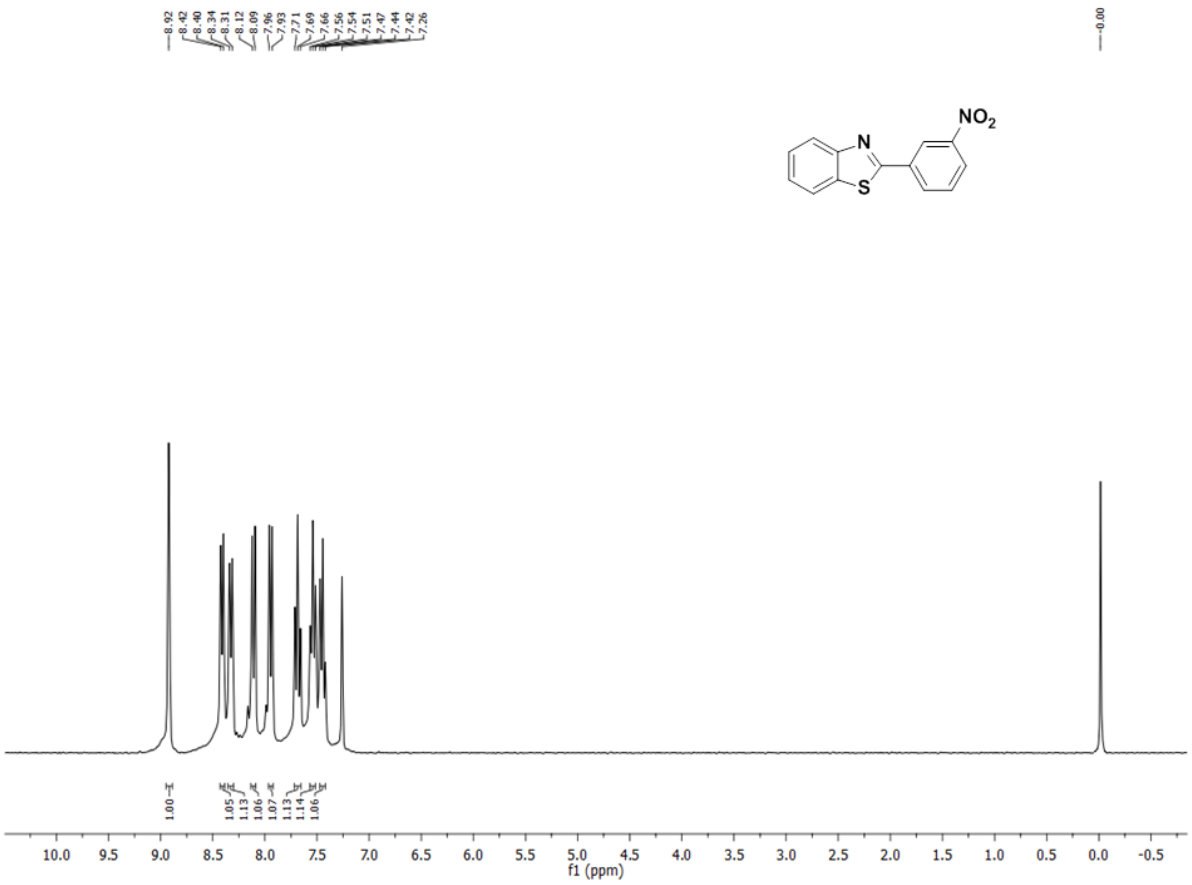


Figure 48. ^{1}H NMR Spectrum of compound **3au**

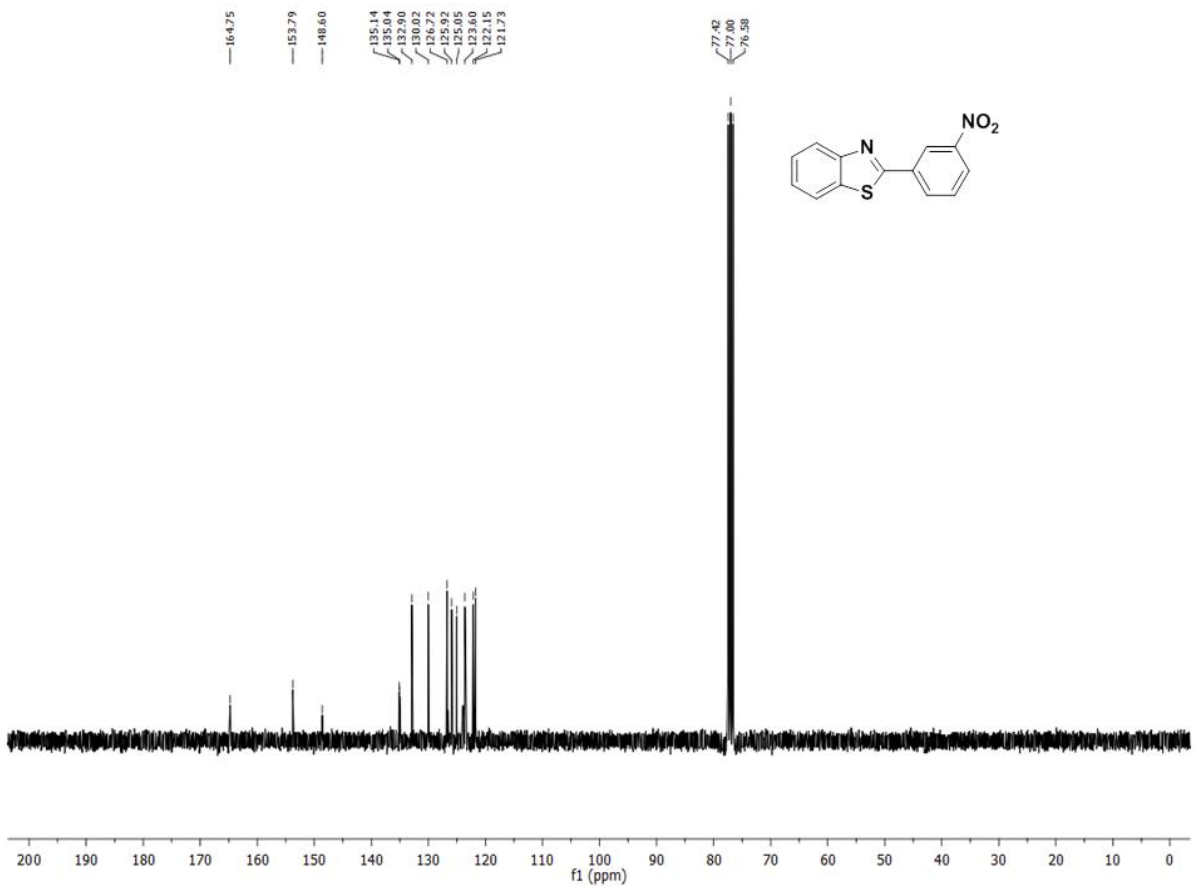


Figure 49. ^{13}C Spectrum of compound **3au**

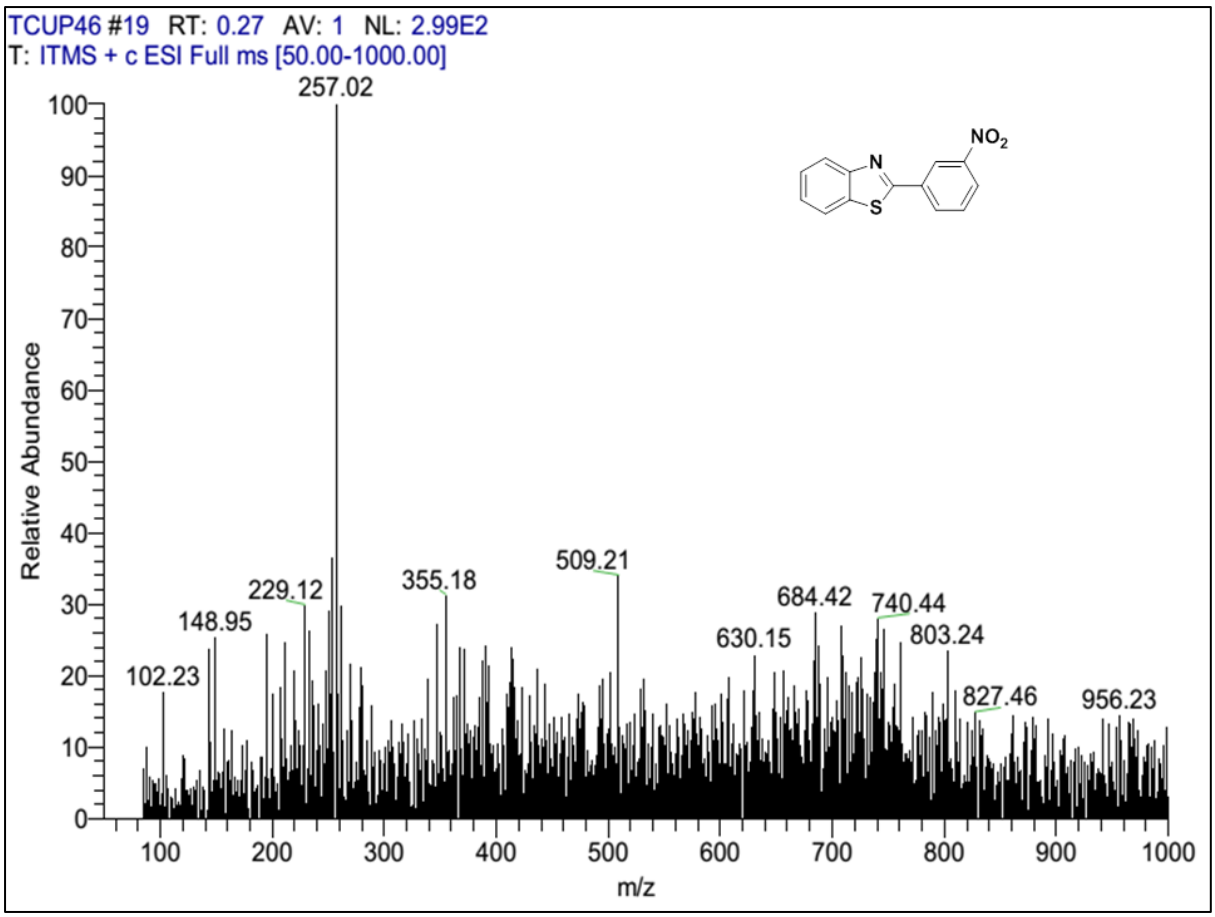


Figure 50. Mass Spectrum of compound **3au**

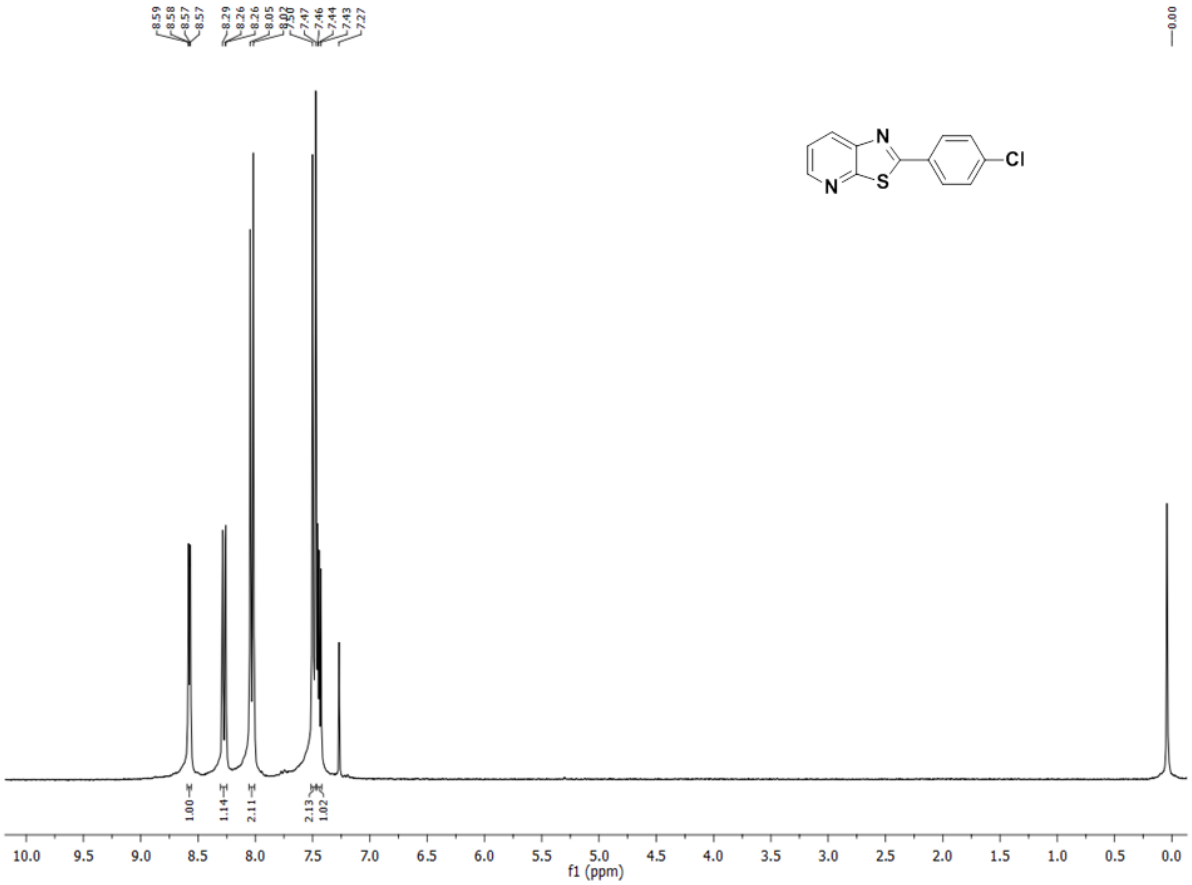


Figure 51. ^{1}H NMR Spectrum of compound **3av**

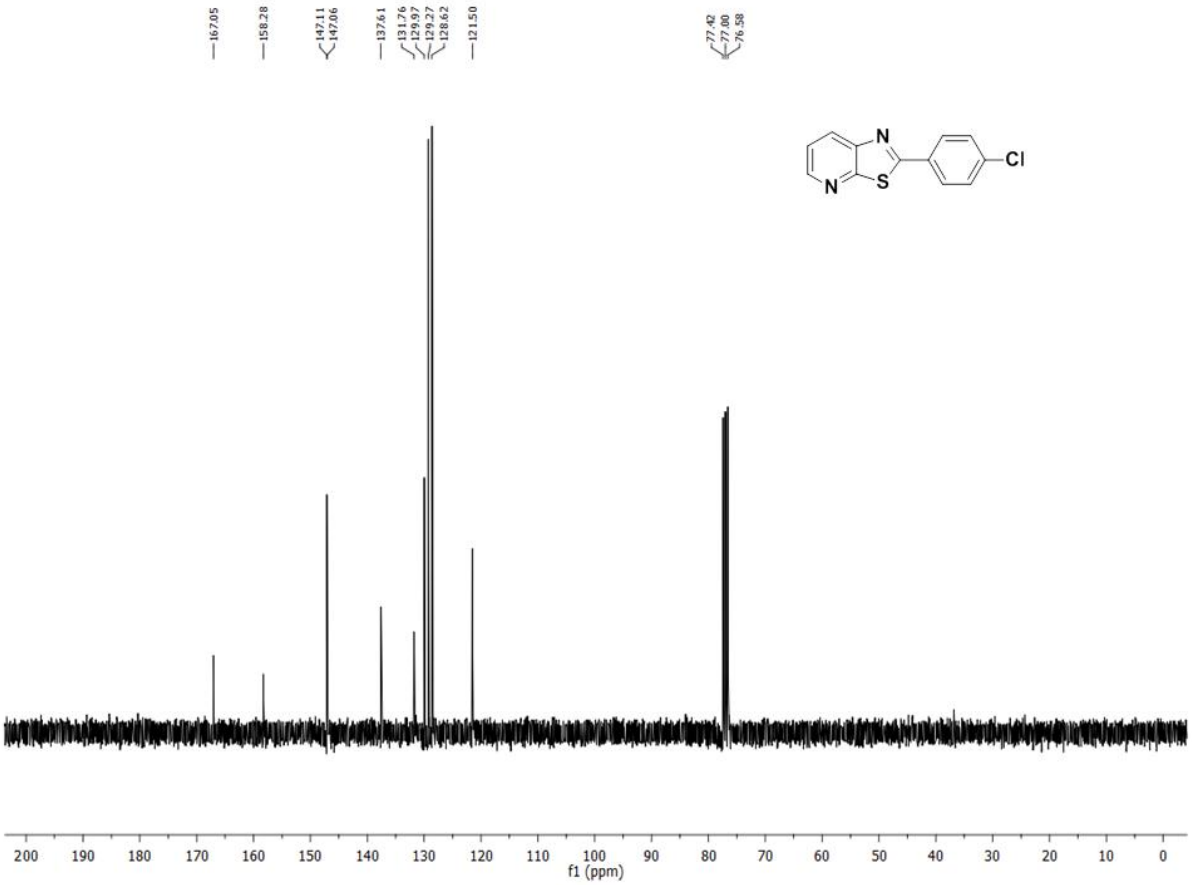


Figure 52. ^{13}C Spectrum of compound **3av**

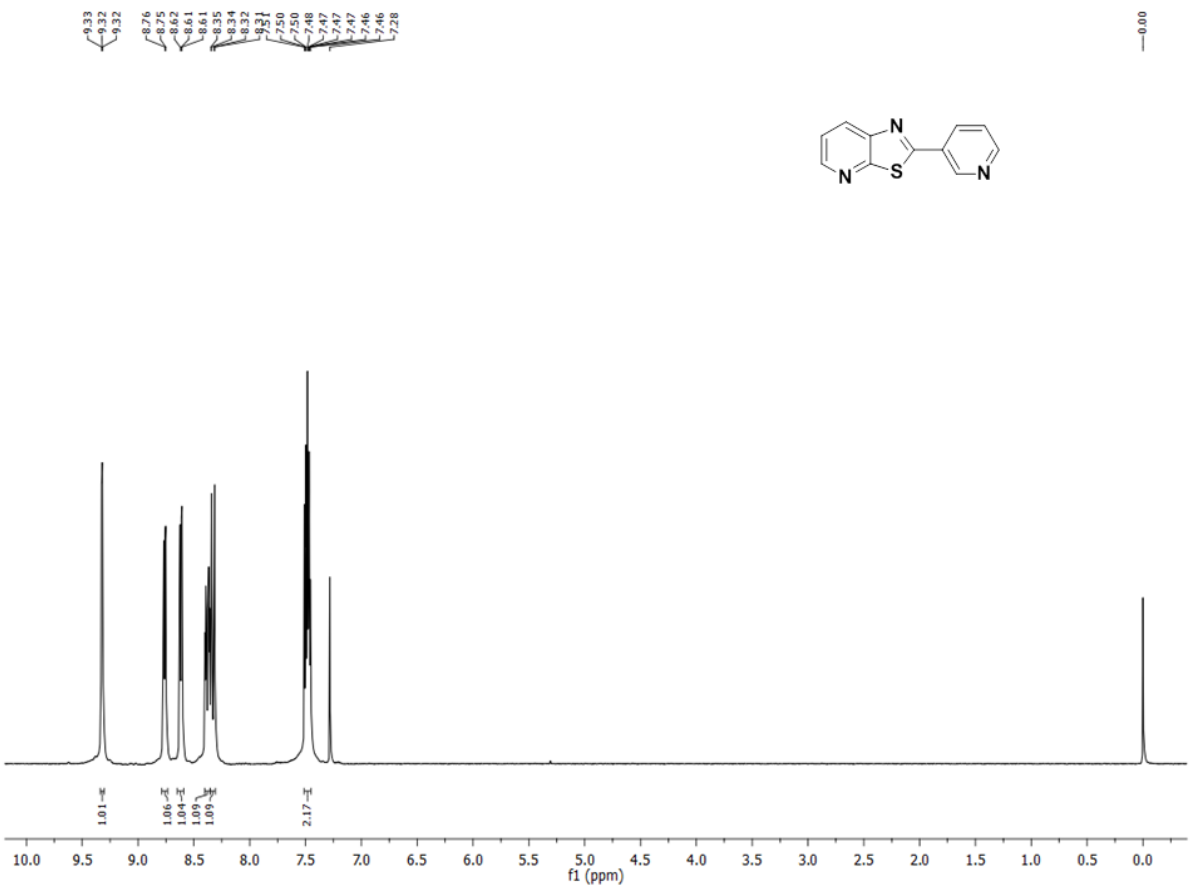


Figure 53. ^{1}H NMR Spectrum of compound **3aw**

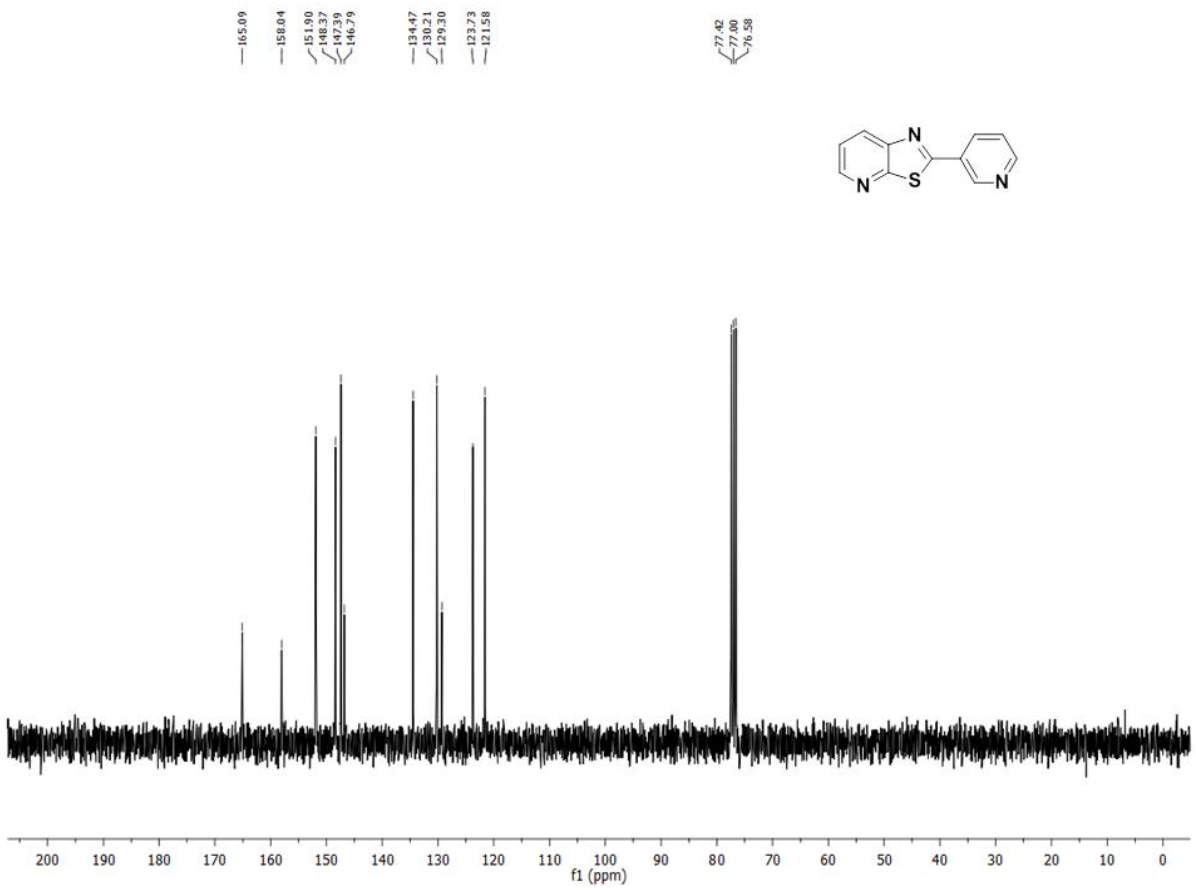


Figure 54. ^{13}C Spectrum of compound **3aw**

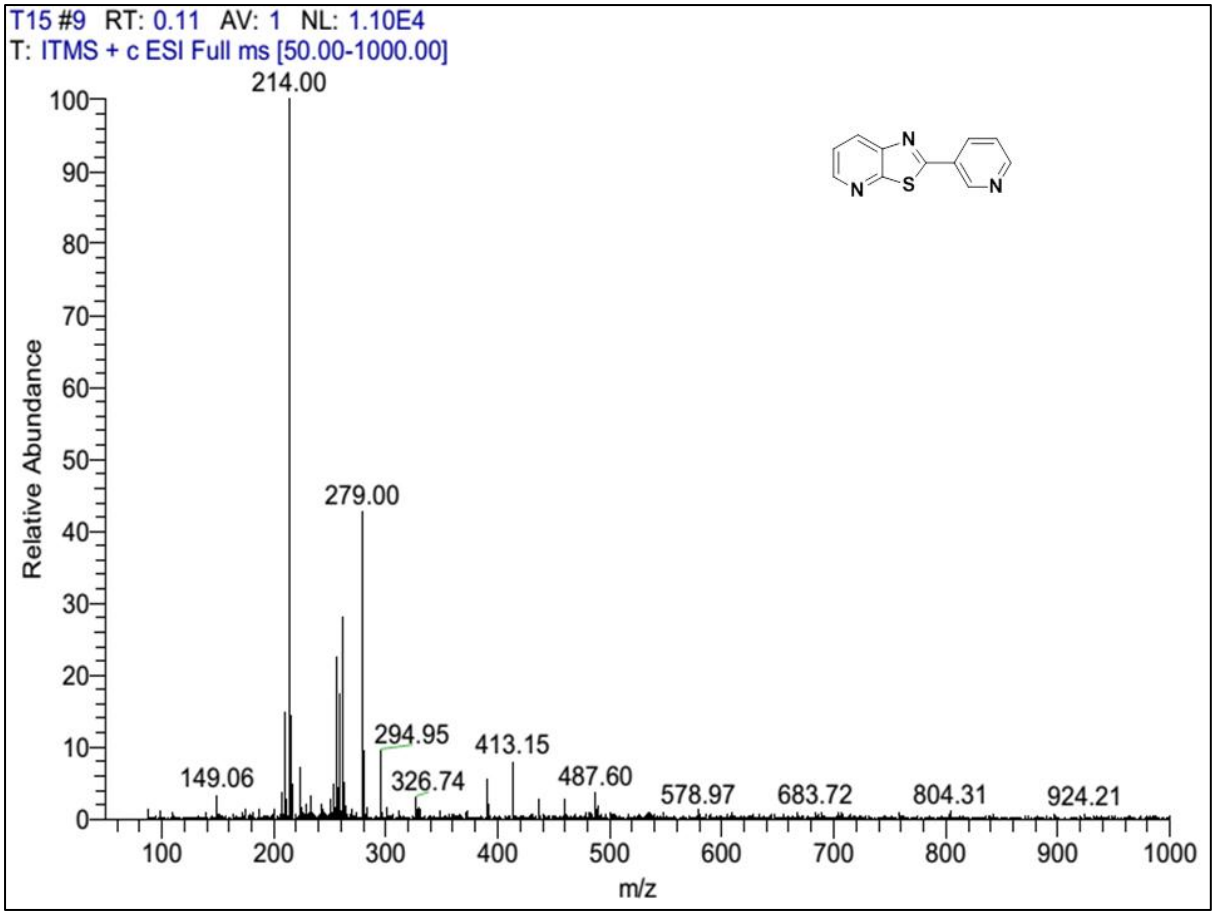


Figure 55. Mass Spectrum of compound **3aw**

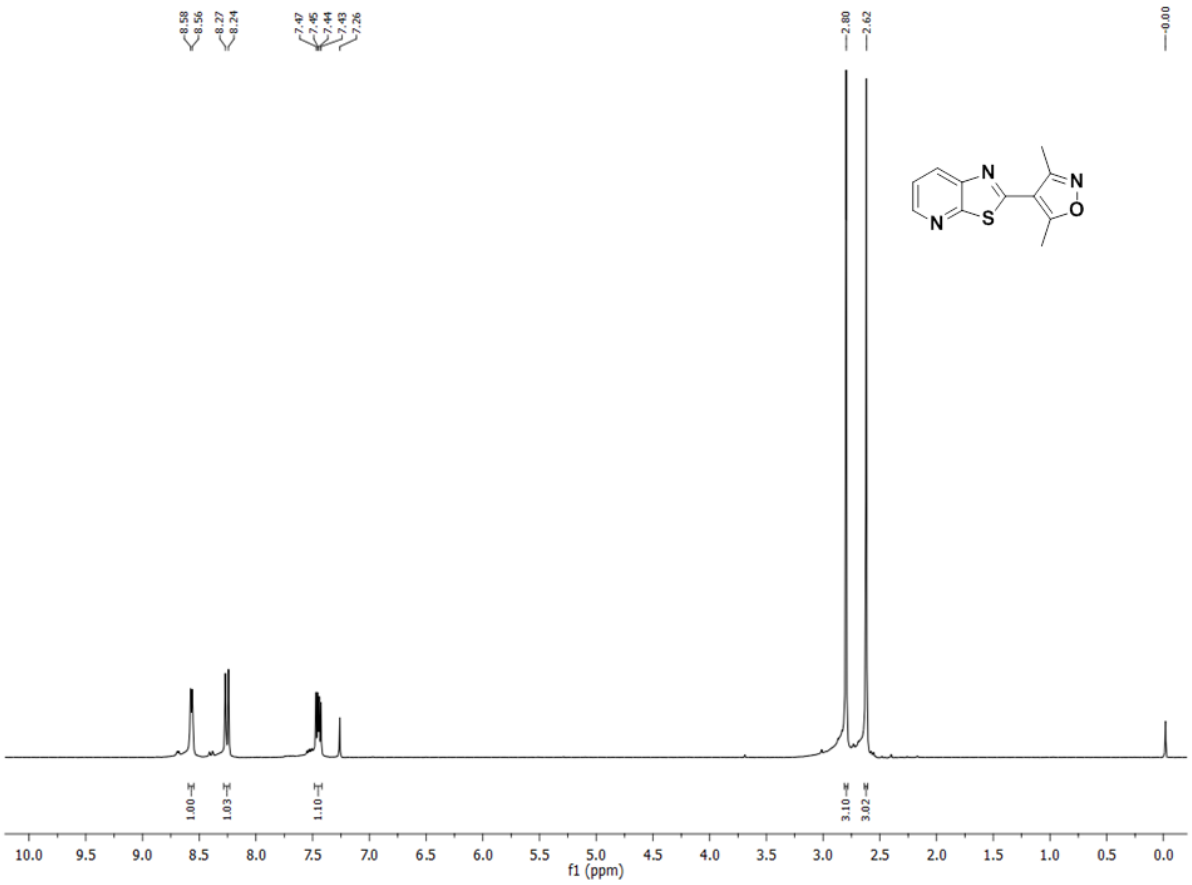


Figure 56. ^{1}H NMR Spectrum of compound **3ax**

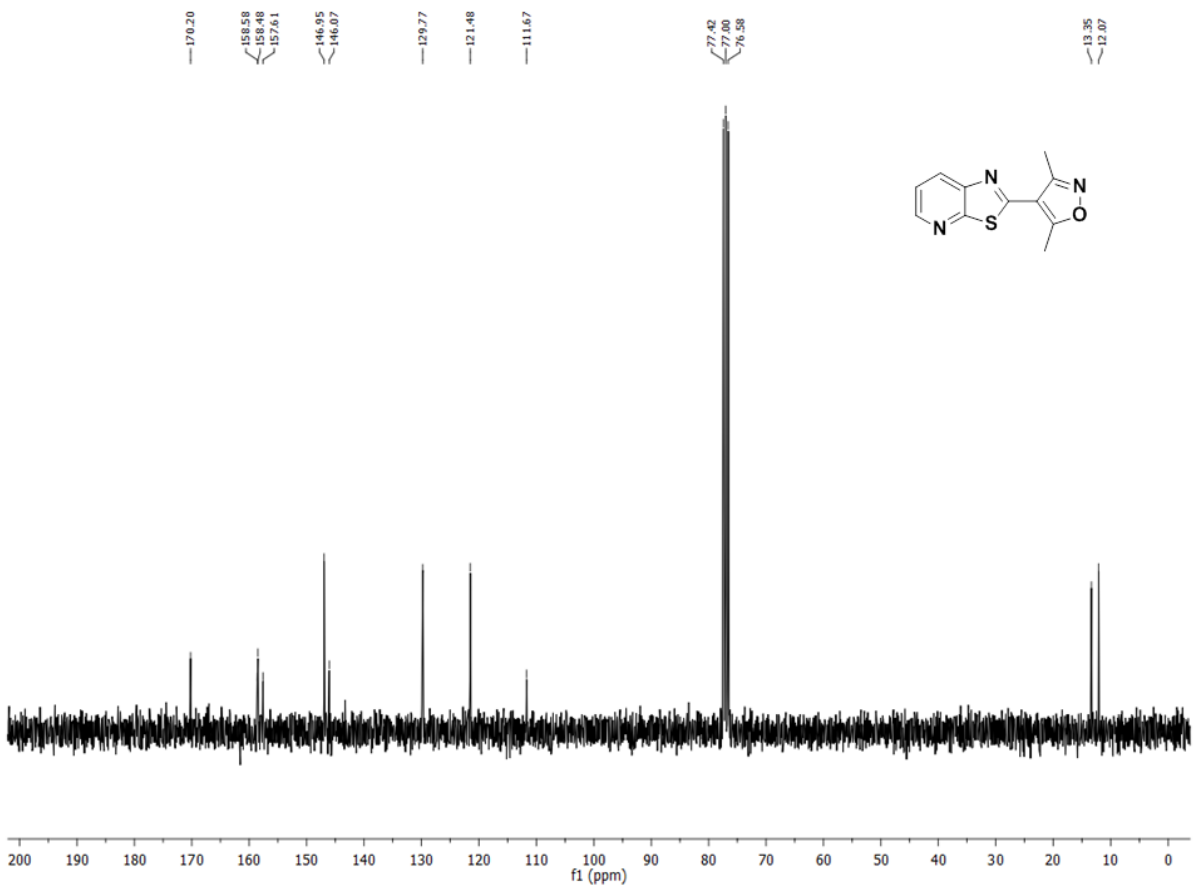


Figure 57. ^{13}C Spectrum of compound **3ax**

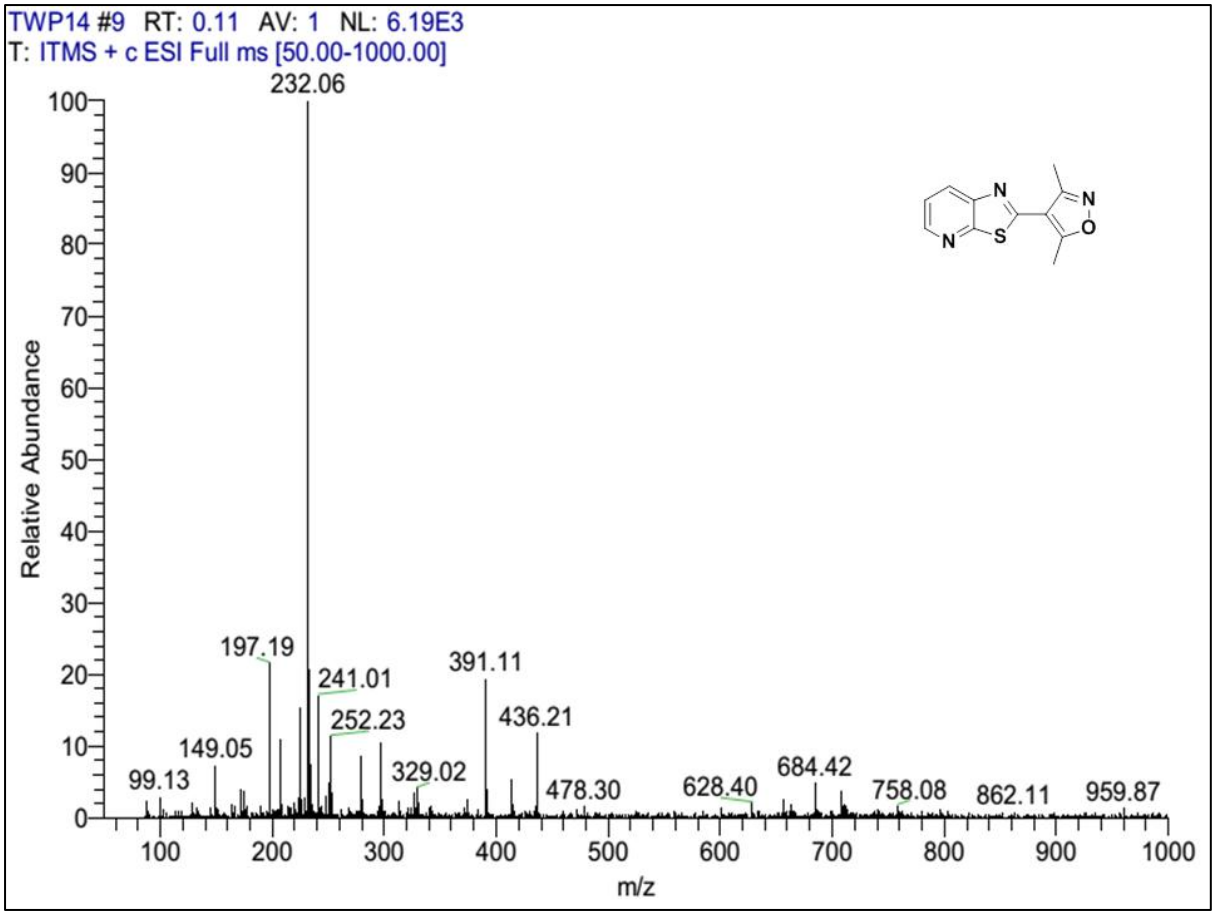


Figure 58. Mass Spectrum of compound **3ax**

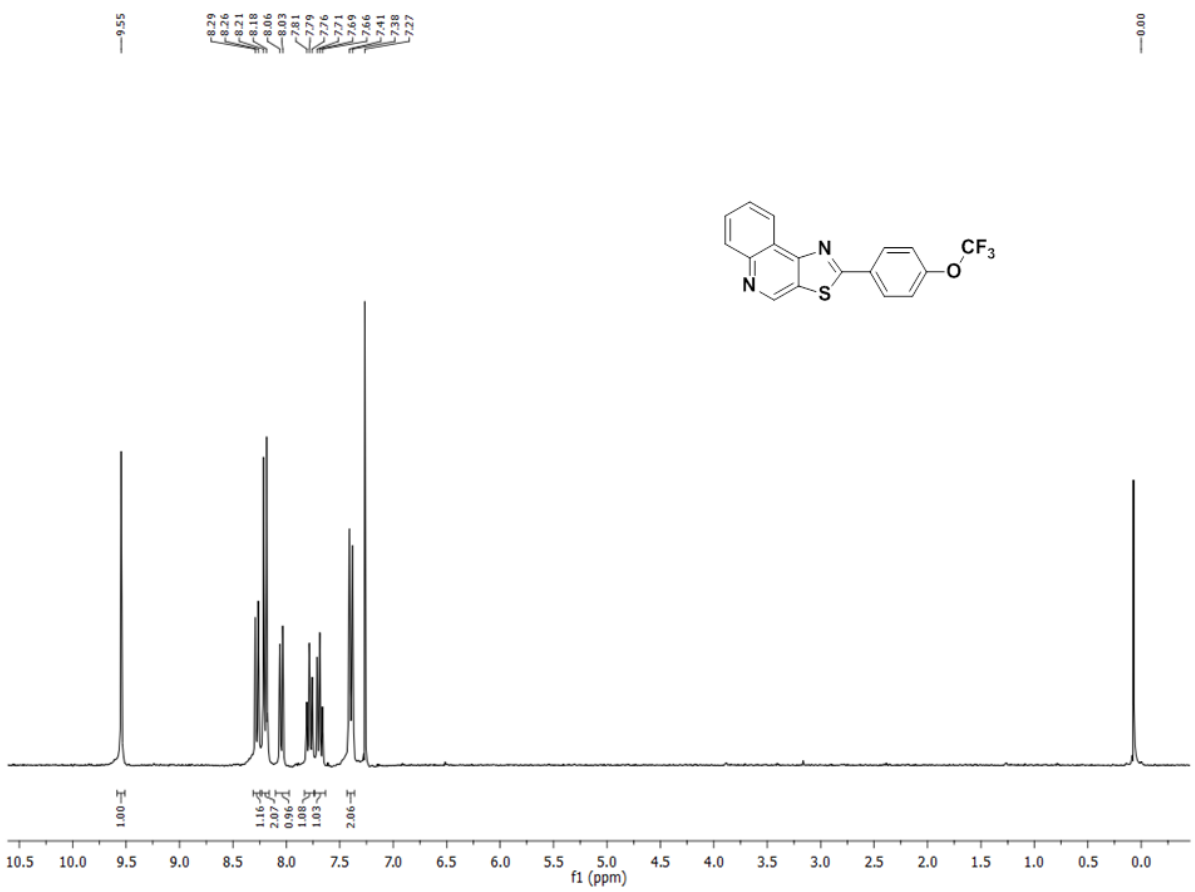


