

BF₃.OEt₂ Catalyzed Synthesis of Functionalized 9-fluorene-9-ylidene Appended Quinazolin-4-ones

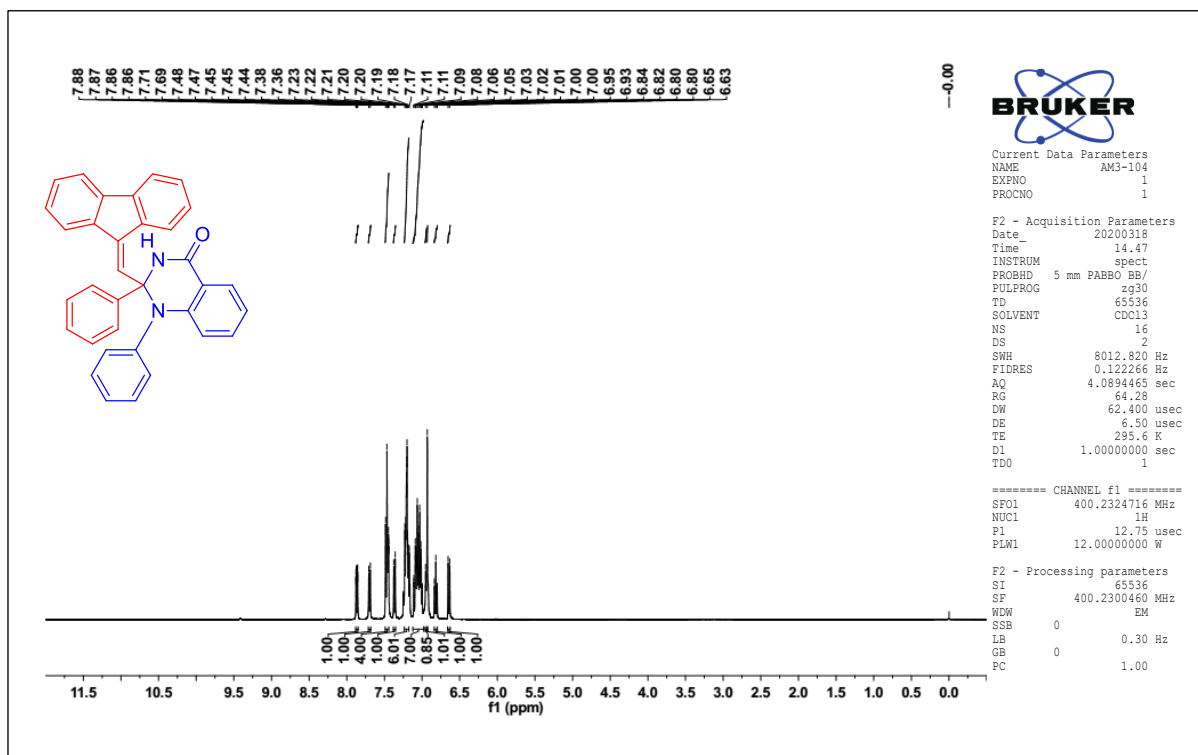
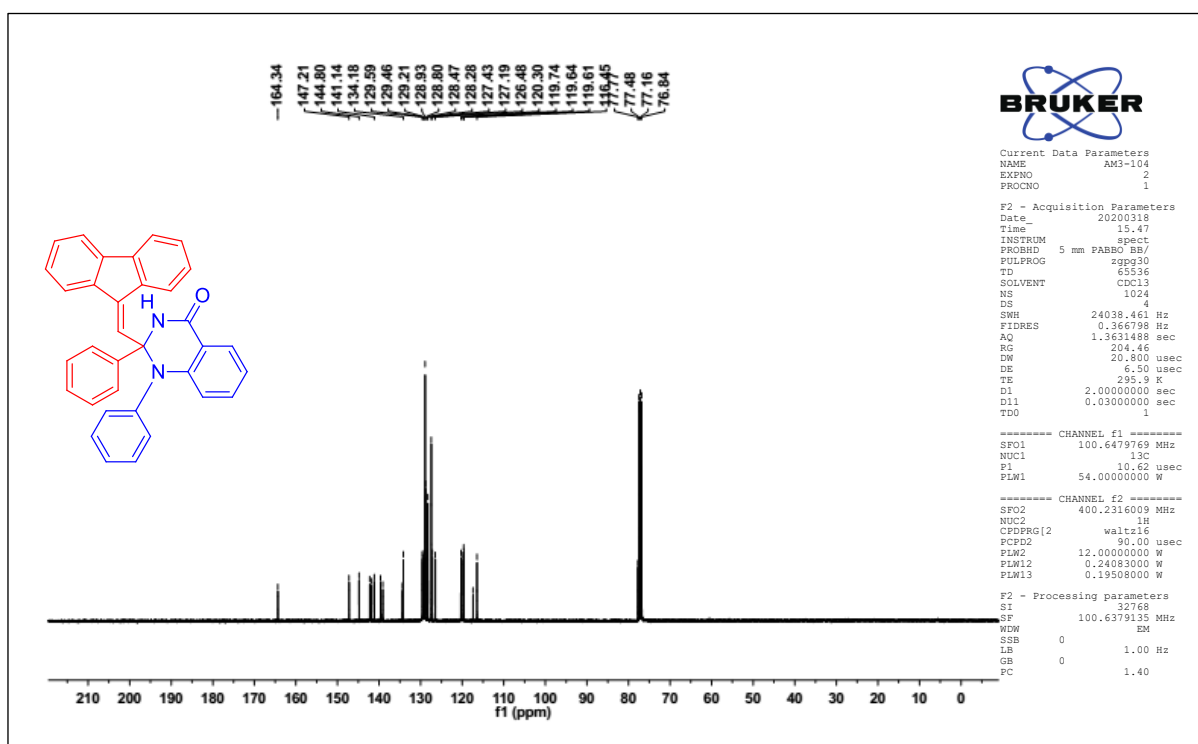
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1. Scanned copies of spectra (^1H and ^{13}C , DEPT-135 NMR, HRMS)Figure 1 ^1H NMR spectrum of compound 3aFigure 2 ^{13}C NMR spectrum of compound 3a

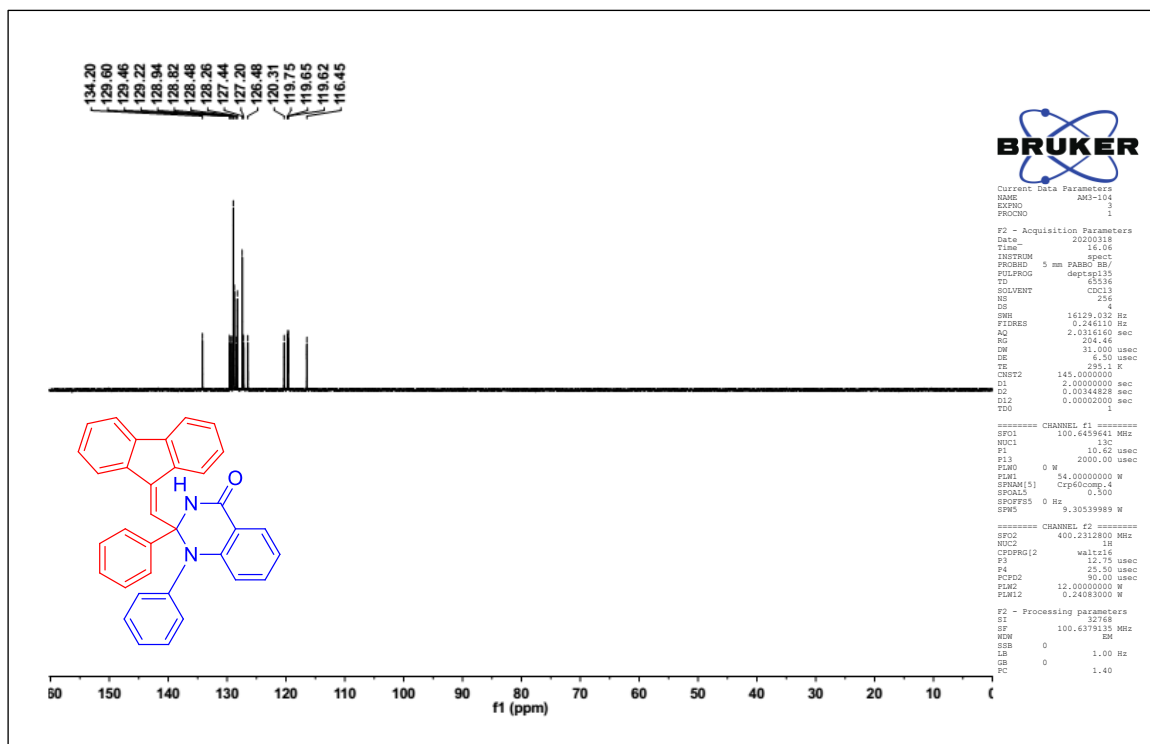


Figure 3 DEPT-135 NMR spectrum of compound 3a

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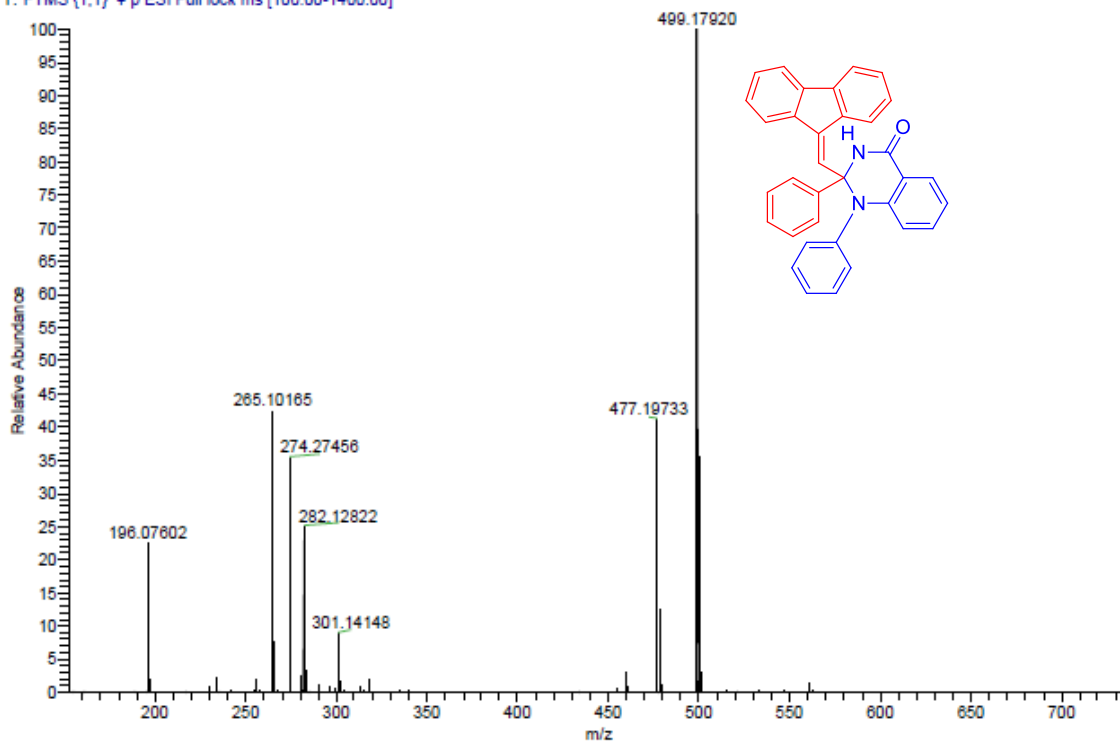


Figure 4 HRMS spectrum of compound 3a

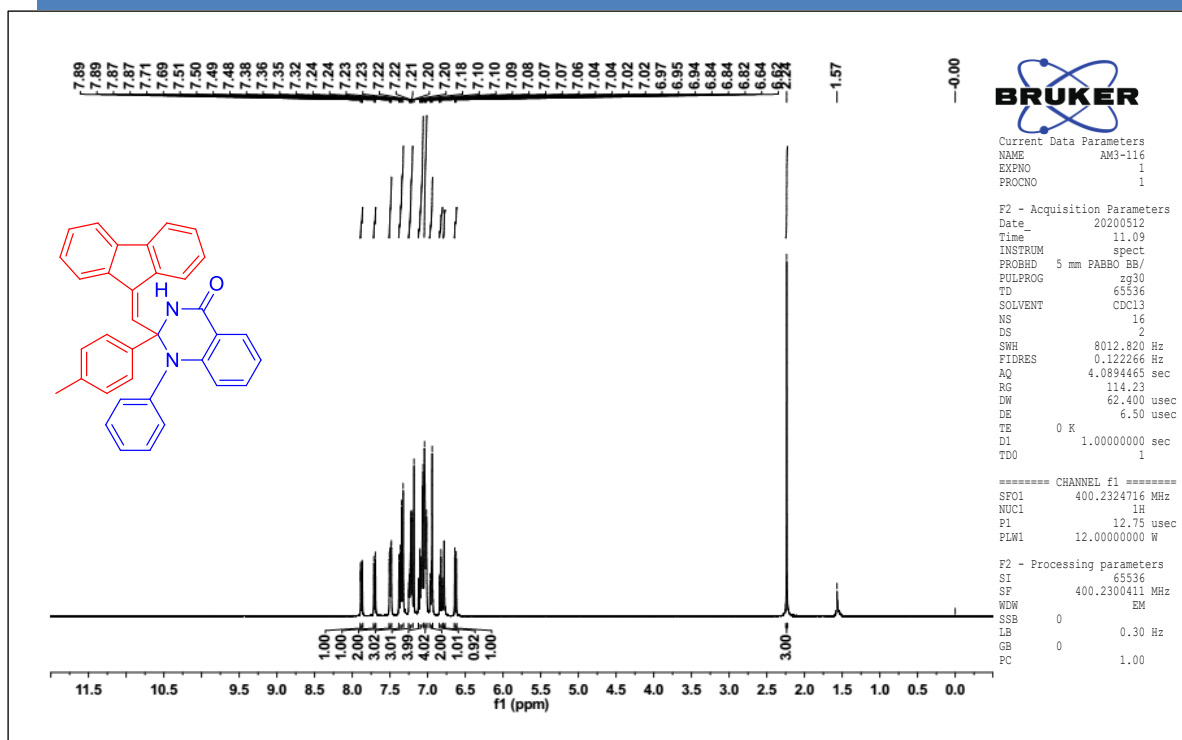


Figure 5 ^1H NMR spectrum of compound **3b**

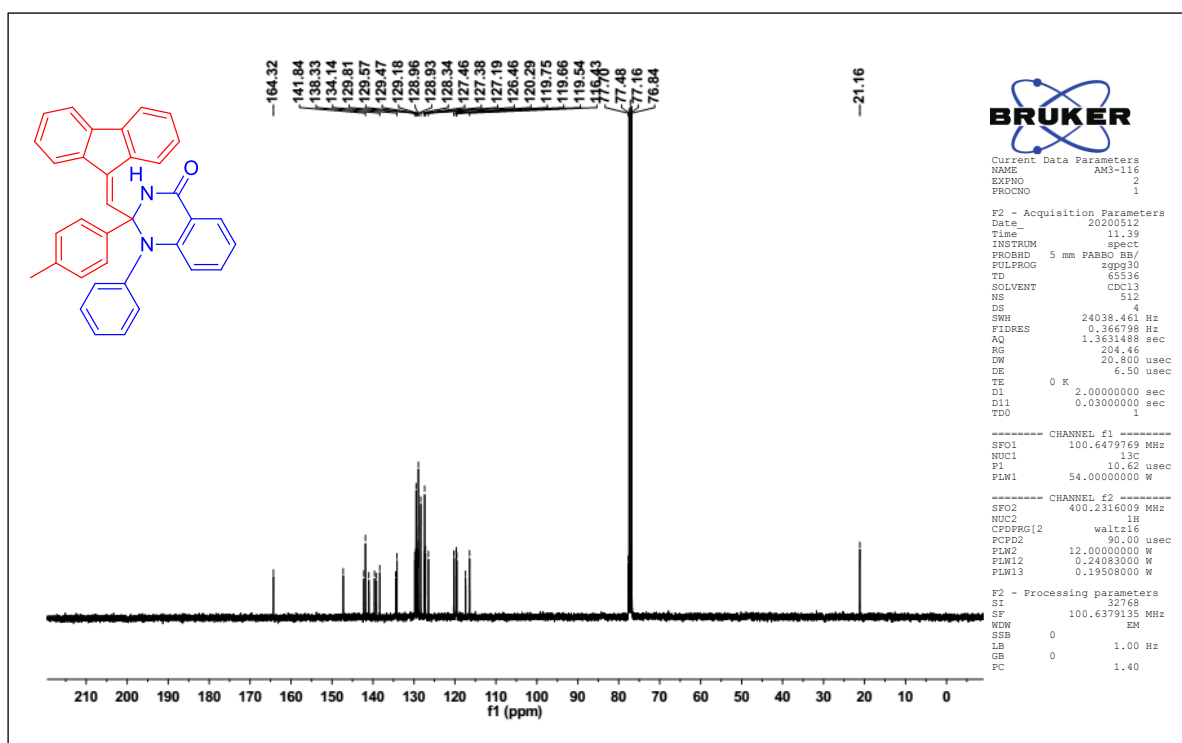


Figure 6 ^{13}C NMR spectrum of compound **3b**

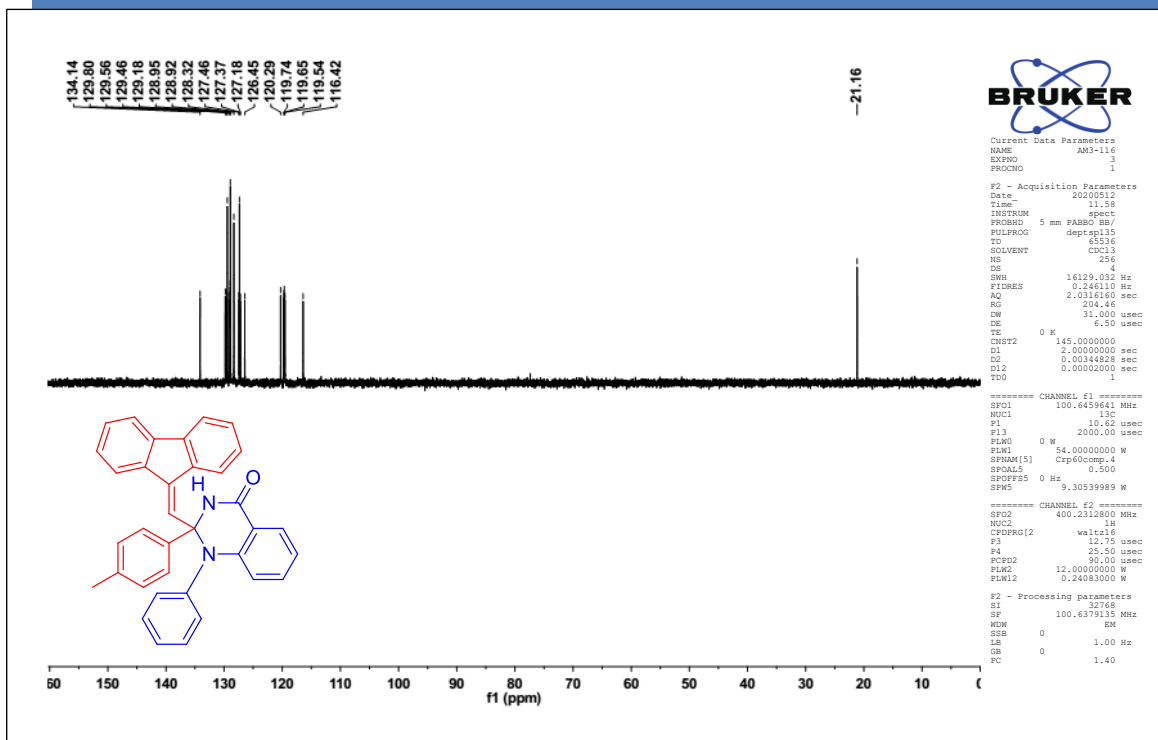


Figure 7 DEPT-135 NMR spectrum of compound 3b

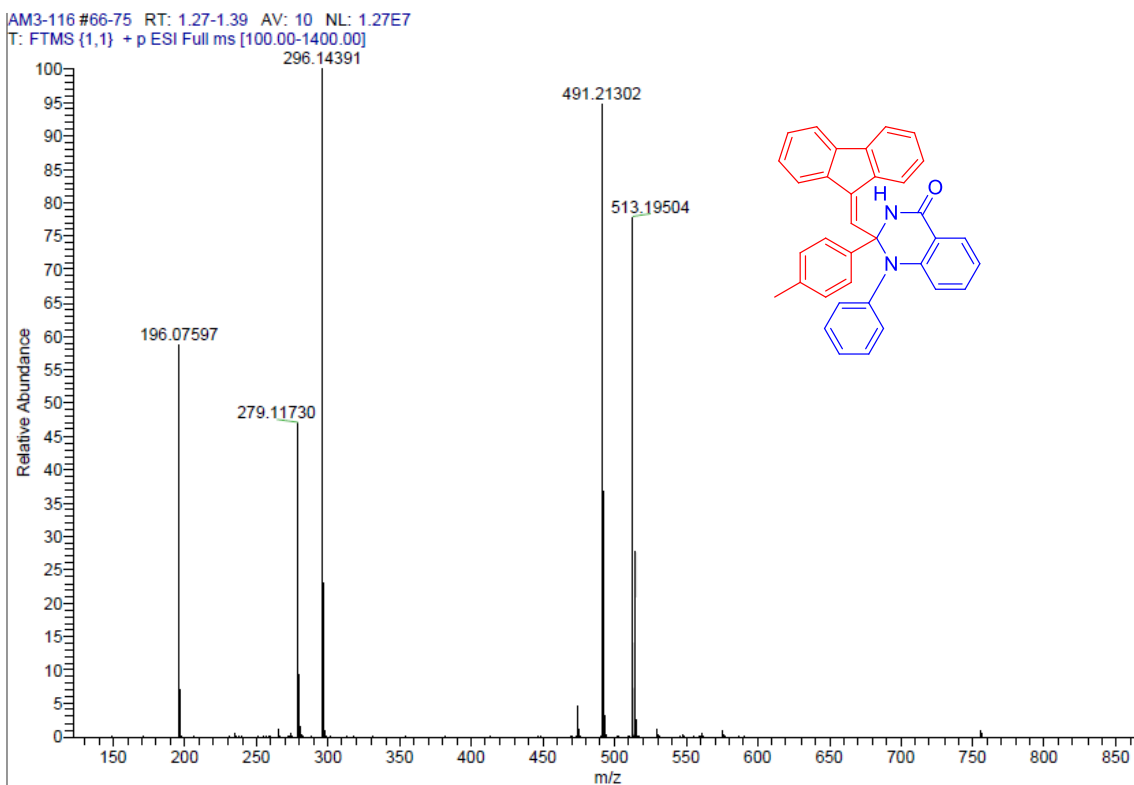
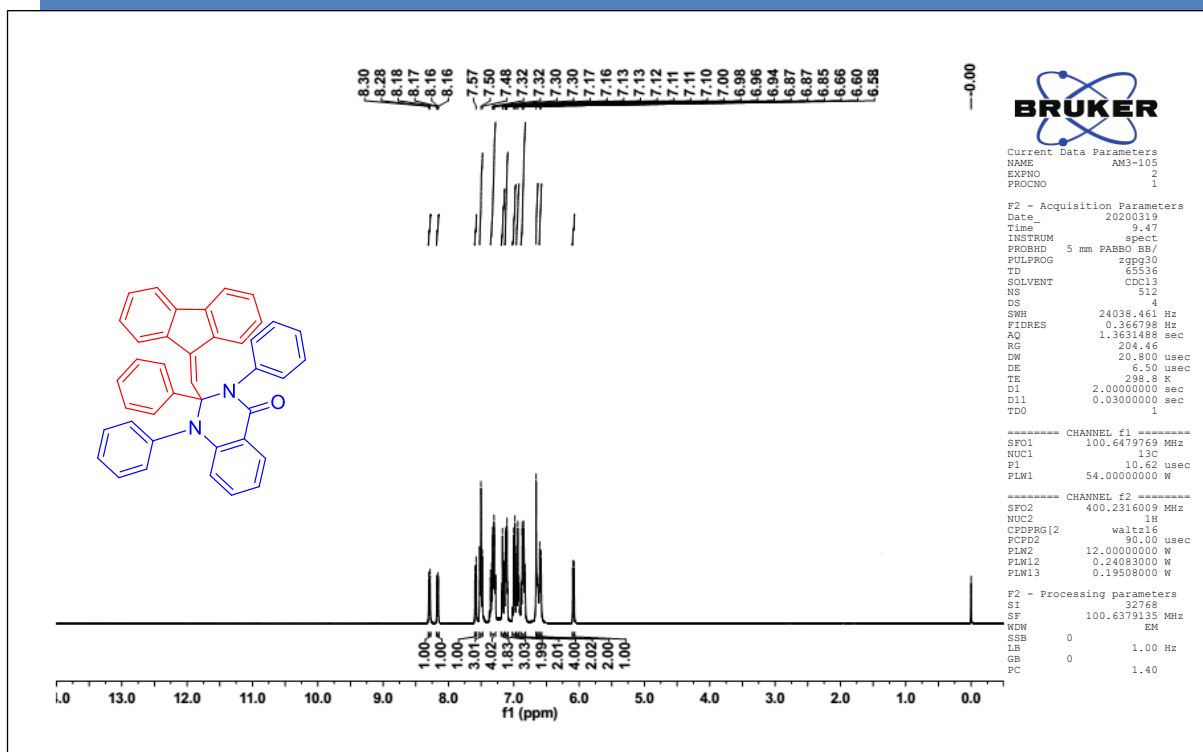
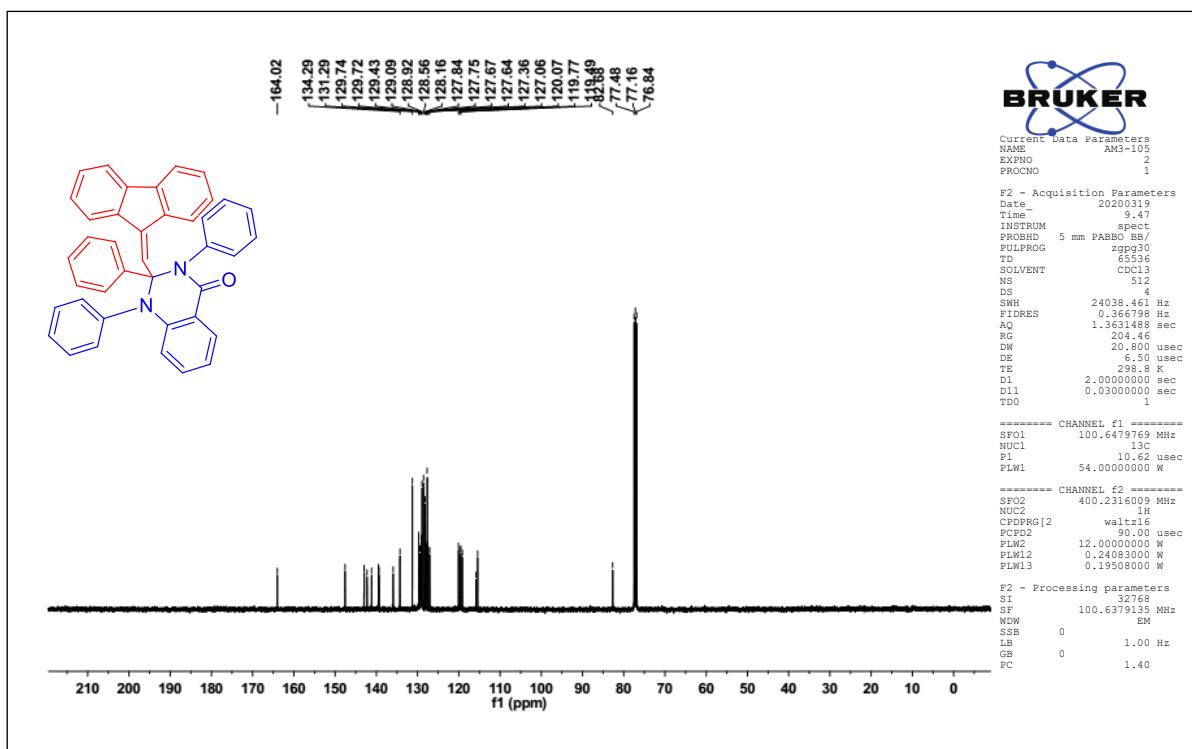


Figure 8 HRMS spectrum of compound 3b

Figure 9 ¹H NMR spectrum of compound 3cFigure 10 ¹³C NMR spectrum of compound 3c

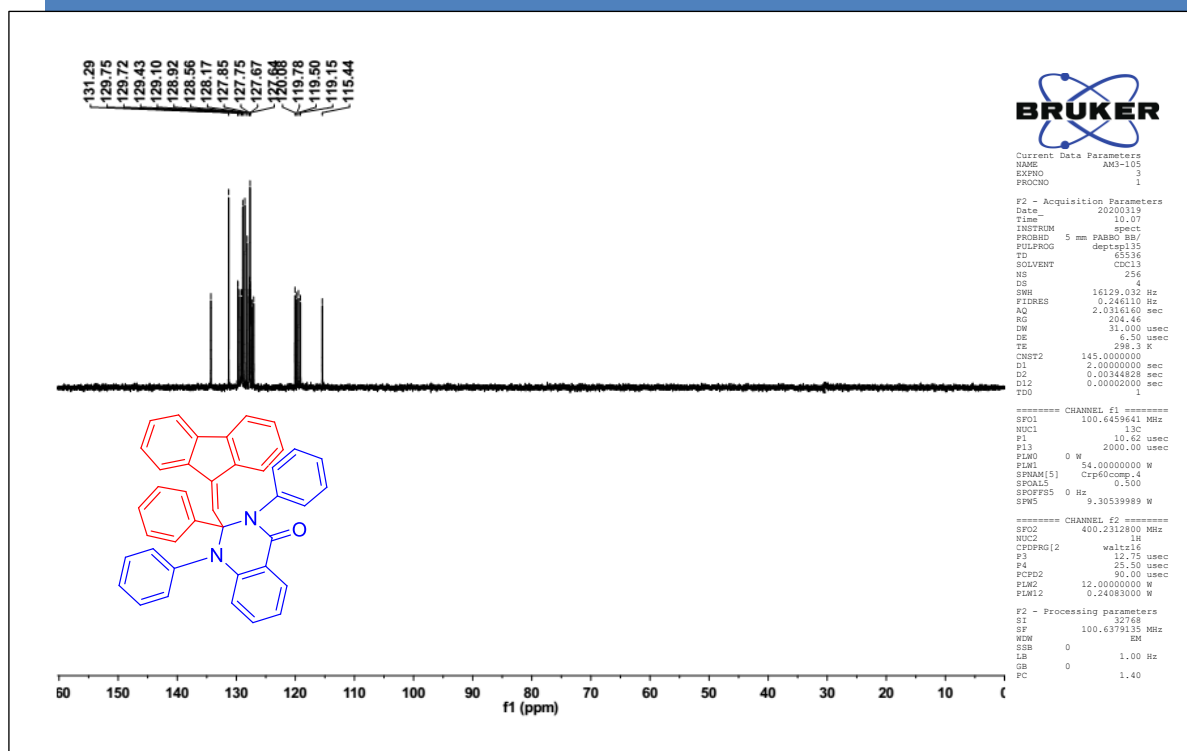


Figure 11 DEPT-135 NMR spectrum of compound **3c**

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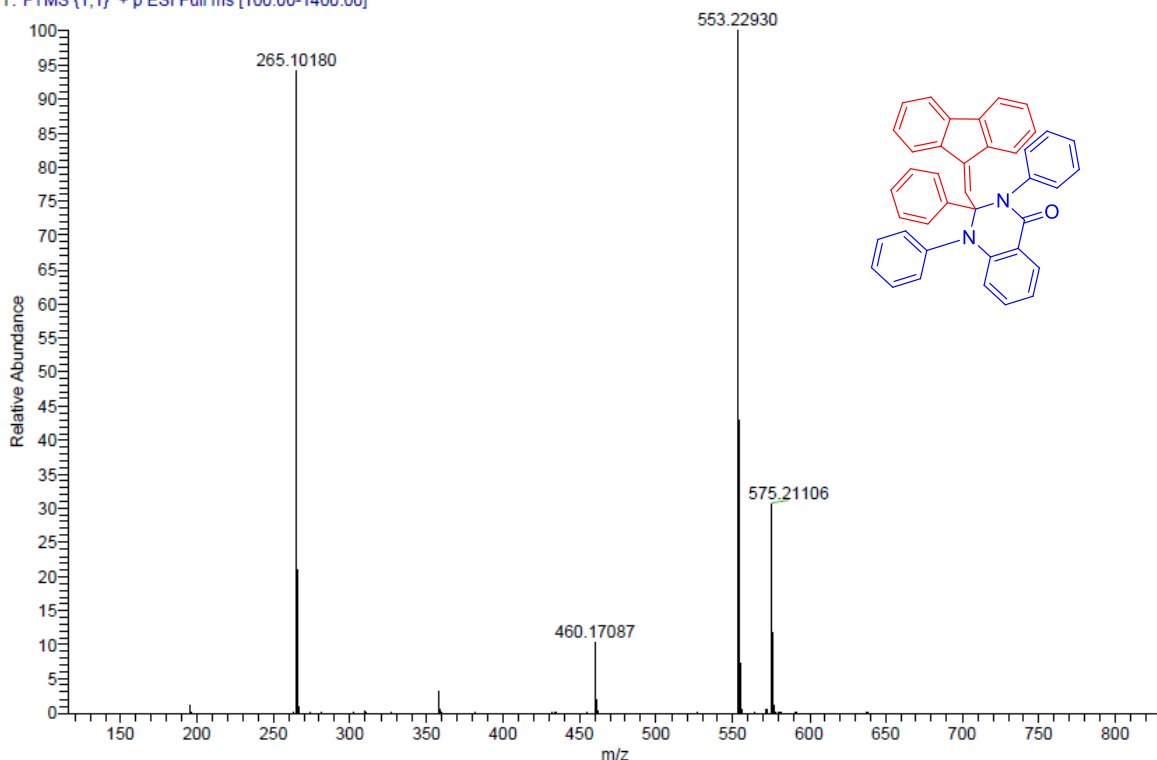
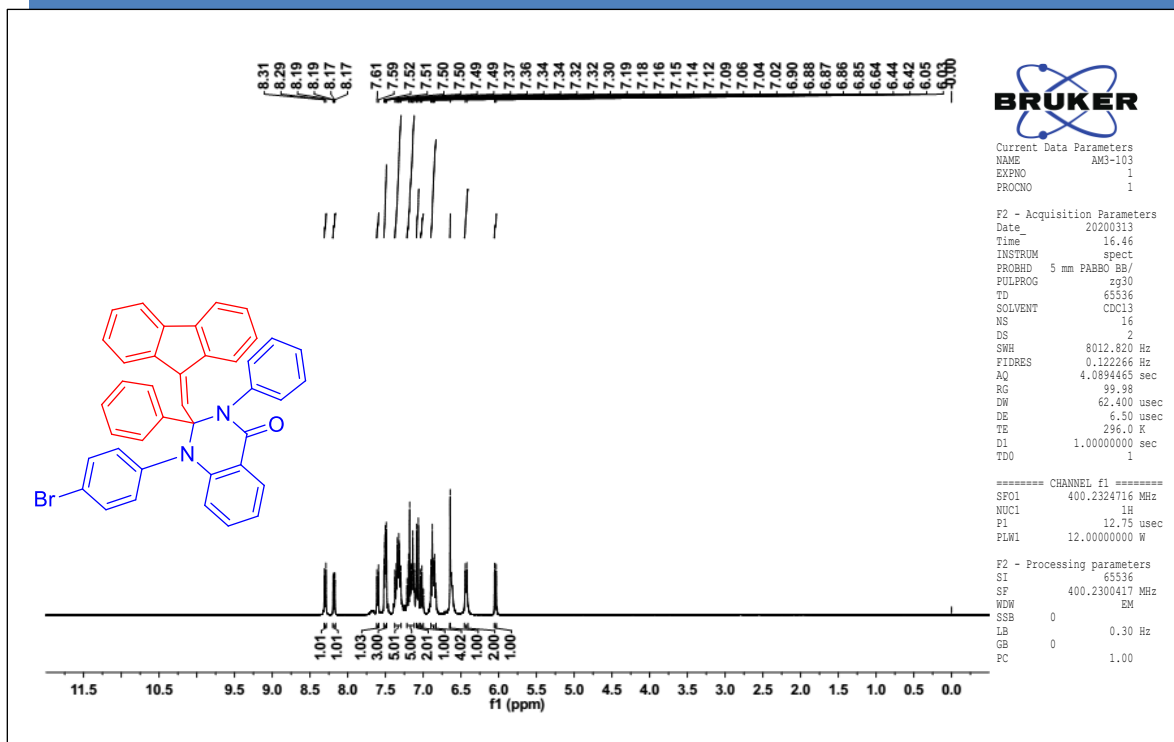
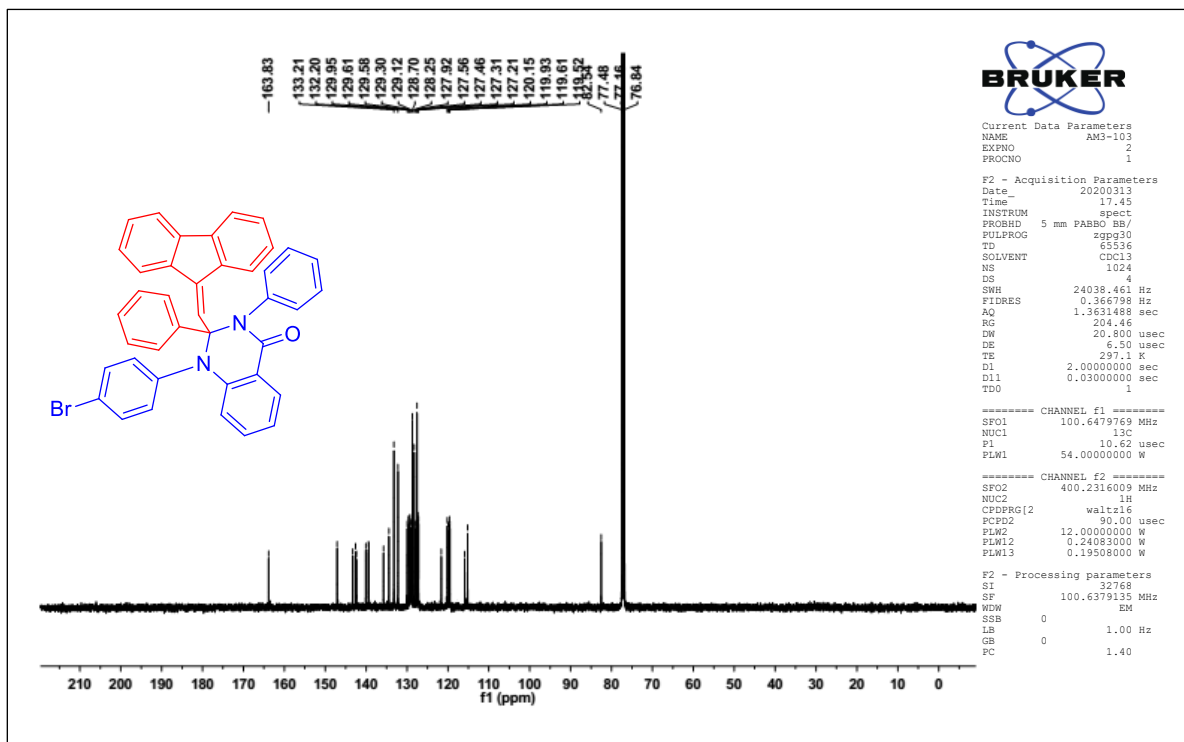
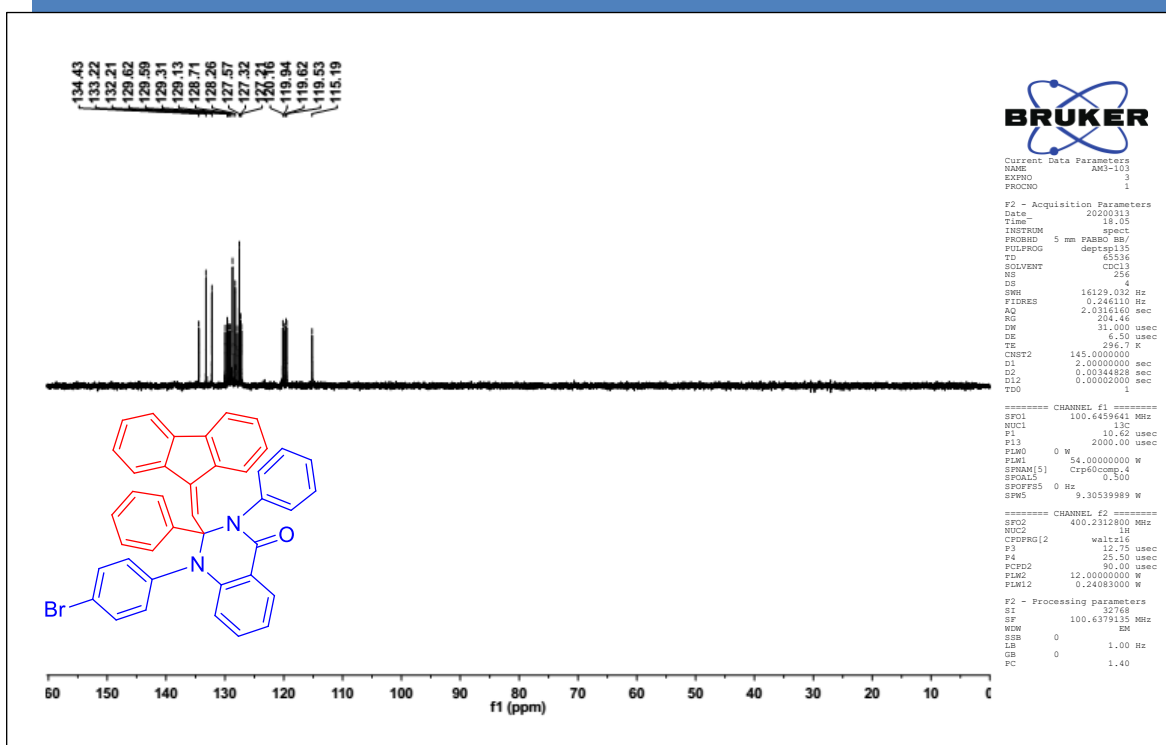
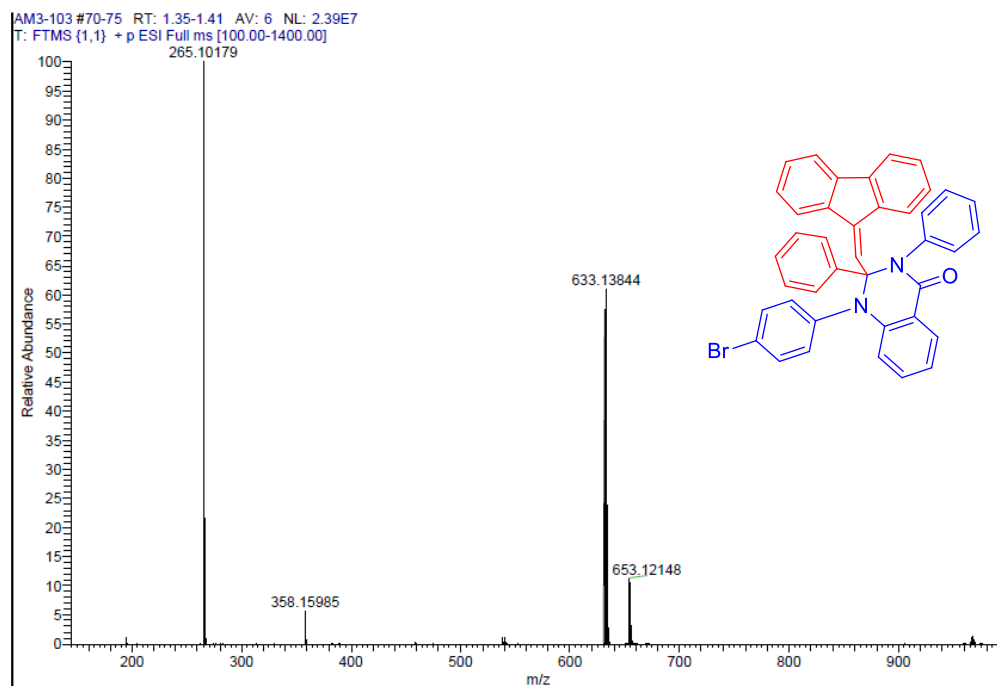