Figure 59. ^{1}H NMR Spectrum of compound **3ay**

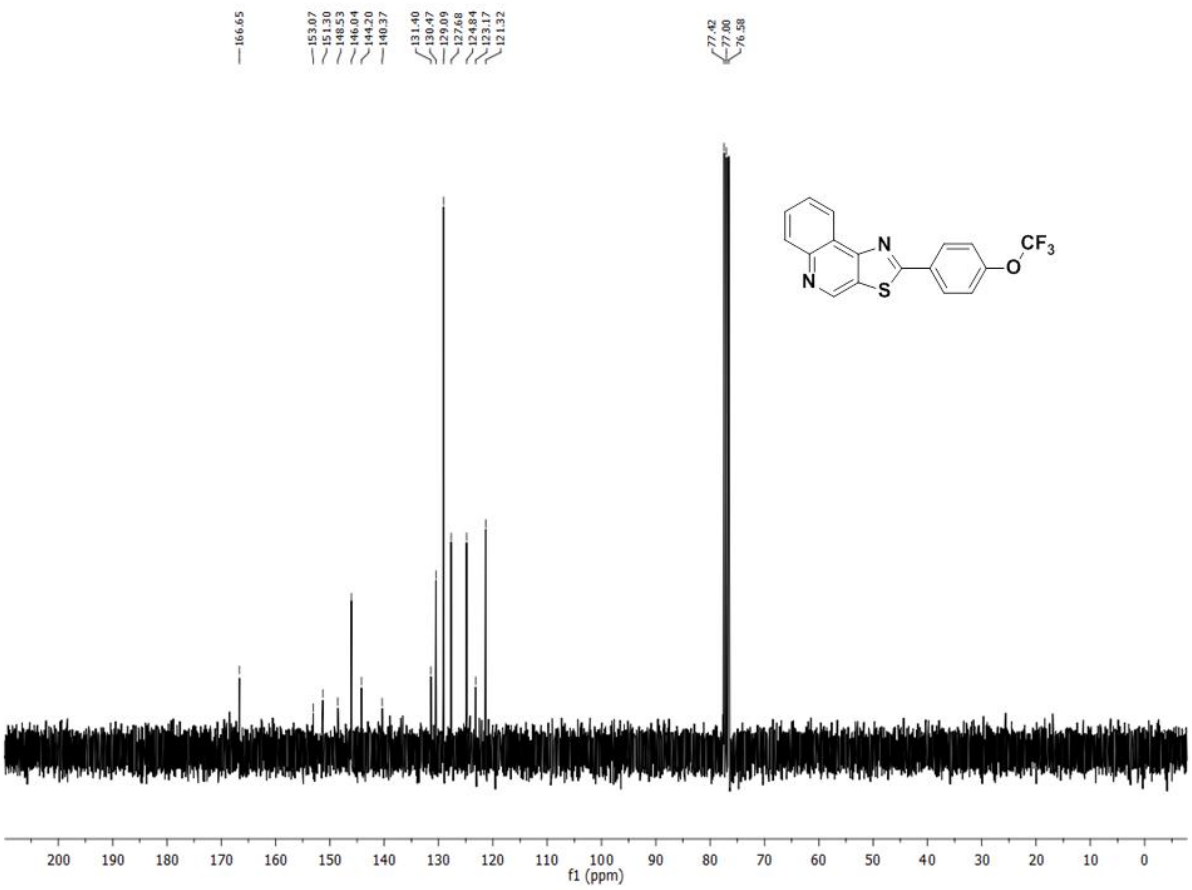


Figure 60. ^{13}C Spectrum of compound **3ay**

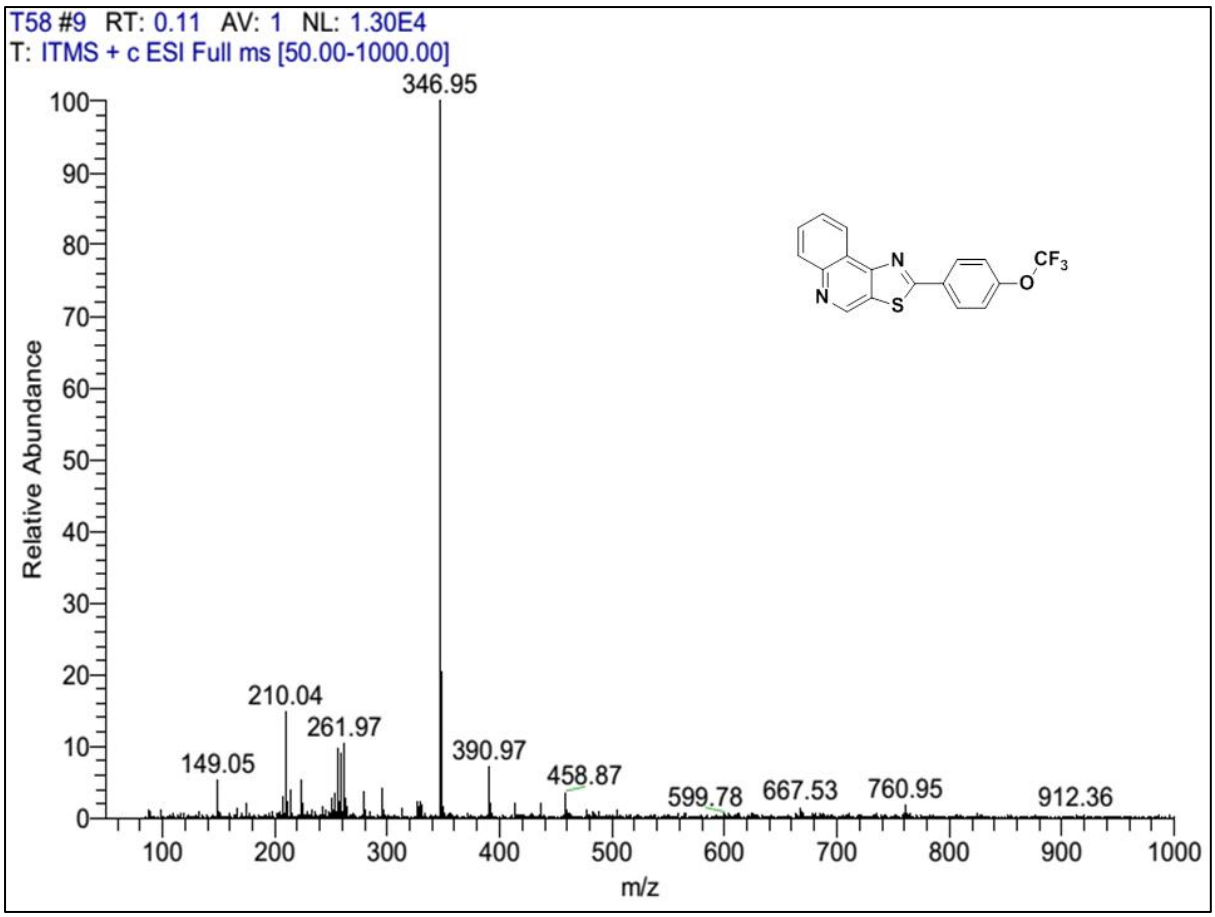


Figure 61. Mass Spectrum of compound **3ay**

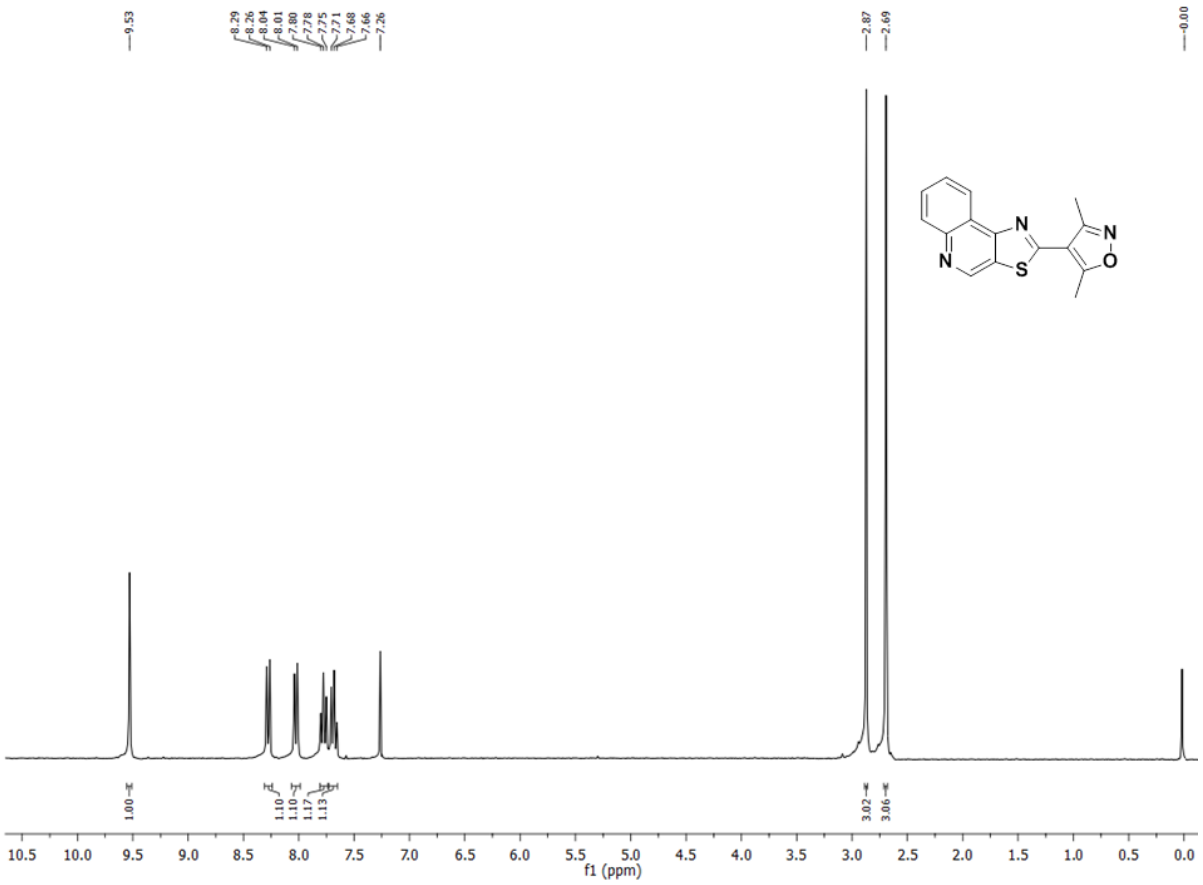


Figure 62. ^{1}H NMR Spectrum of compound **3az**

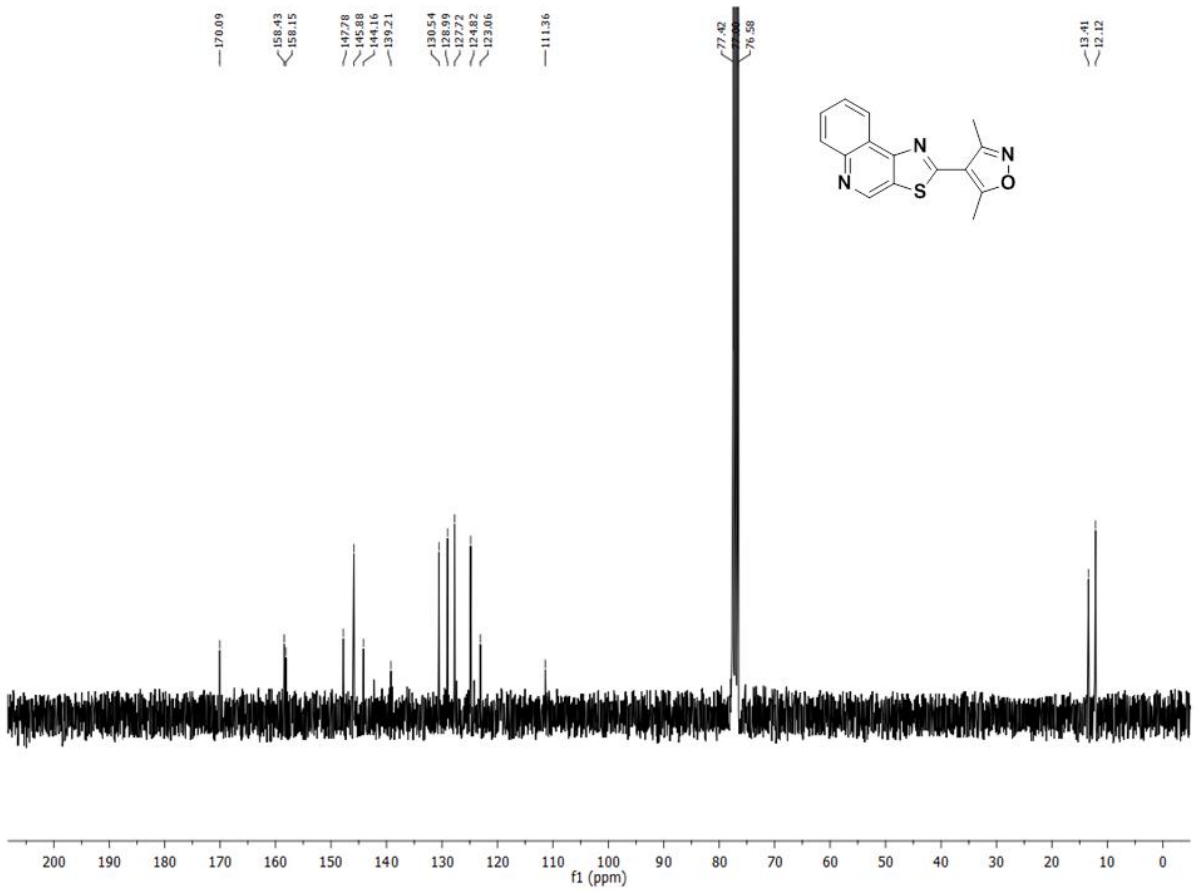


Figure 63. ^{13}C Spectrum of compound **3az**

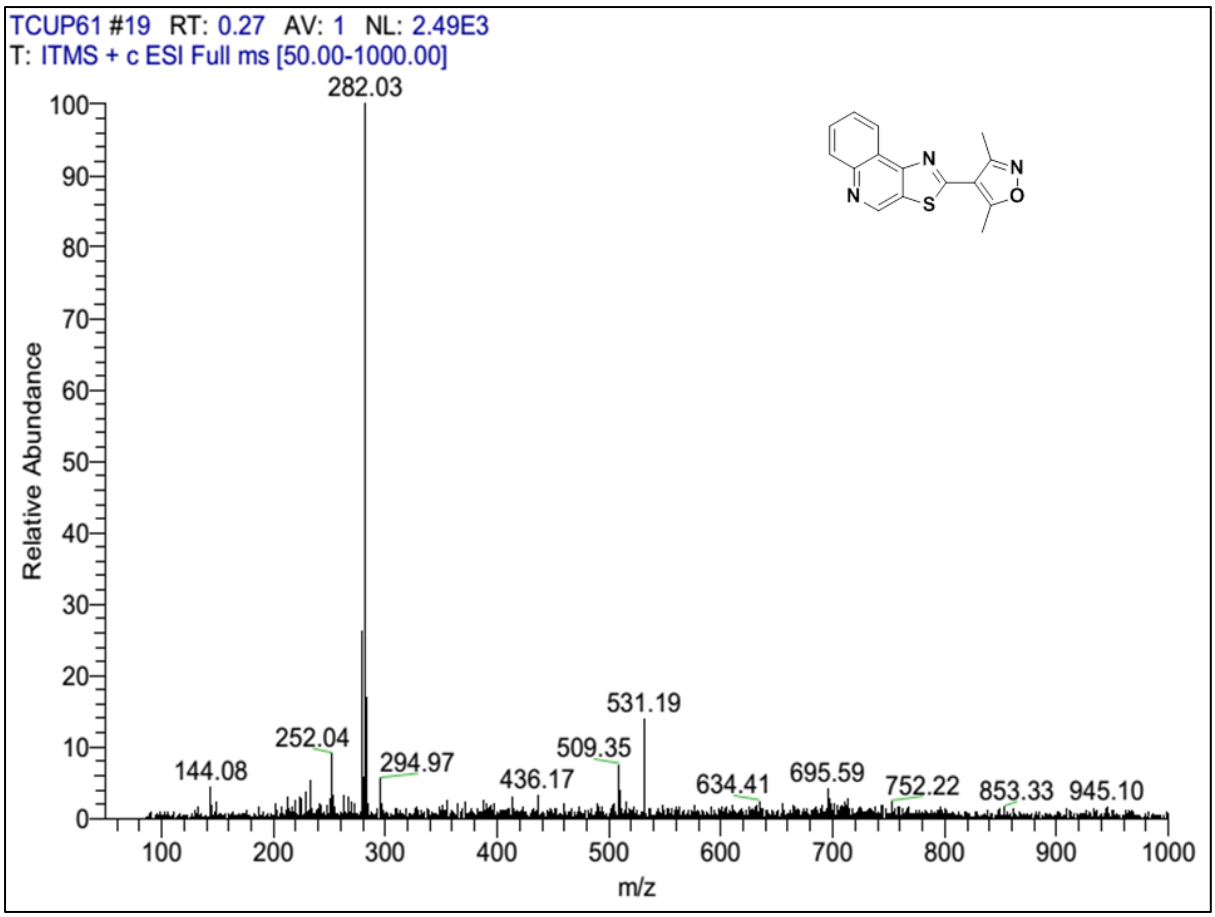


Figure 64. Mass Spectrum of compound **3az**

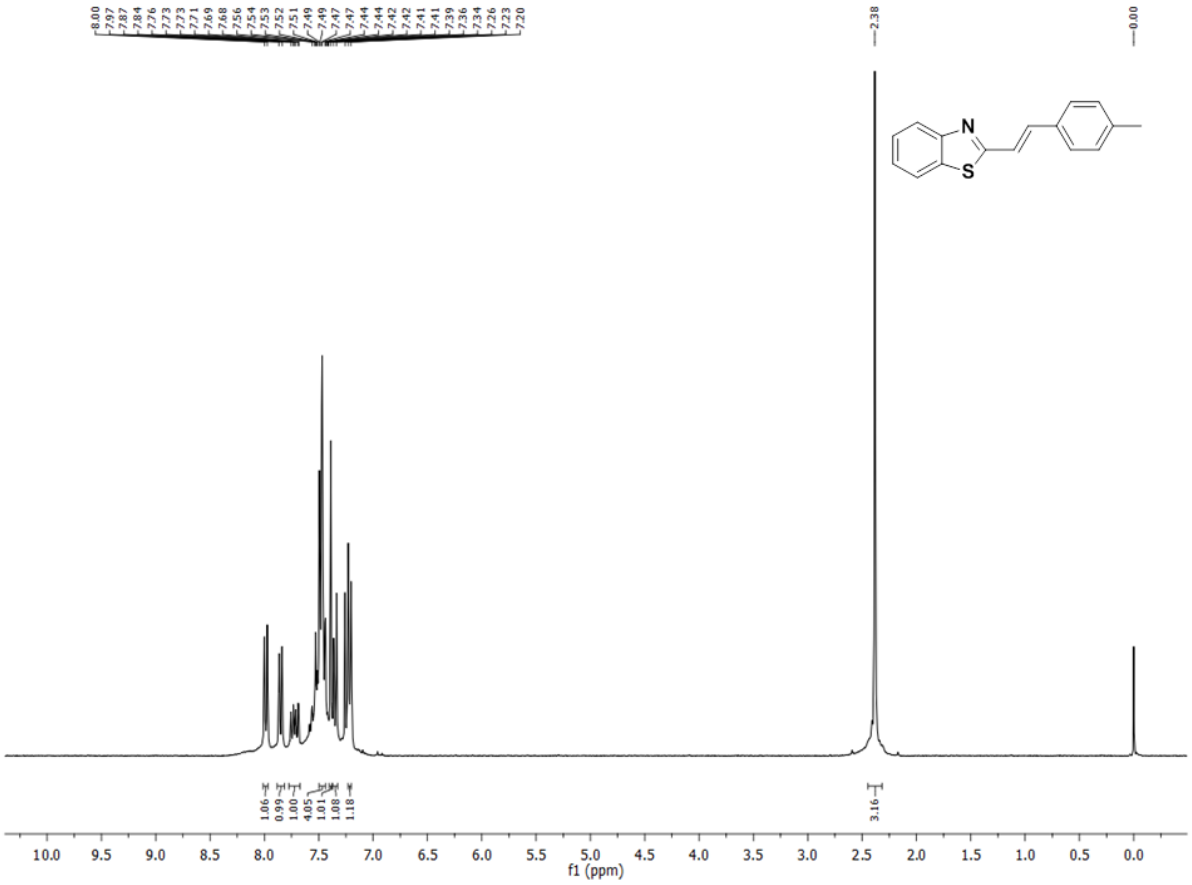


Figure 65. ^{1}H NMR Spectrum of compound **3ba**

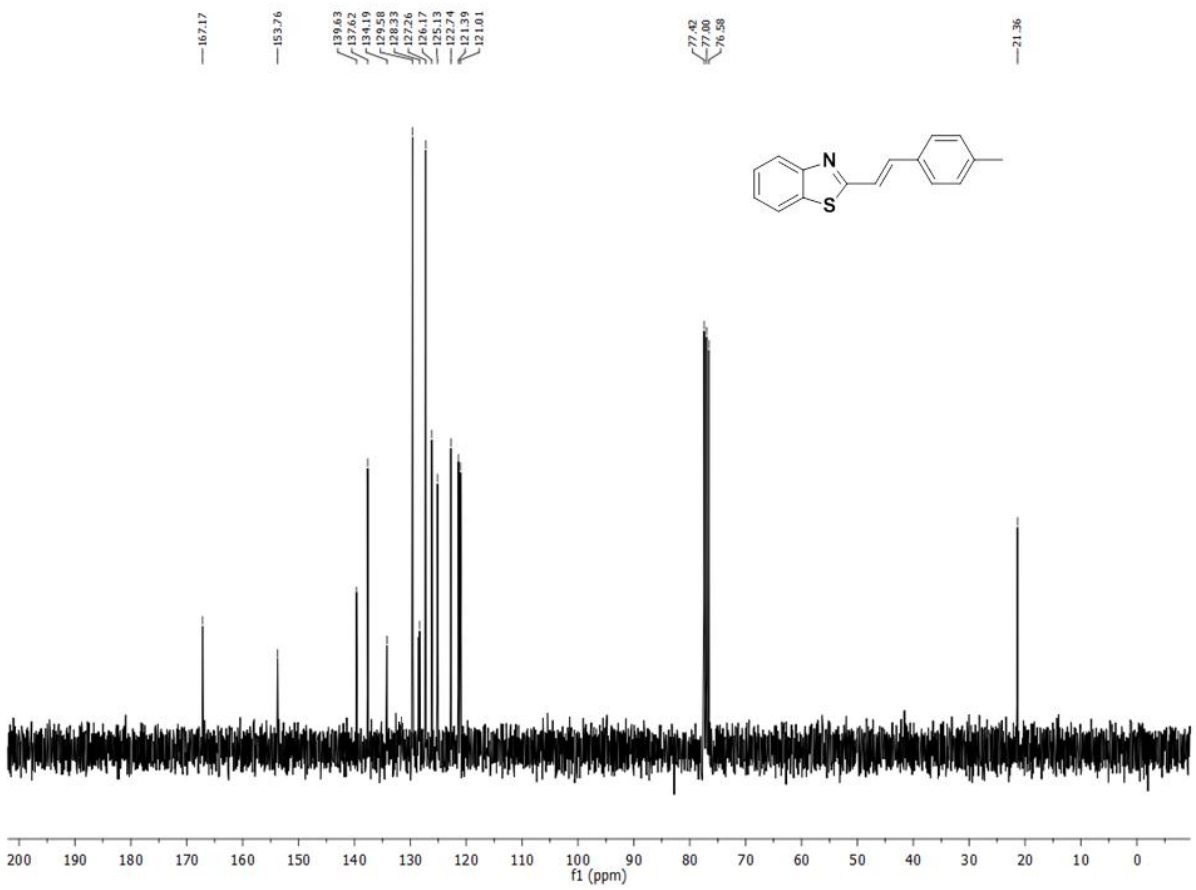


Figure 66. ^{13}C Spectrum of compound **3ba**

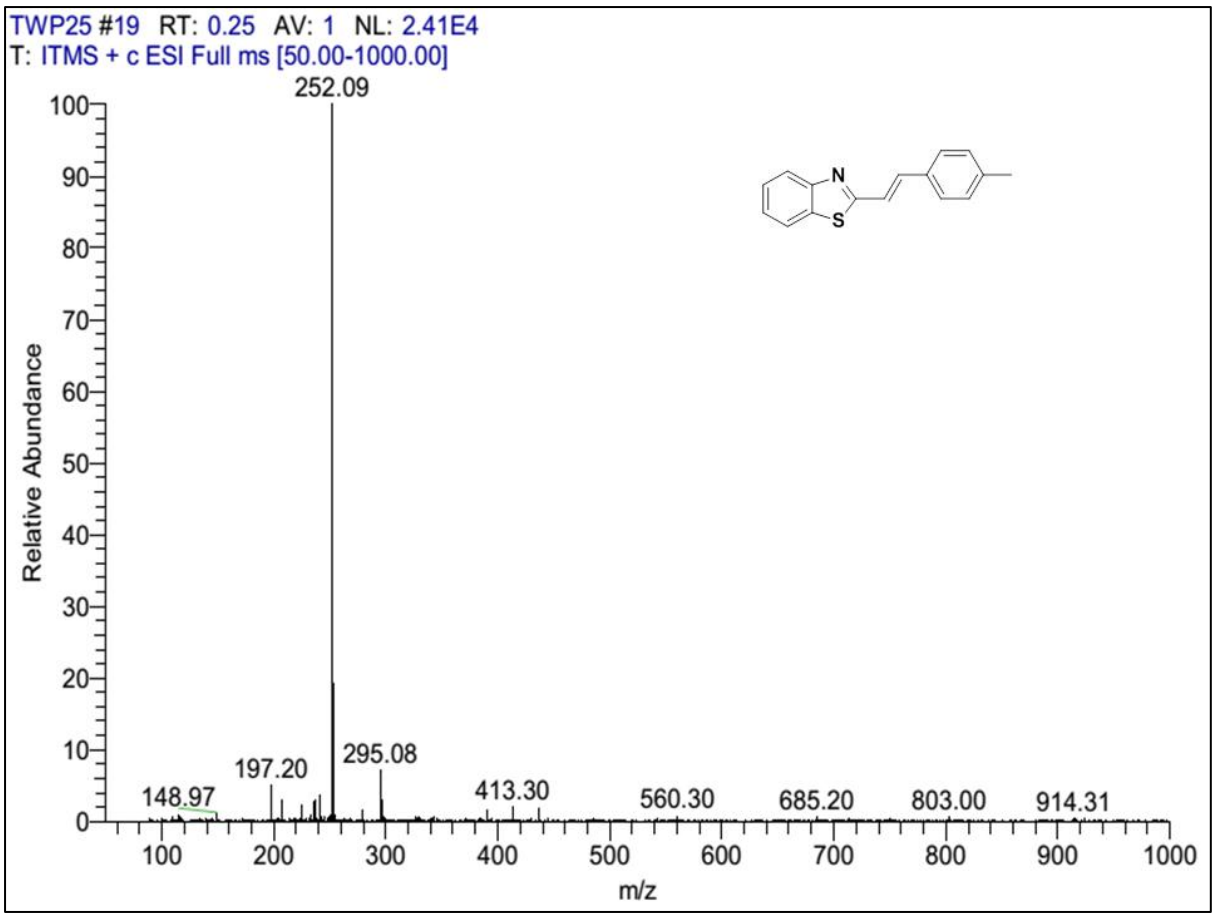


Figure 67. Mass Spectrum of compound **3ba**

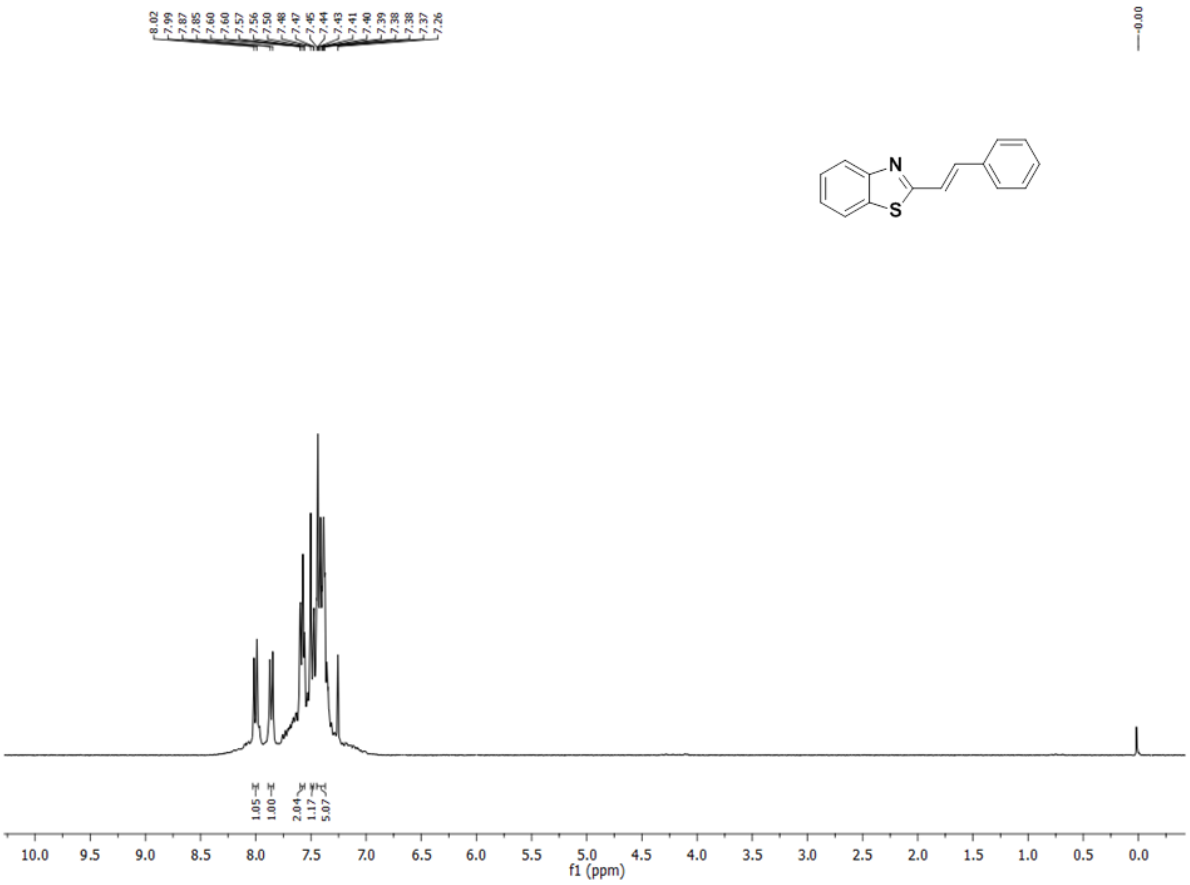


Figure 68. ^{1}H NMR Spectrum of compound **3bb**

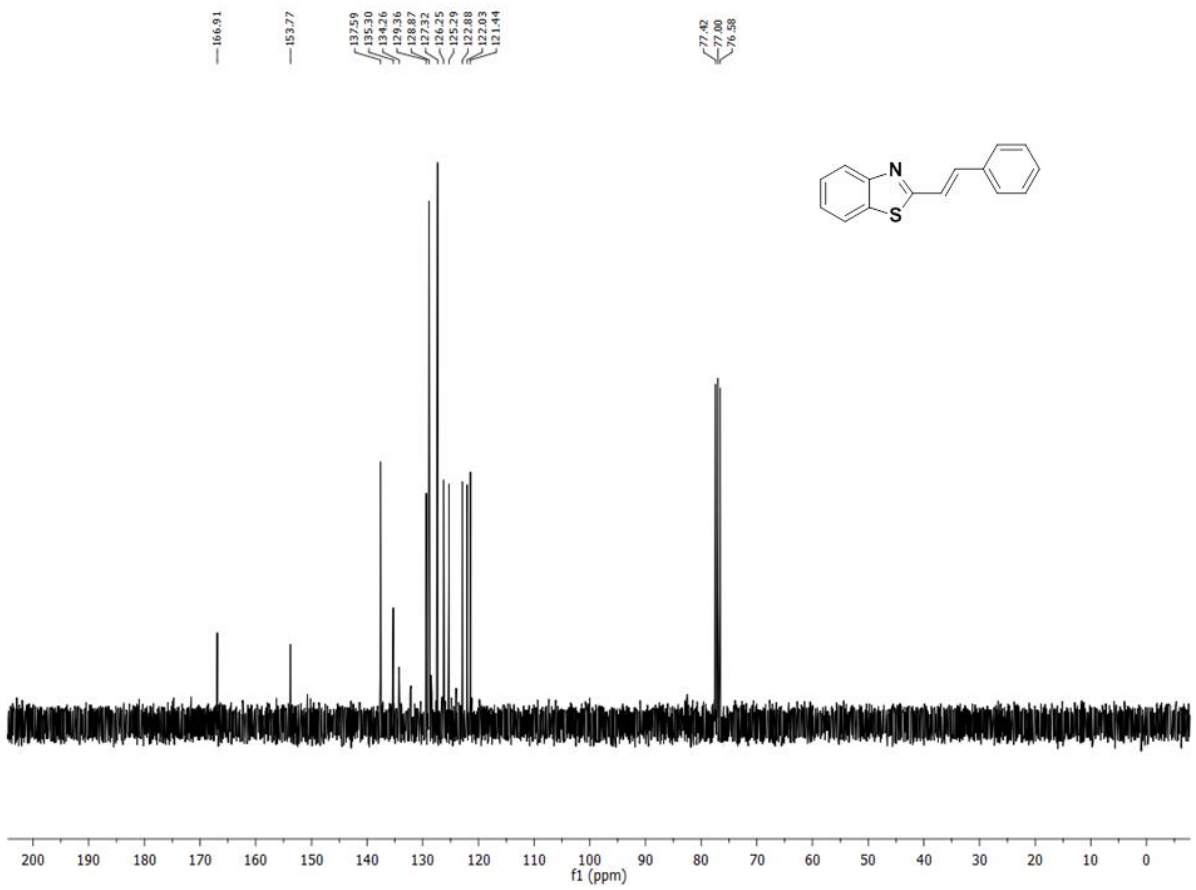


Figure 69. ^{13}C Spectrum of compound **3bb**

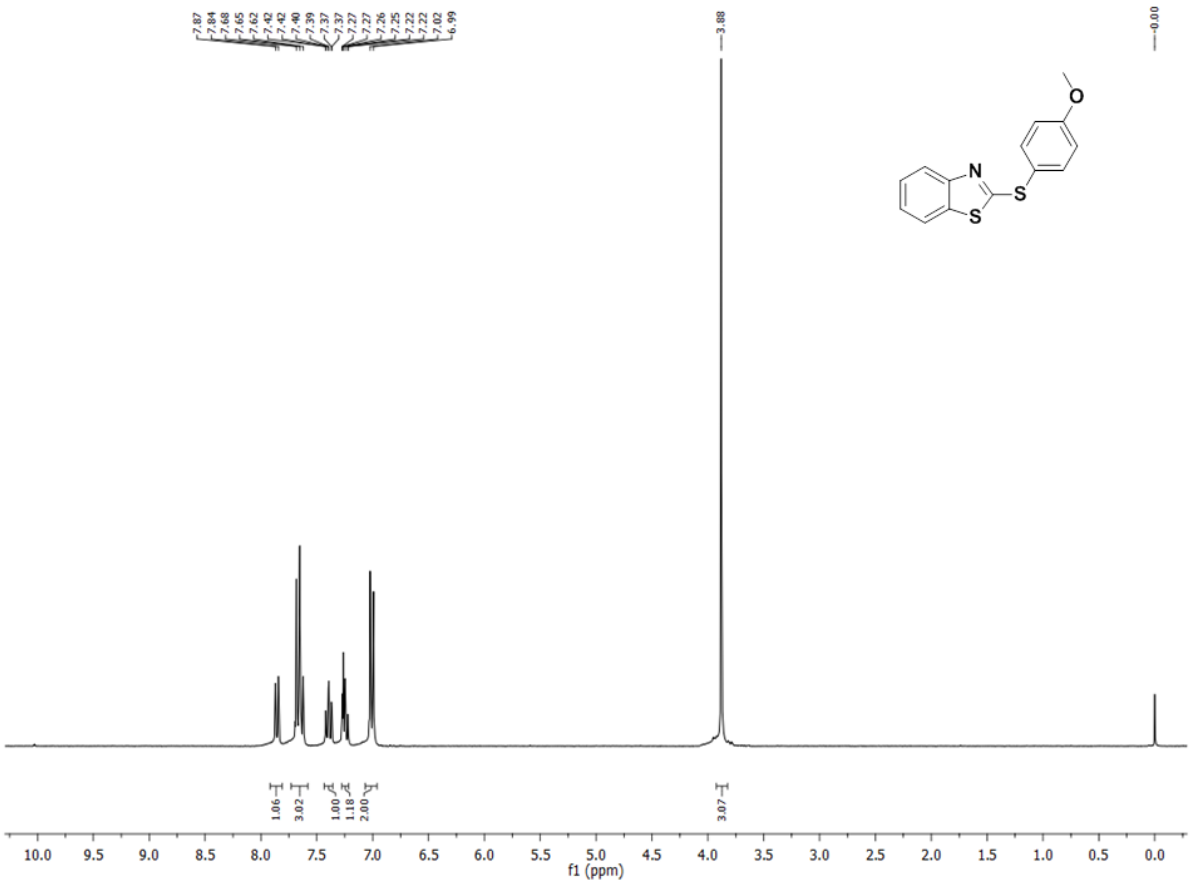


Figure 70. ^{1}H NMR Spectrum of compound **4a**

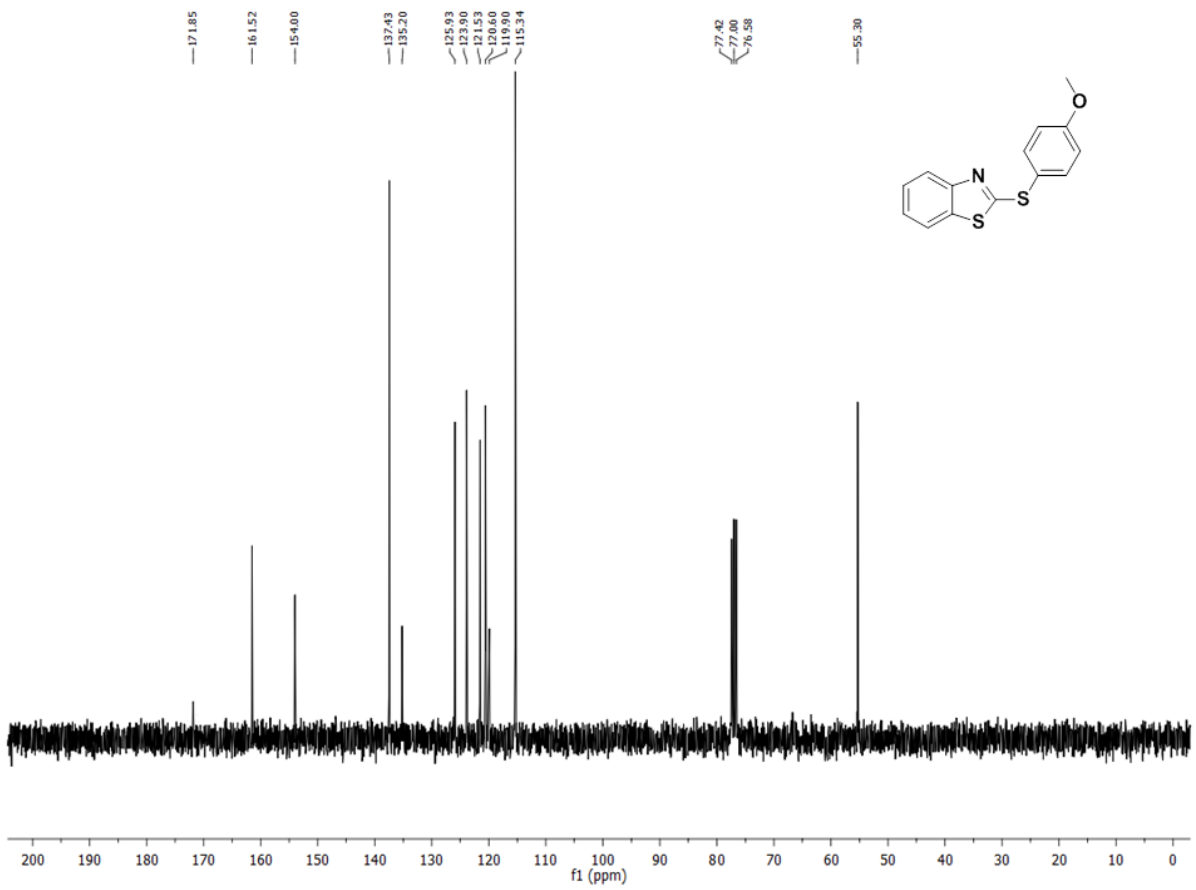


Fig .71. ^{13}C Spectrum of compound **4a**

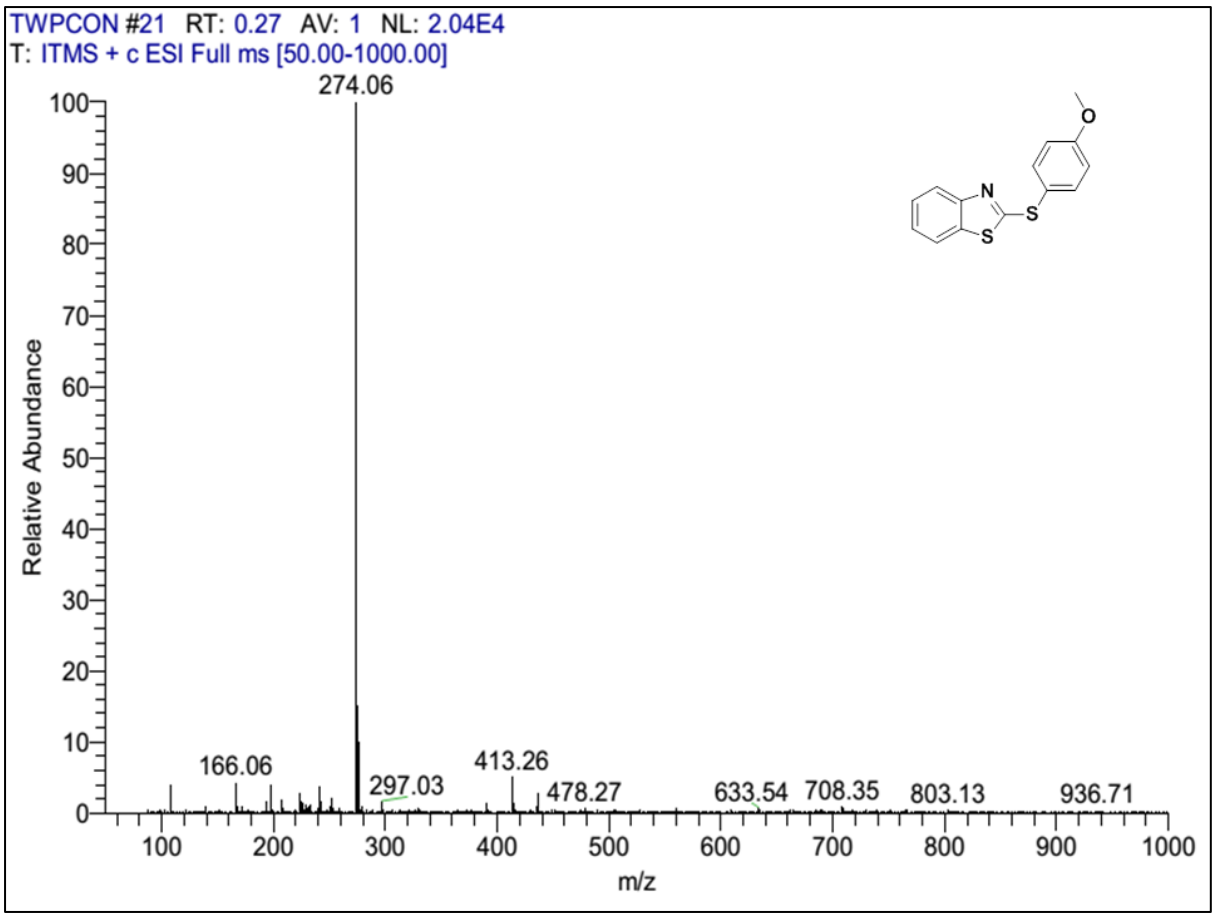


Figure 72. Mass Spectrum of compound **4a**

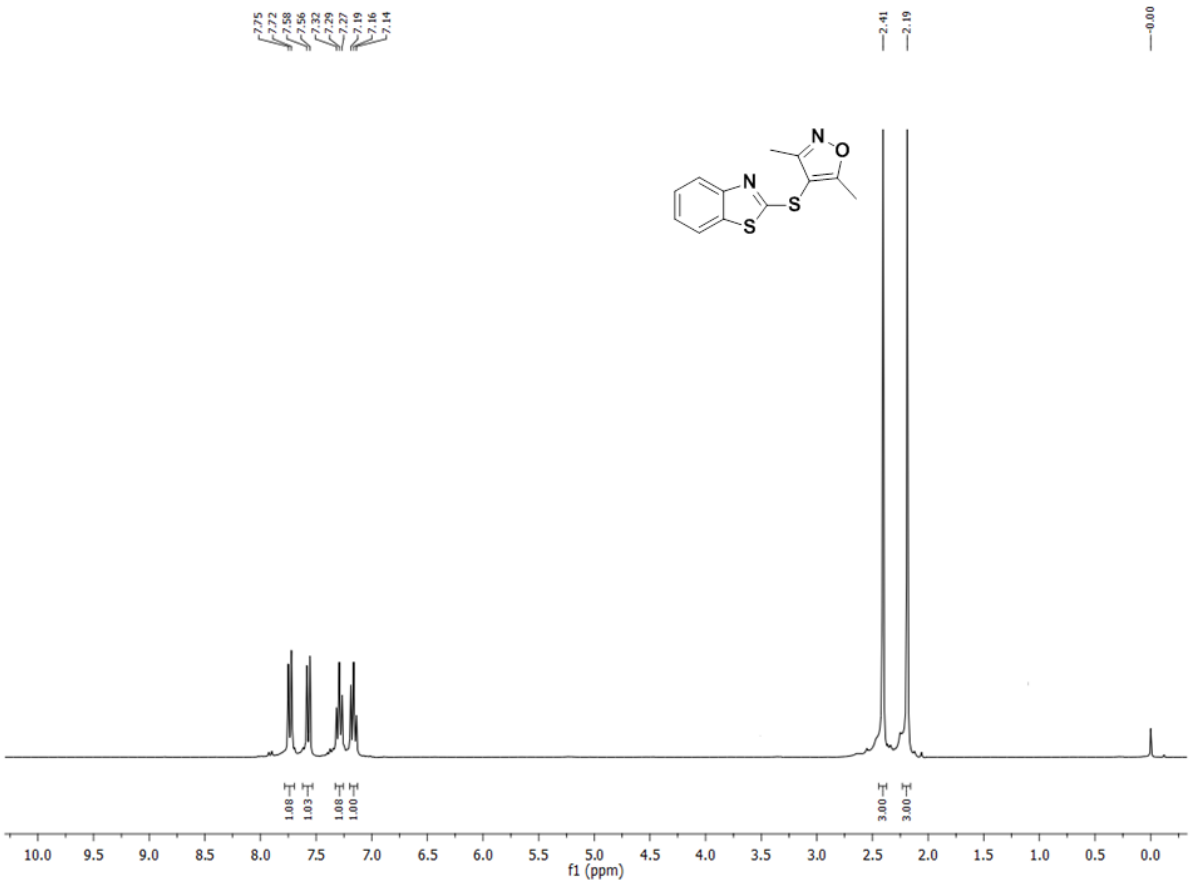


Figure 73. ^{1}H NMR Spectrum of compound **4b**

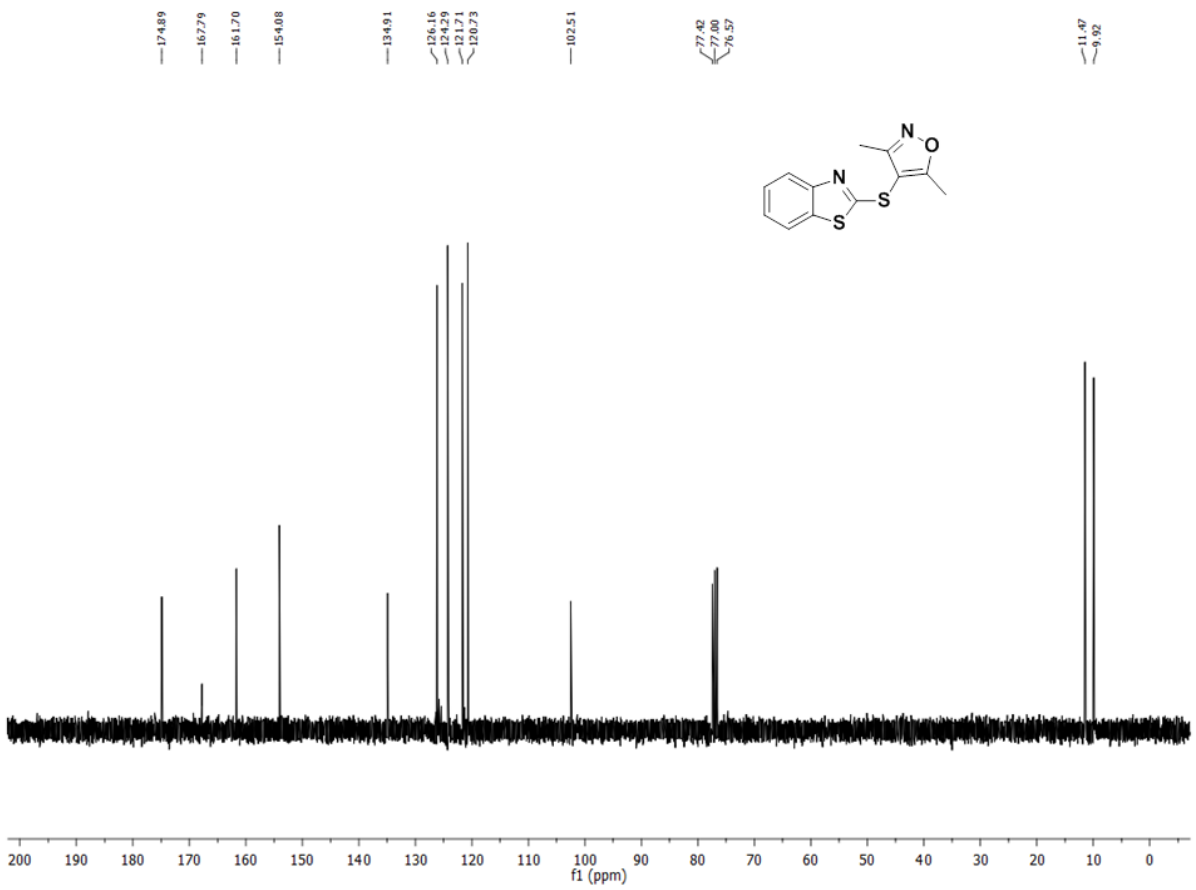


Figure 74. ^{13}C Spectrum of compound **4b**

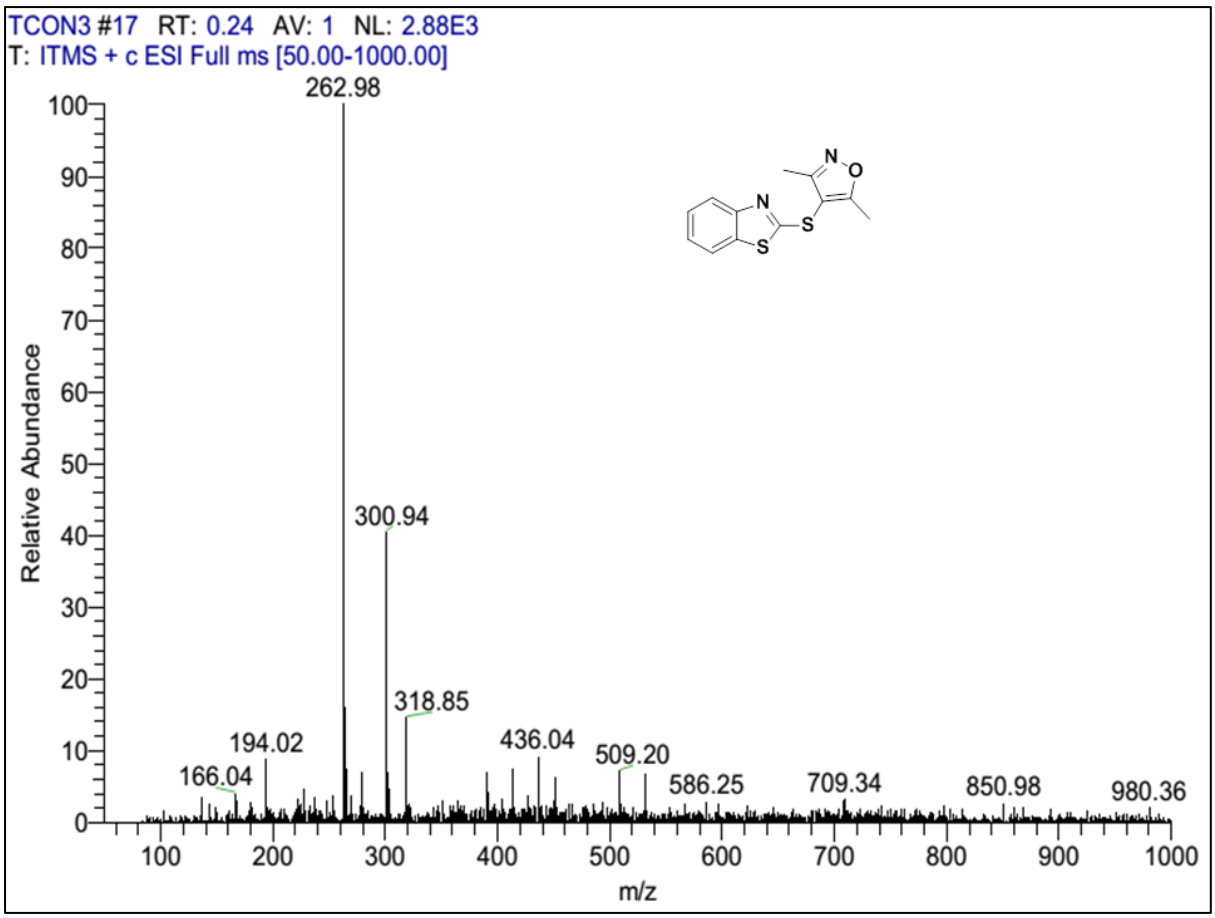


Figure 75. Mass Spectrum of compound **4b**

X-ray Crystallographic Data

of Compound (3ah)

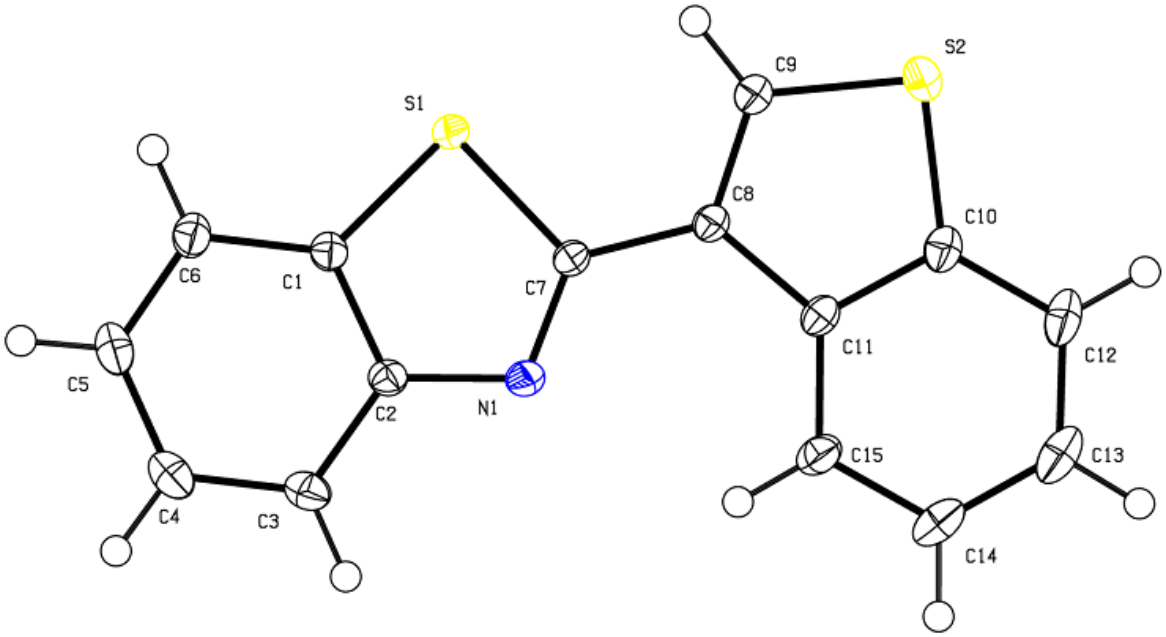


Table 1. Crystal data and structure refinement for SMB_KR_150401_A3_TCUP30.

Identification code	tcup30	
Empirical formula	C15 H9 N S2	
Formula weight	267.35	
Temperature	150.15 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 25.831(3) Å	α= 90°.
	b = 11.8166(11) Å	β= 90°.
	c = 3.9035(4) Å	γ = 90°.
Volume	1191.5(2) $Å^3$	
Z	4	
Density (calculated)	1.490 Mg/m^3	
Absorption coefficient	0.424 mm^{-1}	
F(000)	552	
Crystal size	0.51 x 0.18 x 0.08 mm^3	
Theta range for data collection	1.577 to 38.720°.	
Index ranges	-44<=h<=44, -20<=k<=20, -6<=l<=6	
Reflections collected	55390	