Figure 12 HRMS spectrum of compound **3c**

Figure 13 ¹H NMR spectrum of compound 3dFigure 14 ¹³C NMR spectrum of compound 3d

Figure 15 DEPT-135 NMR spectrum of compound **3d**Figure 16 HRMS spectrum of compound **3d**

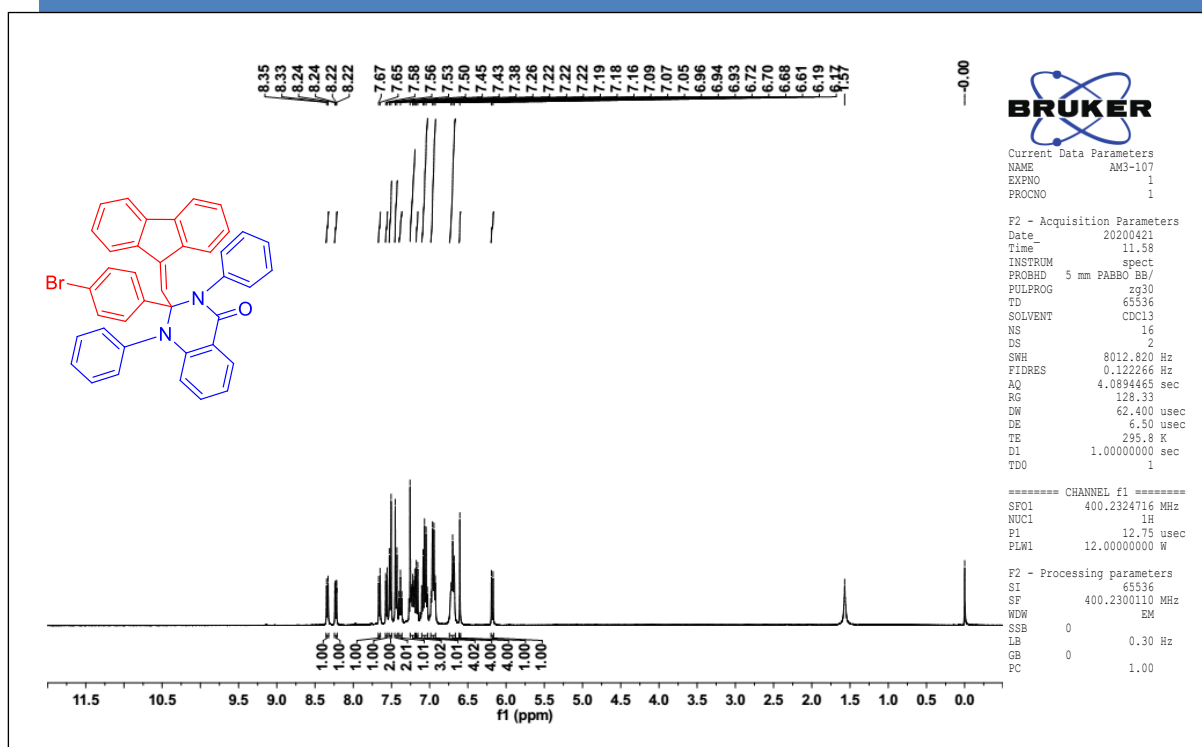


Figure 17 ^1H NMR spectrum of compound **3e**

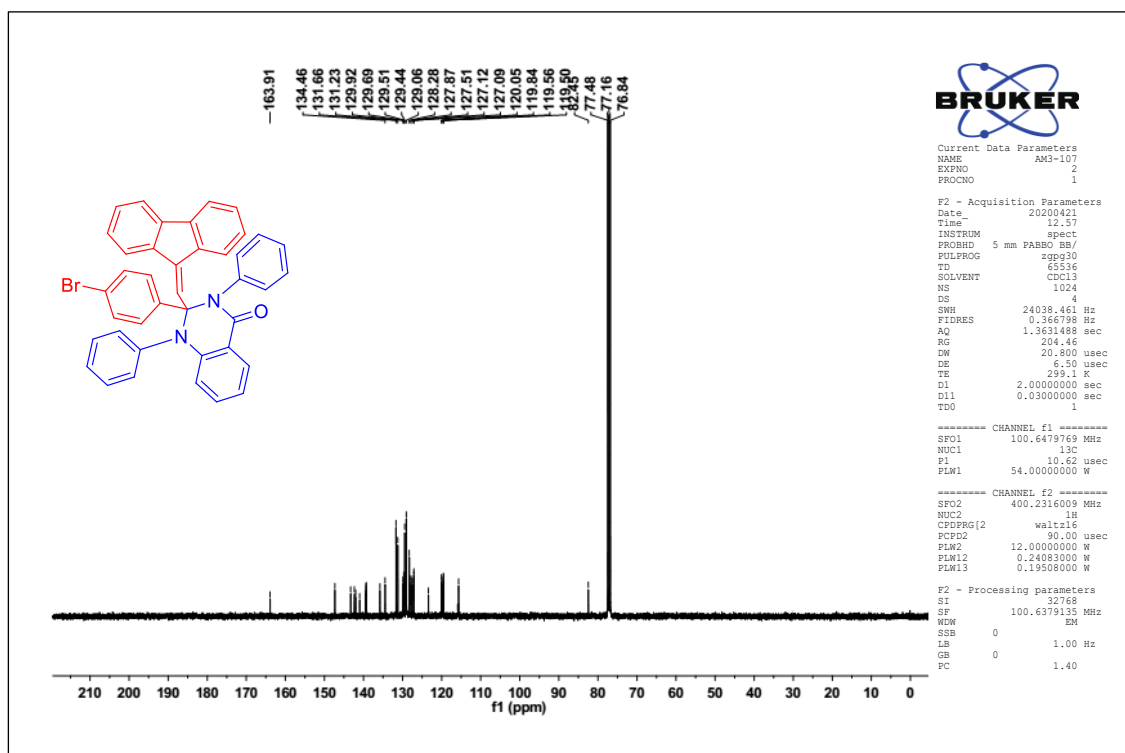


Figure 18 ^{13}C NMR spectrum of compound **3e**

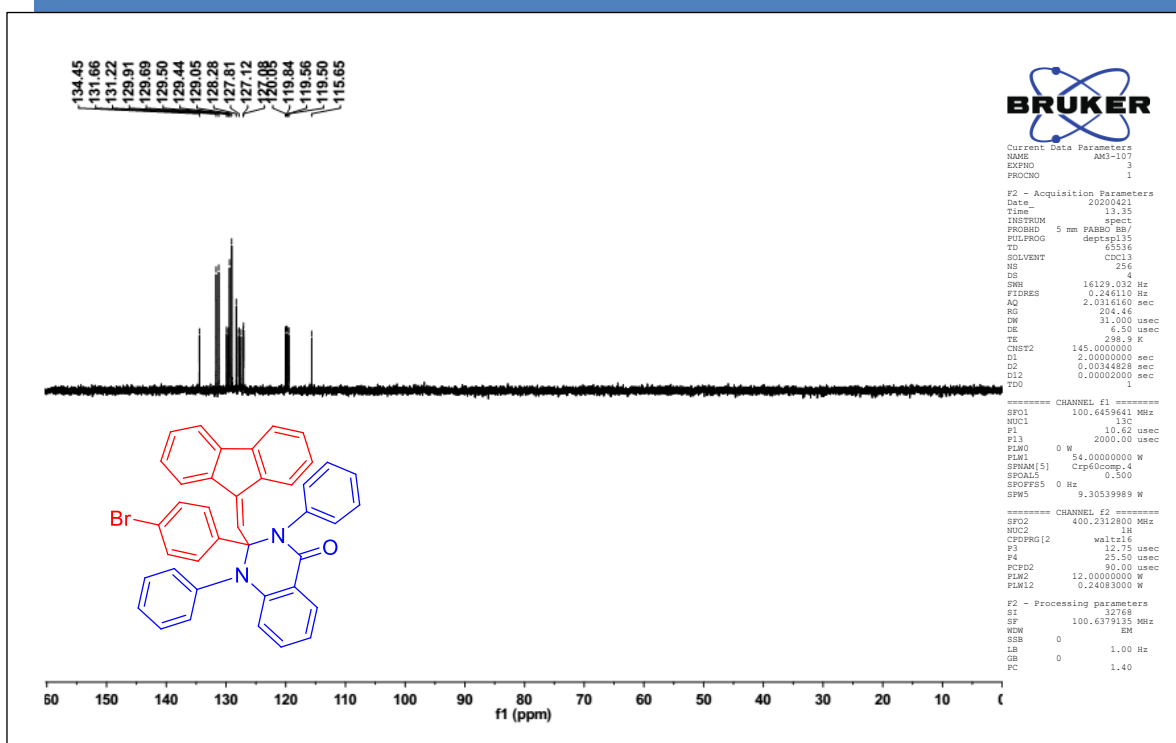


Figure 19 DEPT-135 NMR spectrum of compound 3e

T: FTMS (1,1) + p ESI Full ms [100.00-1400.00]

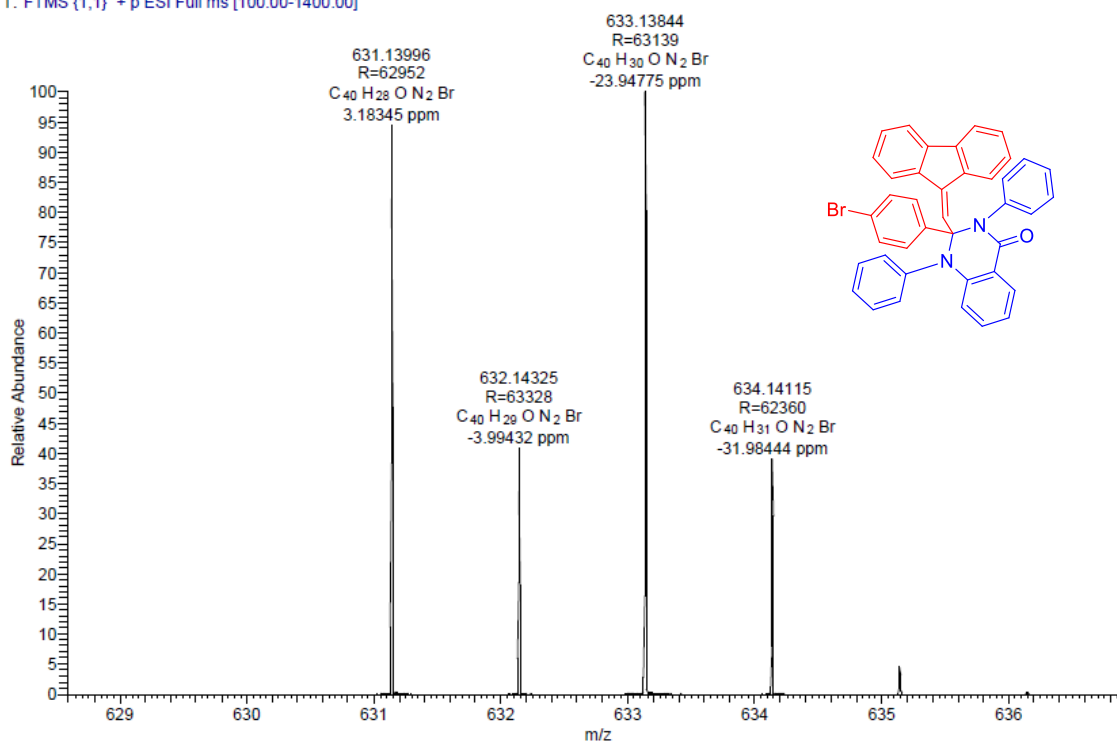
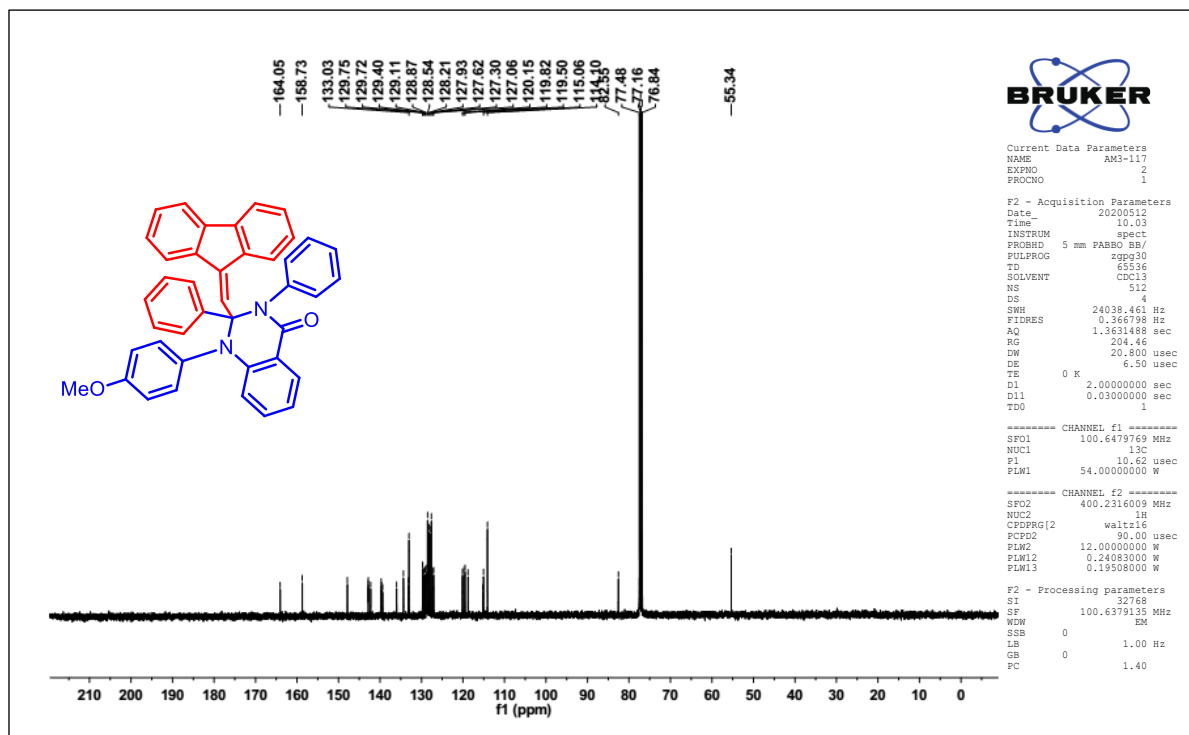
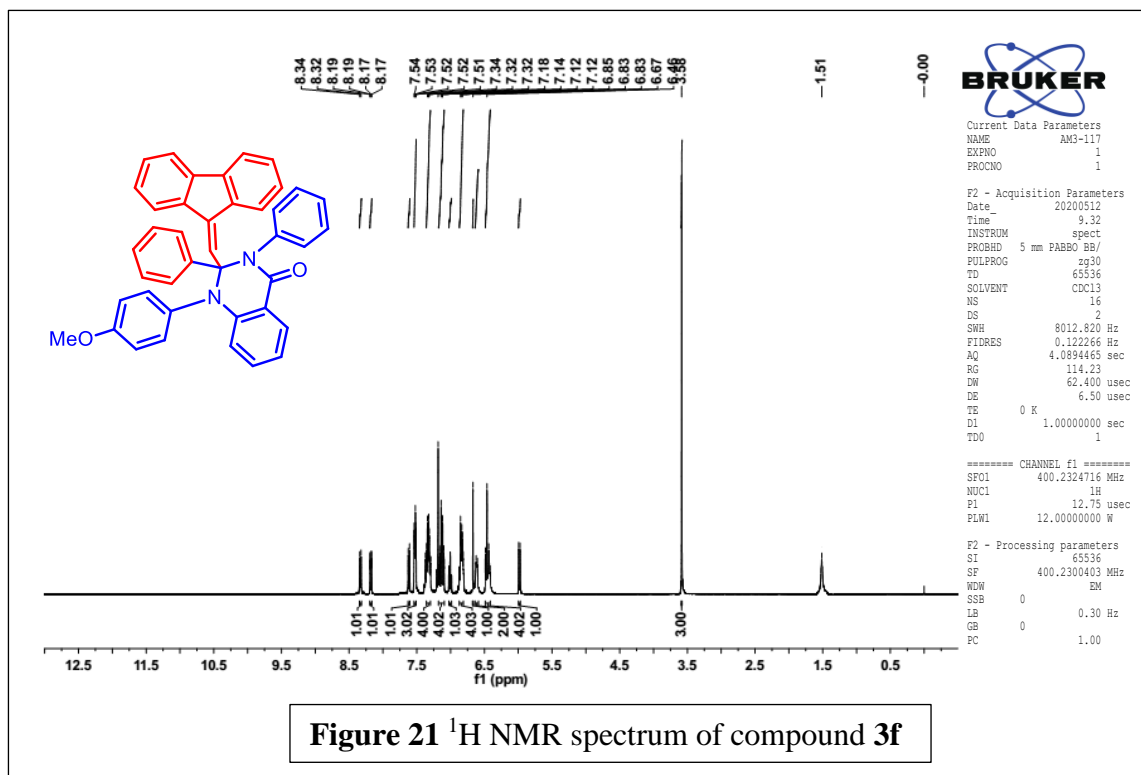


Figure 20 HRMS spectrum of compound 3e



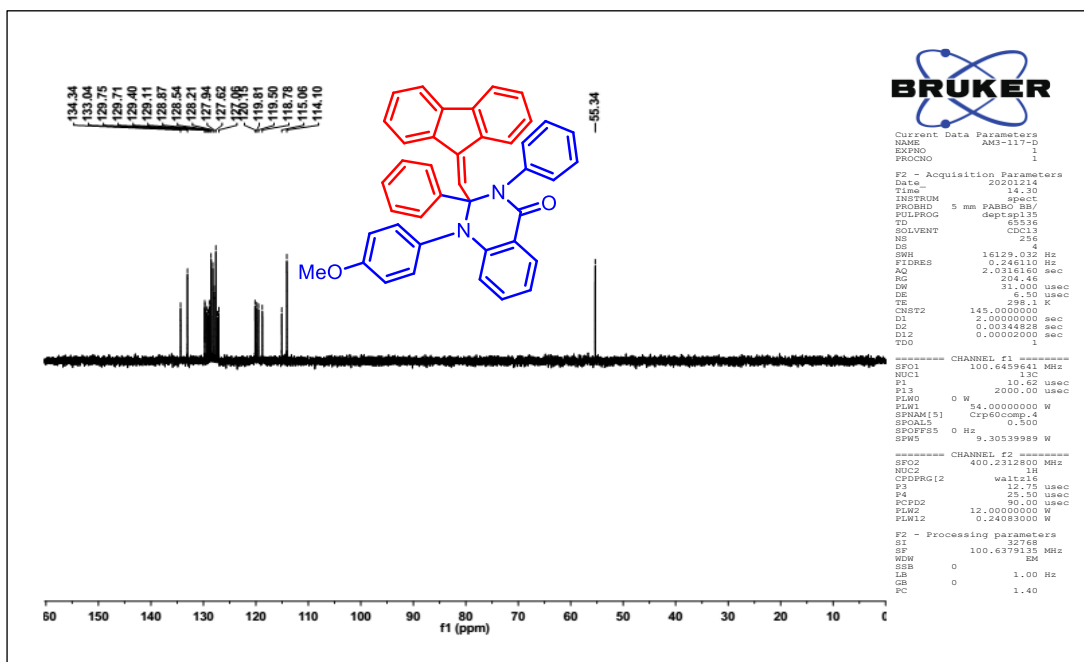


Figure 23 DEPT-135 NMR spectrum of compound 3f

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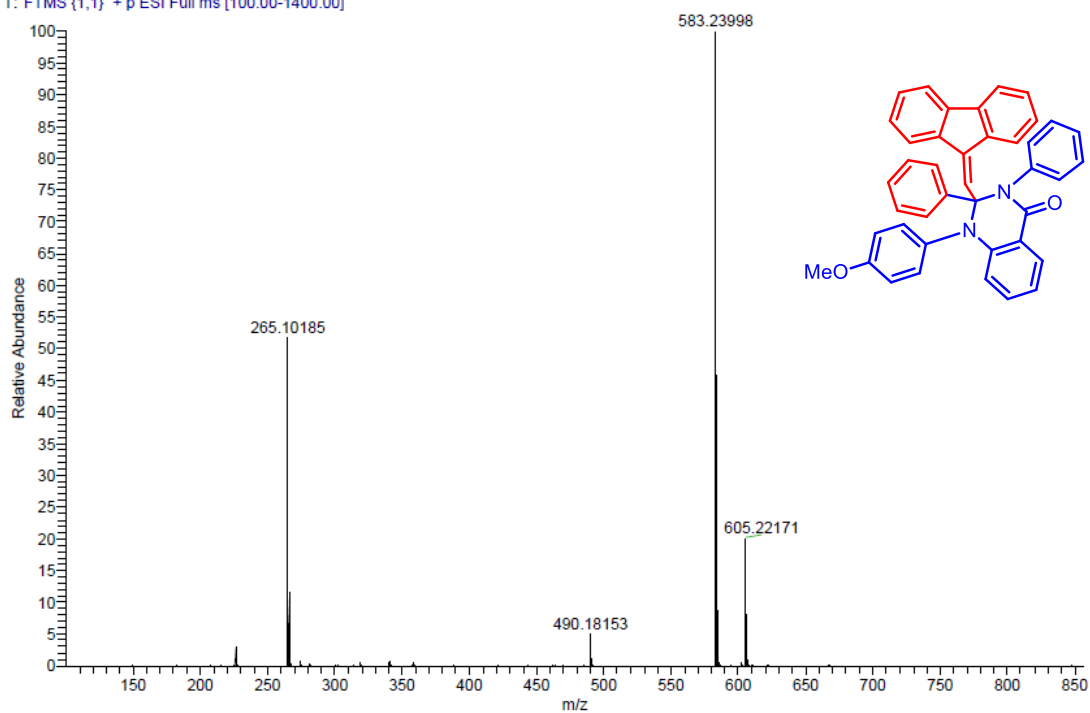
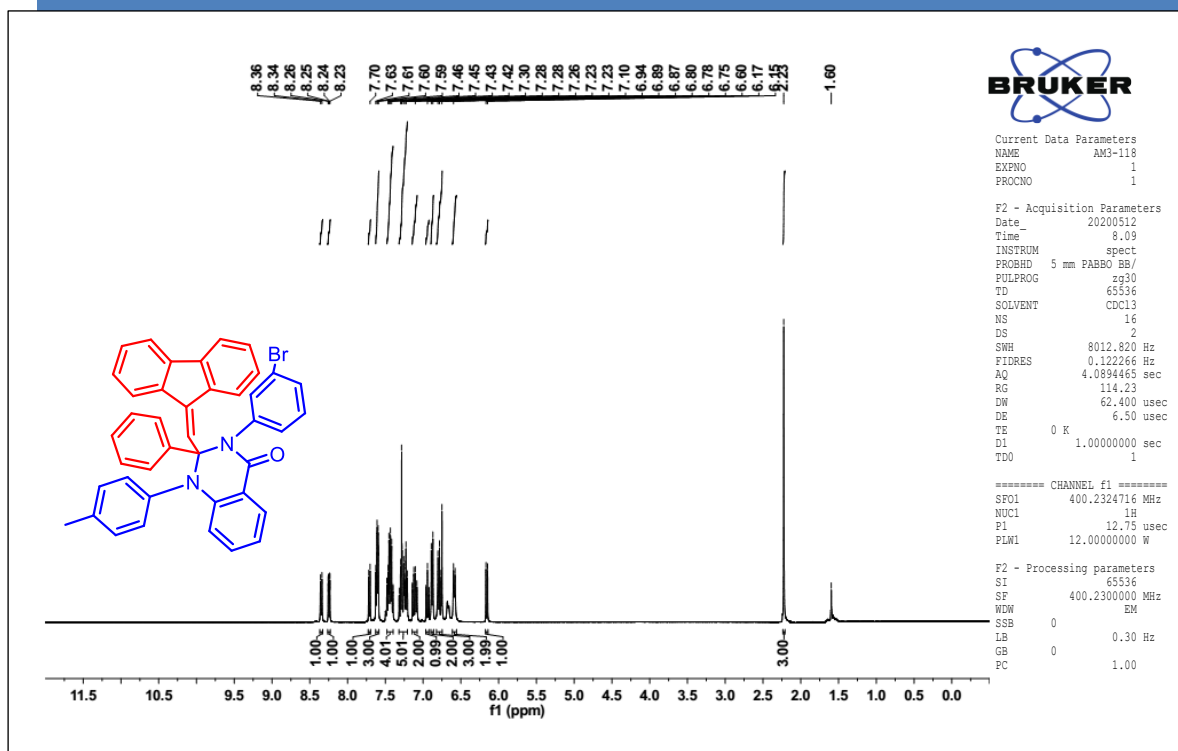
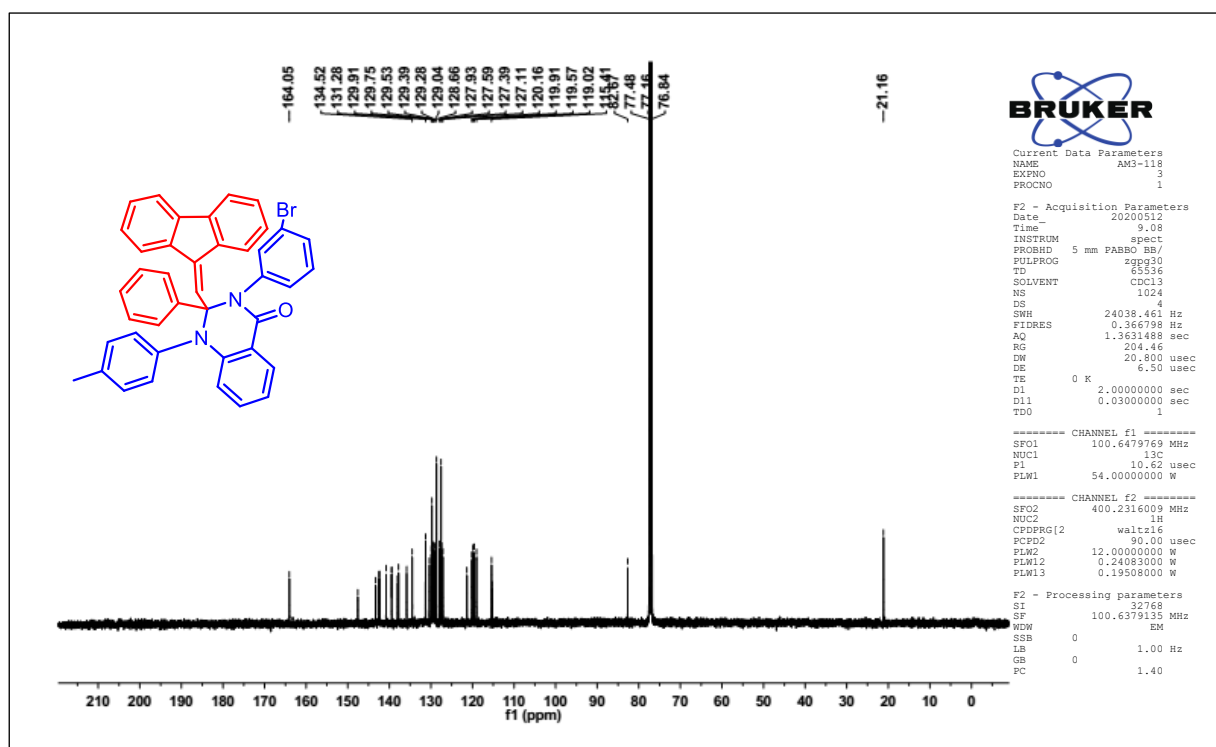


Figure 24 HRMS spectrum of compound 3f

Figure 25 ^1H NMR spectrum of compound 3gFigure 26 ^{13}C NMR spectrum of compound 3g

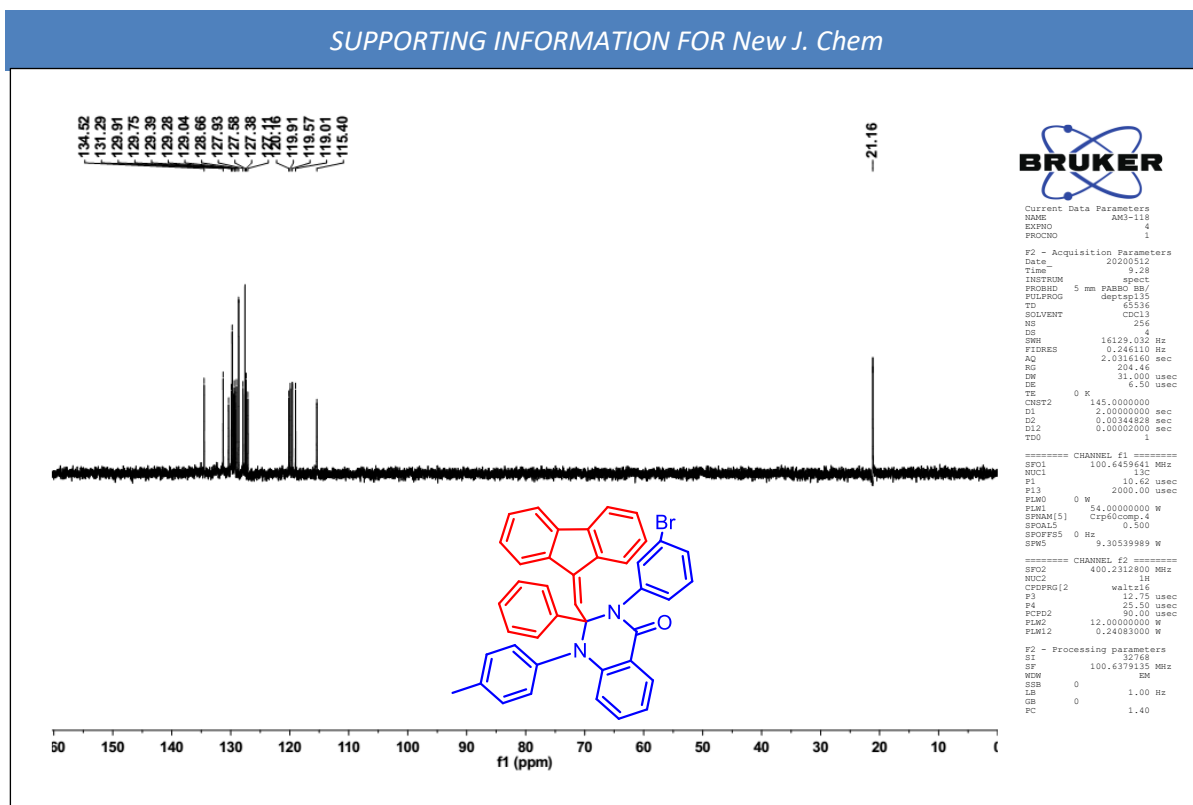


Figure 27 DEPT-135 NMR spectrum of compound 3g

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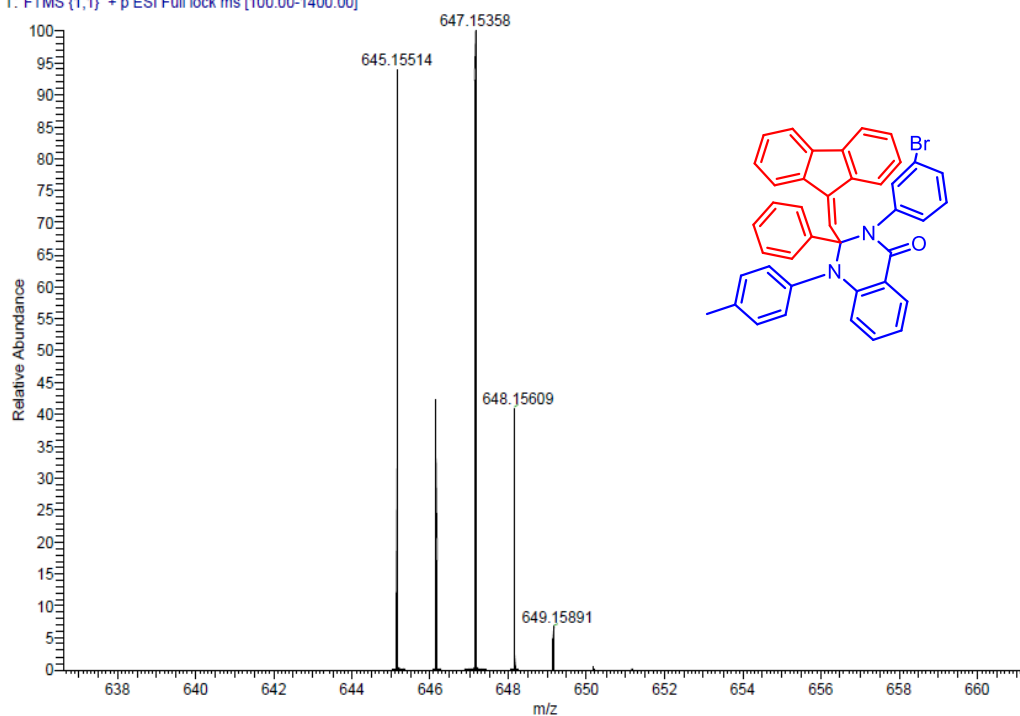


Figure 28 HRMS spectrum of compound 3g

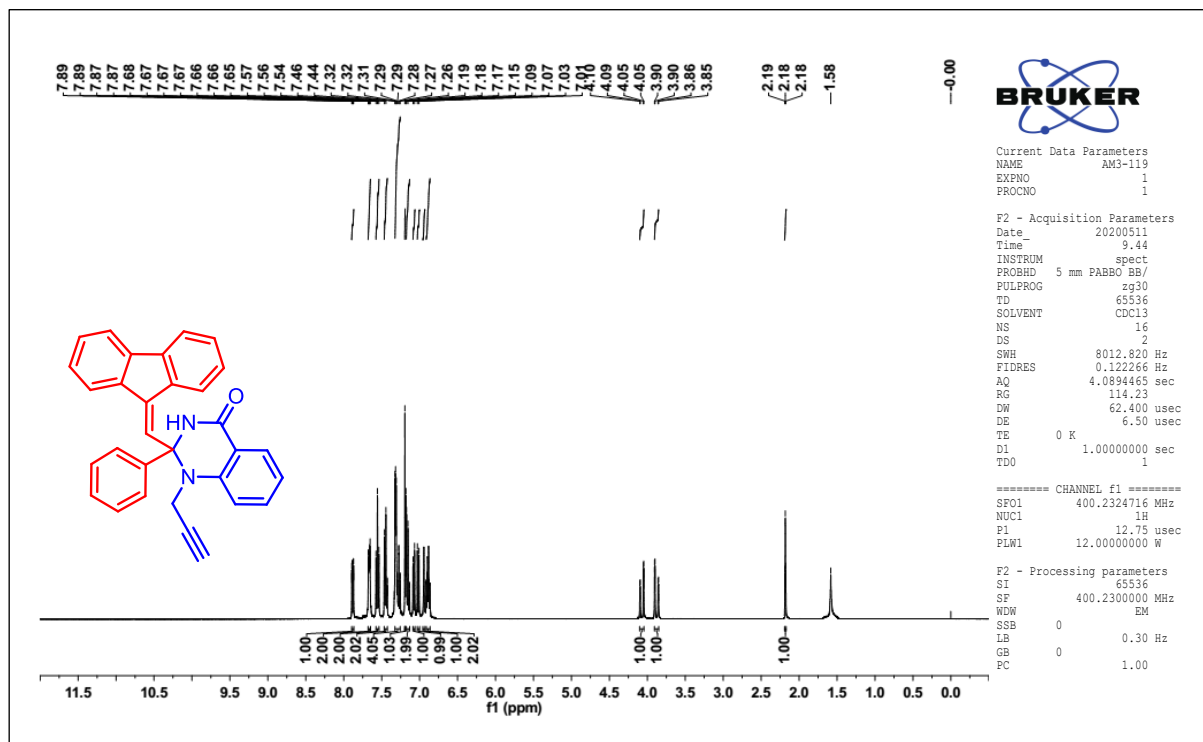


Figure 29 ^1H NMR spectrum of compound **3h**

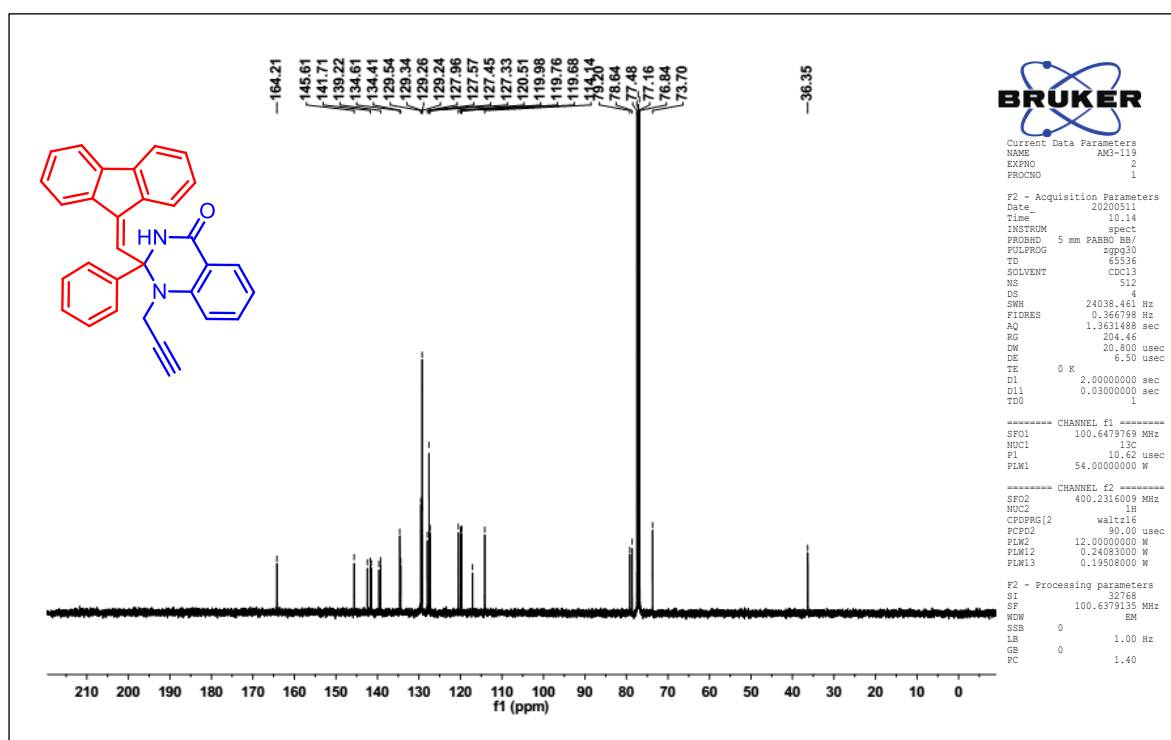


Figure 30 ^{13}C NMR spectrum of compound **3h**

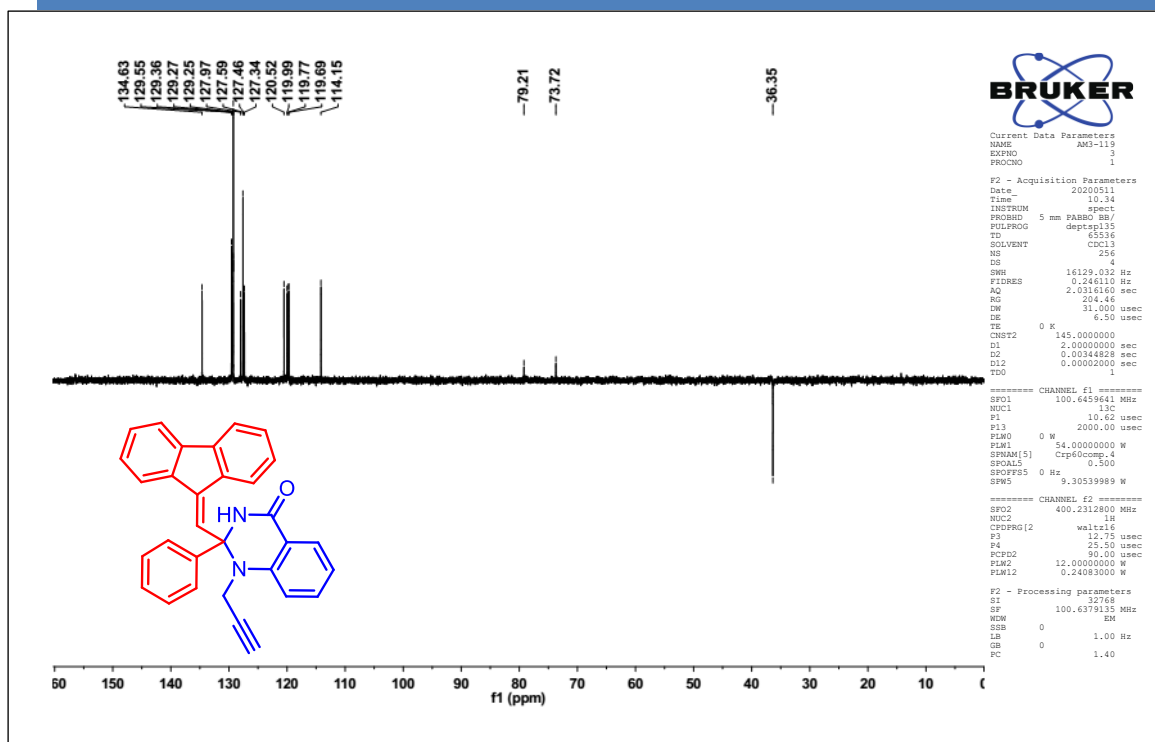


Figure 31 DEPT-135 NMR spectrum of compound 3h

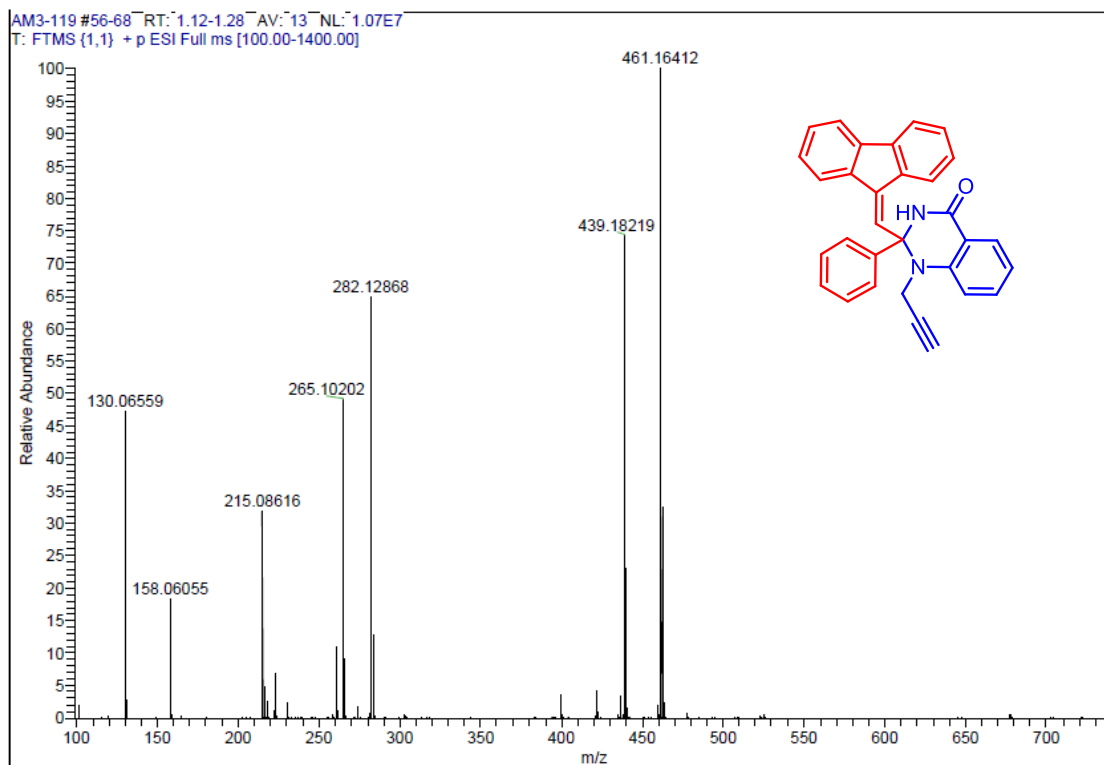
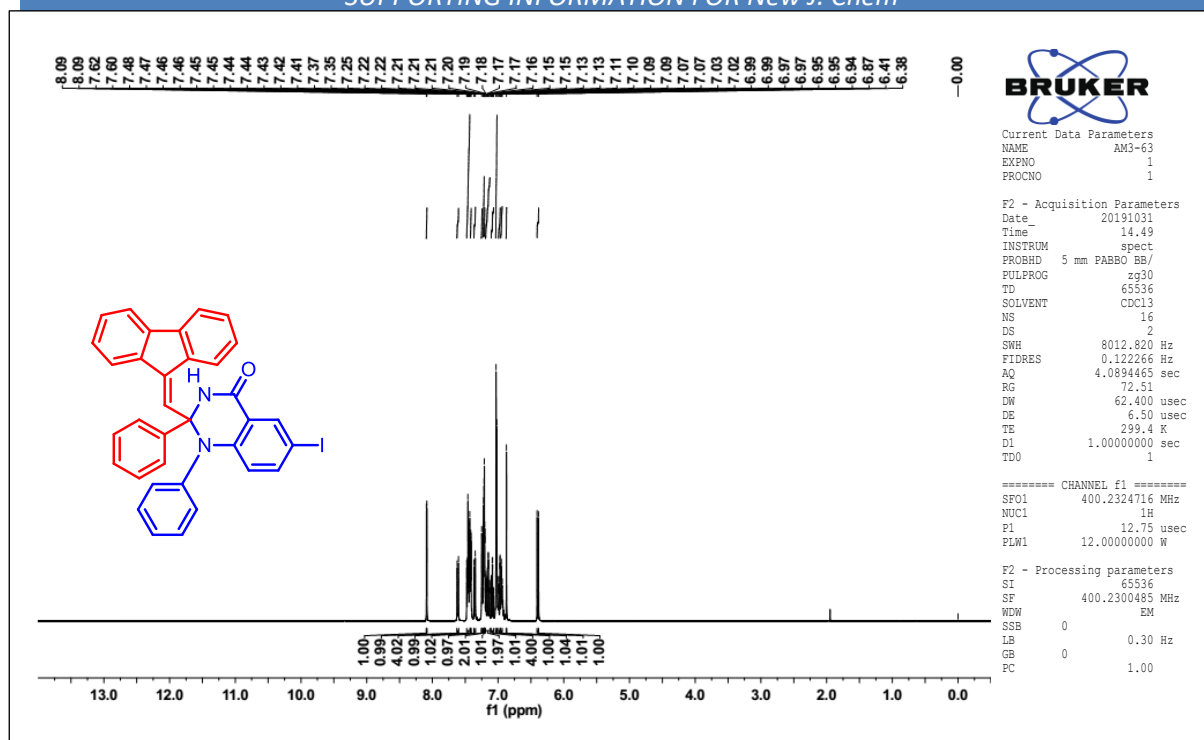
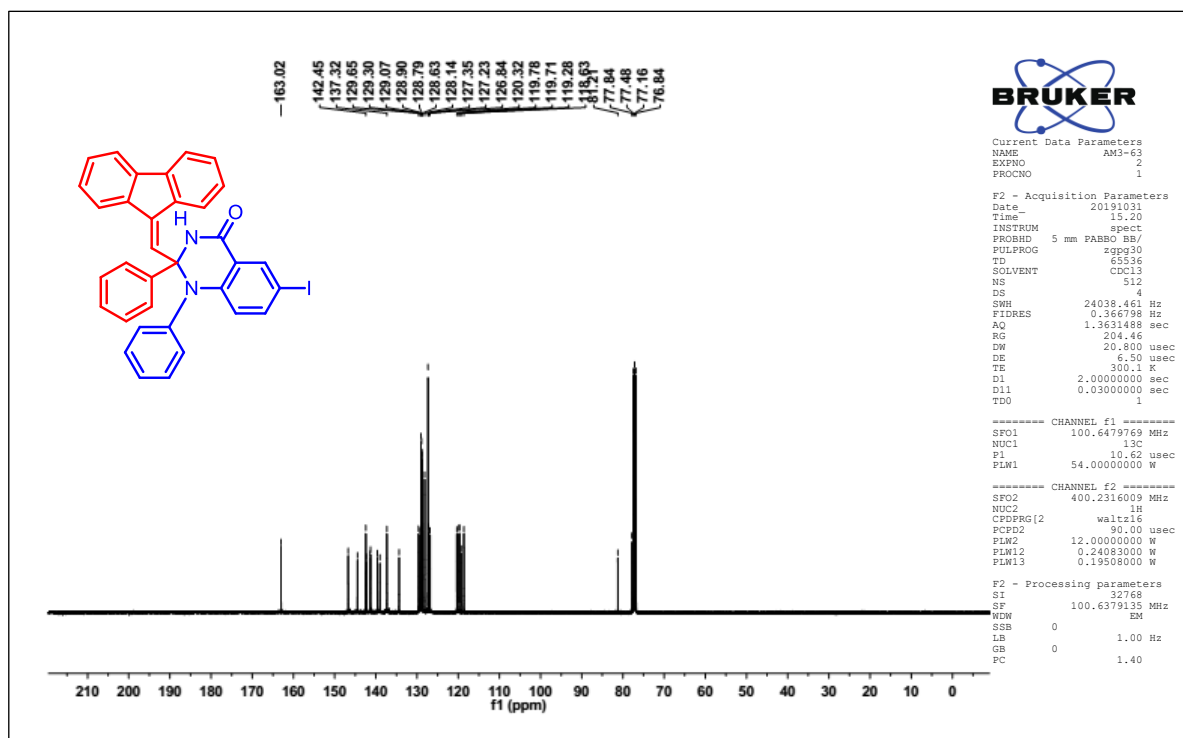
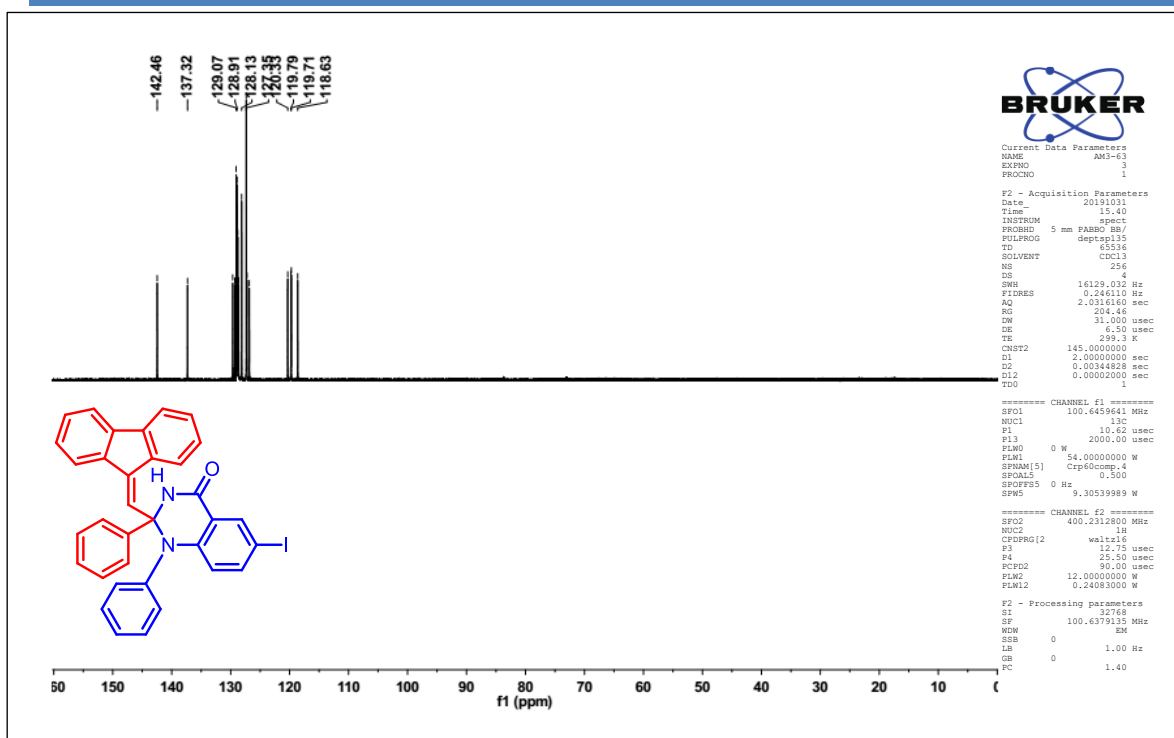
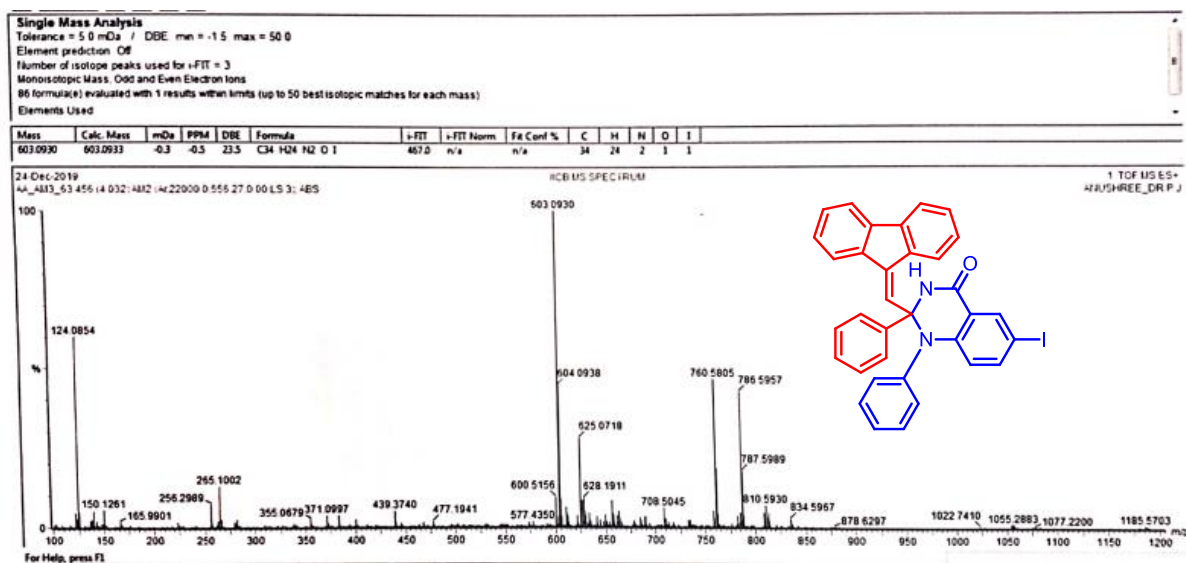
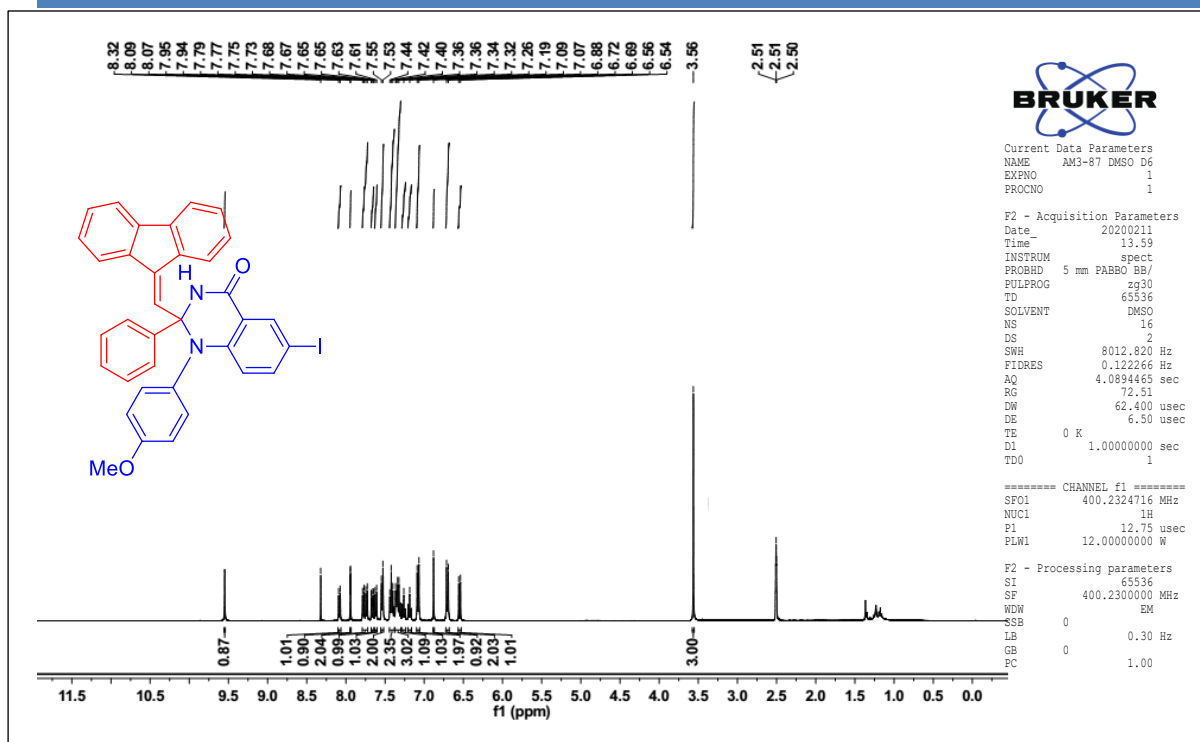
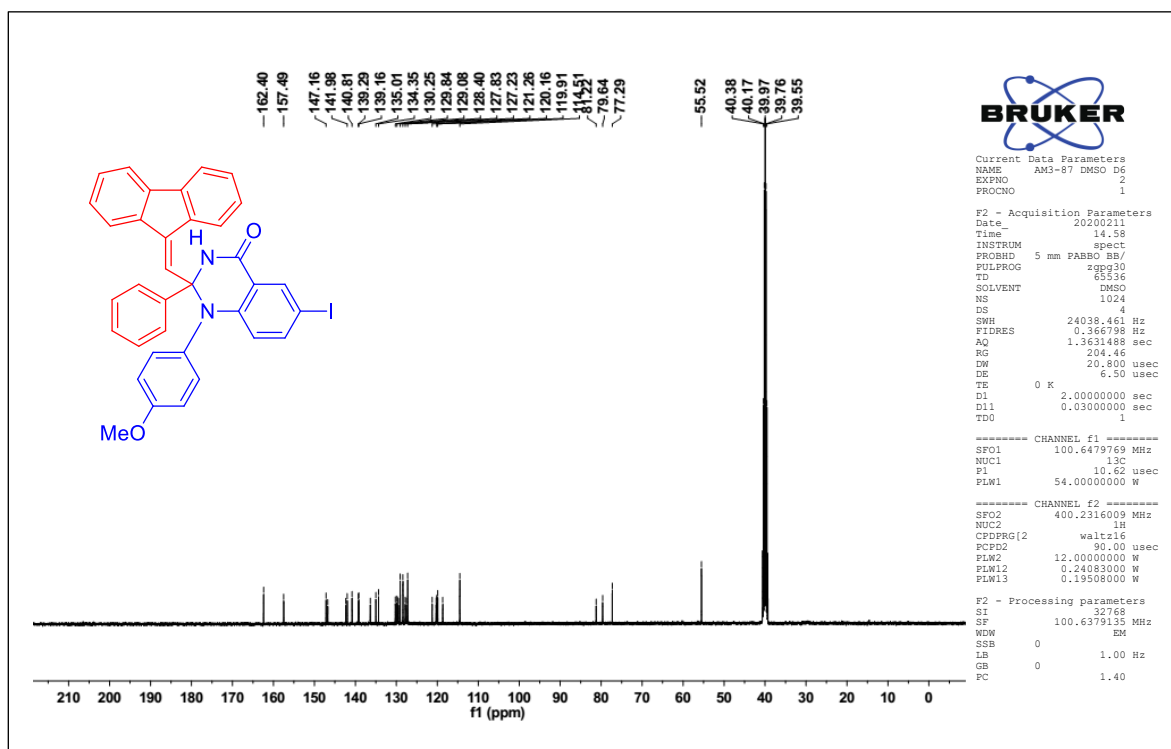


Figure 32 HRMS spectrum of compound 3h

Figure 33 ^1H NMR spectrum of compound **3i**Figure 34 ^{13}C NMR spectrum of compound **3i**

Figure 35 DEPT-135 NMR spectrum of compound **3i**Figure 36 HRMS spectrum of compound **3i**

Figure 37 ^1H NMR spectrum of compound 3jFigure 38 ^{13}C NMR spectrum of compound 3j