Independent reflections	6578 [R(int) = 0.0525]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7476 and 0.6180	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6578 / 1 / 163	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0364, wR2 = 0.0865	
R indices (all data)	R1 = 0.0419, wR2 = 0.0892	
Absolute structure parameter	0.01(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.553 and -0.284 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for SMB_KR_150401_A3_TCUP30. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	4576(1)	5941(1)	2638(1)	15(1)
S(2)	3968(1)	2093(1)	2641(1)	22(1)
N(1)	3686(1)	6186(1)	5707(3)	16(1)
C(1)	4411(1)	7280(1)	4057(4)	15(1)
C(2)	3920(1)	7246(1)	5622(4)	15(1)
C(3)	3707(1)	8241(1)	6987(4)	20(1)
C(4)	3986(1)	9242(1)	6714(5)	23(1)
C(5)	4473(1)	9262(1)	5141(5)	22(1)
C(6)	4695(1)	8284(1)	3817(4)	19(1)
C(7)	3982(1)	5427(1)	4291(4)	14(1)
C(8)	3860(1)	4226(1)	4017(4)	15(1)
C(9)	4202(1)	3455(1)	2691(5)	18(1)
C(10)	3386(1)	2521(1)	4447(4)	19(1)
C(11)	3379(1)	3698(1)	5078(4)	16(1)
C(12)	2964(1)	1826(1)	5260(5)	26(1)