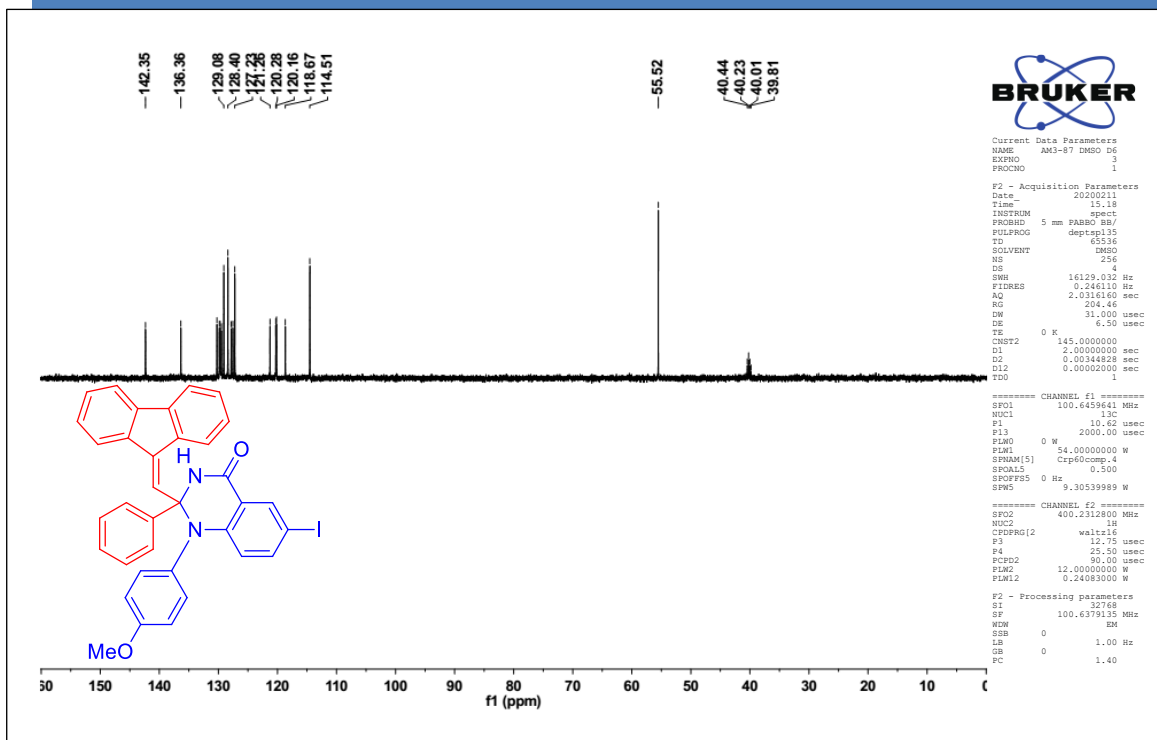


Figure 39 DEPT-135 NMR spectrum of compound 3j

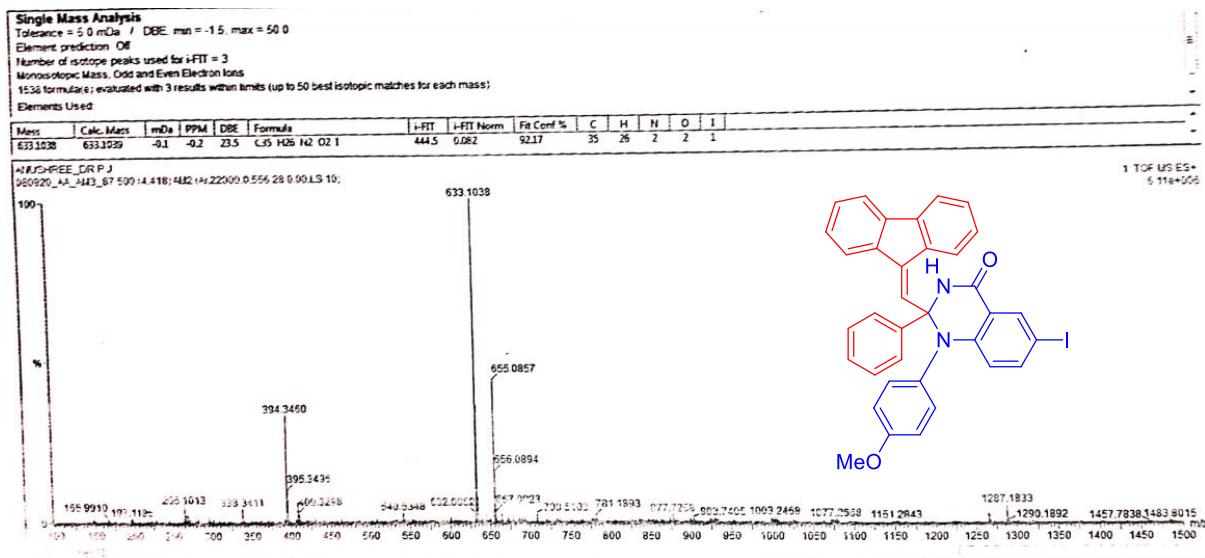
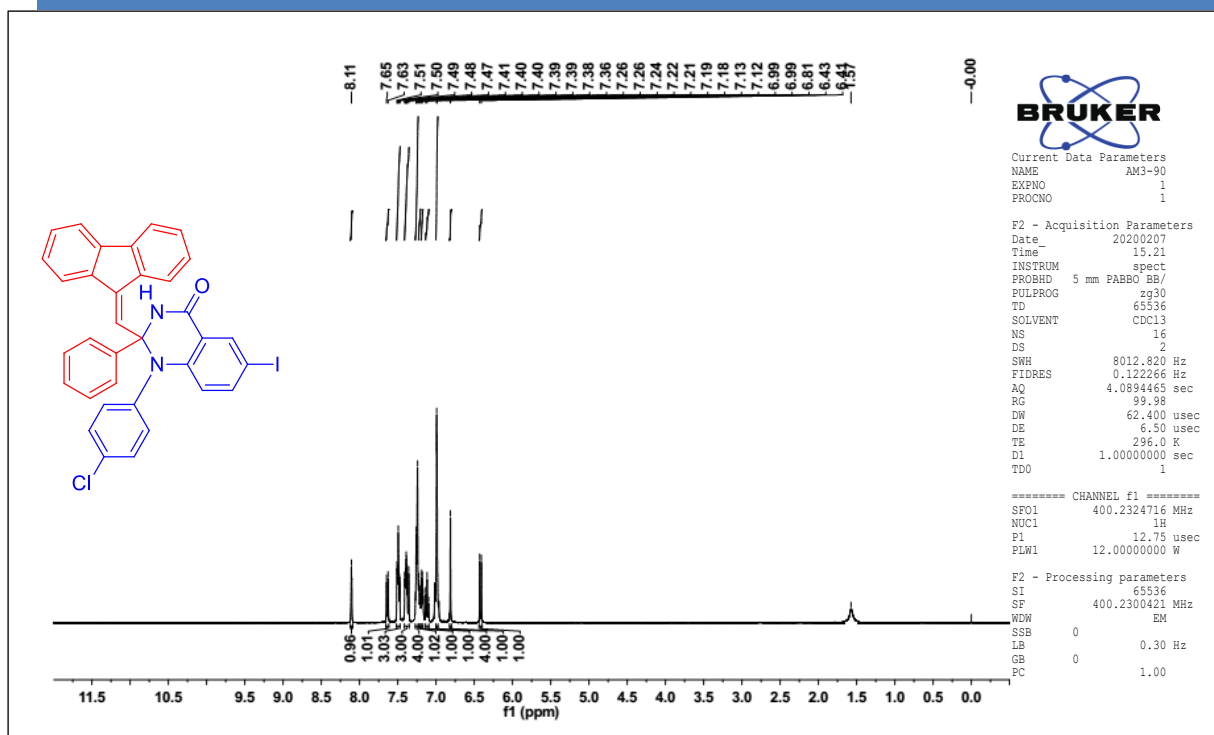
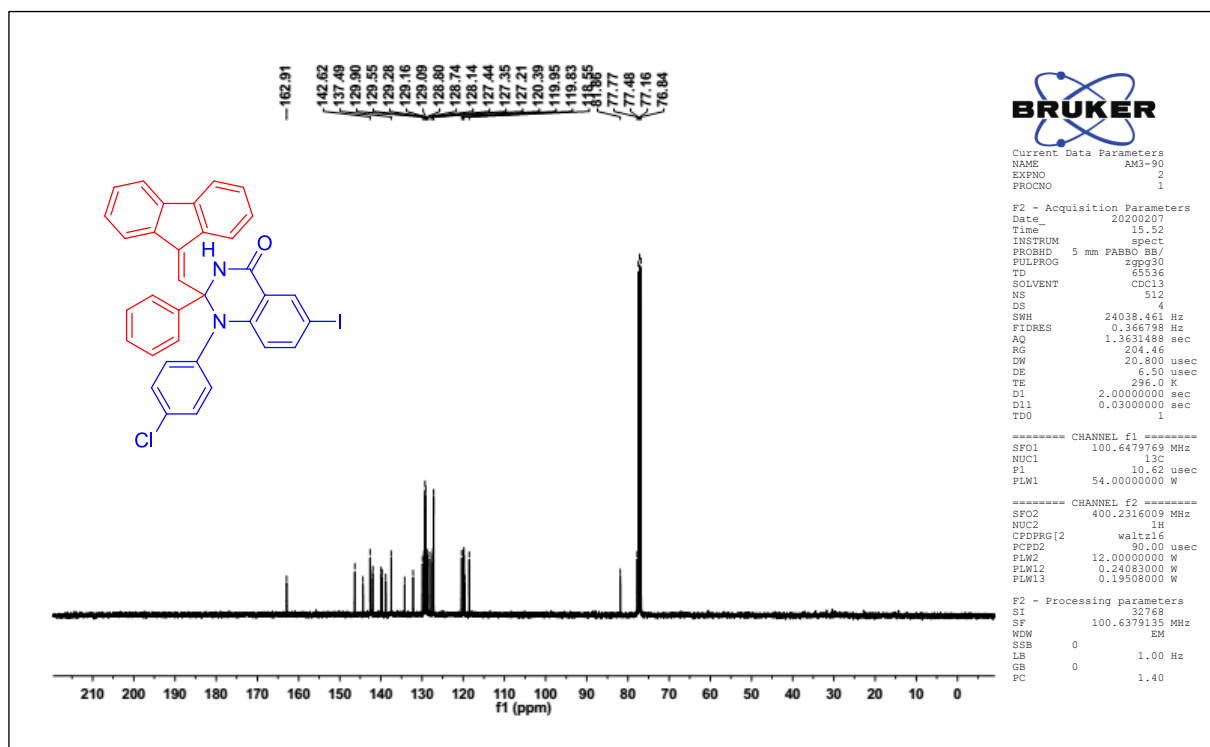
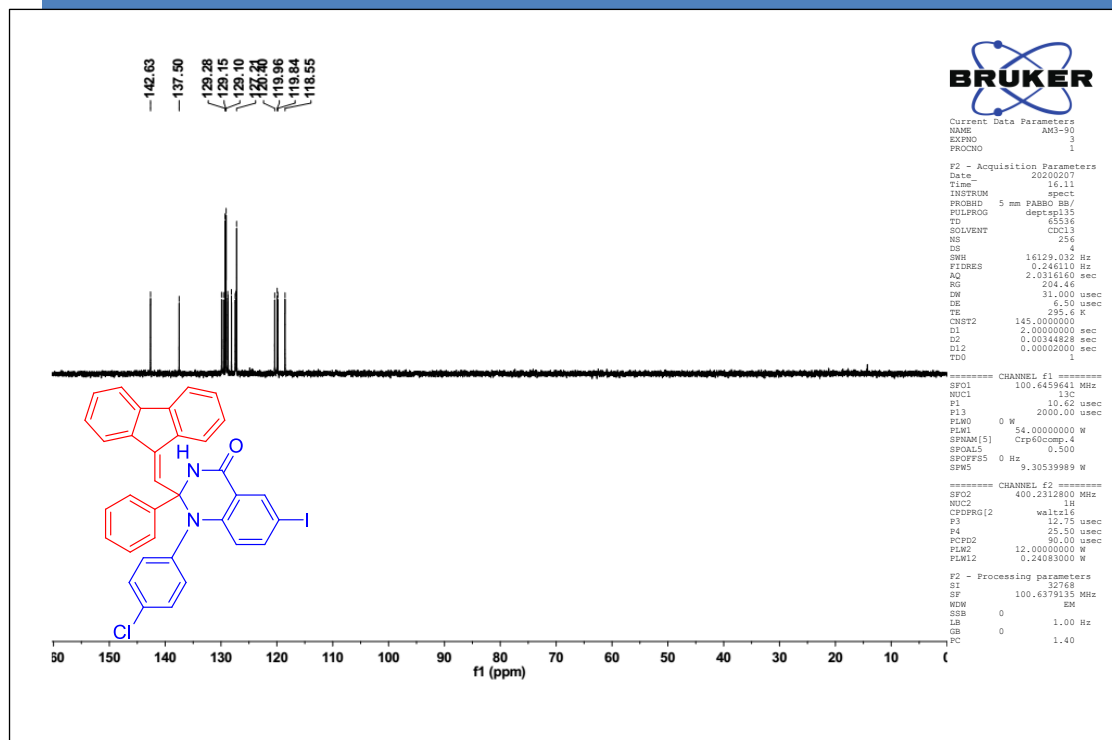
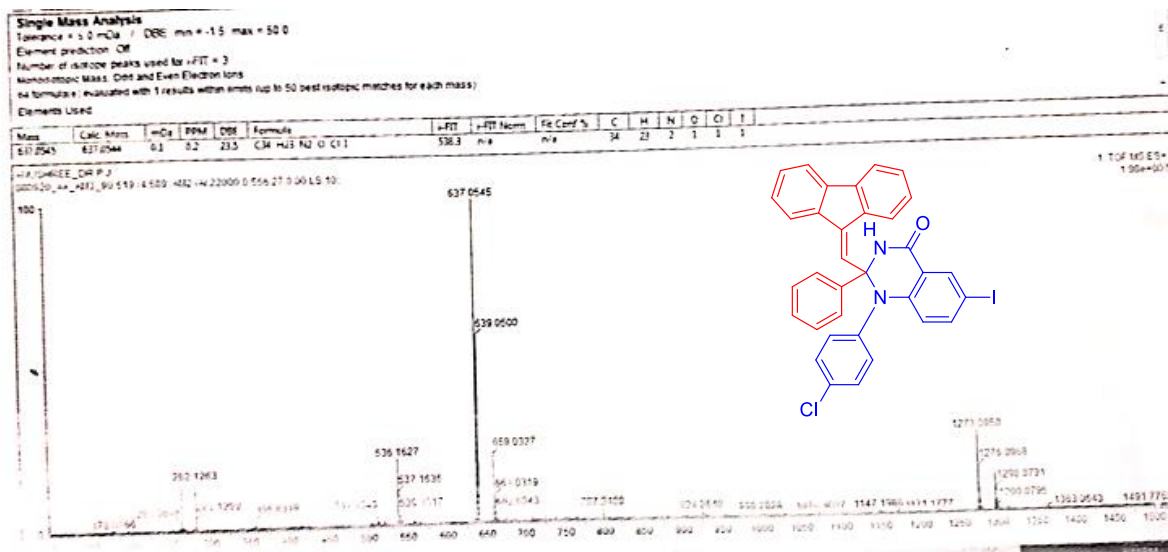
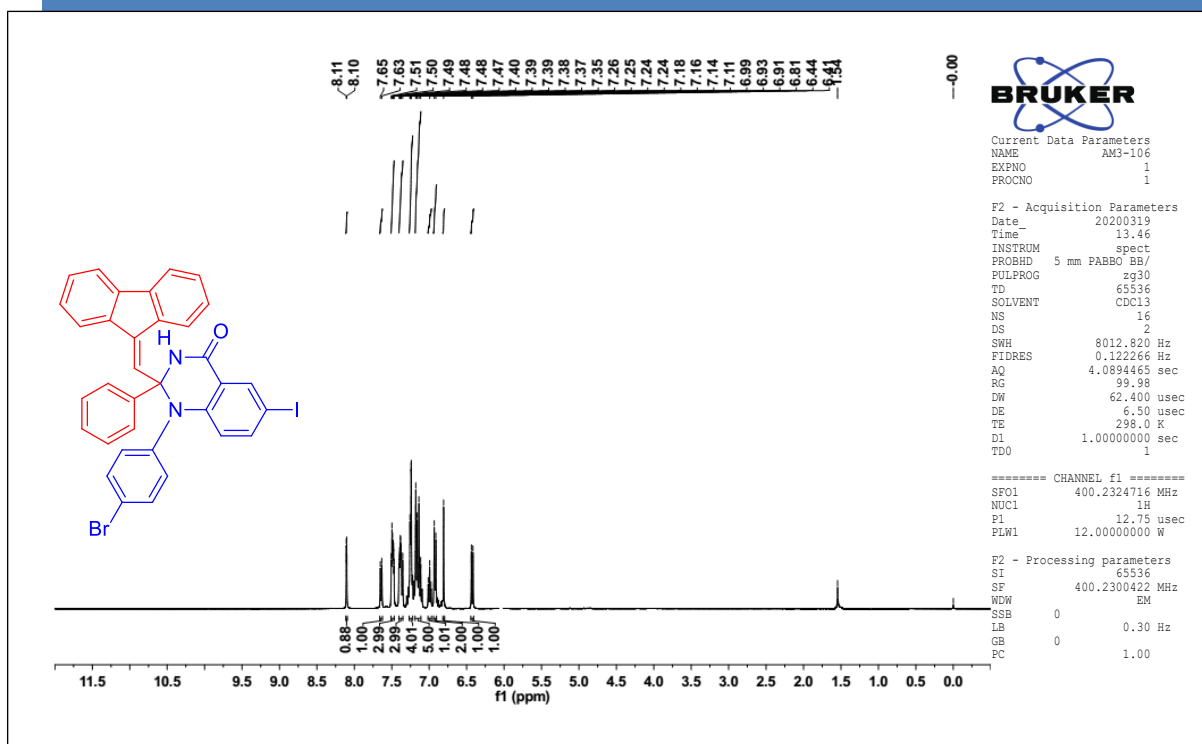
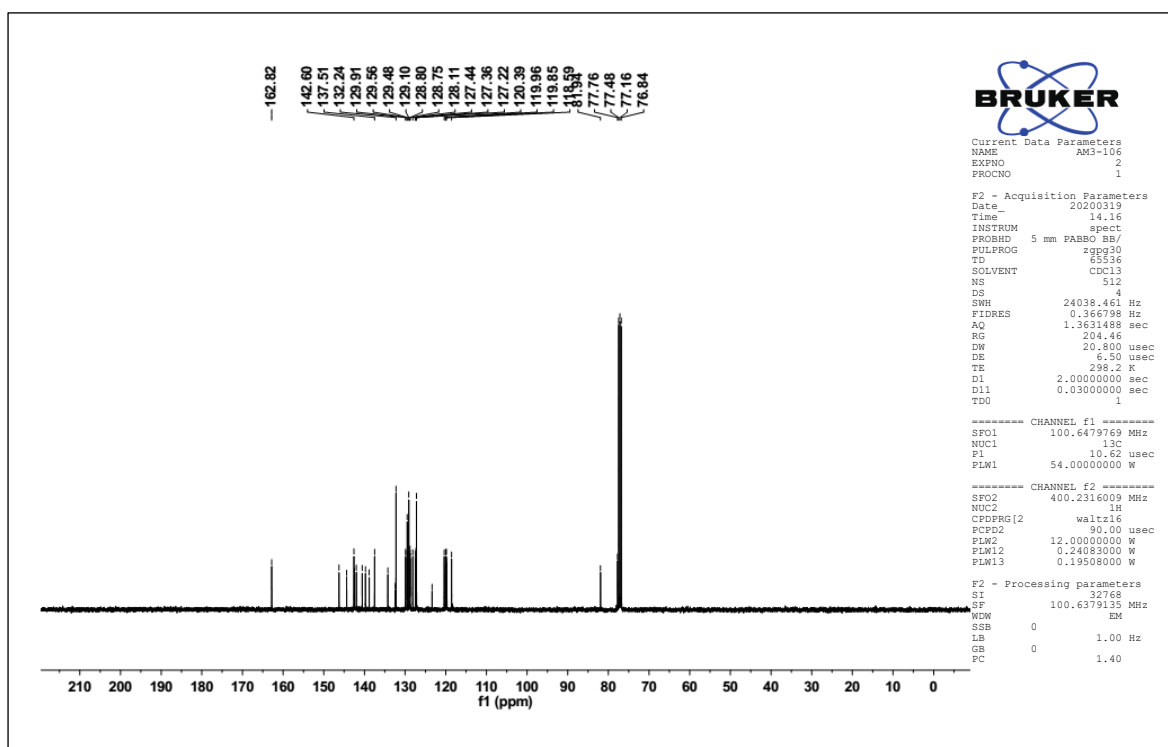


Figure 40 HRMS spectrum of compound 3j

Figure 41 ^1H NMR spectrum of compound **3k**Figure 42 ^{13}C NMR spectrum of compound **3k**

Figure 43 DEPT-135 NMR spectrum of compound **3k**Figure 44 HRMS spectrum of compound **3k**

Figure 45 ^1H NMR spectrum of compound 31Figure 46 ^{13}C NMR spectrum of compound 31

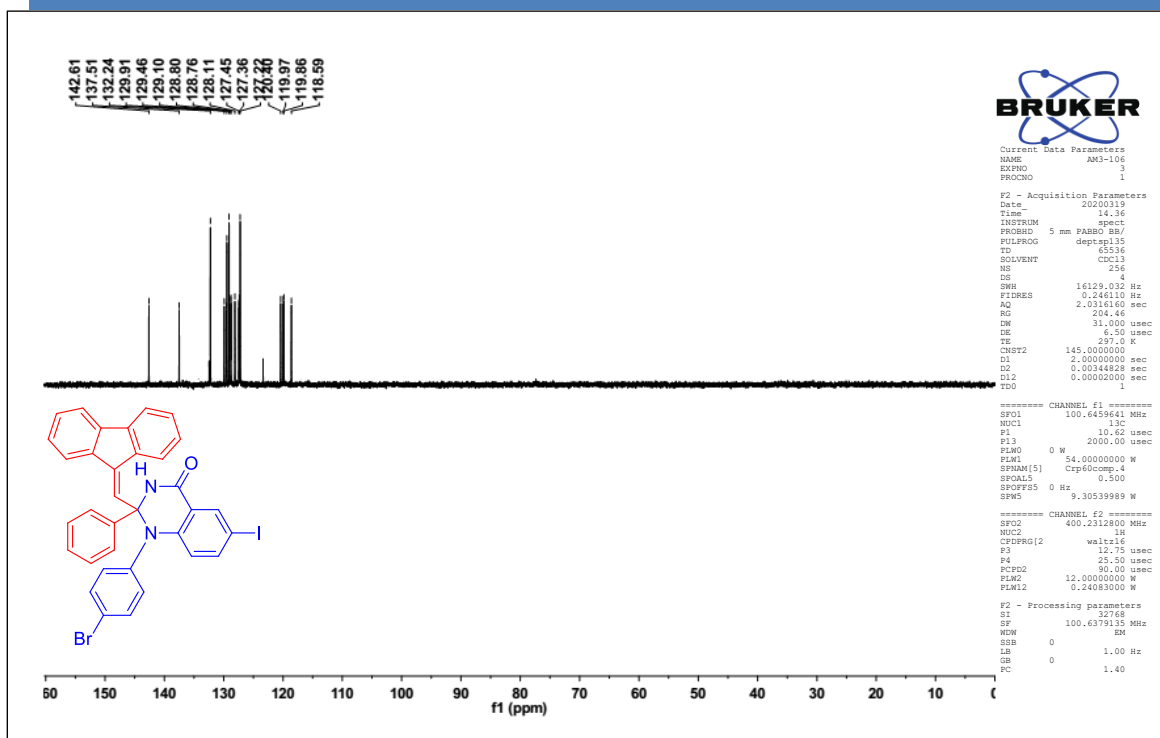


Figure 47 DEPT-135 NMR spectrum of compound 31

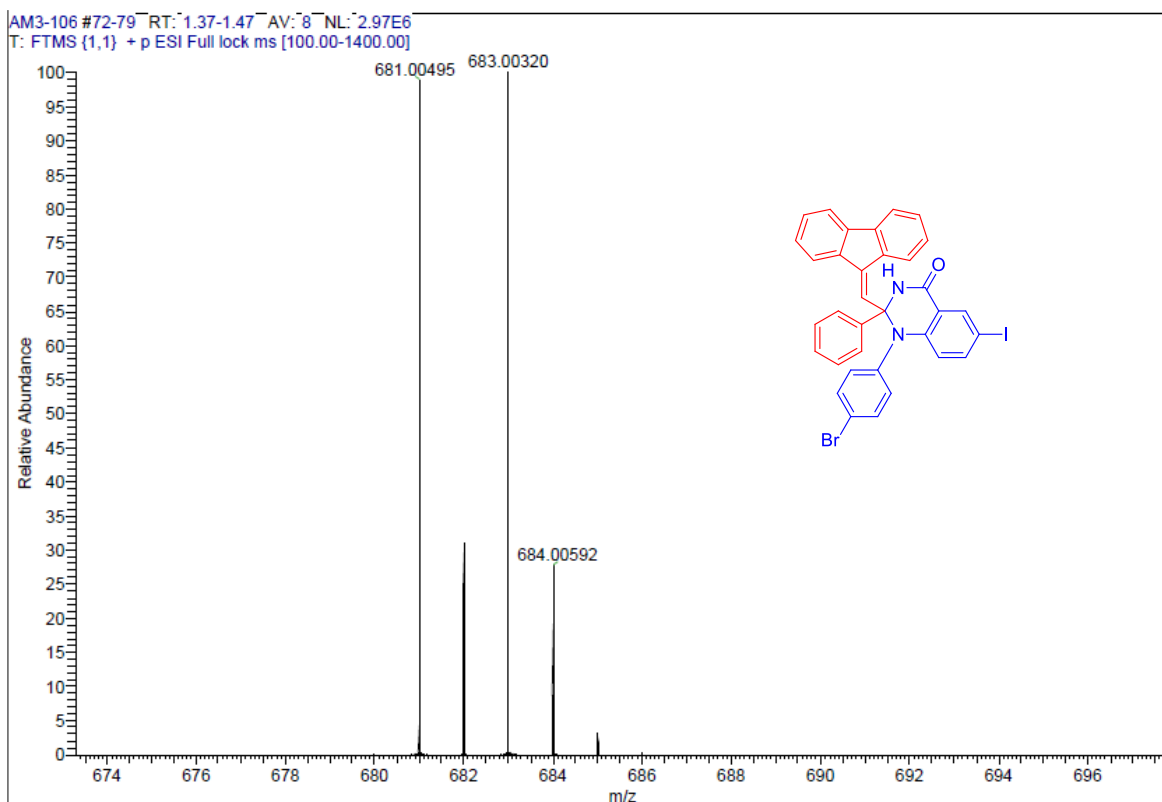


Figure 48 HRMS spectrum of compound 31

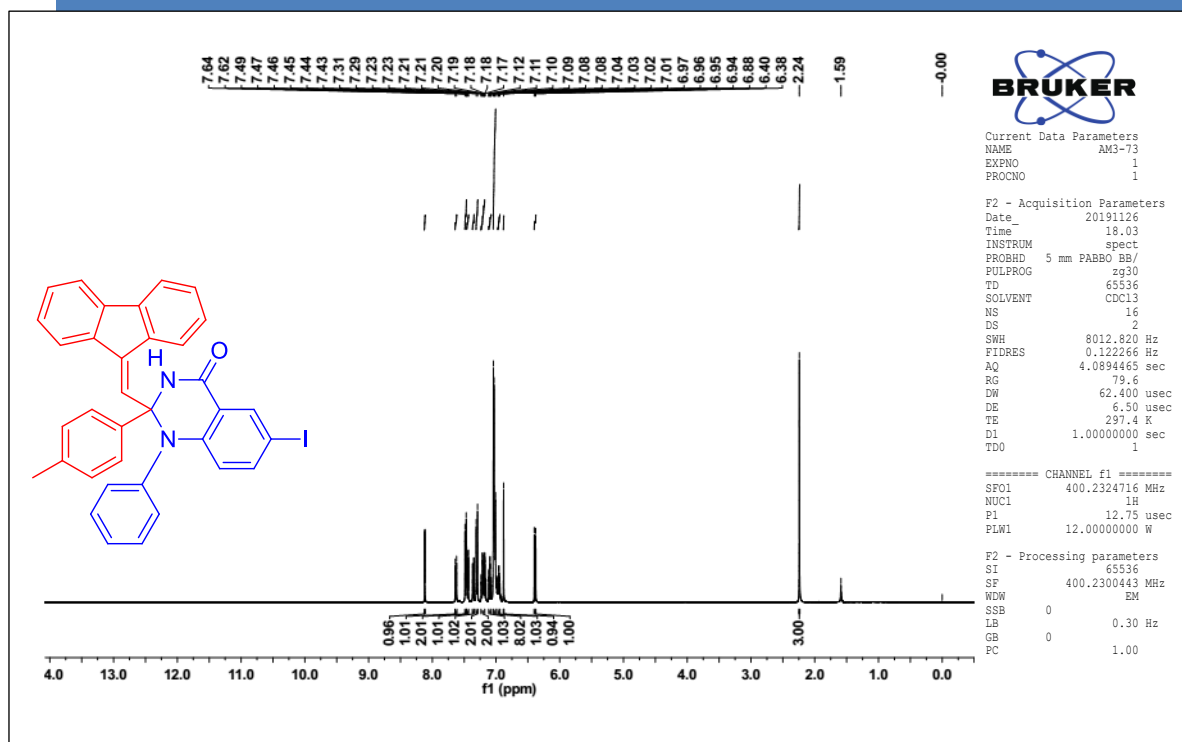


Figure 49 ¹H NMR spectrum of compound 3m

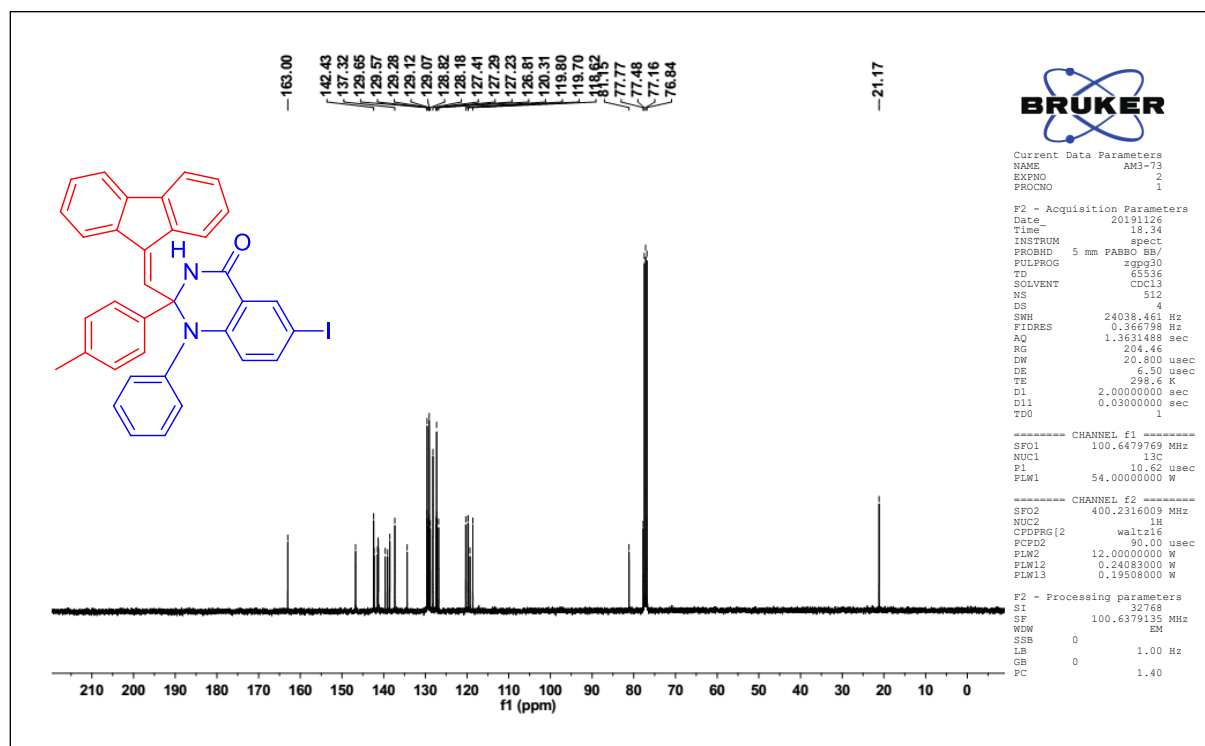
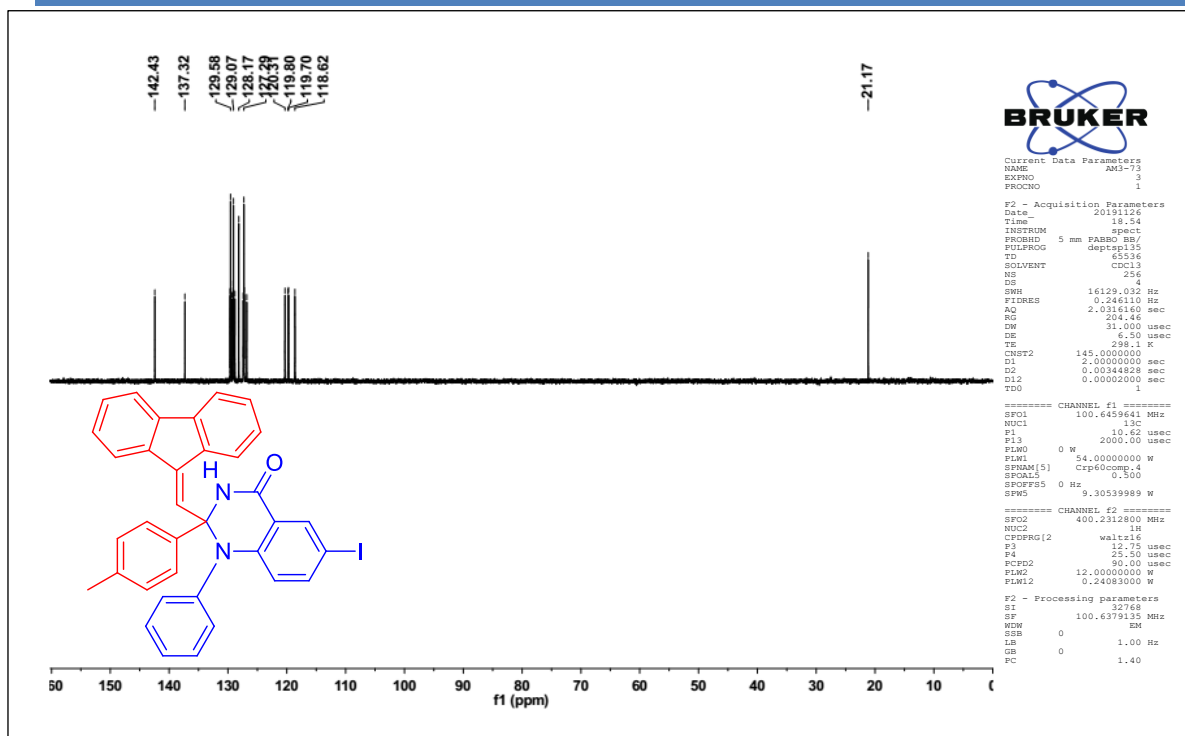
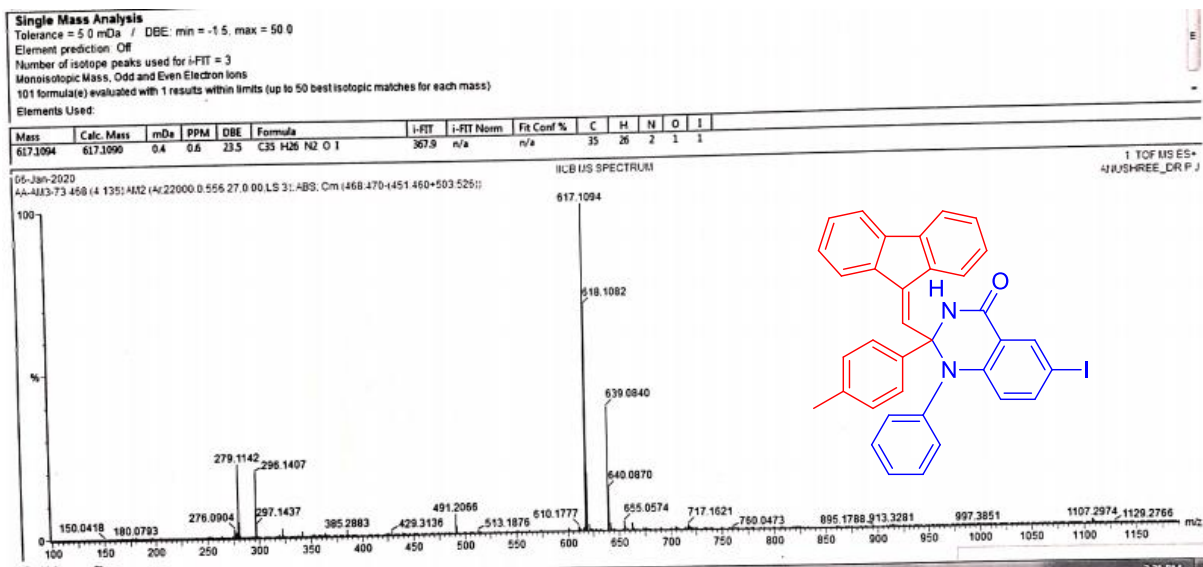


Figure 50 ¹³C NMR spectrum of compound 3m

Figure 51 DEPT-135 NMR spectrum of compound **3m**Figure 52 HRMS spectrum of compound **3m**

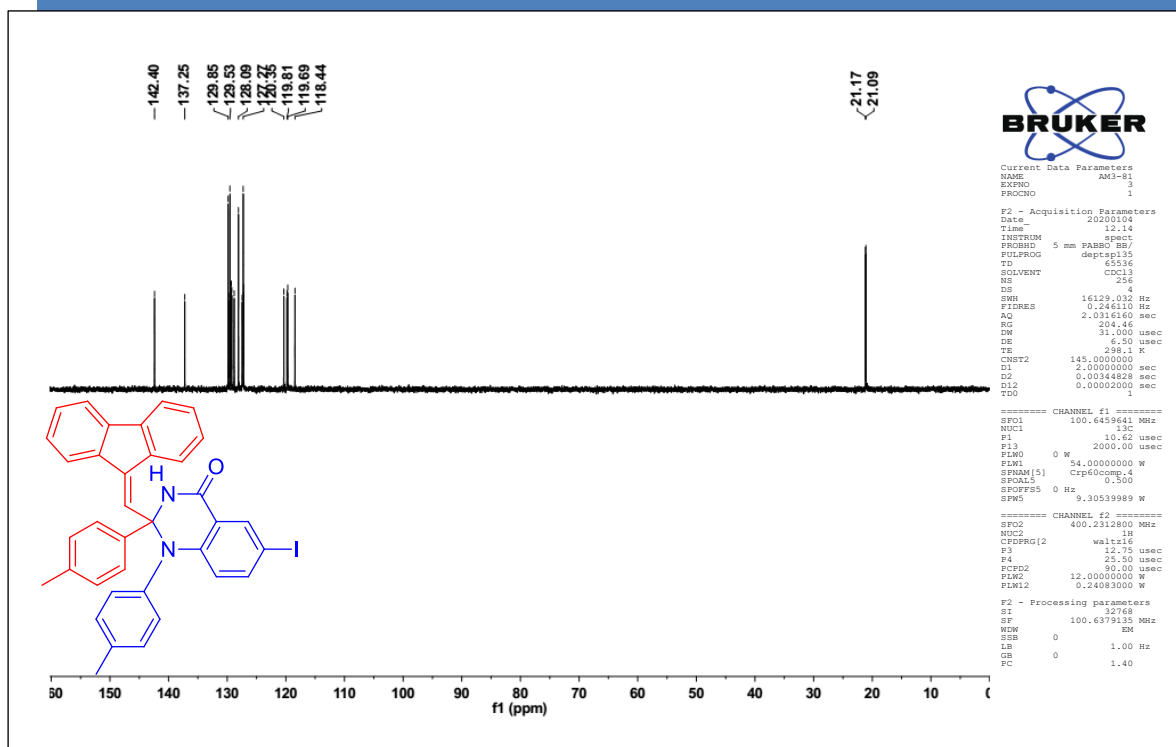


Figure 55 DEPT-135 NMR spectrum of compound 3n

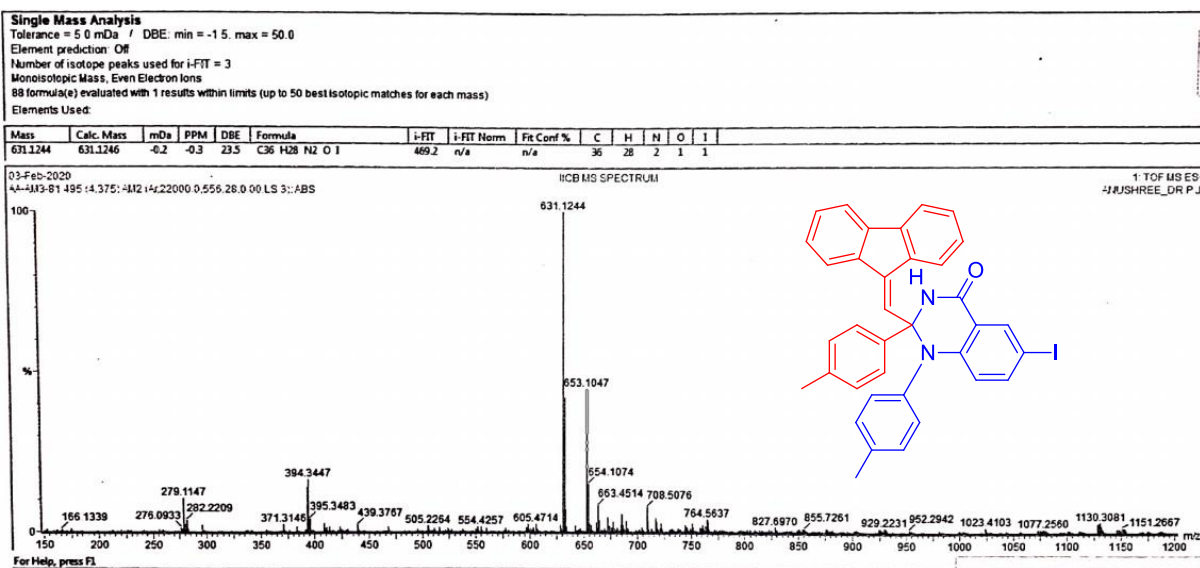
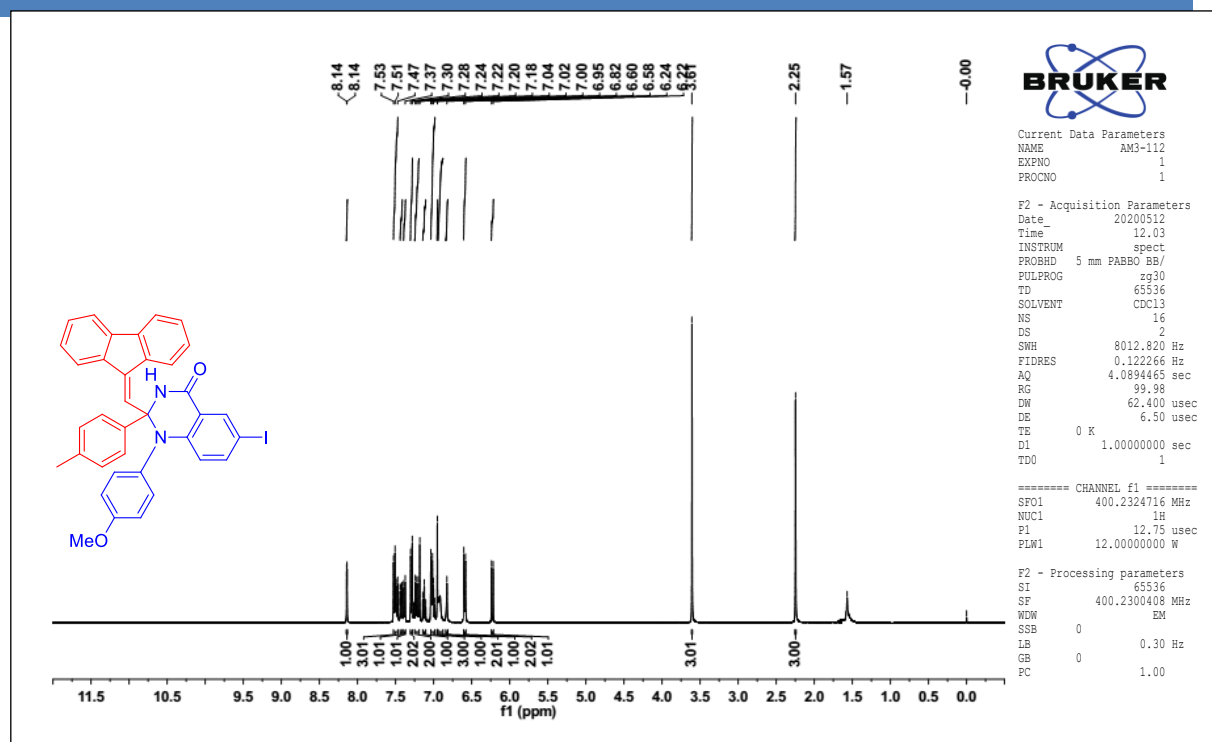
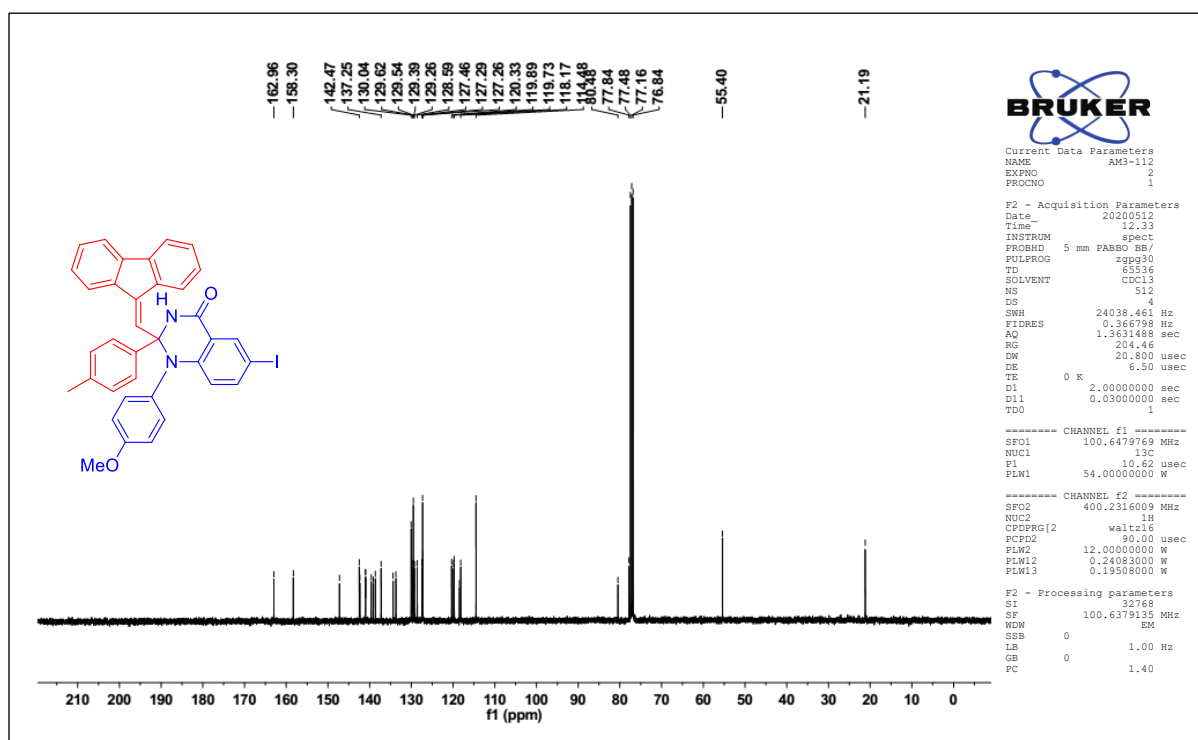


Figure 56 HRMS spectrum of compound 3n

Figure 57 ^1H NMR spectrum of compound **30**Figure 58 ^{13}C NMR spectrum of compound **30**

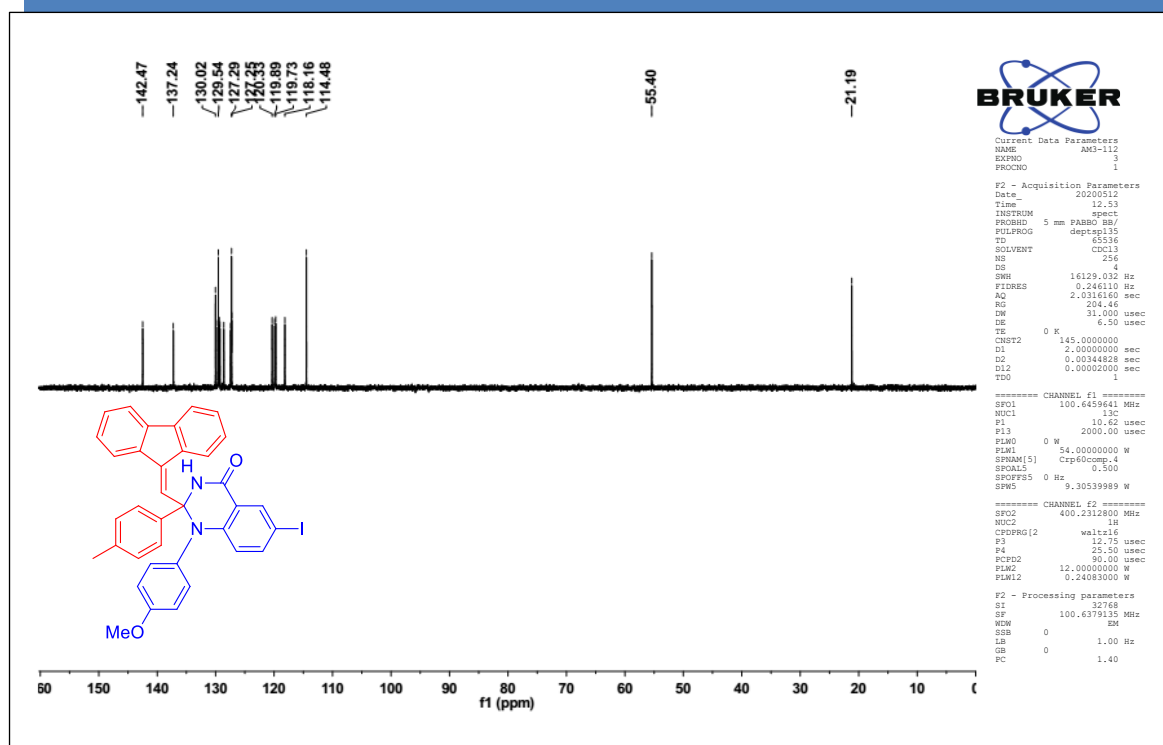


Figure 59 DEPT-135 NMR spectrum of compound 30

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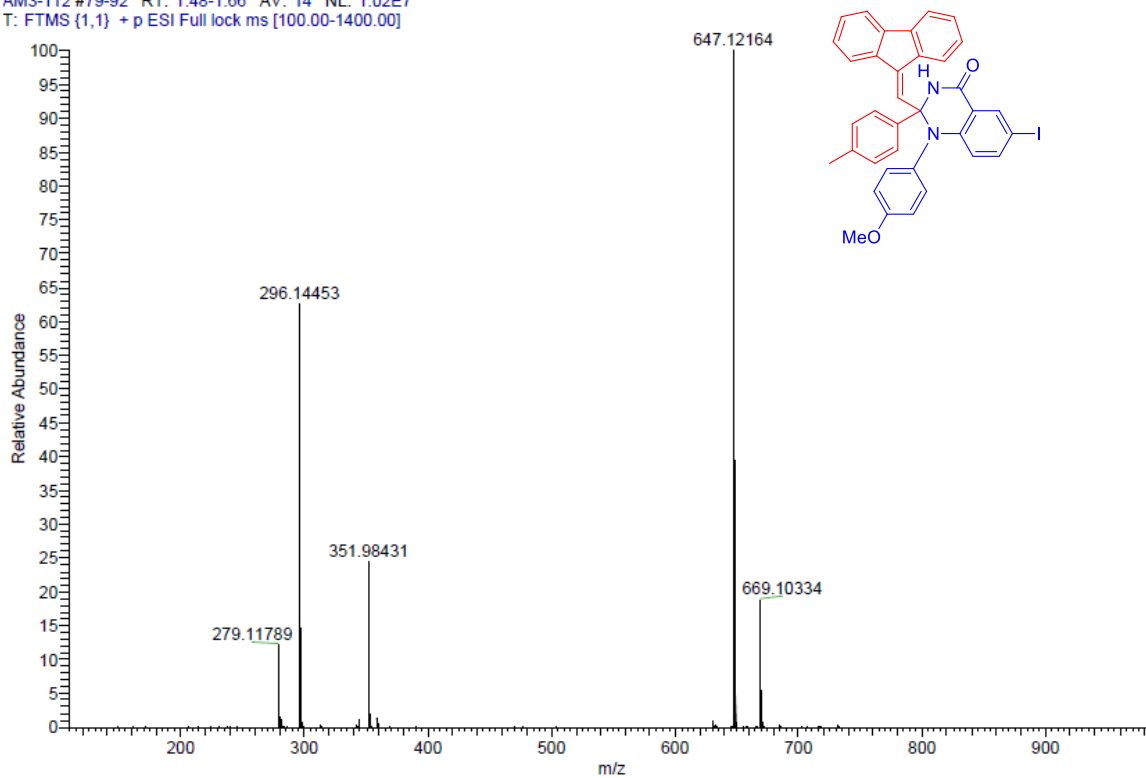


Figure 60 HRMS spectrum of compound 30

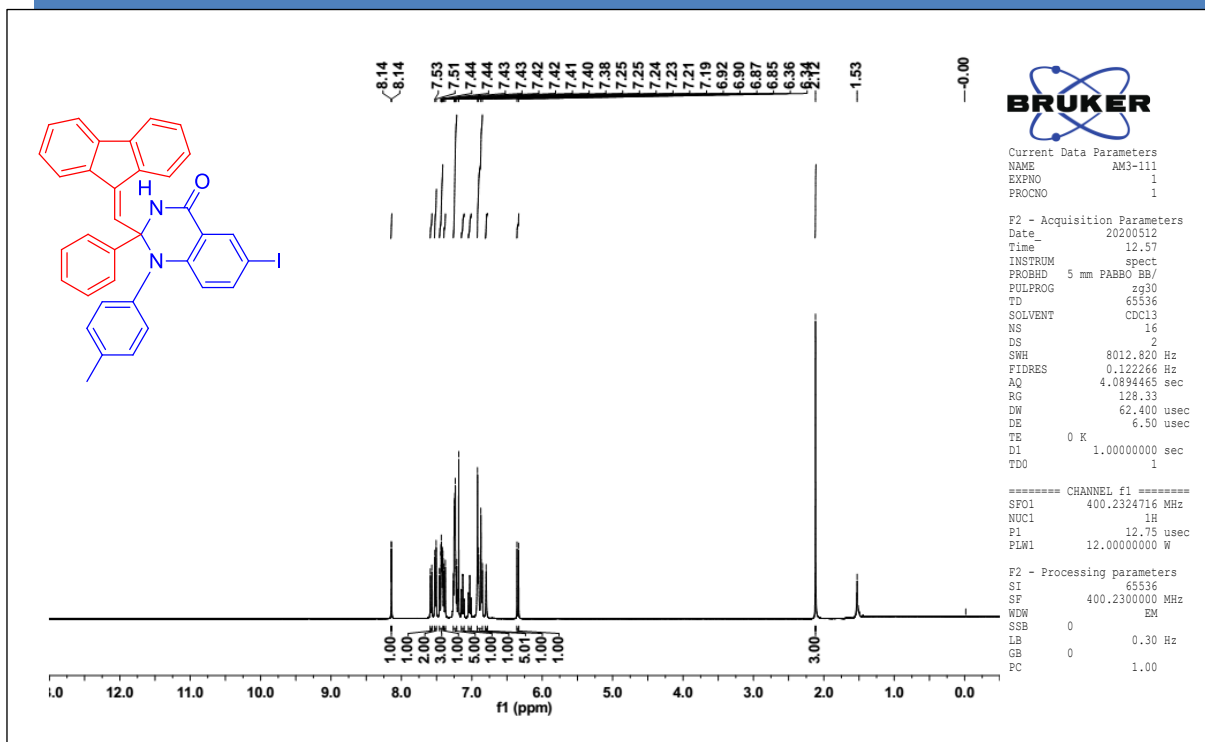


Figure 61 ^1H NMR spectrum of compound **3p**

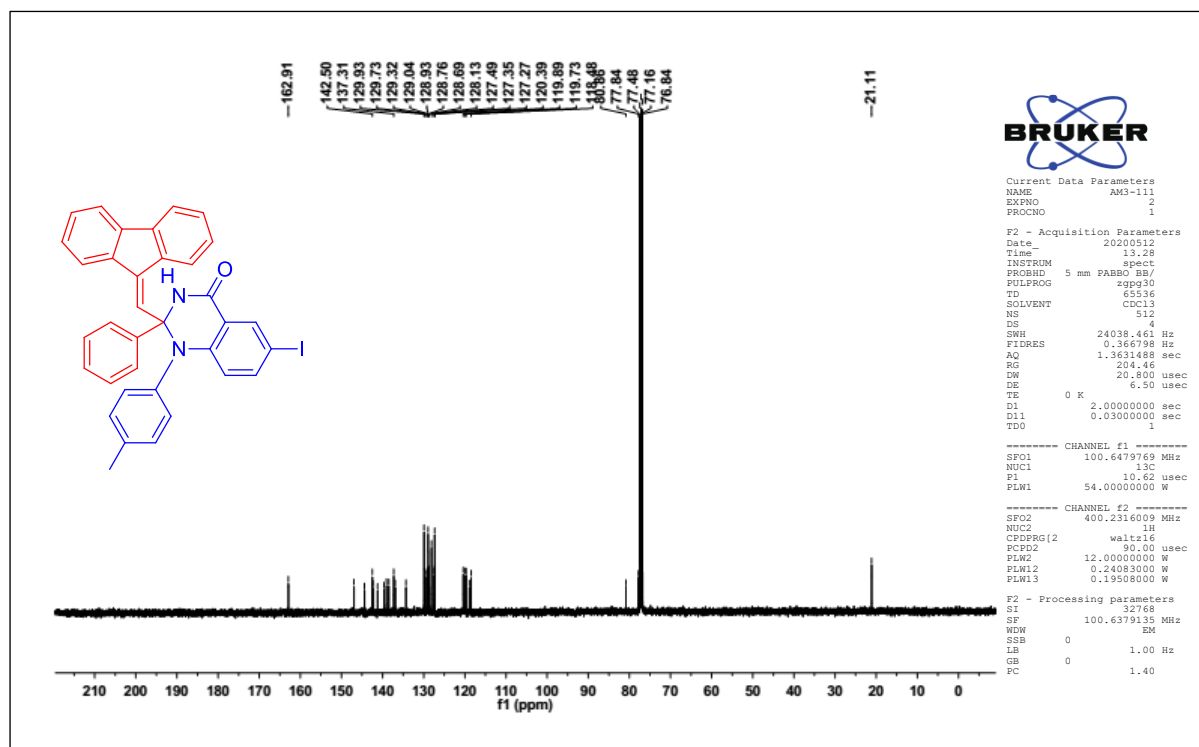


Figure 62 ^{13}C NMR spectrum of compound **3p**

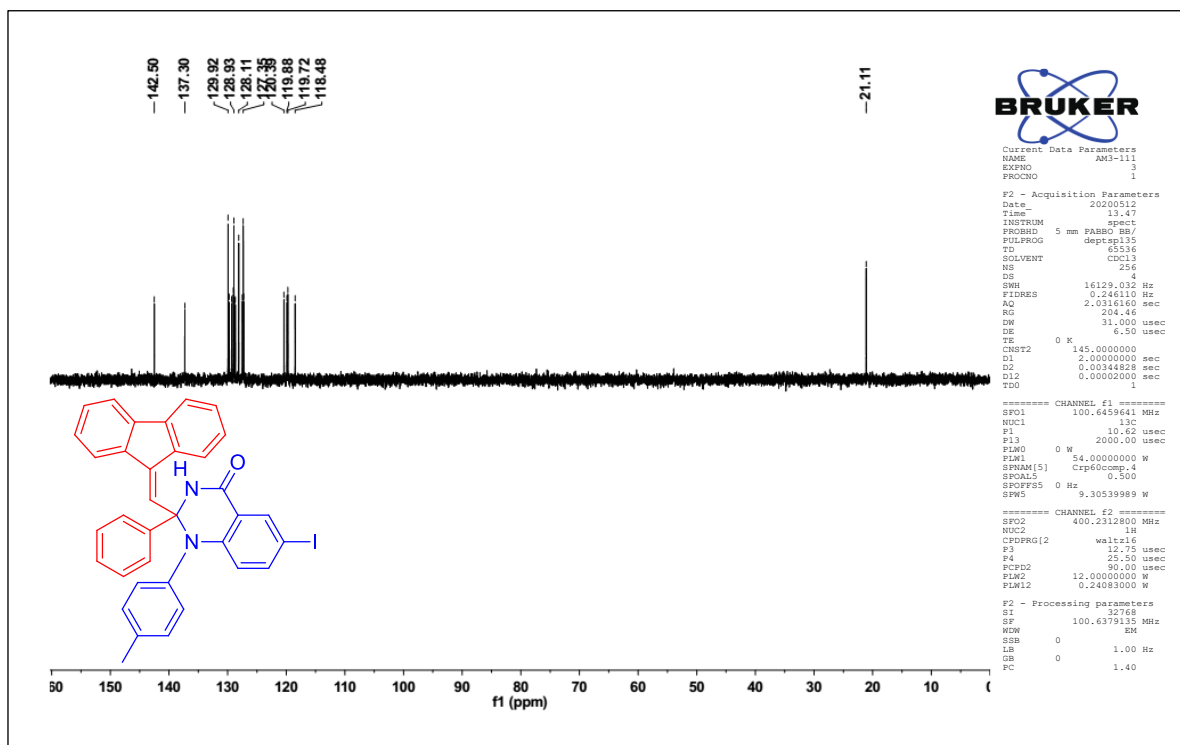


Figure 63 DEPT-135 NMR spectrum of compound 3p

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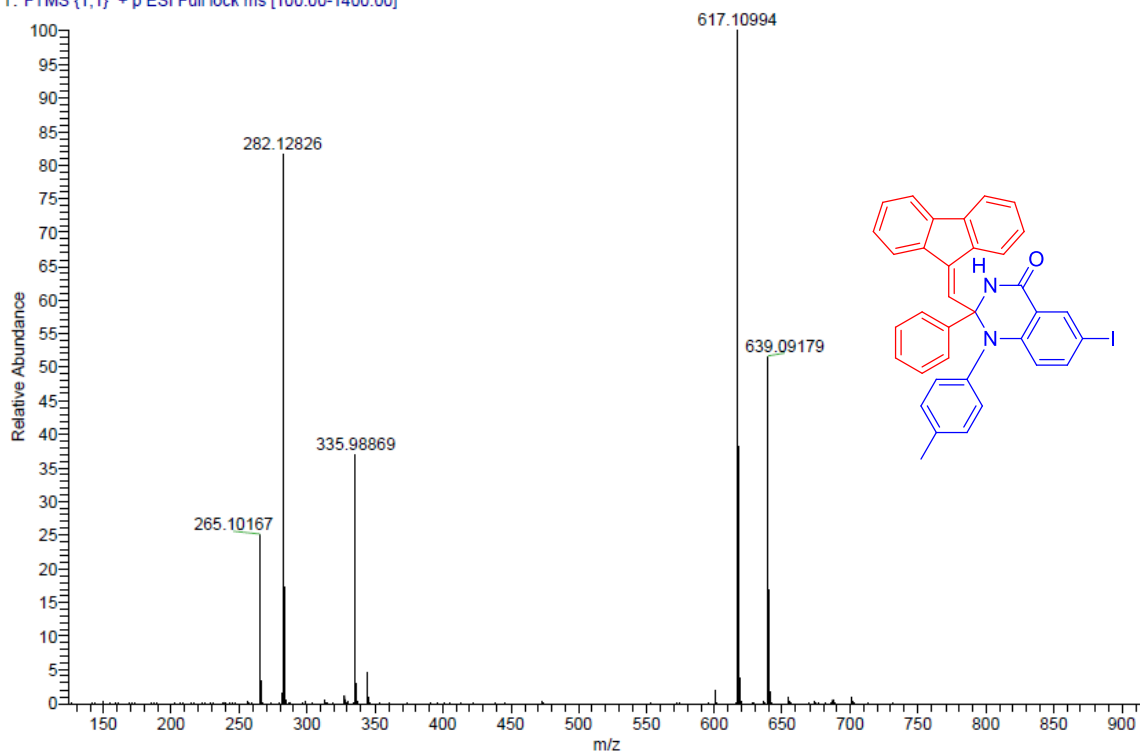


Figure 64 HRMS spectrum of compound 3p

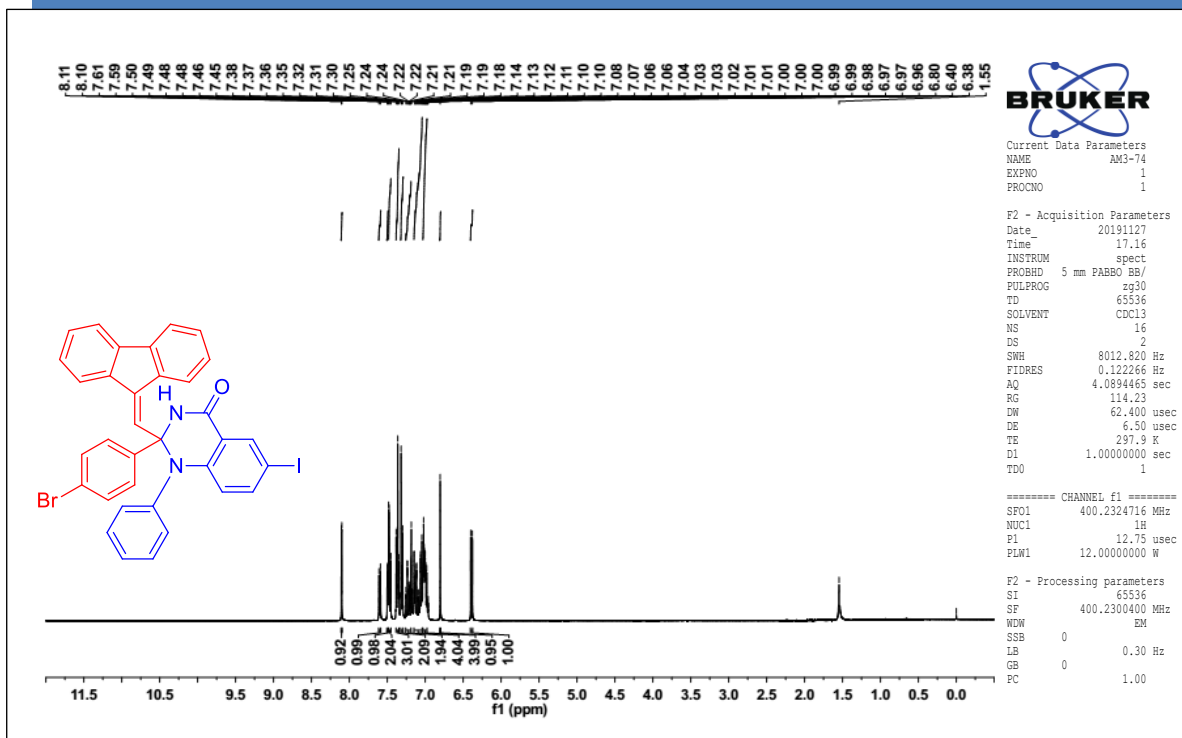


Figure 65 ^1H NMR spectrum of compound **3q**

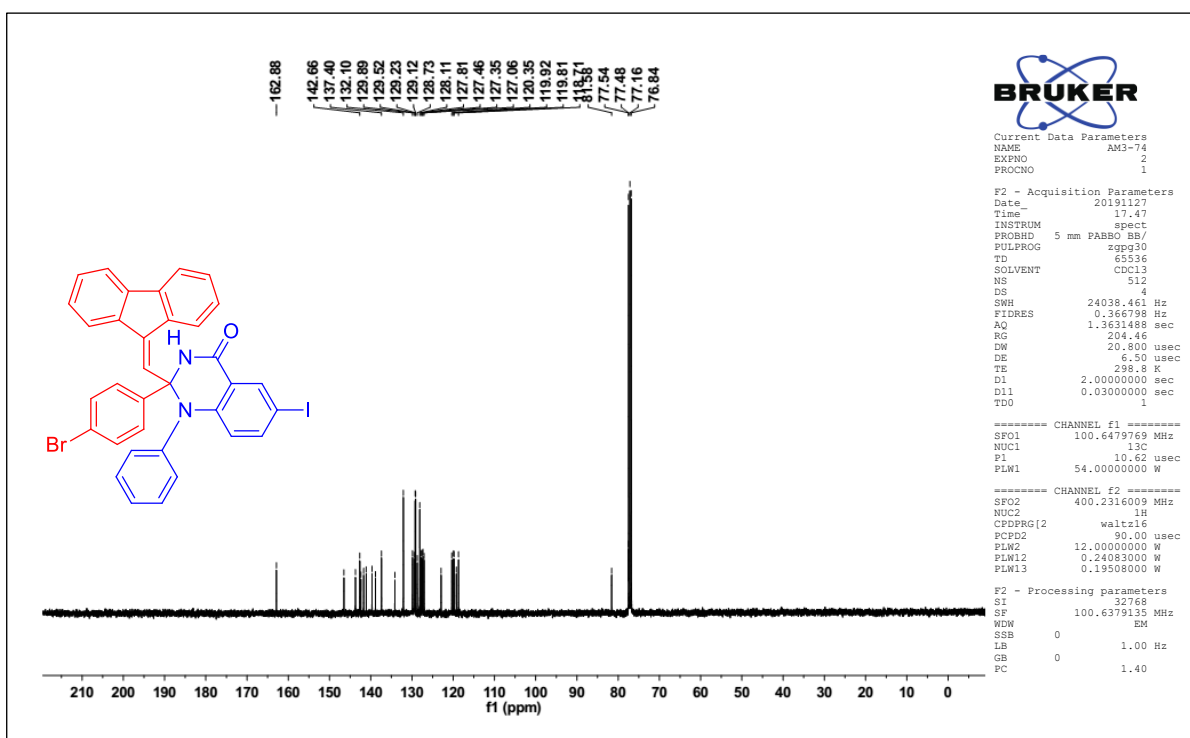


Figure 66 ^{13}C NMR spectrum of compound **3q**

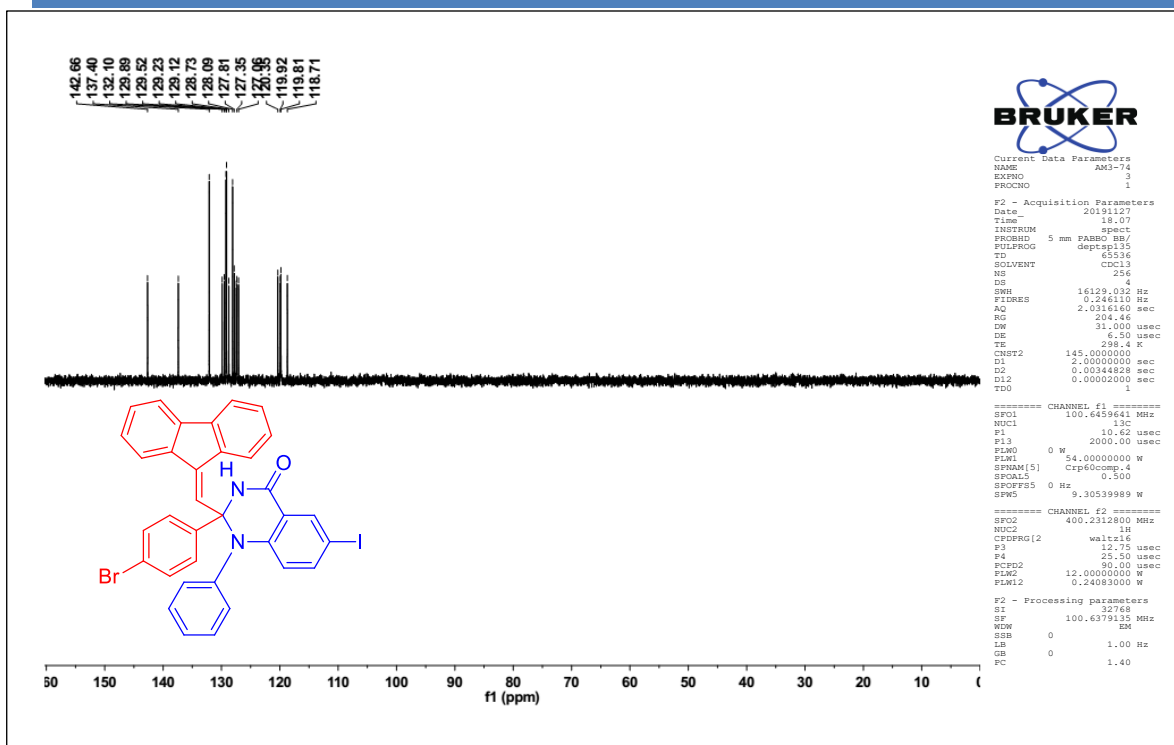


Figure 67 DEPT-135 NMR spectrum of compound 3q

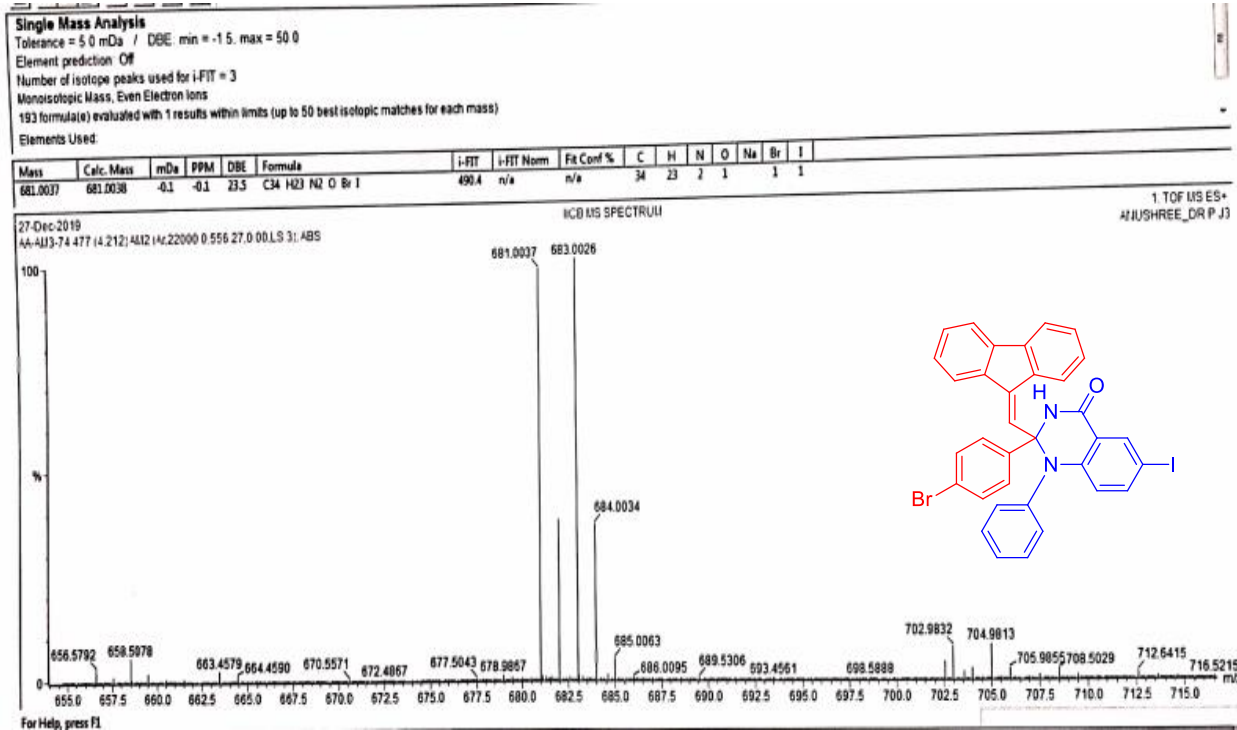
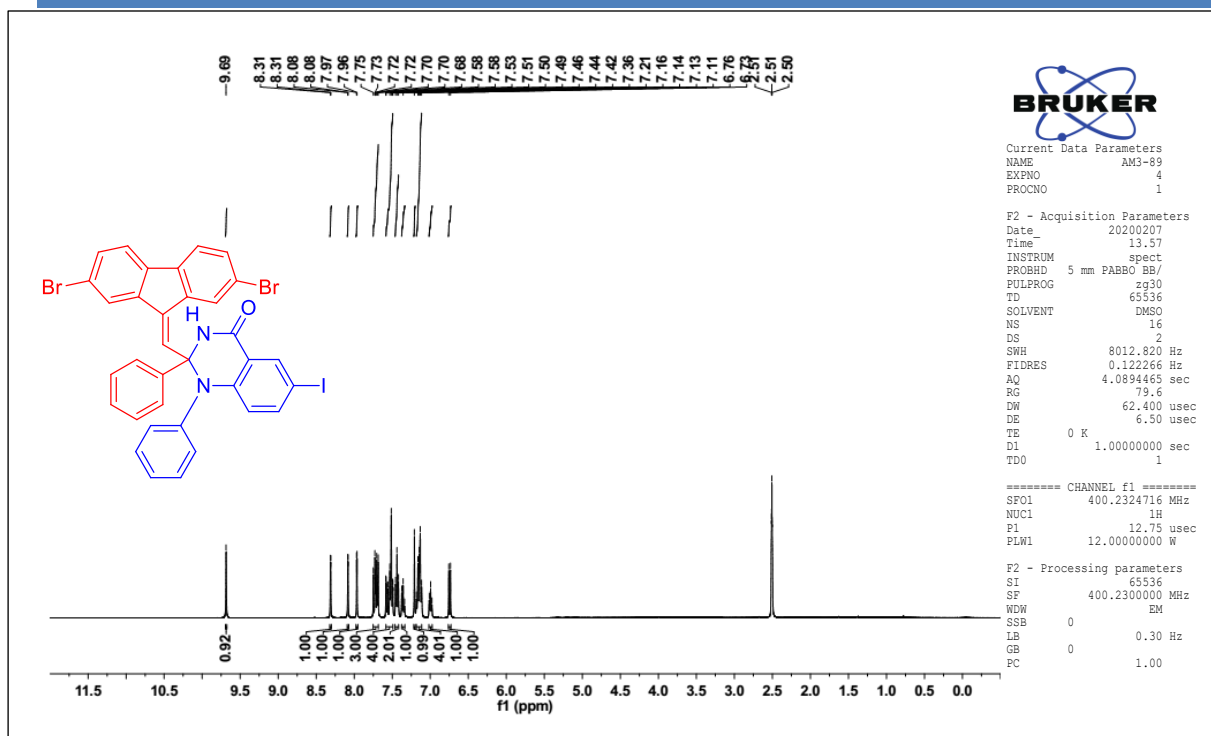
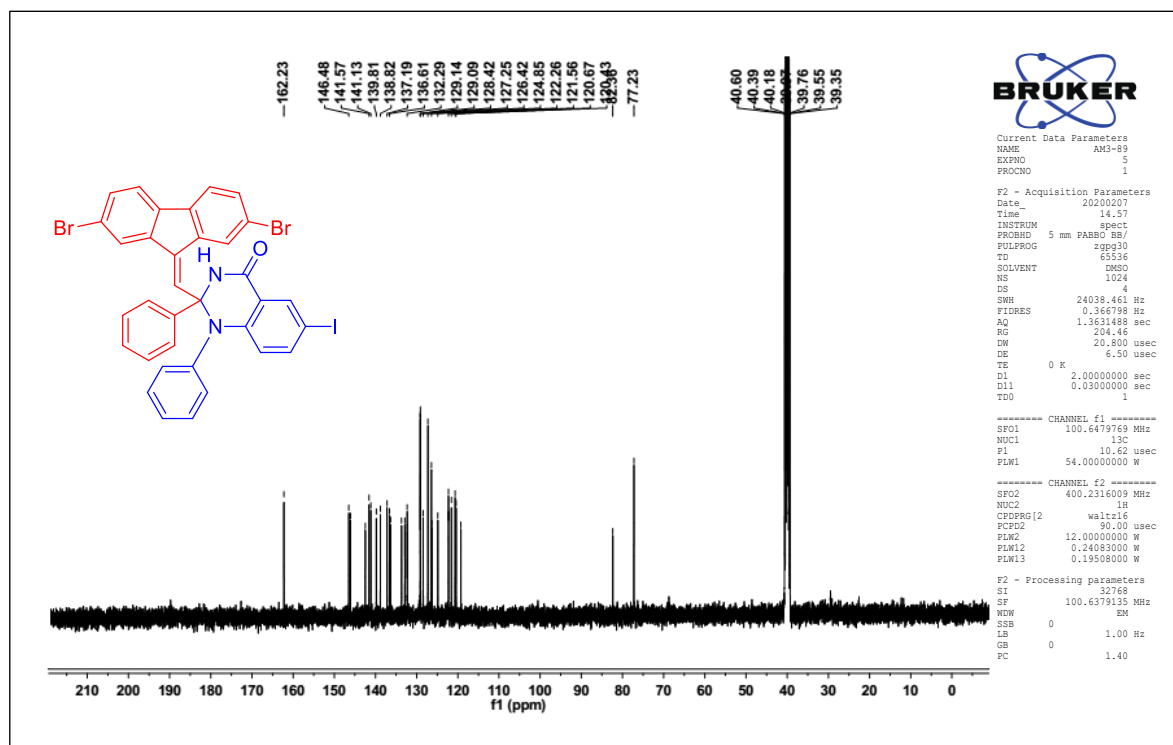


Figure 68 HRMS spectrum of compound 3q

Figure 69 ^1H NMR spectrum of compound **3r**Figure 70 ^{13}C NMR spectrum of compound **3r**