C(13)	2532(1)	2326(2)	6731(5)	29(1)
C(14)	2518(1)	3491(2)	7361(5)	27(1)
C(15)	2936(1)	4184(1)	6556(4)	21(1)

Table 3. Bond lengths [Å] and angles [°] for SMB_KR_150401_A3_TCUP30.

S(1)-C(1)	1.7294(14)
S(1)-C(7)	1.7713(13)
S(2)-C(9)	1.7195(13)
S(2)-C(10)	1.7358(16)
N(1)-C(2)	1.3910(18)
N(1)-C(7)	1.3028(18)
C(1)-C(2)	1.409(2)
C(1)-C(6)	1.3987(19)
C(2)-C(3)	1.4036(19)
C(3)-H(3)	0.9500
C(3)-C(4)	1.390(2)
C(4)-H(4)	0.9500
C(4)-C(5)	1.400(3)
C(5)-H(5)	0.9500
C(5)-C(6)	1.391(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.4577(19)
C(8)-C(9)	1.3698(19)
C(8)-C(11)	1.4494(19)
C(9)-H(9)	0.9500
C(10)-C(11)	1.413(2)
C(10)-C(12)	1.403(2)
C(11)-C(15)	1.406(2)
C(12)-H(12)	0.9500
C(12)-C(13)	1.385(3)
C(13)-H(13)	0.9500
C(13)-C(14)	1.399(3)
C(14)-H(14)	0.9500
C(14)-C(15)	1.390(2)
C(15)-H(15)	0.9500
C(1)-S(1)-C(7)	89.11(6)
C(9)-S(2)-C(10)	91.48(7)
C(7)-N(1)-C(2)	110.77(12)
C(2)-C(1)-S(1)	109.52(10)
C(6)-C(1)-S(1)	128.75(11)
C(6)-C(1)-C(2)	121.73(13)

N(1)-C(2)-C(1)	115.33(12)
N(1)-C(2)-C(3)	125.01(13)
C(3)-C(2)-C(1)	119.66(13)
C(2)-C(3)-H(3)	120.7
C(4)-C(3)-C(2)	118.66(14)