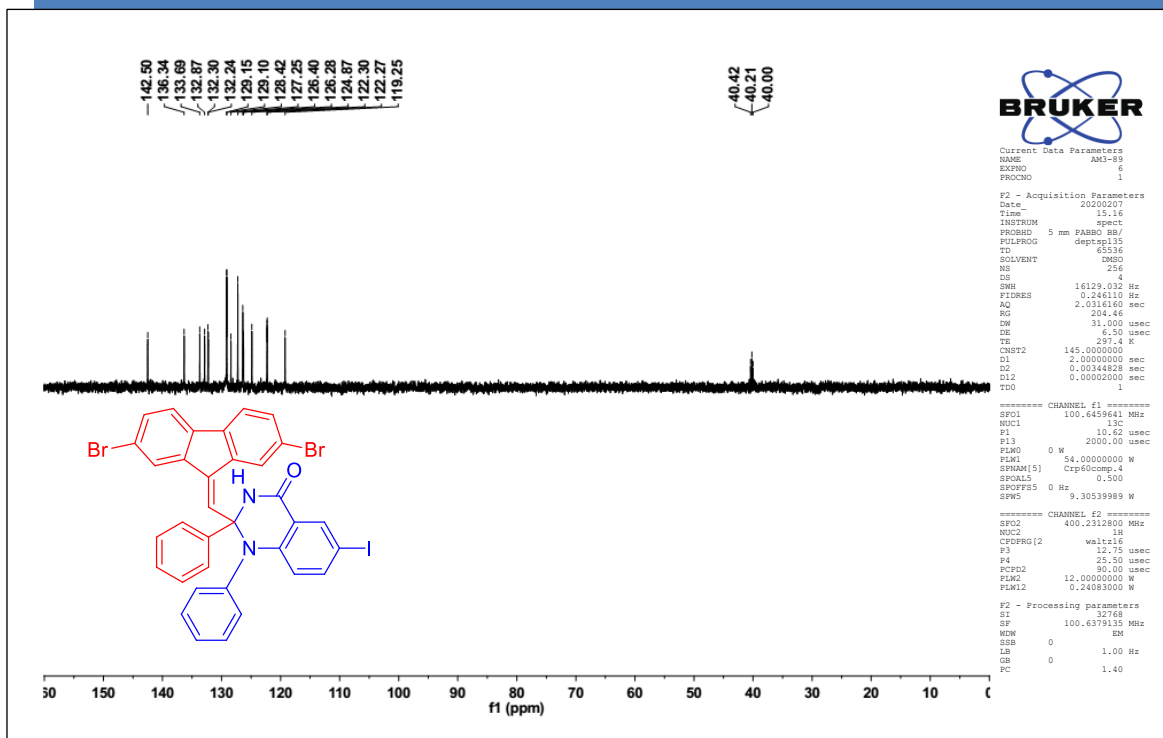


Figure 71 DEPT-135 NMR spectrum of compound 3r

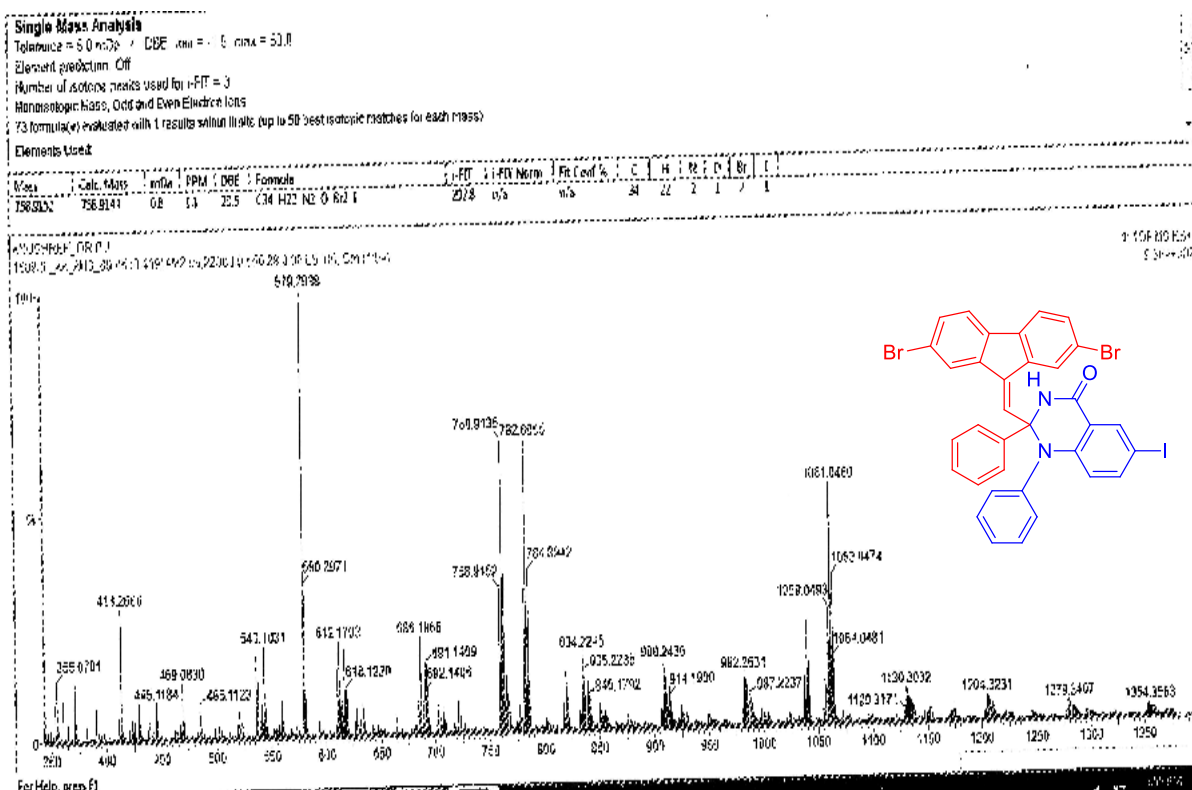


Figure 72 HRMS spectrum of compound 3r

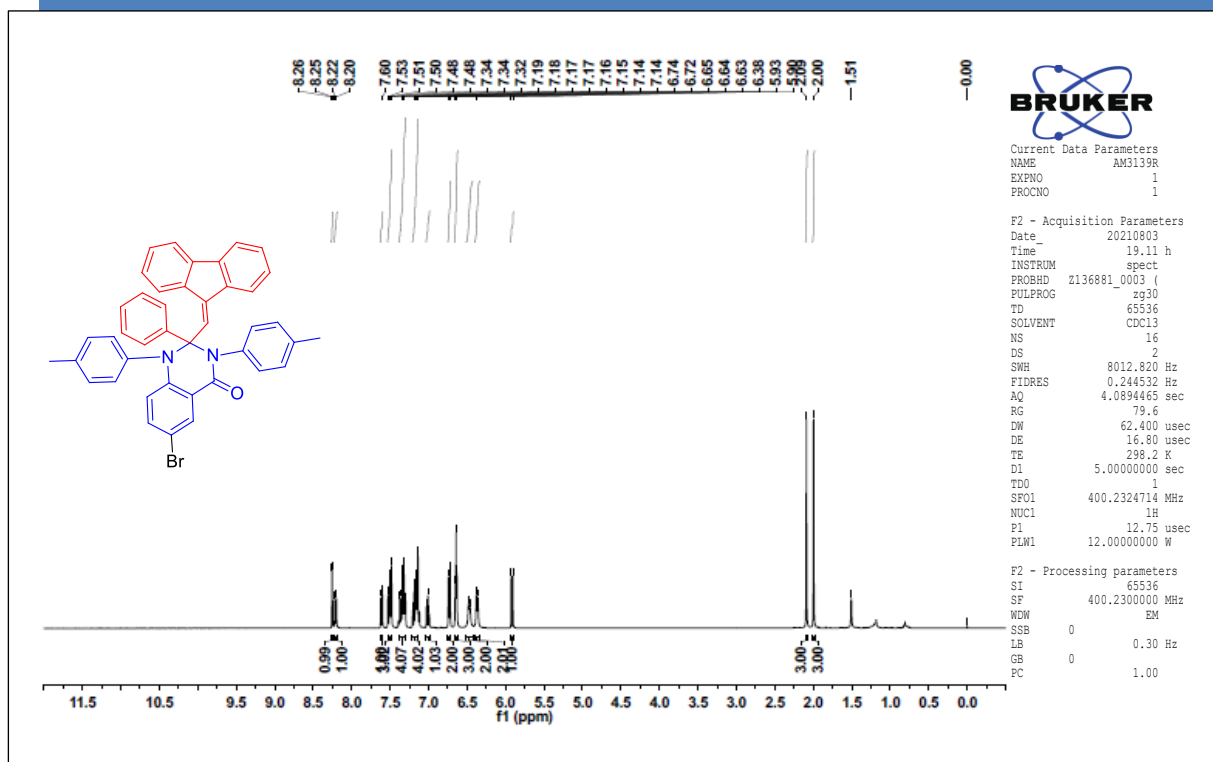


Figure 73 ^1H NMR spectrum of compound 4a

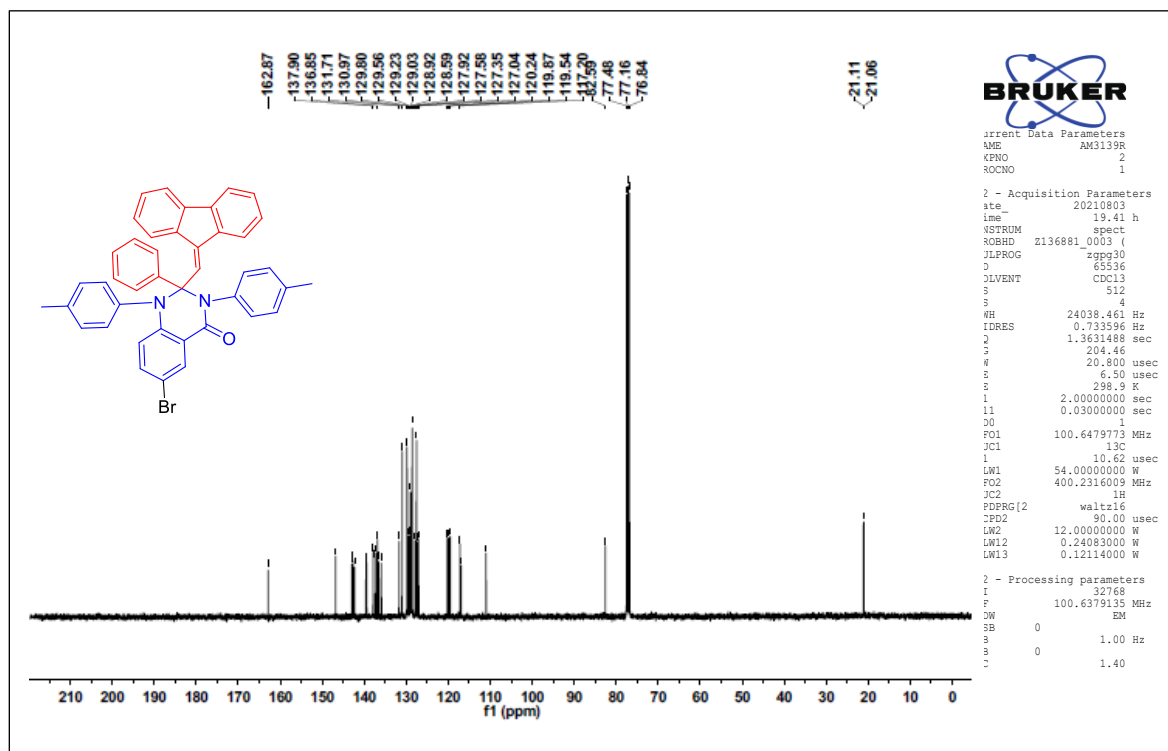
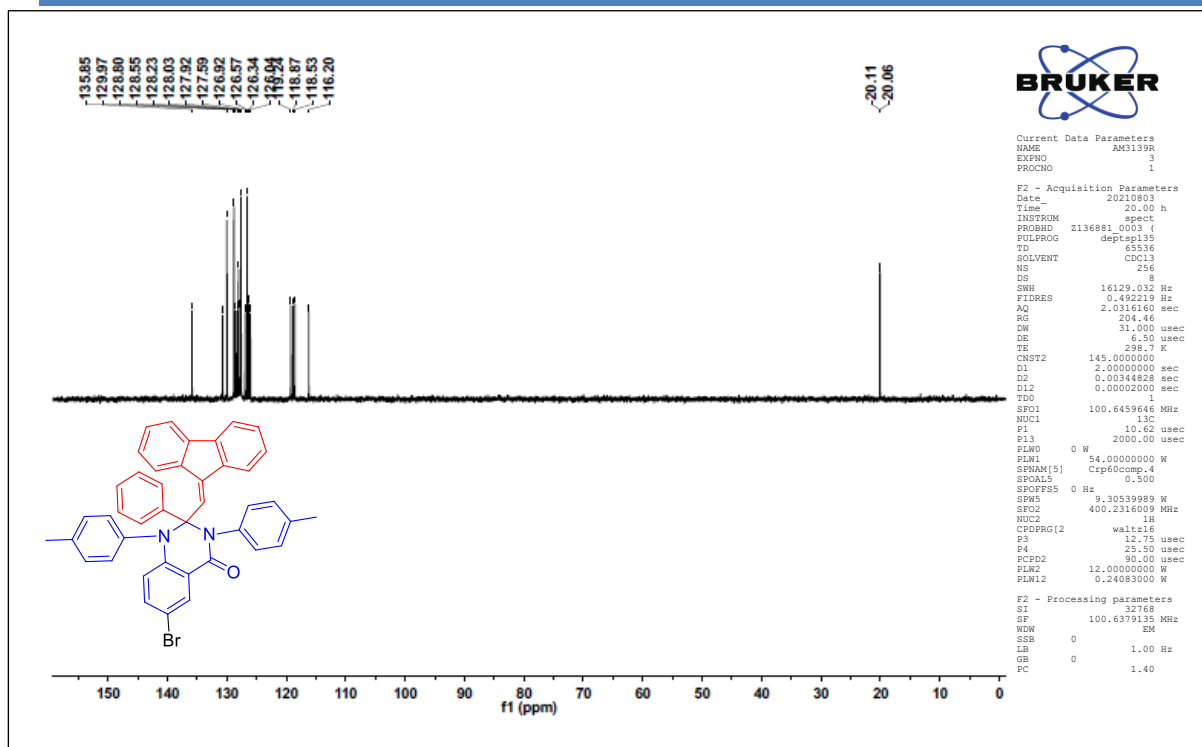
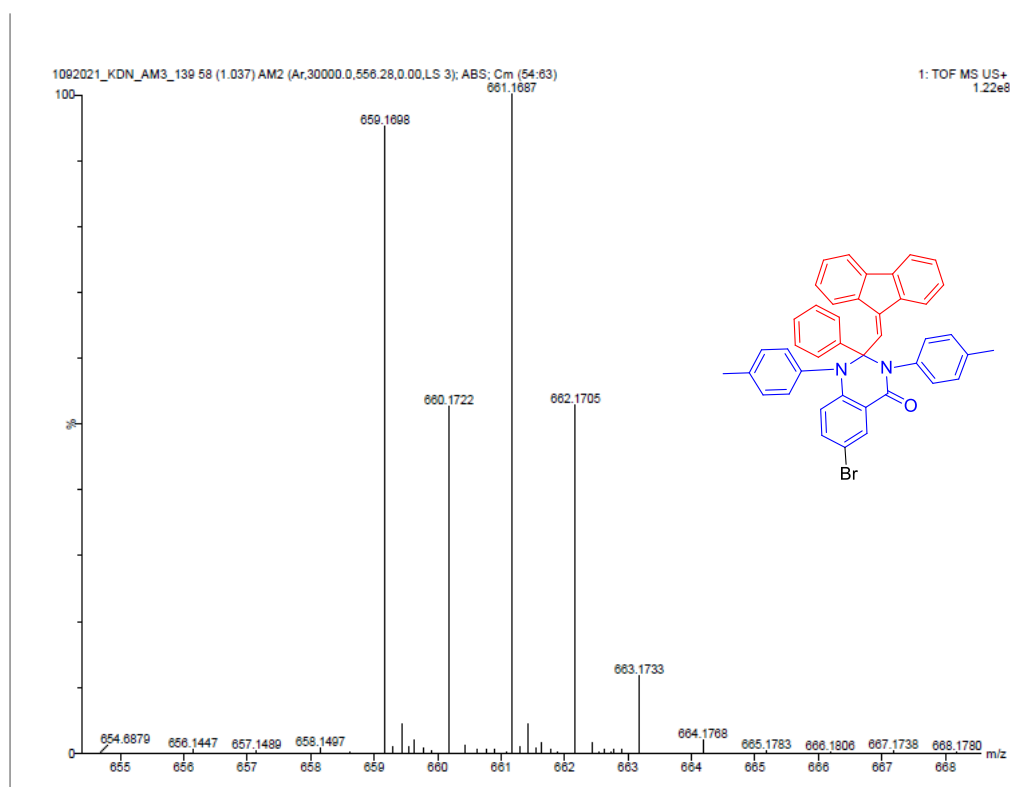


Figure 74 ^{13}C NMR spectrum of compound 4a

Figure 75 DEPT-135 NMR spectrum of compound **4a**Figure 76 HRMS spectrum of compound **4a**

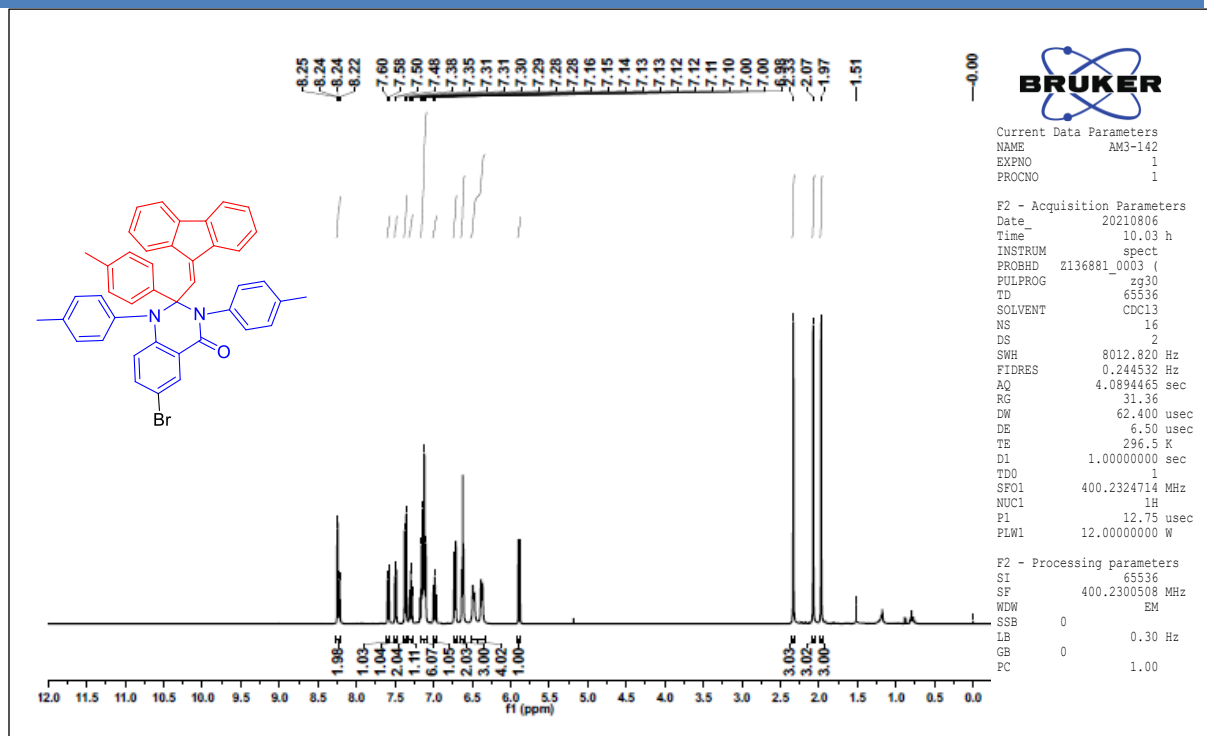


Figure 77 ^1H NMR spectrum of compound **4b**

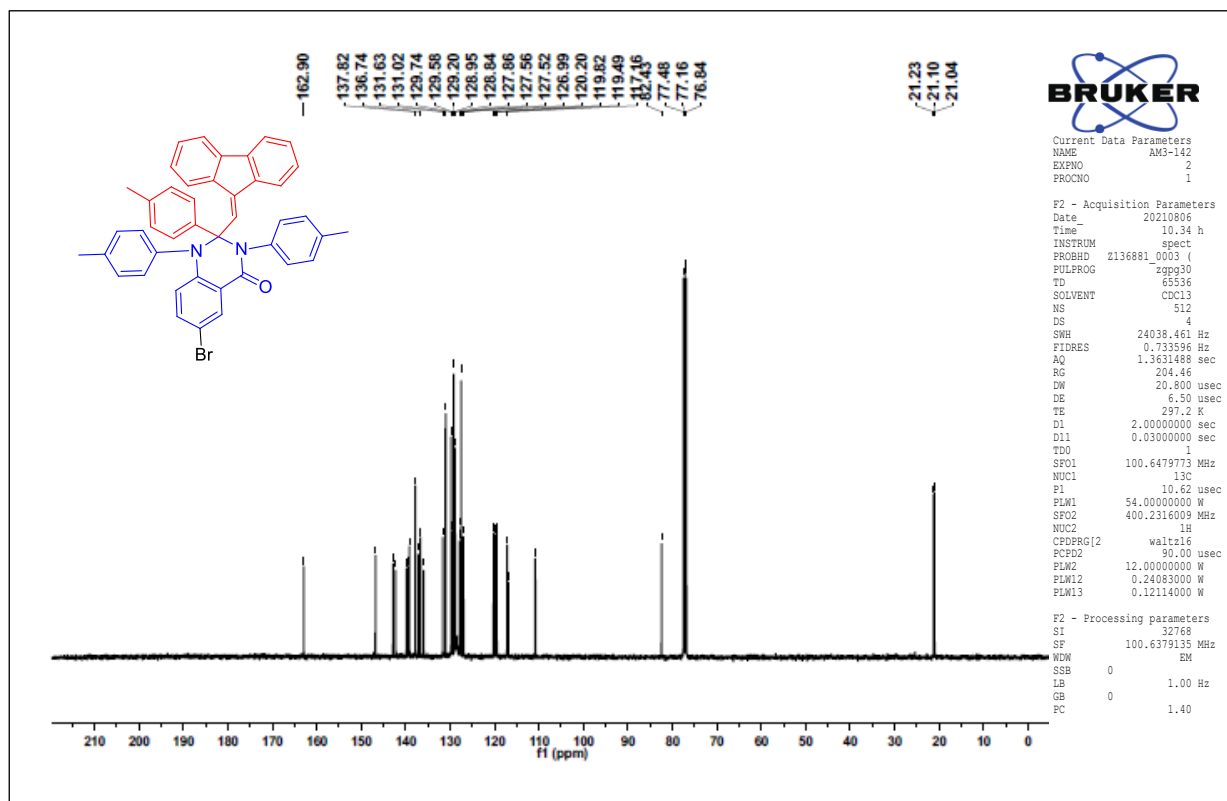


Figure 78 ^{13}C NMR spectrum of compound **4b**

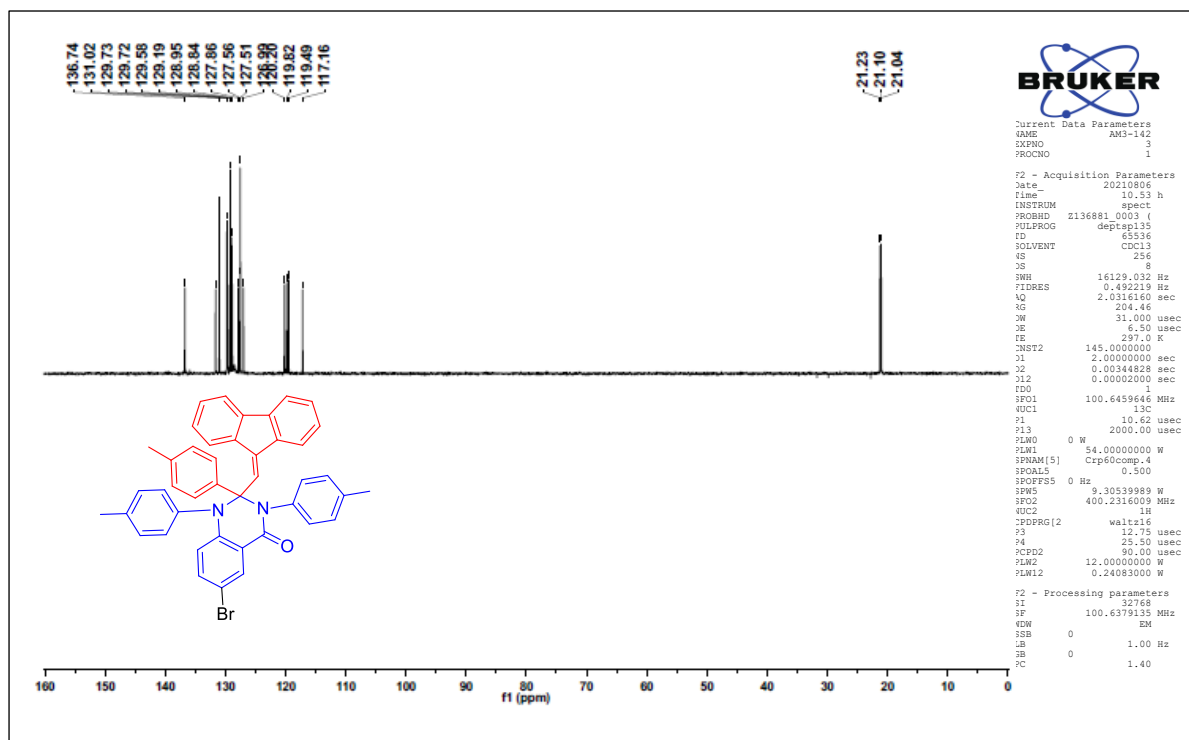


Figure 79 DEPT-135 NMR spectrum of compound **4b**

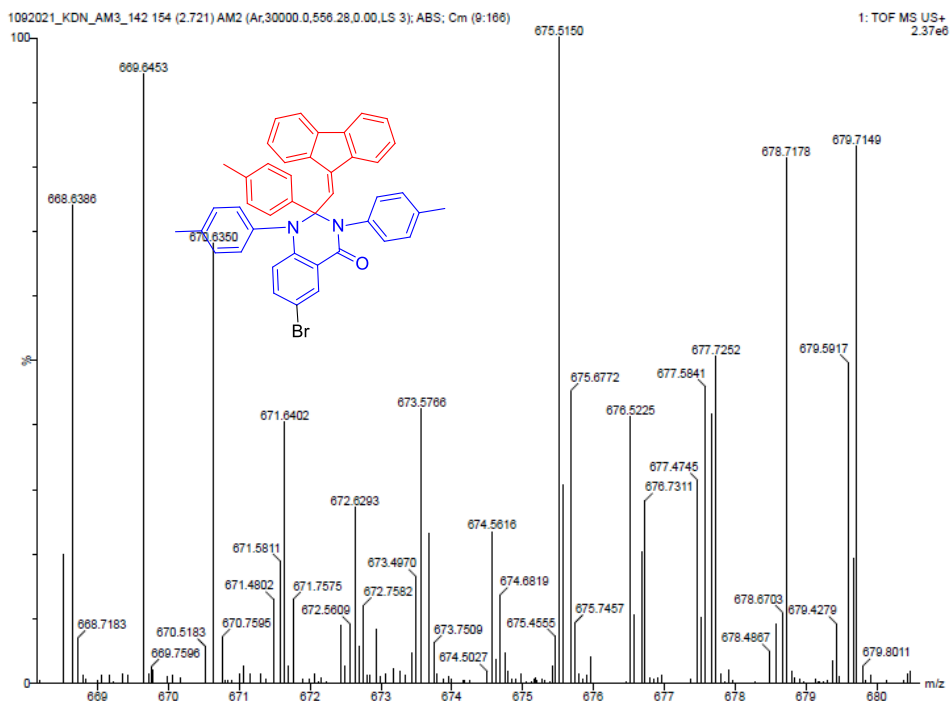


Figure 80 HRMS spectrum of compound **4b**

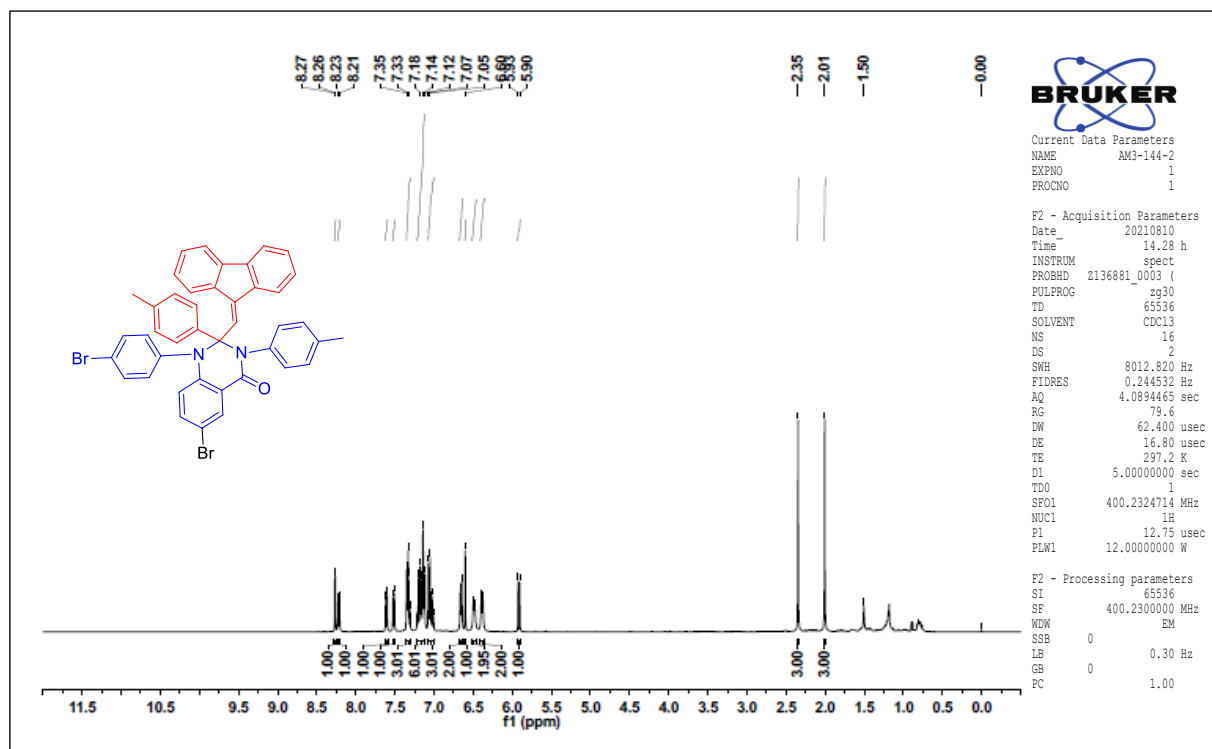


Figure 81 ^1H NMR spectrum of compound **4c**

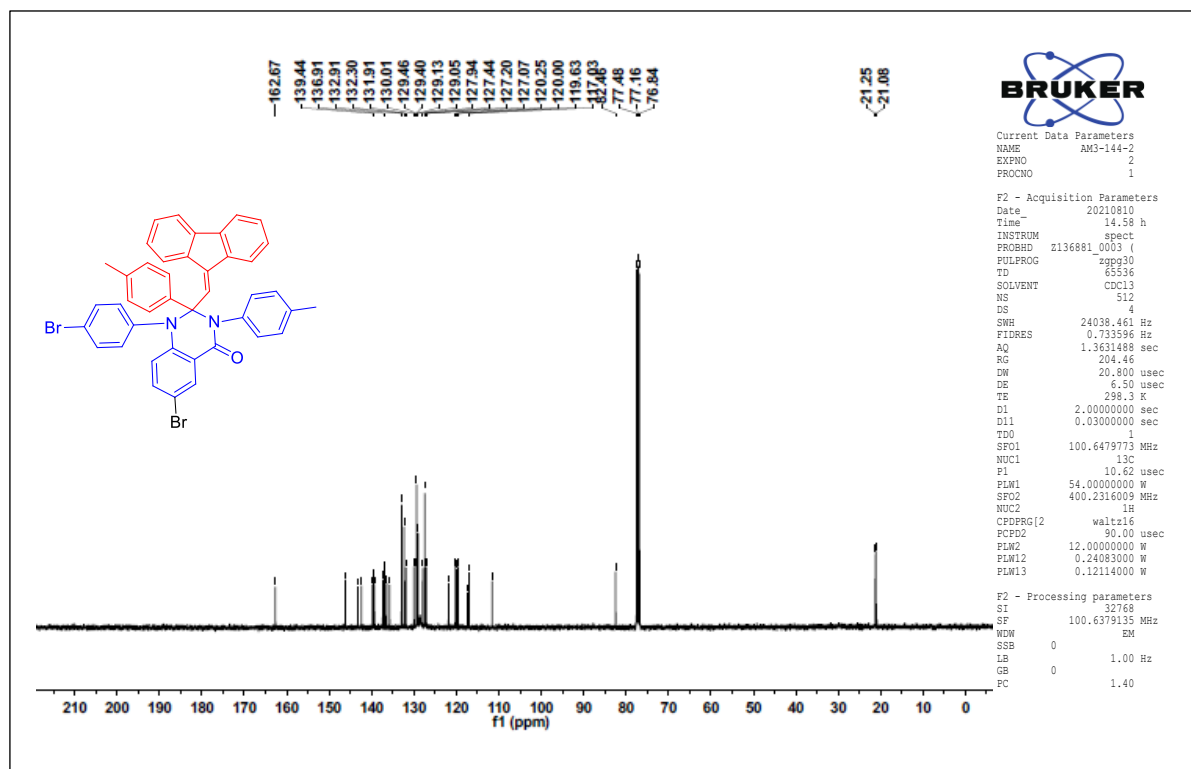


Figure 82 ^{13}C NMR spectrum of compound **4c**

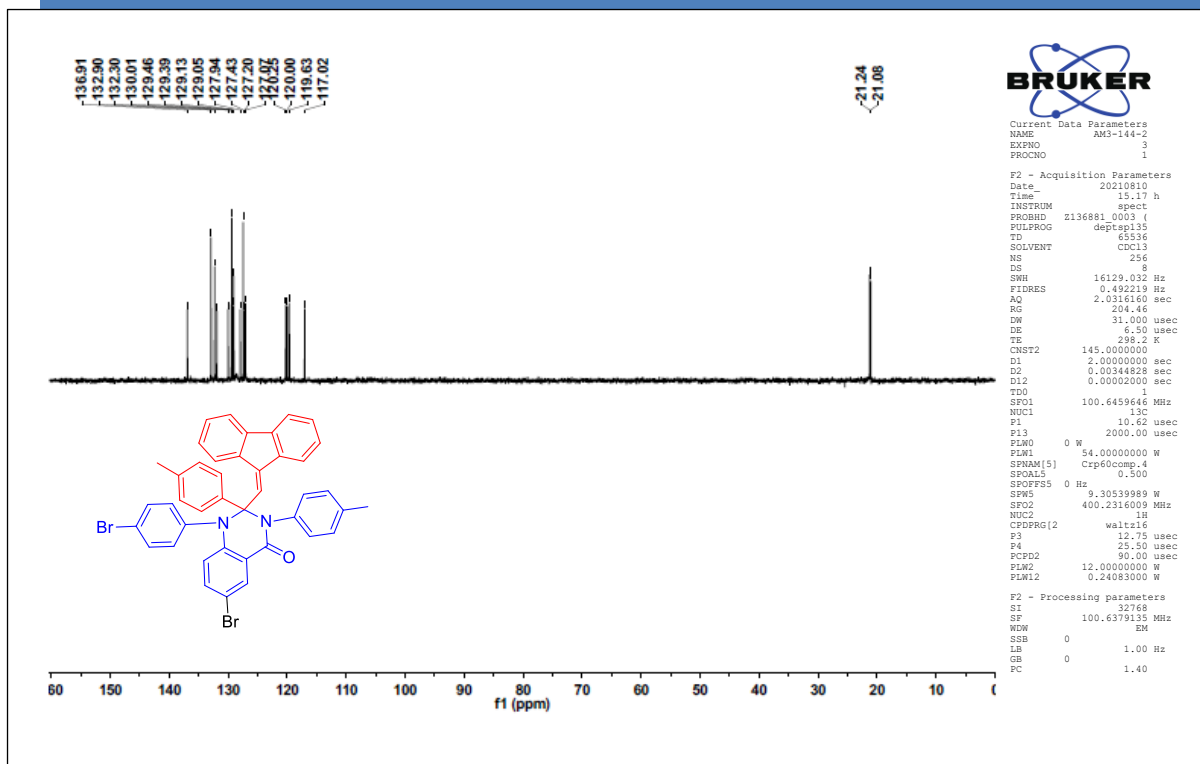


Figure 83 DEPT-135 NMR spectrum of compound **4c**

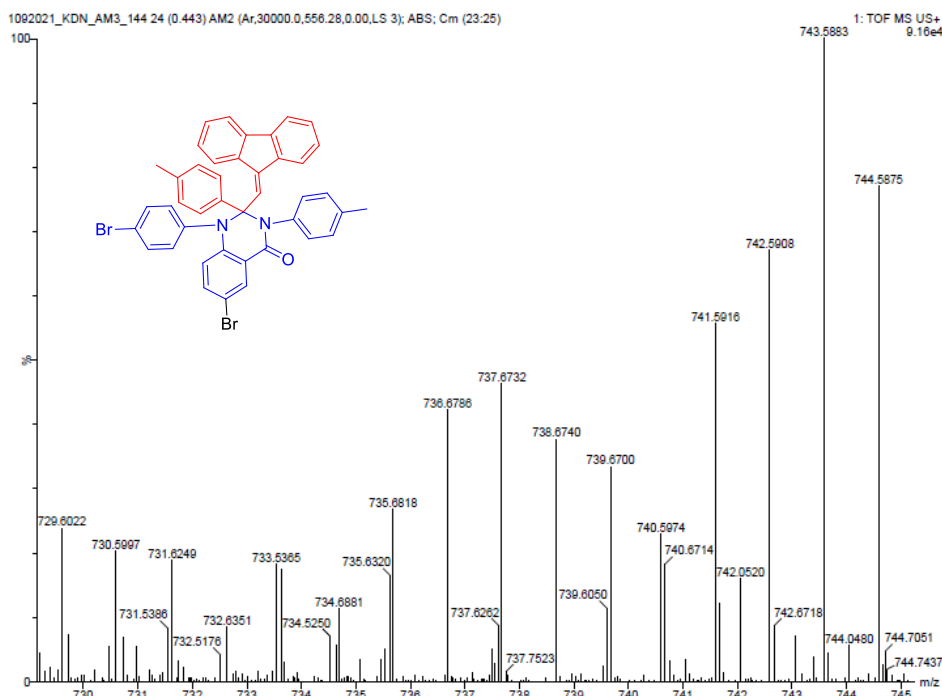
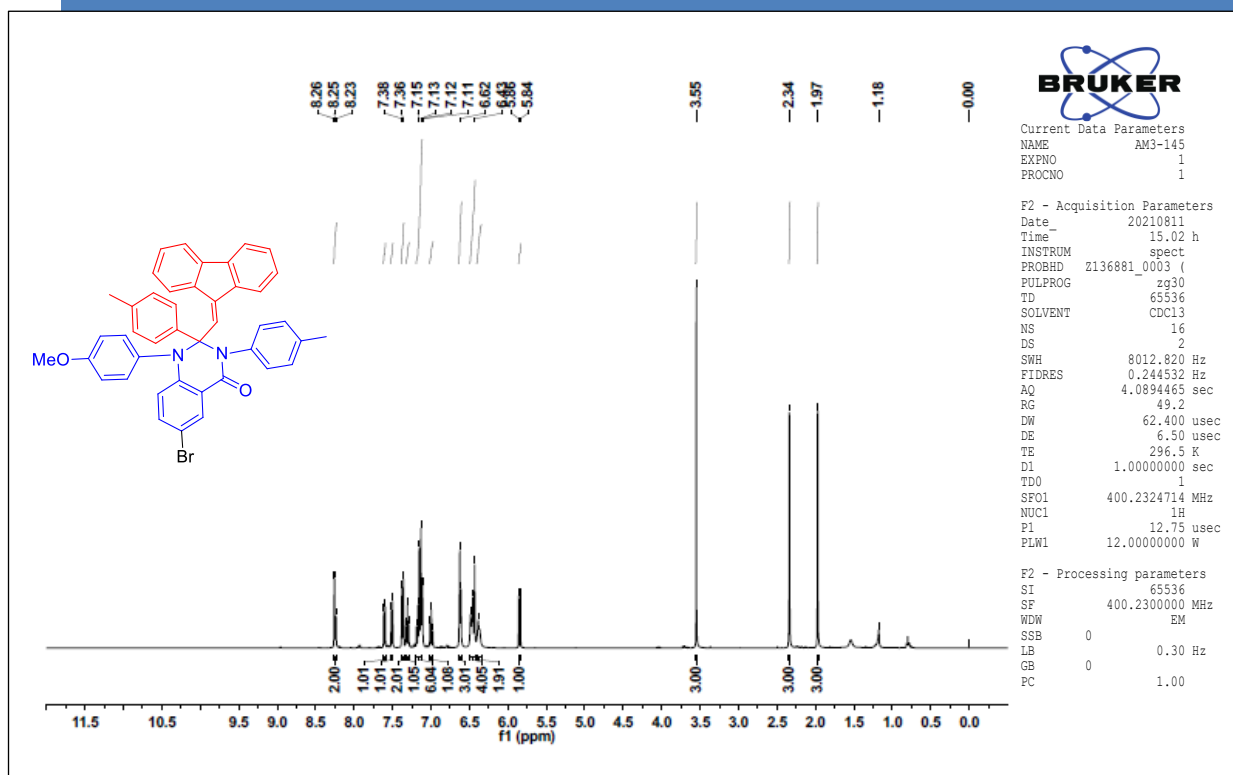
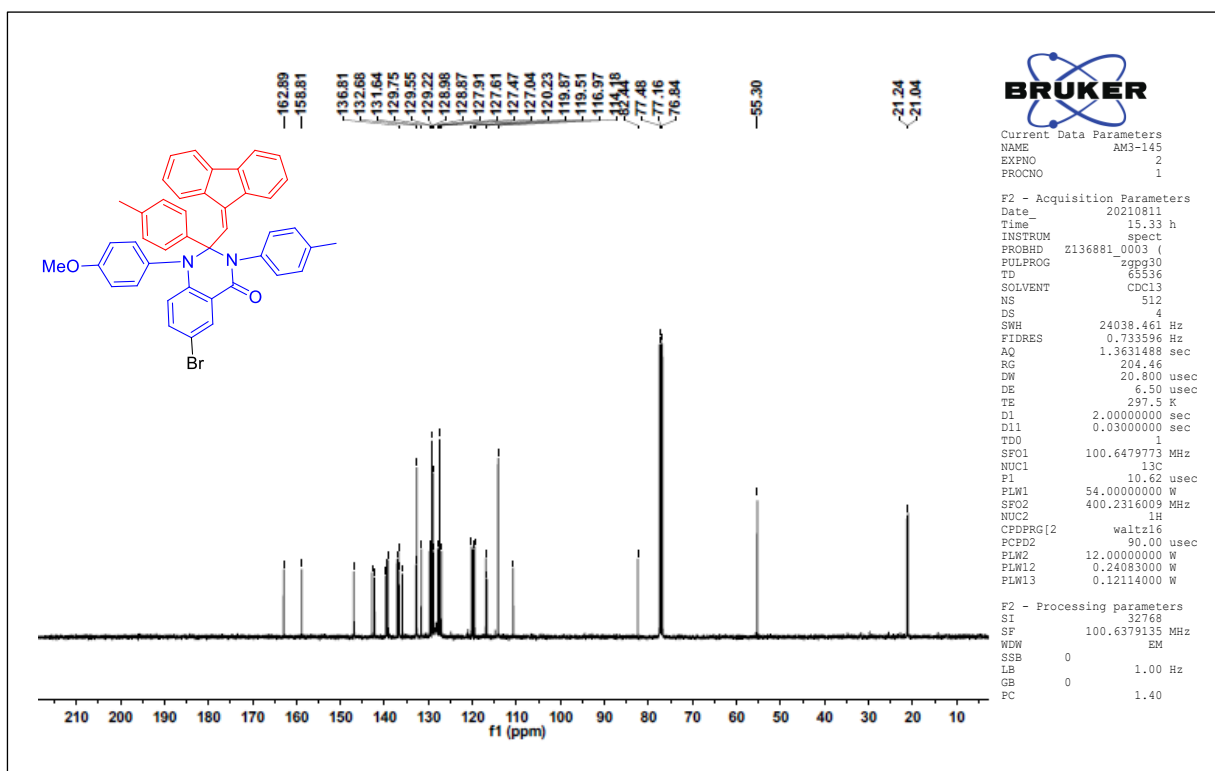