C(4)-C(3)-H(3)	120.7
C(3)-C(4)-H(4)	119.5
C(3)-C(4)-C(5)	120.97(14)
C(5)-C(4)-H(4)	119.5
C(4)-C(5)-H(5)	119.3
C(6)-C(5)-C(4)	121.37(14)
C(6)-C(5)-H(5)	119.3
C(1)-C(6)-H(6)	121.2
C(5)-C(6)-C(1)	117.60(14)
C(5)-C(6)-H(6)	121.2
N(1)-C(7)-S(1)	115.25(10)
N(1)-C(7)-C(8)	125.10(12)
C(8)-C(7)-S(1)	119.64(10)
C(9)-C(8)-C(7)	122.36(12)
C(9)-C(8)-C(11)	111.98(12)
C(11)-C(8)-C(7)	125.67(12)
S(2)-C(9)-H(9)	123.2
C(8)-C(9)-S(2)	113.62(10)
C(8)-C(9)-H(9)	123.2
C(11)-C(10)-S(2)	111.67(10)
C(12)-C(10)-S(2)	126.55(13)
C(12)-C(10)-C(11)	121.78(15)
C(10)-C(11)-C(8)	111.26(13)
C(15)-C(11)-C(8)	129.76(14)
C(15)-C(11)-C(10)	118.98(13)
C(10)-C(12)-H(12)	121.0
C(13)-C(12)-C(10)	118.05(16)
C(13)-C(12)-H(12)	121.0
C(12)-C(13)-H(13)	119.5
C(12)-C(13)-C(14)	120.90(15)
C(14)-C(13)-H(13)	119.5
C(13)-C(14)-H(14)	119.3
C(15)-C(14)-C(13)	121.33(16)

C(15)-C(14)-H(14)	119.3
C(11)-C(15)-H(15)	120.5
C(14)-C(15)-C(11)	118.96(15)
C(14)-C(15)-H(15)	120.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for SMB_KR_150401_A3_TCUP30. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	12(1)	15(1)	19(1)	0(1)	2(1)	0(1)
S(2)	22(1)	15(1)	28(1)	-3(1)	1(1)	-1(1)
N(1)	12(1)	17(1)	19(1)	-1(1)	0(1)	0(1)
C(1)	14(1)	14(1)	17(1)	2(1)	-2(1)	1(1)
C(2)	13(1)	16(1)	17(1)	0(1)	-2(1)	2(1)
C(3)	19(1)	20(1)	22(1)	-2(1)	-1(1)	5(1)
C(4)	26(1)	17(1)	25(1)	-4(1)	-5(1)	4(1)
C(5)	26(1)	14(1)	27(1)	0(1)	-6(1)	-2(1)
C(6)	16(1)	16(1)	25(1)	3(1)	-2(1)	-2(1)
C(7)	12(1)	15(1)	15(1)	0(1)	-1(1)	0(1)
C(8)	13(1)	16(1)	16(1)	0(1)	-1(1)	-1(1)
C(9)	15(1)	18(1)	21(1)	-1(1)	1(1)	-2(1)
C(10)	18(1)	19(1)	21(1)	2(1)	-2(1)	-4(1)
C(11)	13(1)	19(1)	16(1)	1(1)	-2(1)	-2(1)
C(12)	23(1)	22(1)	32(1)	5(1)	-4(1)	-10(1)
C(13)	20(1)	34(1)	32(1)	8(1)	-1(1)	-11(1)
C(14)	16(1)	37(1)	28(1)	3(1)	4(1)	-6(1)
C(15)	14(1)	26(1)	24(1)	-1(1)	2(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for SMB_KR_150401_A3_TCUP30.

	x	y	z	U(eq)
H(3)	3378	8230	8076	24
H(4)	3844	9923	7609	28
H(5)	4655	9959	4974	27
H(6)	5029	8298	2788	23
H(9)	4536	3655	1875	22
H(12)	2973	1036	4814	31
H(13)	2243	1872	7321	34
H(14)	2217	3815	8358	33
H(15)	2921	4974	6998	25

Table 6. Torsion angles [°] for SMB_KR_150401_A3_TCUP30.