Figure 84 HRMS spectrum of compound **4c**

Figure 85 ¹H NMR spectrum of compound 4dFigure 86 ¹³C NMR spectrum of compound 4d

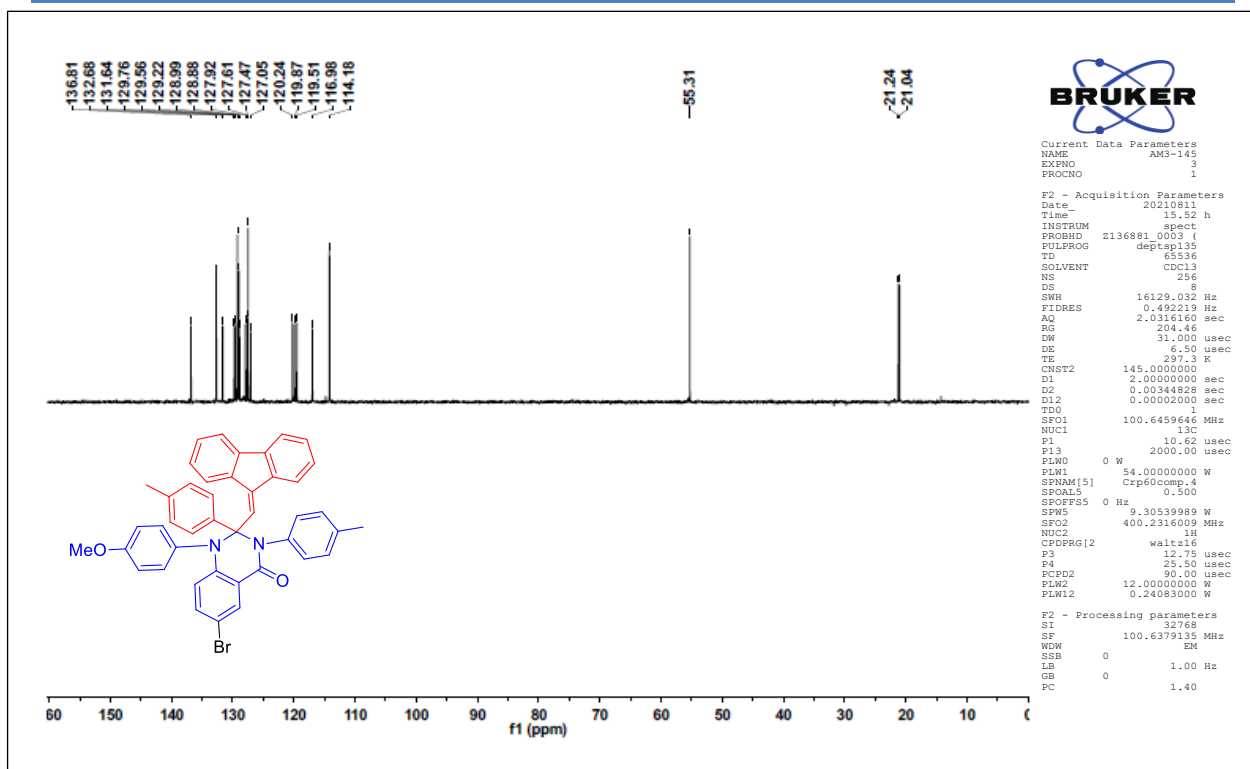


Figure 87 DEPT-135 NMR spectrum of compound **4c**

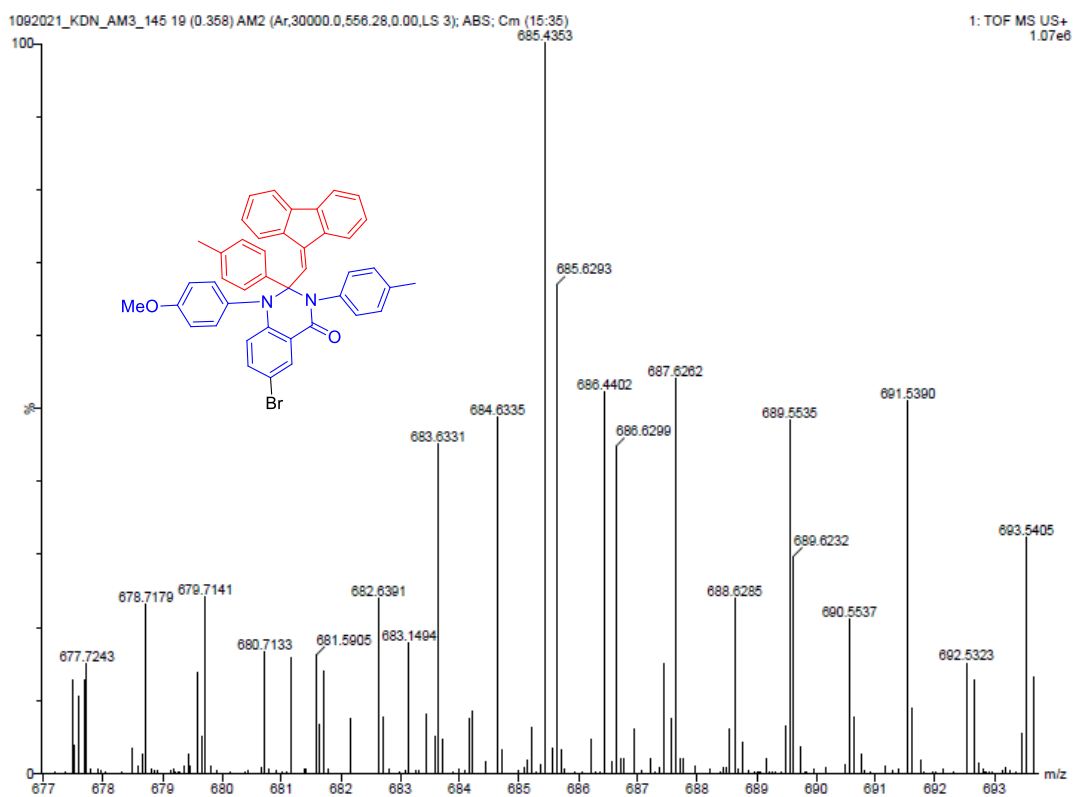
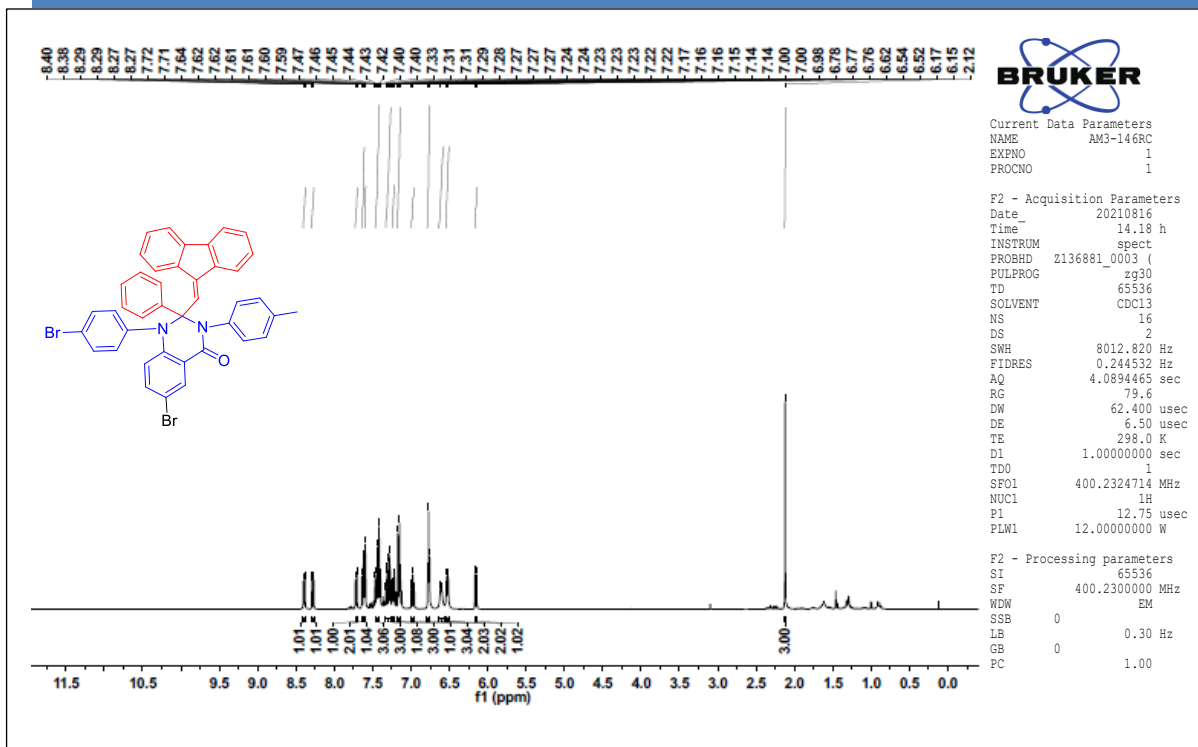
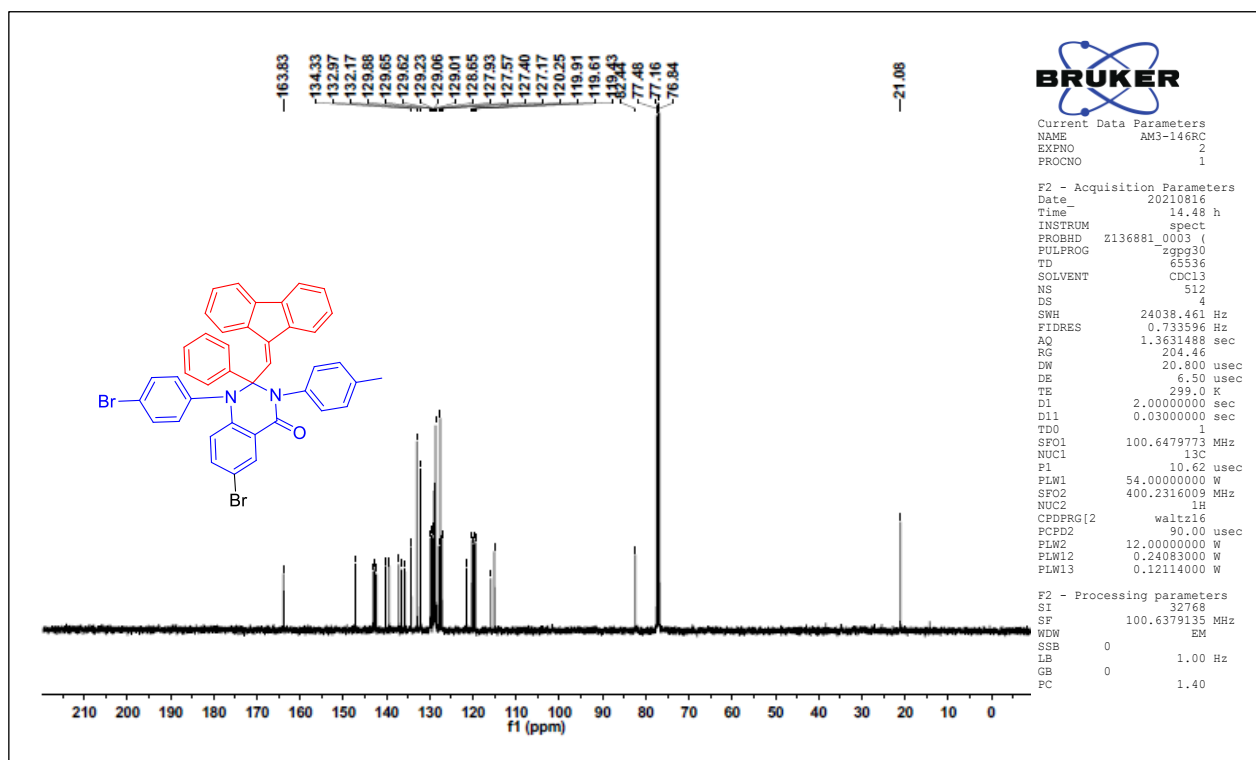


Figure 88 HRMS spectrum of compound **4d**

Figure 89 ^1H NMR spectrum of compound **4e**Figure 90 ^{13}C NMR spectrum of compound **4e**

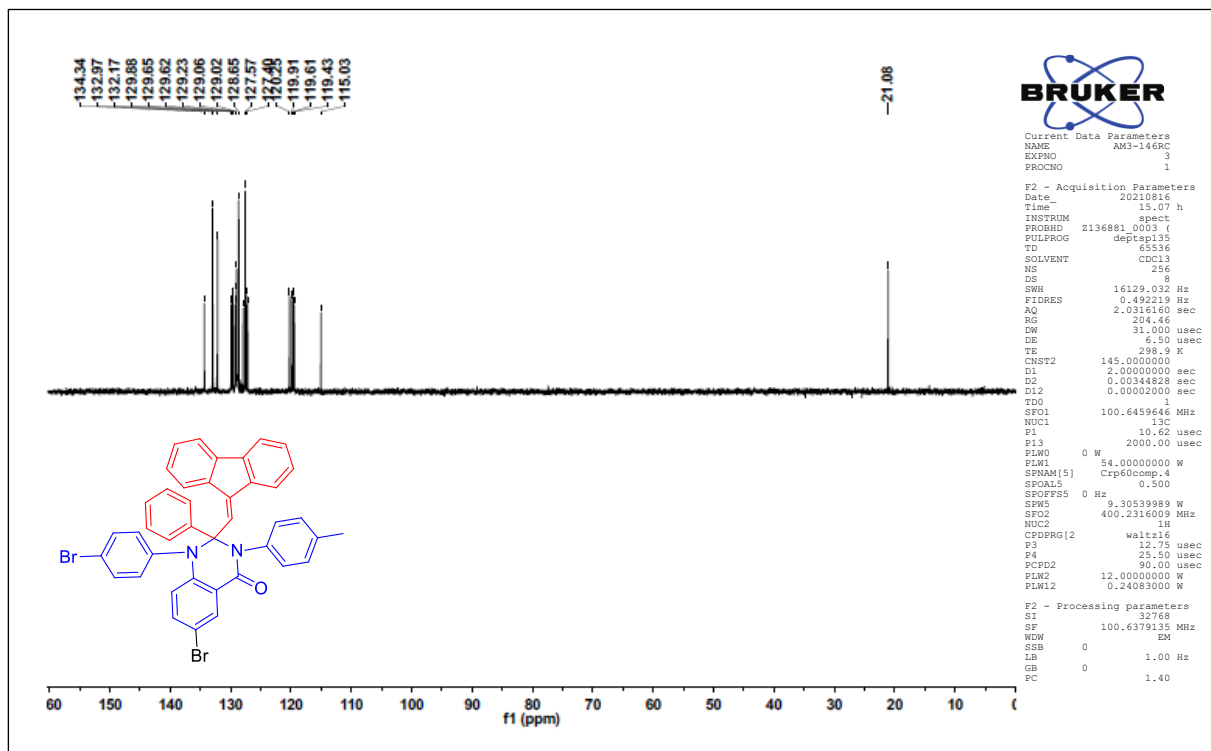


Figure 91 DEPT-135 NMR spectrum of compound 4e

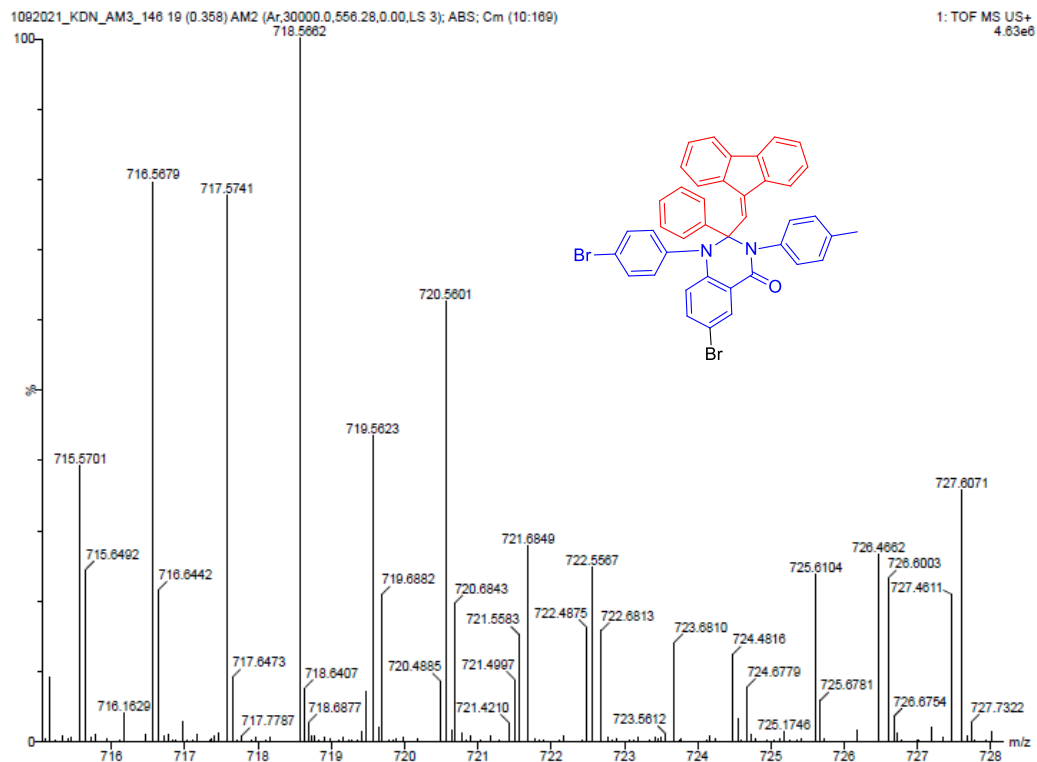
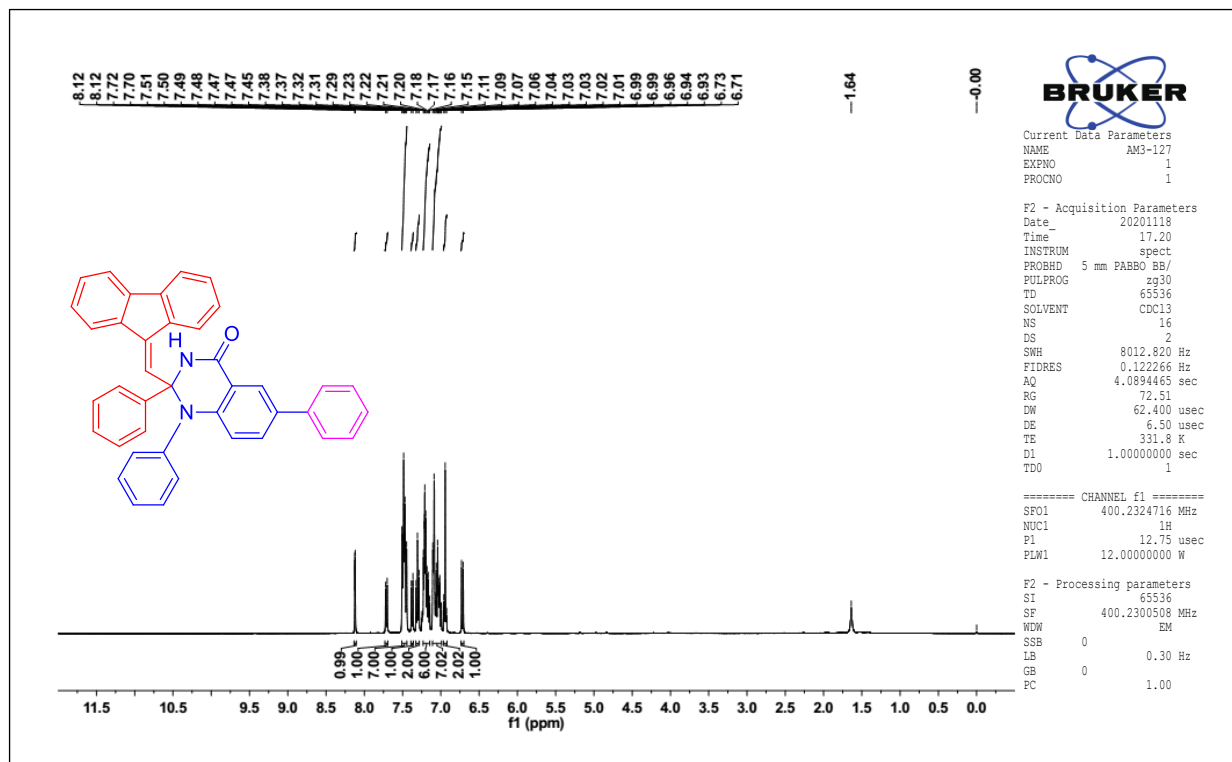
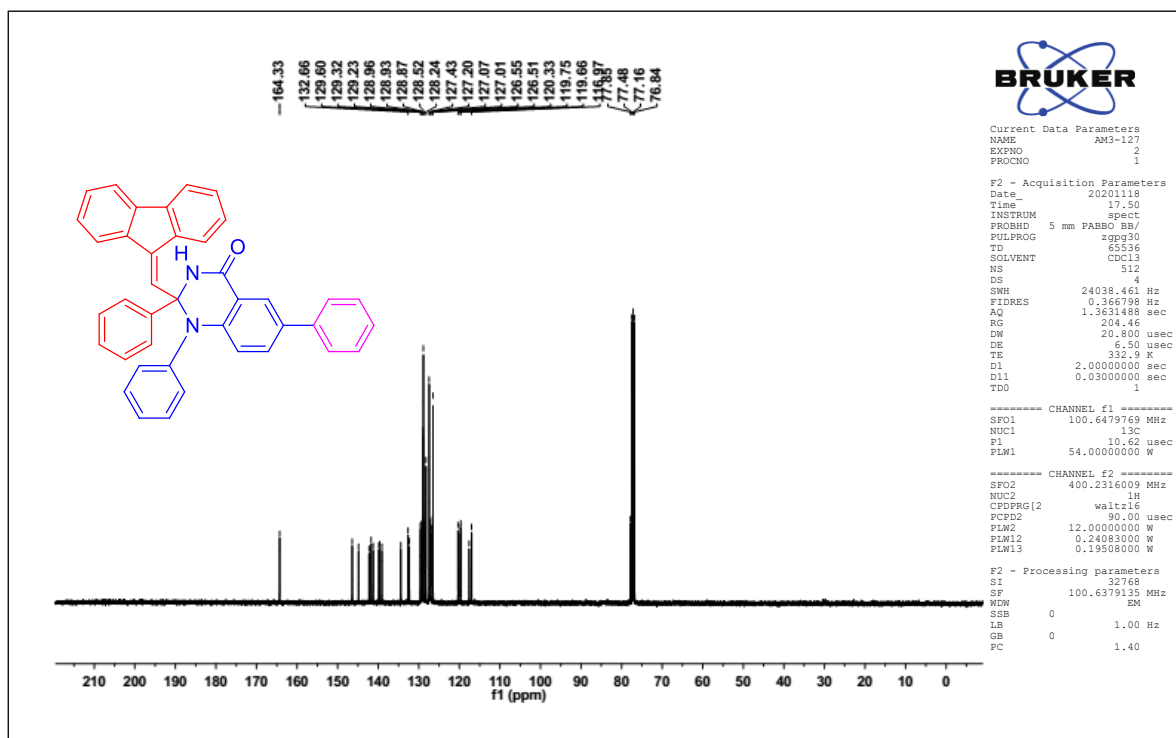


Figure 92 HRMS spectrum of compound 4e

Figure 93 ^1H NMR spectrum of compound 5Figure 94 ^{13}C NMR spectrum of compound 5

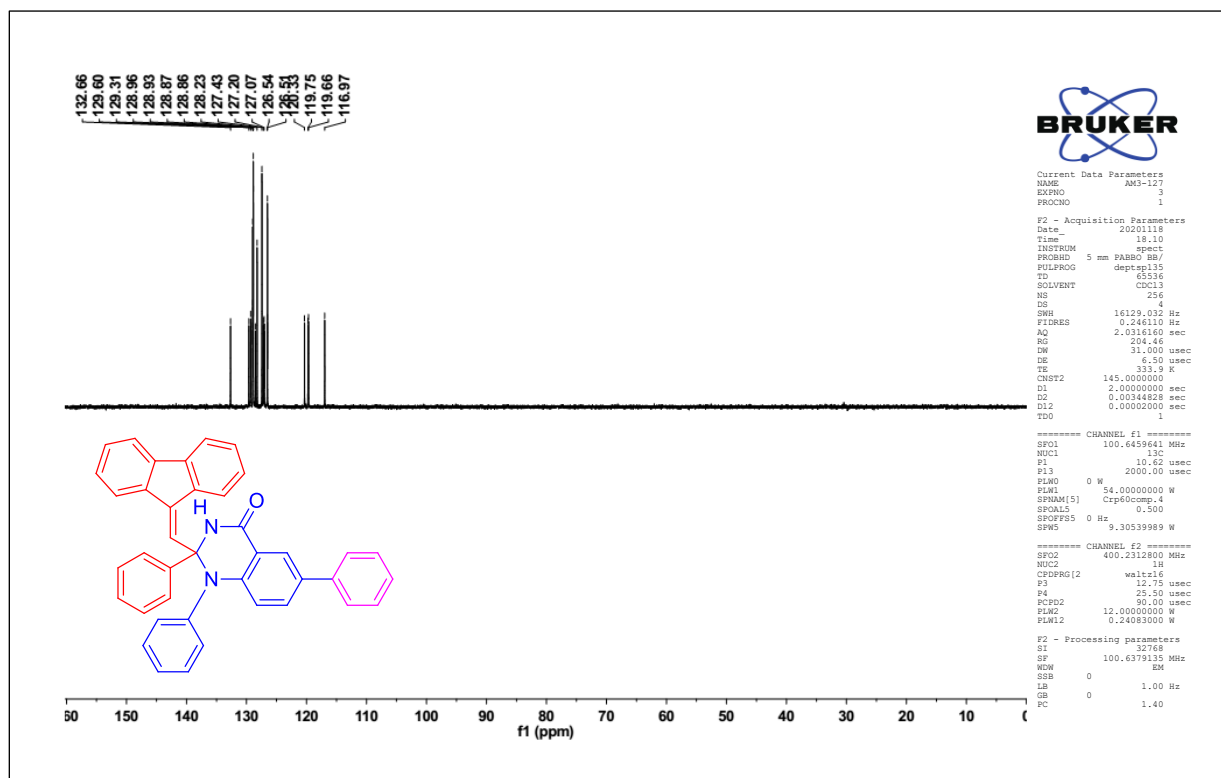


Figure 95 DEPT-135 NMR spectrum of compound 5

AM3-127 #74 RT: 1.36 AV: 1 NL: 5.21E6
 T: FTMS (1,1) + p ESI Full lock ms [100.00-1400.00]

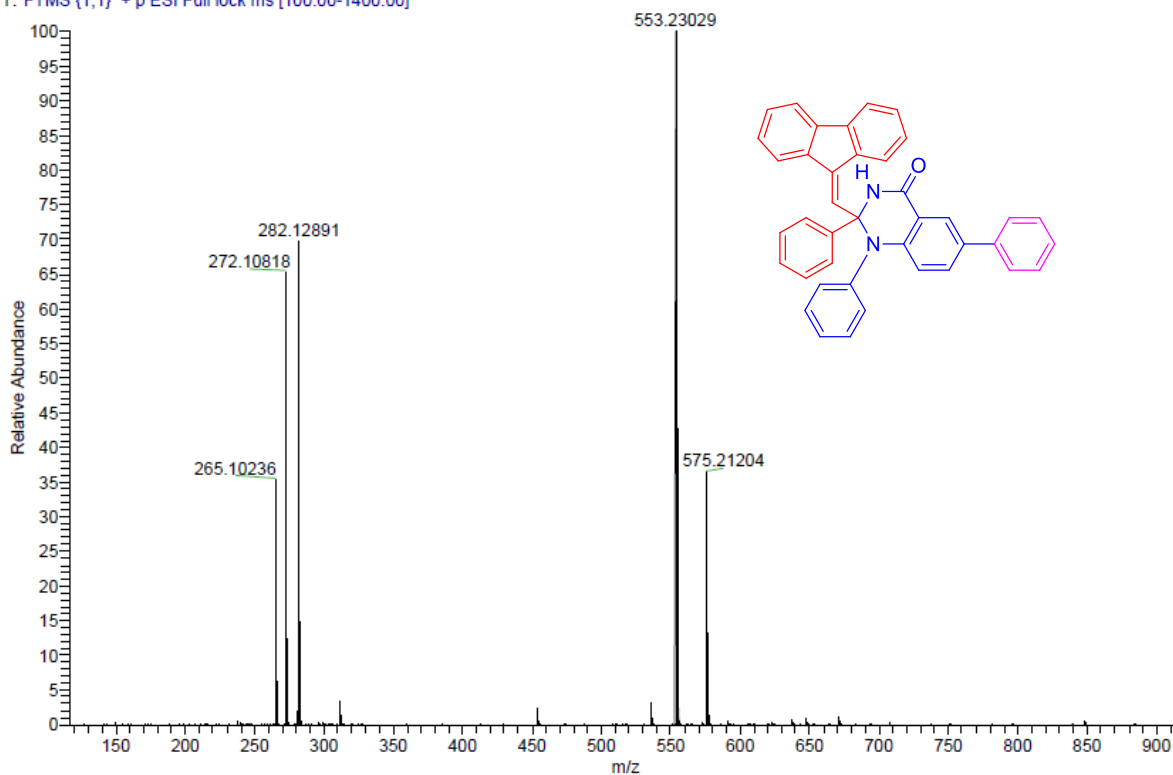
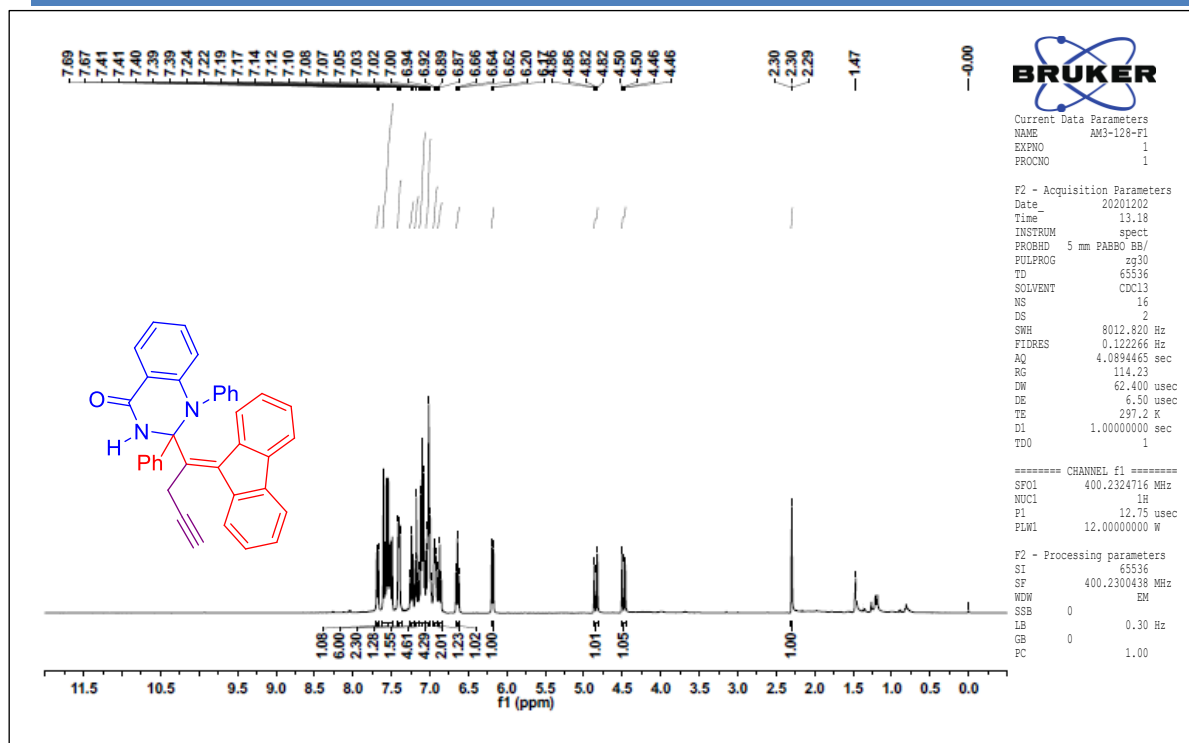
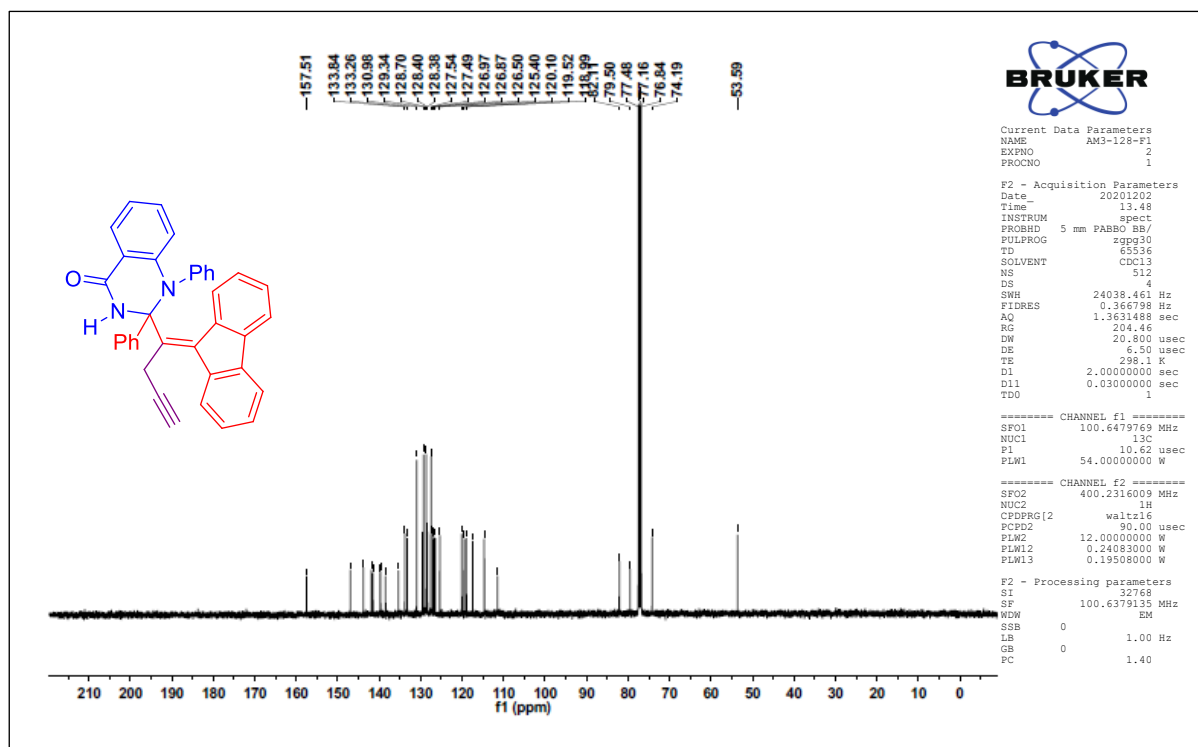


Figure 96 HRMS spectrum of compound 5

Figure 97 ^1H NMR spectrum of compound 6aFigure 98 ^{13}C NMR spectrum of compound 6a

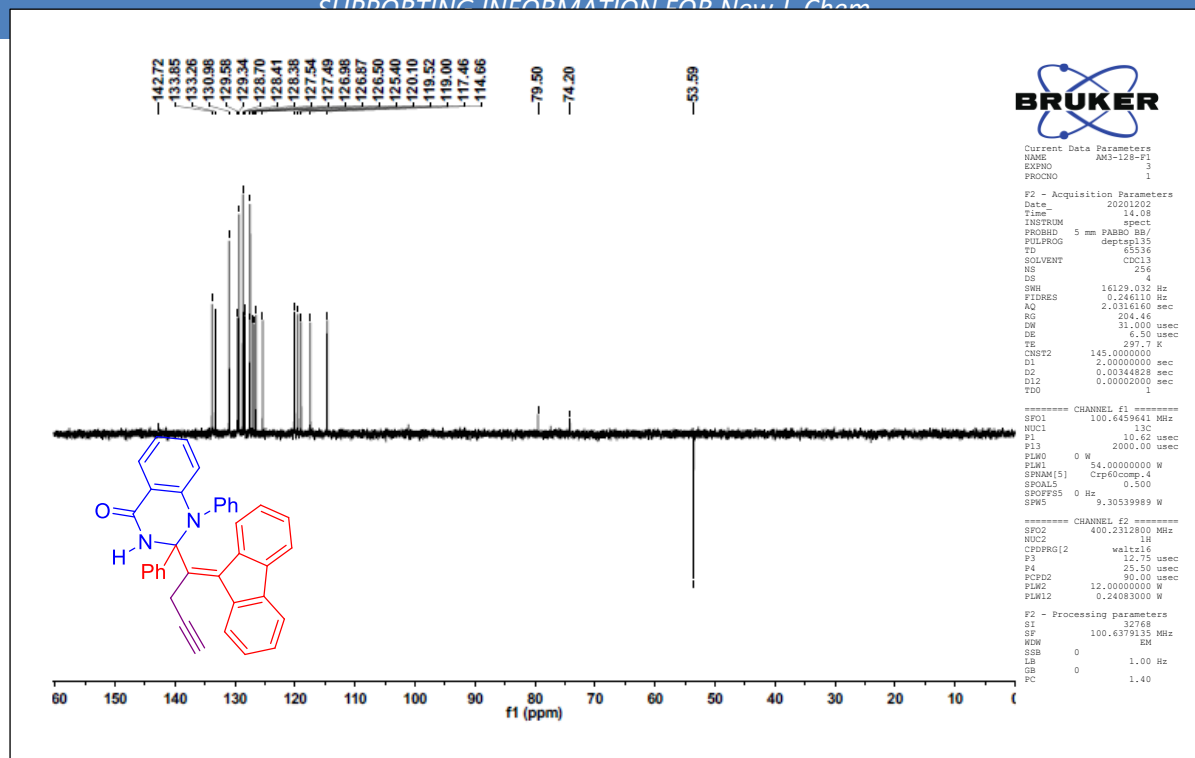


Figure 99 DEPT-135 NMR spectrum of compound 6a

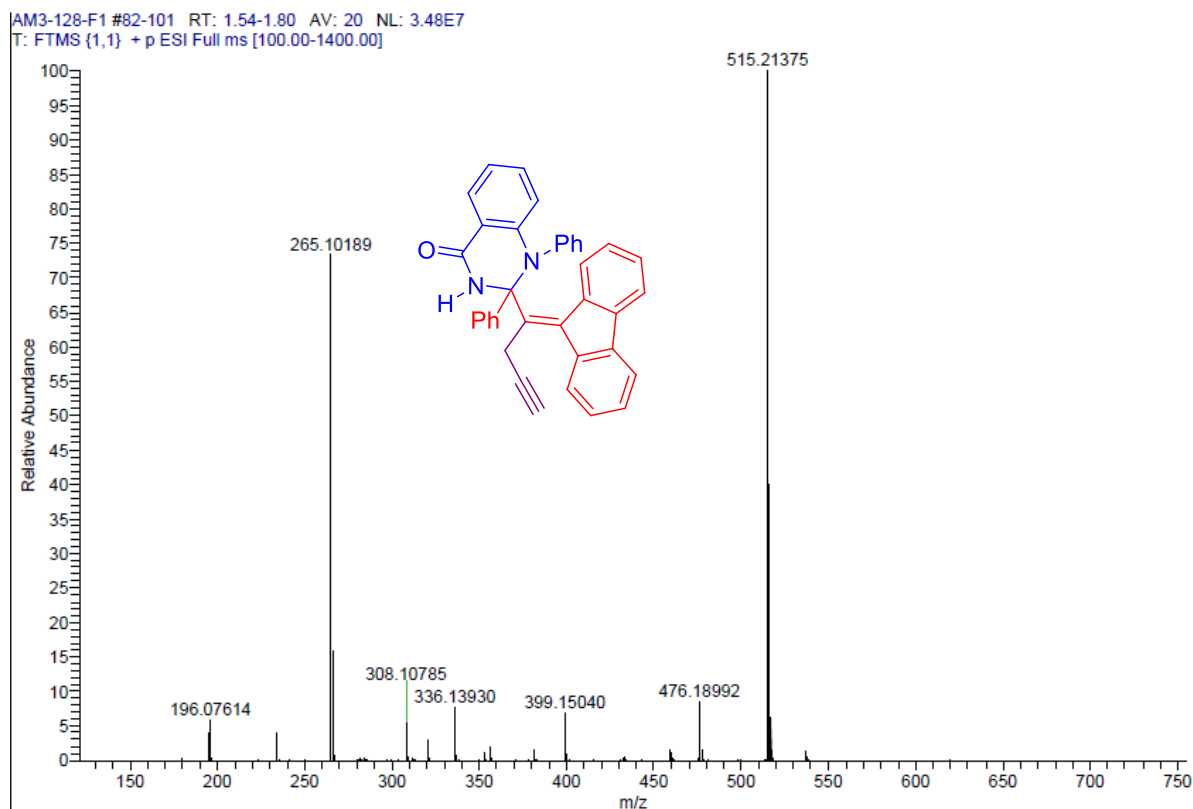
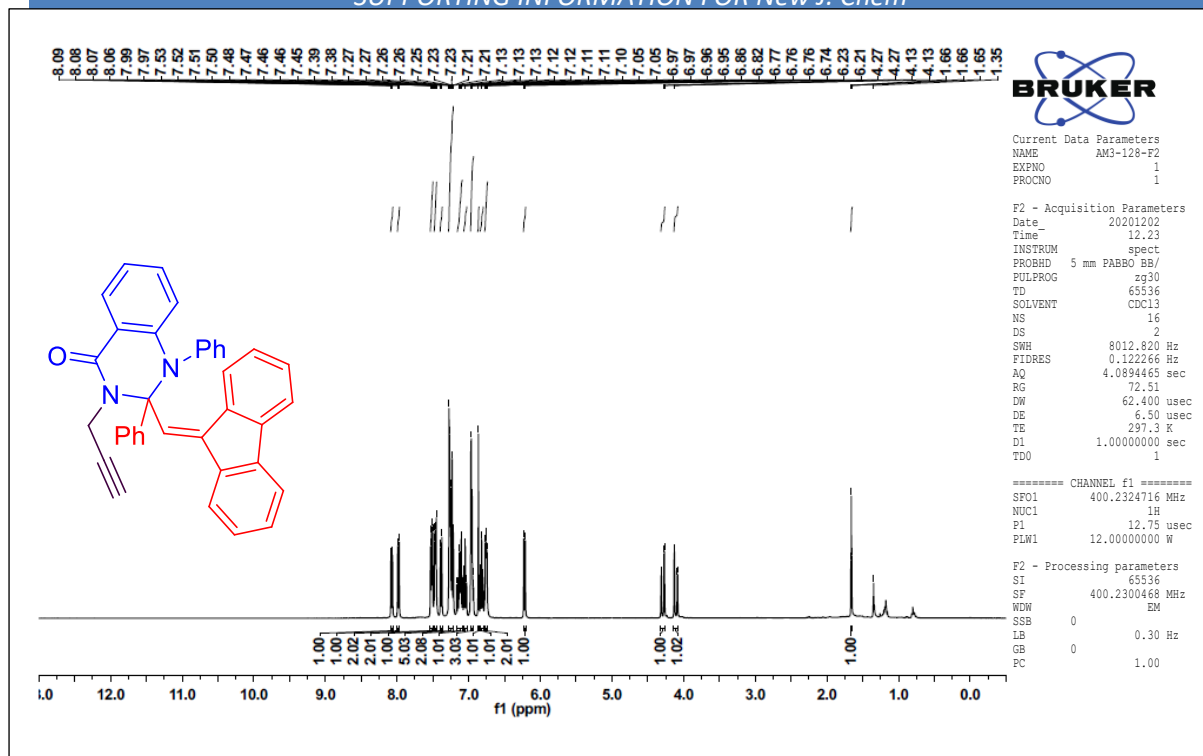
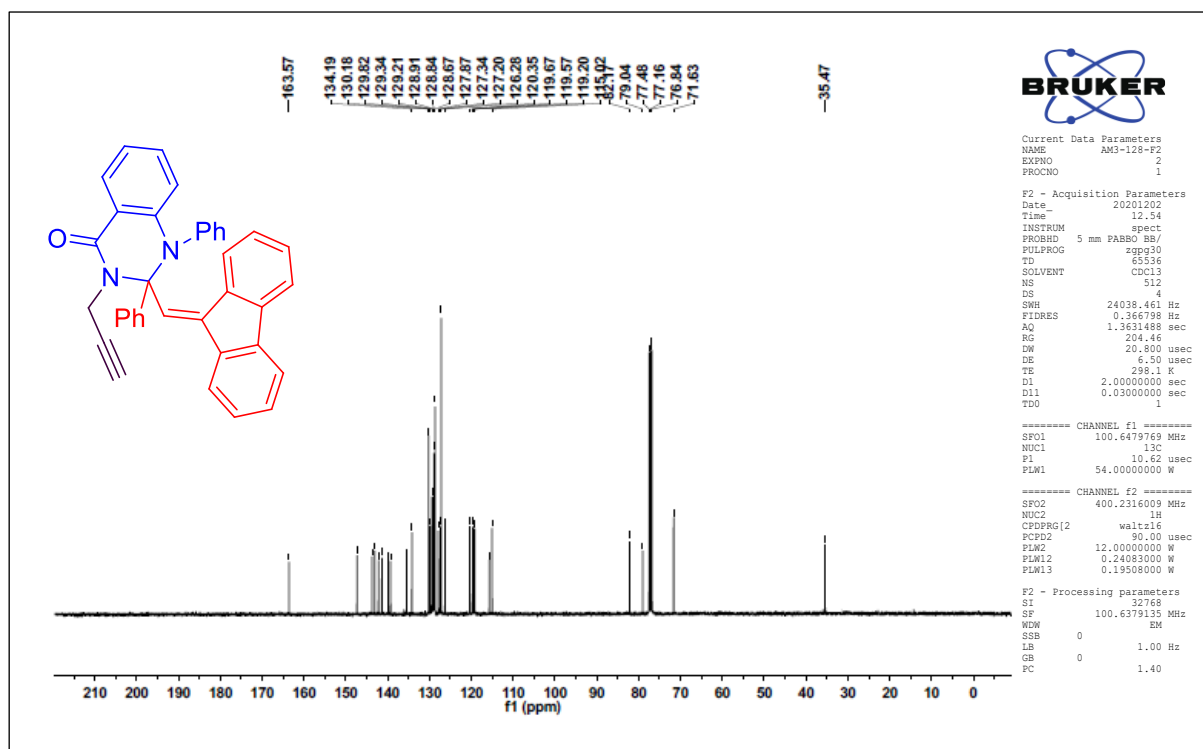
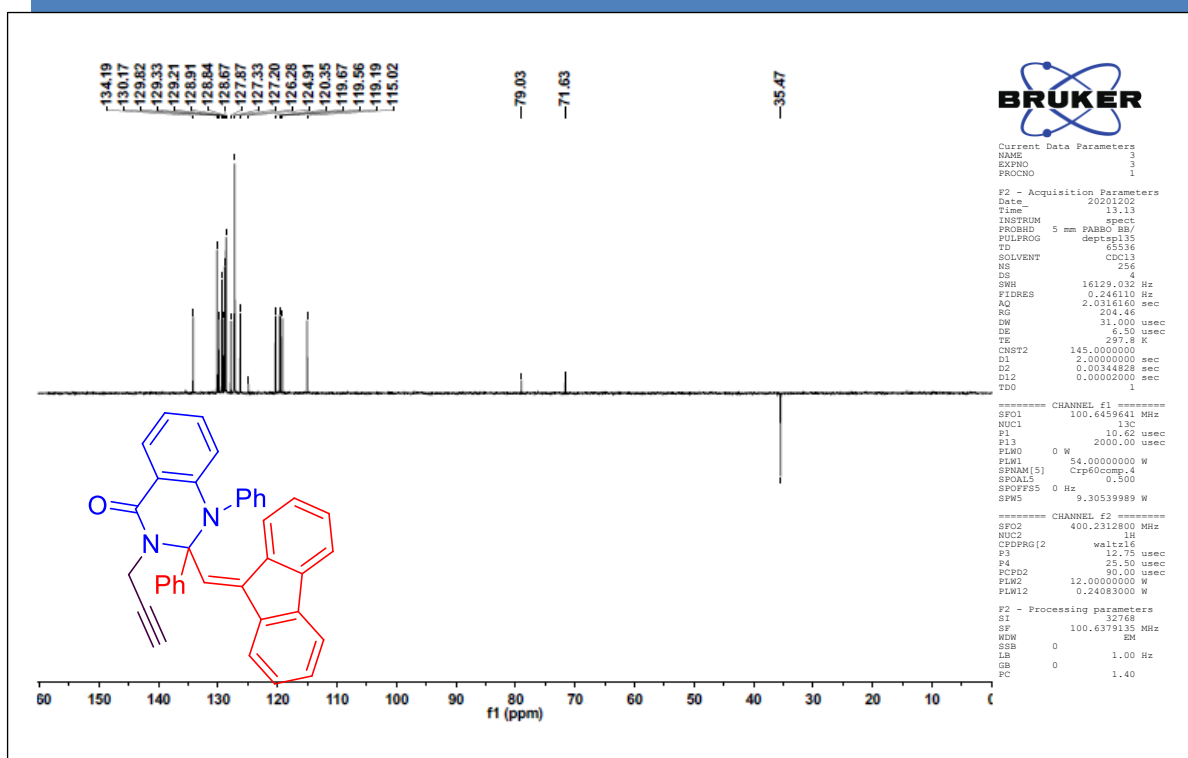
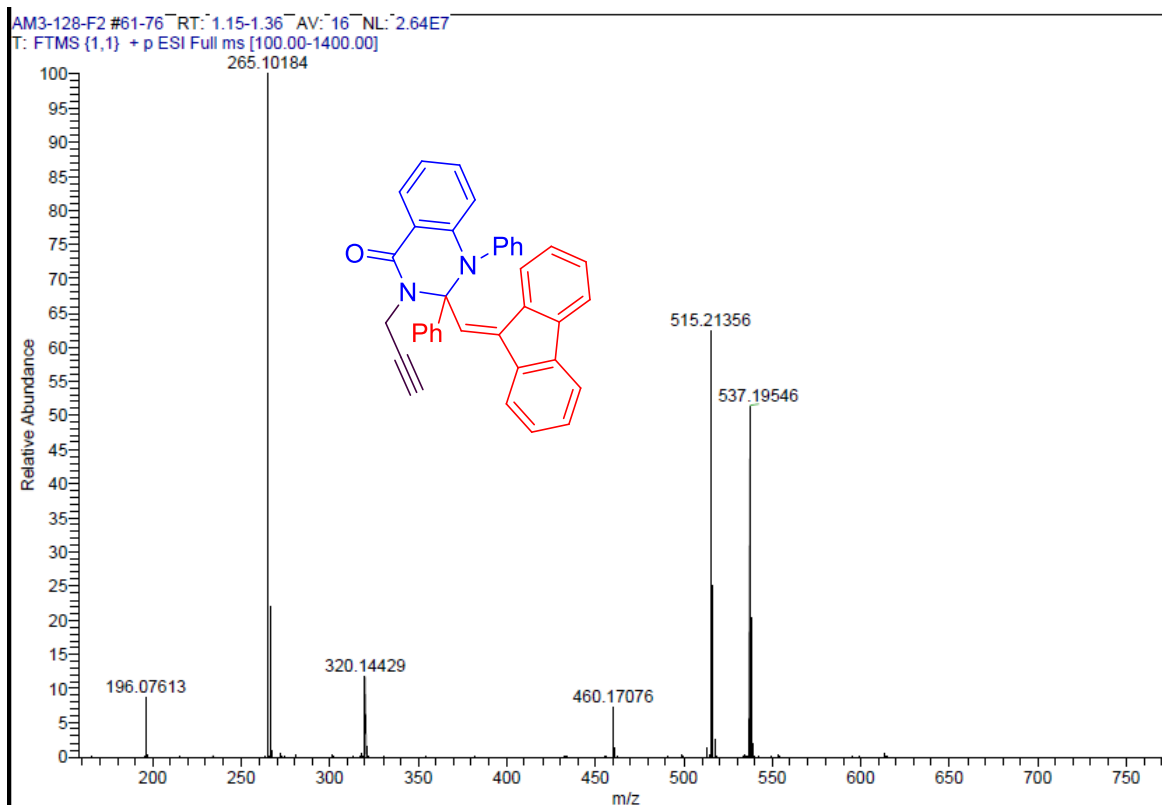
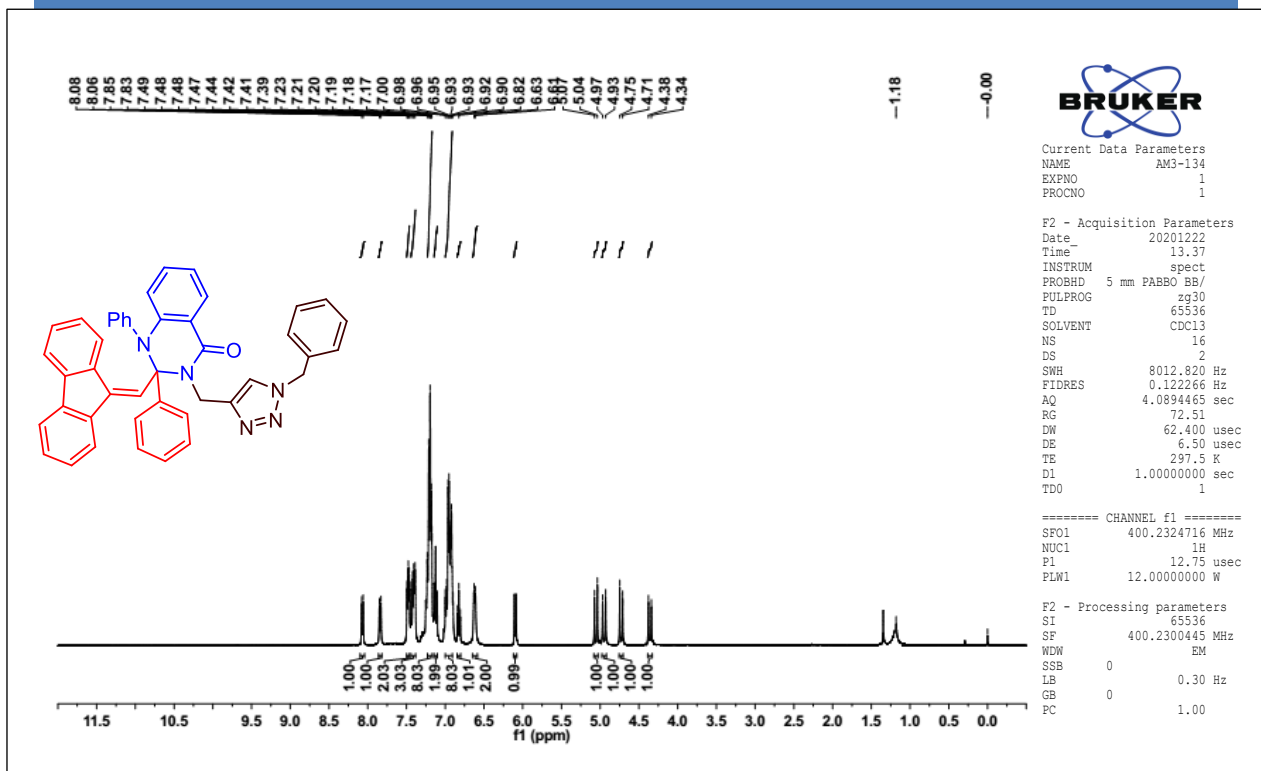
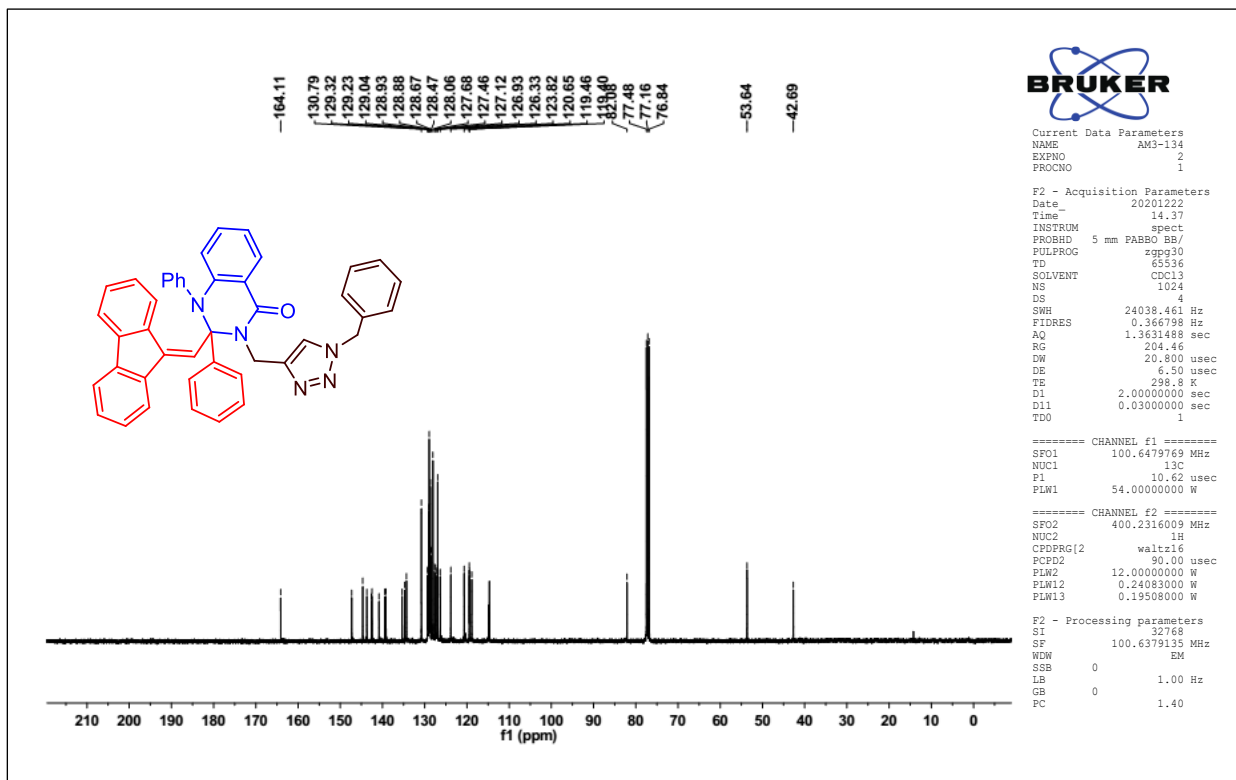


Figure 100 HRMS spectrum of compound 6a

Figure 101 ^1H NMR spectrum of compound **6b**Figure 102 ^{13}C NMR spectrum of compound **6b**

Figure 103 DEPT-135 NMR spectrum of compound **6b**Figure 104 HRMS spectrum of compound **6b**

Figure 105 ^1H NMR spectrum of compound 7Figure 106 ^{13}C NMR spectrum of compound 7

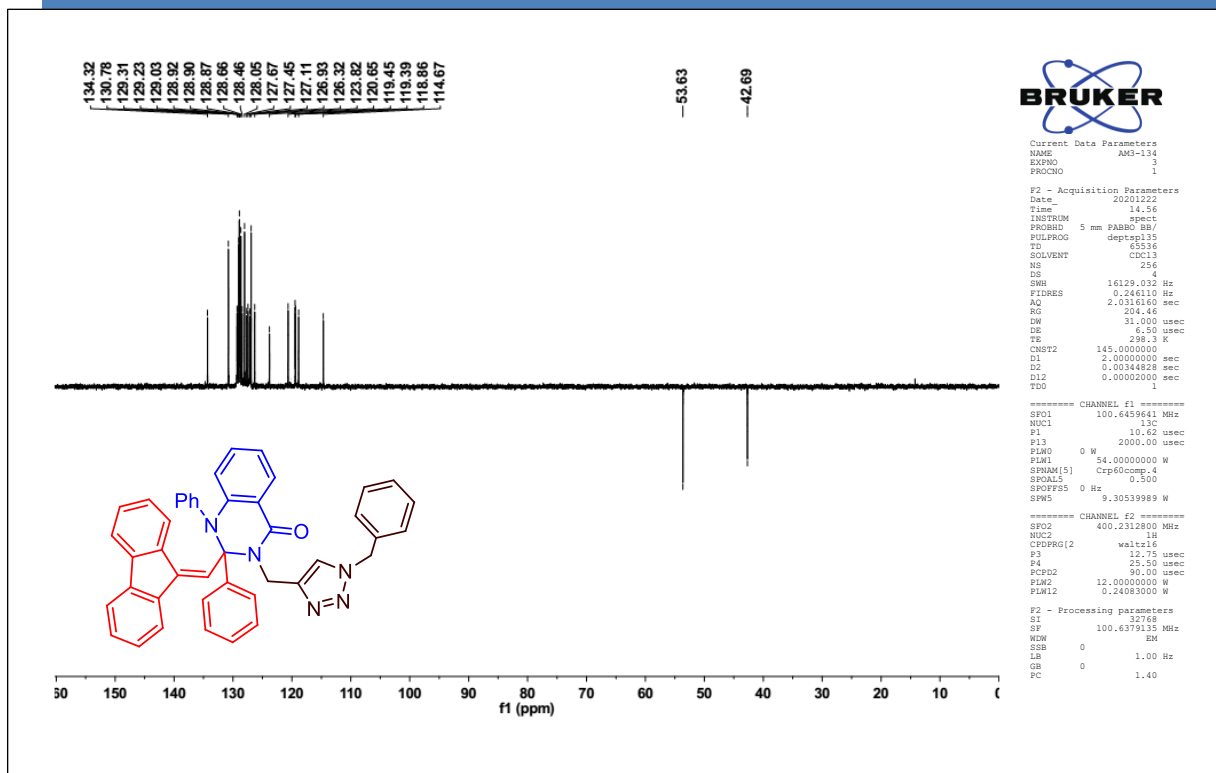


Figure 107 DEPT-135 NMR spectrum of compound 7

AM3-134 #59-77 RT: 1.16-1.40 AV: 19 NL: 8.36E7
 T: FTMS (1,1) + p ESI Full ms [100.00-1400.00]

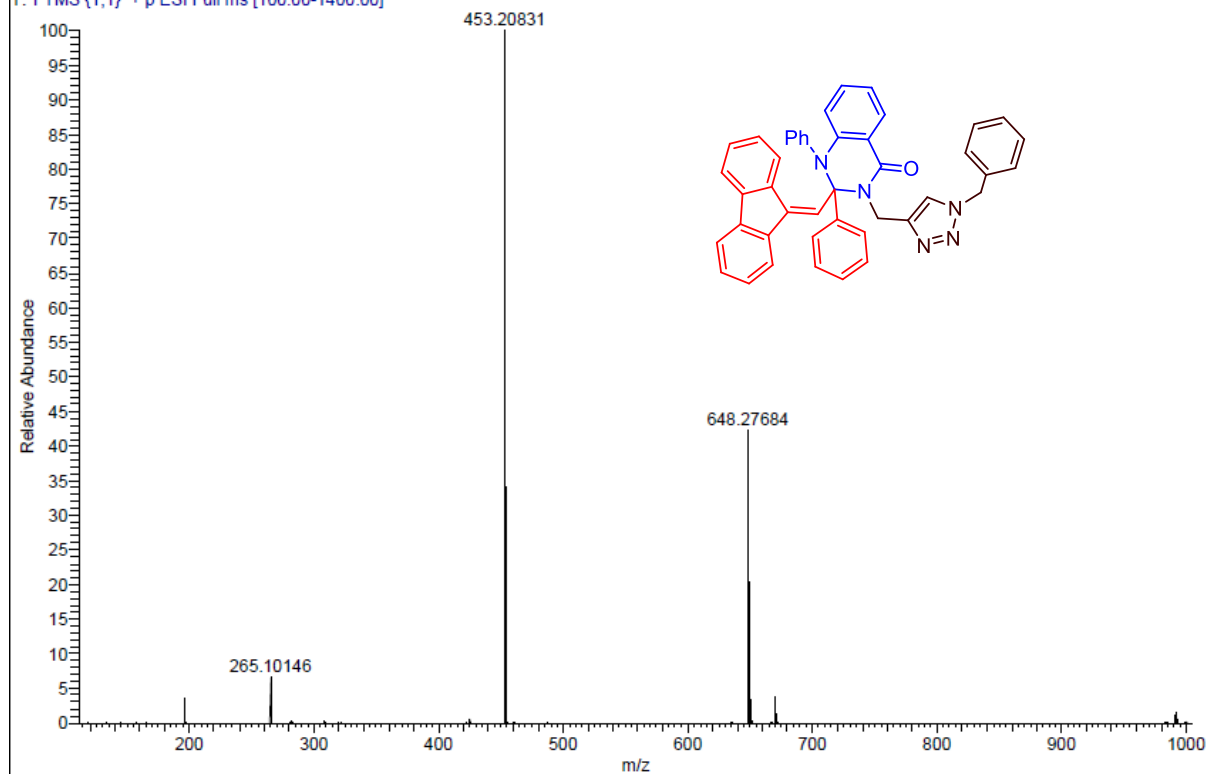
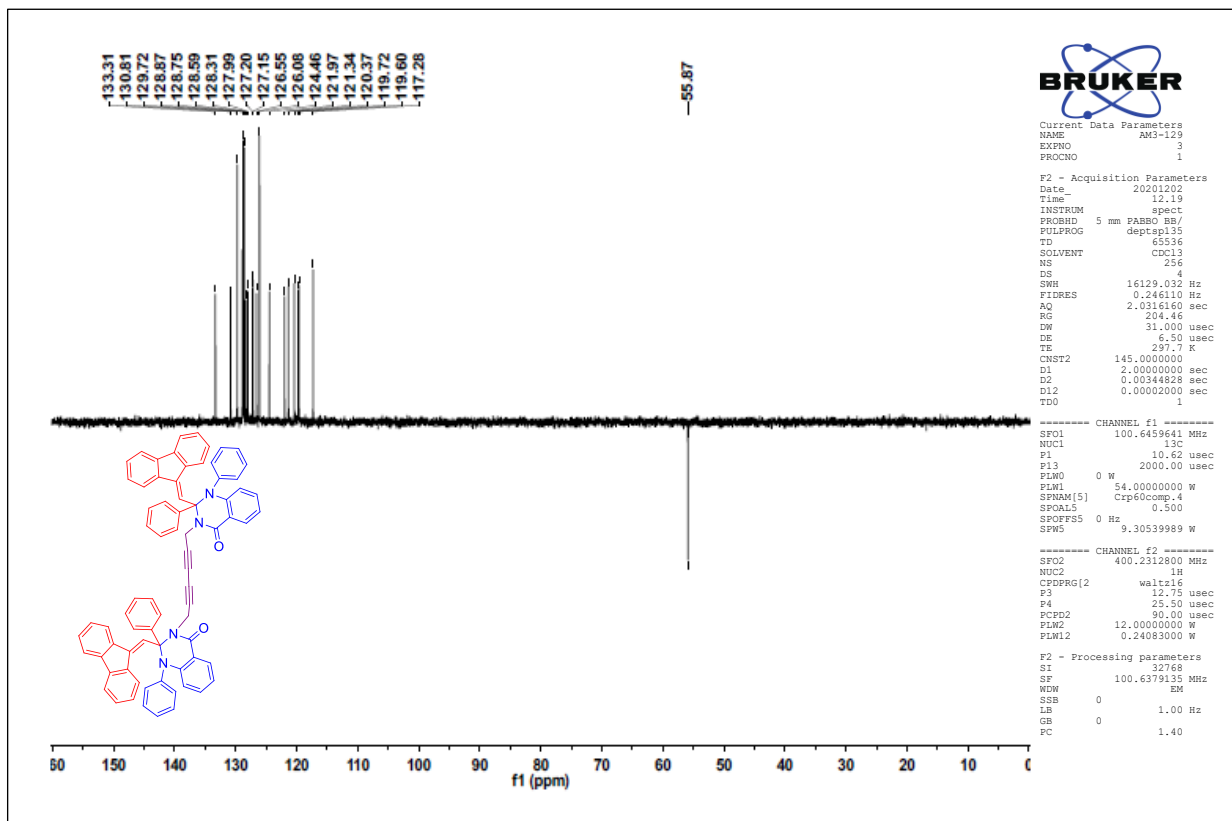
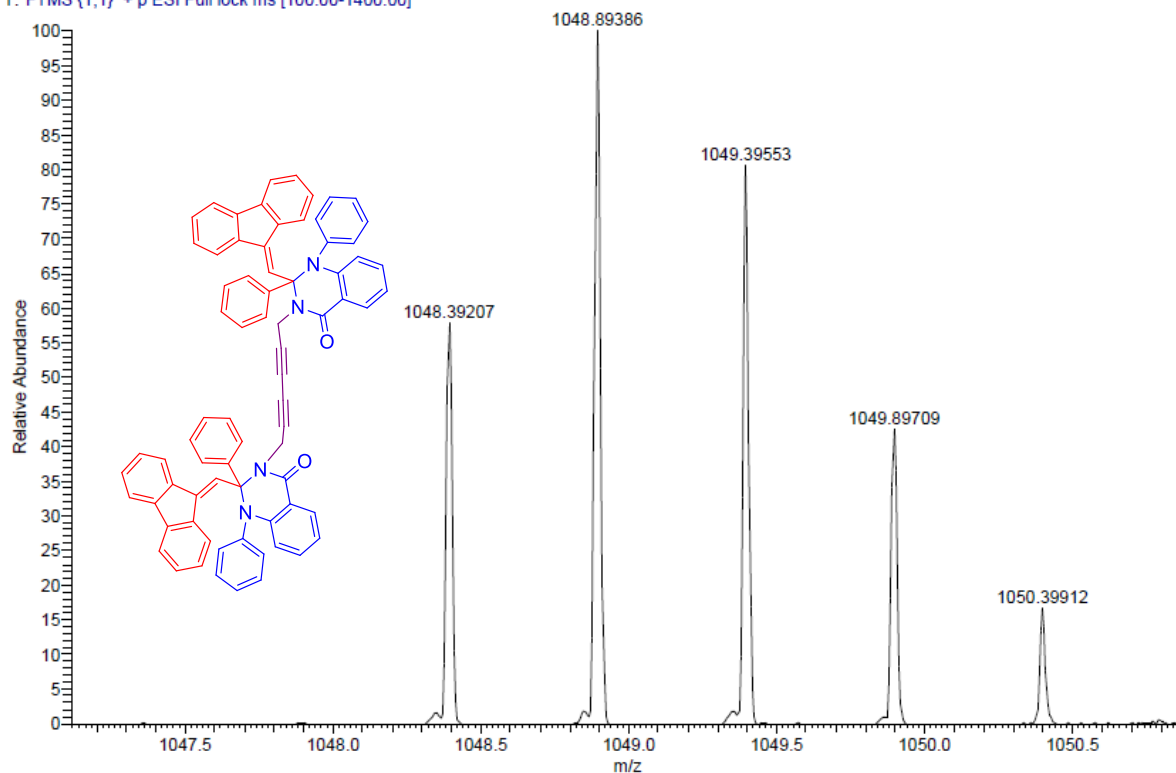
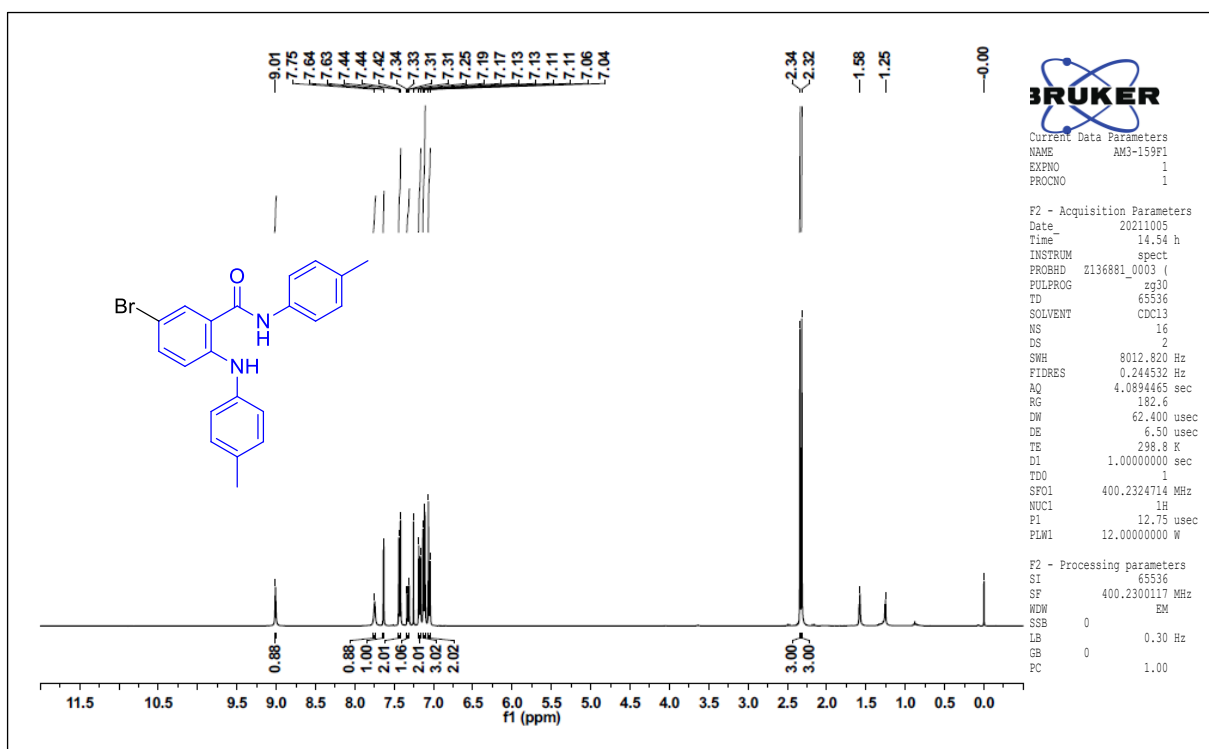
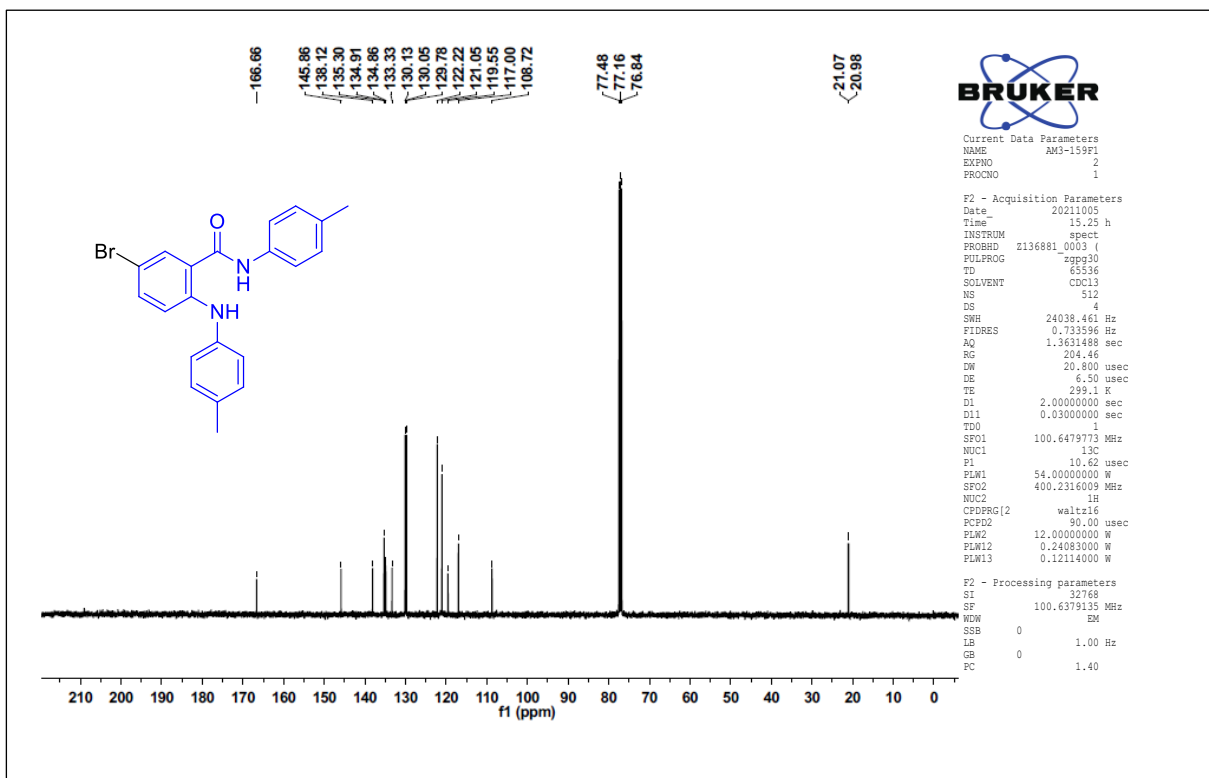


Figure 108 HRMS spectrum of compound 7

Figure 111 DEPT-135 NMR spectrum of compound **8**

AM3-129 #76-94 RT: 1.39-1.64 AV: 19 NL: 2.42E5
 T: FTMS (1,1) + p ESI Full lock ms [100.00-1400.00]

Figure 112 HRMS spectrum of compound **8**

Figure 113 ¹H NMR spectrum of compound **2f**Figure 114 ¹³C NMR spectrum of compound **2f**