S(1)-C(1)-C(2)-N(1)	0.45(16)
S(1)-C(1)-C(2)-C(3)	179.74(11)
S(1)-C(1)-C(6)-C(5)	179.35(12)
S(1)-C(7)-C(8)-C(9)	3.8(2)
S(1)-C(7)-C(8)-C(11)	-176.41(12)
S(2)-C(10)-C(11)-C(8)	0.43(16)
S(2)-C(10)-C(11)-C(15)	-179.71(12)
S(2)-C(10)-C(12)-C(13)	179.29(14)
N(1)-C(2)-C(3)-C(4)	179.99(14)
N(1)-C(7)-C(8)-C(9)	-175.77(16)
N(1)-C(7)-C(8)-C(11)	4.0(2)
C(1)-S(1)-C(7)-N(1)	1.11(12)
C(1)-S(1)-C(7)-C(8)	-178.51(12)
C(1)-C(2)-C(3)-C(4)	0.8(2)
C(2)-N(1)-C(7)-S(1)	-1.03(16)
C(2)-N(1)-C(7)-C(8)	178.56(13)
C(2)-C(1)-C(6)-C(5)	-0.9(2)
C(2)-C(3)-C(4)-C(5)	-0.6(2)

C(3)-C(4)-C(5)-C(6)	-0.4(3)
C(4)-C(5)-C(6)-C(1)	1.2(2)
C(6)-C(1)-C(2)-N(1)	-179.30(14)
C(6)-C(1)-C(2)-C(3)	0.0(2)
C(7)-S(1)-C(1)-C(2)	-0.82(11)
C(7)-S(1)-C(1)-C(6)	178.92(15)
C(7)-N(1)-C(2)-C(1)	0.37(18)
C(7)-N(1)-C(2)-C(3)	-178.88(14)
C(7)-C(8)-C(9)-S(2)	179.98(12)
C(7)-C(8)-C(11)-C(10)	179.81(14)
C(7)-C(8)-C(11)-C(15)	0.0(3)
C(8)-C(11)-C(15)-C(14)	-179.95(16)
C(9)-S(2)-C(10)-C(11)	-0.29(12)
C(9)-S(2)-C(10)-C(12)	-179.87(17)
C(9)-C(8)-C(11)-C(10)	-0.38(19)
C(9)-C(8)-C(11)-C(15)	179.77(16)
C(10)-S(2)-C(9)-C(8)	0.07(14)
C(10)-C(11)-C(15)-C(14)	0.2(2)
C(10)-C(12)-C(13)-C(14)	0.5(3)
C(11)-C(8)-C(9)-S(2)	0.17(19)
C(11)-C(10)-C(12)-C(13)	-0.3(3)
C(12)-C(10)-C(11)-C(8)	-179.96(15)
C(12)-C(10)-C(11)-C(15)	-0.1(2)
C(12)-C(13)-C(14)-C(15)	-0.4(3)
C(13)-C(14)-C(15)-C(11)	0.0(3)

Symmetry transformations used to generate equivalent atoms:

X-ray Crystallographic Data

of Compound (3aw)

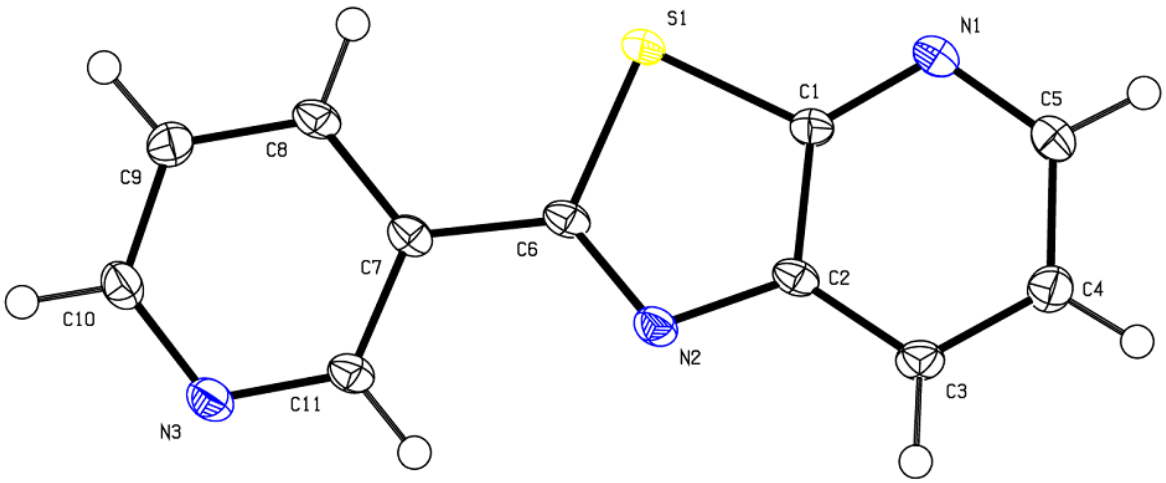


Table 1. Crystal data and structure refinement for SMB_KR_150401_A3_TCUP15.

Identification code	tcup15	
Empirical formula	C11 H7 N3 S	
Formula weight	213.26	
Temperature	150.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 13.203(6) Å	α= 90°.
	b = 6.233(3) Å	β= 104.518(4)°.
	c = 11.730(6) Å	γ = 90°.
Volume	934.5(8) $Å^3$	
Z	4	
Density (calculated)	1.516 Mg/m^3	
Absorption coefficient	0.309 mm^{-1}	
F(000)	440	
Crystal size	0.54 x 0.54 x 0.16 mm^3	
Theta range for data collection	1.593 to 27.553°.	
Index ranges	-17<=h<=16, -8<=k<=8, -15<=l<=15	
Reflections collected	10092	
Independent reflections	2146 [R(int) = 0.0615]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.4502	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2146 / 0 / 137	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0387, wR2 = 0.1033	
R indices (all data)	R1 = 0.0420, wR2 = 0.1066	
Extinction coefficient	0.025(4)	
Largest diff. peak and hole	0.514 and -0.356 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for SMB_KR_150401_A3_TCUP15. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2066(1)	3854(1)	5911(1)	19(1)
N(2)	2470(1)	3378(2)	3849(1)	16(1)
N(3)	4197(1)	-2367(2)	4655(1)	20(1)
N(1)	943(1)	7387(2)	4942(1)	22(1)
C(7)	3294(1)	622(2)	5266(1)	15(1)
C(8)	3613(1)	-47(2)	6440(1)	17(1)
C(2)	1838(1)	5179(2)	3771(1)	15(1)
C(6)	2650(1)	2549(2)	4903(1)	15(1)
C(1)	1535(1)	5713(2)	4808(1)	16(1)
C(11)	3606(1)	-600(2)	4411(1)	17(1)
C(9)	4225(1)	-1884(2)	6707(1)	20(1)
C(4)	860(1)	8231(3)	2903(1)	20(1)
C(10)	4496(1)	-2980(2)	5793(1)	20(1)
C(3)	1483(1)	6494(2)	2788(1)	18(1)
C(5)	618(1)	8622(2)	3985(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for SMB_KR_150401_A3_TCUP15.

S(1)-C(6)	1.7636(15)
S(1)-C(1)	1.7473(16)
N(2)-C(2)	1.3880(19)
N(2)-C(6)	1.3048(19)
N(3)-C(11)	1.3391(19)
N(3)-C(10)	1.349(2)
N(1)-C(1)	1.337(2)
N(1)-C(5)	1.341(2)
C(7)-C(8)	1.399(2)
C(7)-C(6)	1.471(2)
C(7)-C(11)	1.401(2)
C(8)-H(8)	0.9500
C(8)-C(9)	1.391(2)
C(2)-C(1)	1.4118(19)
C(2)-C(3)	1.397(2)
C(11)-H(11)	0.9500
C(9)-H(9)	0.9500
C(9)-C(10)	1.392(2)
C(4)-H(4)	0.9500
C(4)-C(3)	1.387(2)
C(4)-C(5)	1.405(2)
C(10)-H(10)	0.9500
C(3)-H(3)	0.9500
C(5)-H(5)	0.9500
C(1)-S(1)-C(6)	88.37(7)
C(6)-N(2)-C(2)	110.28(12)
C(11)-N(3)-C(10)	117.04(12)
C(1)-N(1)-C(5)	115.04(13)
C(8)-C(7)-C(6)	122.56(12)
C(8)-C(7)-C(11)	118.21(13)
C(11)-C(7)-C(6)	119.23(13)
C(7)-C(8)-H(8)	120.6
C(9)-C(8)-C(7)	118.81(13)
C(9)-C(8)-H(8)	120.6
N(2)-C(2)-C(1)	115.43(12)
N(2)-C(2)-C(3)	126.91(12)

C(3)-C(2)-C(1)	117.65(13)
N(2)-C(6)-S(1)	116.45(11)
N(2)-C(6)-C(7)	123.54(12)
C(7)-C(6)-S(1)	120.00(10)
N(1)-C(1)-S(1)	124.66(11)
N(1)-C(1)-C(2)	125.88(13)
C(2)-C(1)-S(1)	109.46(11)
N(3)-C(11)-C(7)	123.67(13)
N(3)-C(11)-H(11)	118.2
C(7)-C(11)-H(11)	118.2
C(8)-C(9)-H(9)	120.7
C(8)-C(9)-C(10)	118.50(13)
C(10)-C(9)-H(9)	120.7
C(3)-C(4)-H(4)	120.0
C(3)-C(4)-C(5)	119.90(14)
C(5)-C(4)-H(4)	120.0
N(3)-C(10)-C(9)	123.75(14)
N(3)-C(10)-H(10)	118.1
C(9)-C(10)-H(10)	118.1
C(2)-C(3)-H(3)	121.2
C(4)-C(3)-C(2)	117.51(13)
C(4)-C(3)-H(3)	121.2
N(1)-C(5)-C(4)	124.01(14)
N(1)-C(5)-H(5)	118.0
C(4)-C(5)-H(5)	118.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for SMB_KR_150401_A3_TCUP15. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	24(1)	22(1)	16(1)	2(1)	12(1)	8(1)
N(2)	16(1)	17(1)	18(1)	-1(1)	9(1)	1(1)
N(3)	21(1)	19(1)	22(1)	-2(1)	10(1)	2(1)
N(1)	24(1)	25(1)	20(1)	0(1)	11(1)	8(1)
C(7)	13(1)	15(1)	20(1)	-1(1)	9(1)	-2(1)
C(8)	17(1)	17(1)	20(1)	-1(1)	12(1)	-2(1)
C(2)	14(1)	16(1)	18(1)	-2(1)	9(1)	-2(1)
C(6)	15(1)	16(1)	18(1)	-2(1)	9(1)	-3(1)
C(1)	17(1)	18(1)	15(1)	1(1)	8(1)	1(1)
C(11)	17(1)	18(1)	18(1)	-2(1)	9(1)	-1(1)
C(9)	21(1)	20(1)	20(1)	4(1)	9(1)	0(1)
C(4)	18(1)	23(1)	21(1)	4(1)	7(1)	2(1)
C(10)	19(1)	17(1)	25(1)	1(1)	10(1)	3(1)
C(3)	17(1)	22(1)	17(1)	1(1)	9(1)	-1(1)
C(5)	21(1)	22(1)	22(1)	0(1)	9(1)	6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for SMB_KR_150401_A3_TCUP15.

	x	y	z	U(eq)
H(8)	3416	740	7044	20
H(11)	3385	-149	3613	20
H(9)	4453	-2379	7496	23
H(4)	597	9155	2252	24
H(10)	4915	-4232	5981	23
H(3)	1661	6209	2067	22
H(5)	198	9836	4040	26

Table 6. Torsion angles [°] for SMB_KR_150401_A3_TCUP15.

N(2)-C(2)-C(1)-S(1)	-0.38(16)
N(2)-C(2)-C(1)-N(1)	179.06(14)
N(2)-C(2)-C(3)-C(4)	-179.59(13)
C(7)-C(8)-C(9)-C(10)	0.1(2)
C(8)-C(7)-C(6)-S(1)	-10.75(19)
C(8)-C(7)-C(6)-N(2)	169.70(13)
C(8)-C(7)-C(11)-N(3)	-0.4(2)
C(8)-C(9)-C(10)-N(3)	-0.1(2)
C(2)-N(2)-C(6)-S(1)	0.36(15)
C(2)-N(2)-C(6)-C(7)	179.92(12)
C(6)-S(1)-C(1)-N(1)	-178.99(14)
C(6)-S(1)-C(1)-C(2)	0.45(11)
C(6)-N(2)-C(2)-C(1)	0.02(18)
C(6)-N(2)-C(2)-C(3)	179.70(14)
C(6)-C(7)-C(8)-C(9)	-179.74(13)
C(6)-C(7)-C(11)-N(3)	179.52(13)
C(1)-S(1)-C(6)-N(2)	-0.49(12)
C(1)-S(1)-C(6)-C(7)	179.93(12)
C(1)-N(1)-C(5)-C(4)	0.4(2)
C(1)-C(2)-C(3)-C(4)	0.1(2)

C(11)-N(3)-C(10)-C(9)	-0.1(2)
C(11)-C(7)-C(8)-C(9)	0.1(2)
C(11)-C(7)-C(6)-S(1)	169.38(10)
C(11)-C(7)-C(6)-N(2)	-10.2(2)
C(10)-N(3)-C(11)-C(7)	0.3(2)
C(3)-C(2)-C(1)-S(1)	179.92(11)
C(3)-C(2)-C(1)-N(1)	-0.6(2)
C(3)-C(4)-C(5)-N(1)	-0.9(2)
C(5)-N(1)-C(1)-S(1)	179.78(12)
C(5)-N(1)-C(1)-C(2)	0.4(2)
C(5)-C(4)-C(3)-C(2)	0.6(2)

Symmetry transformations used to generate equivalent atoms: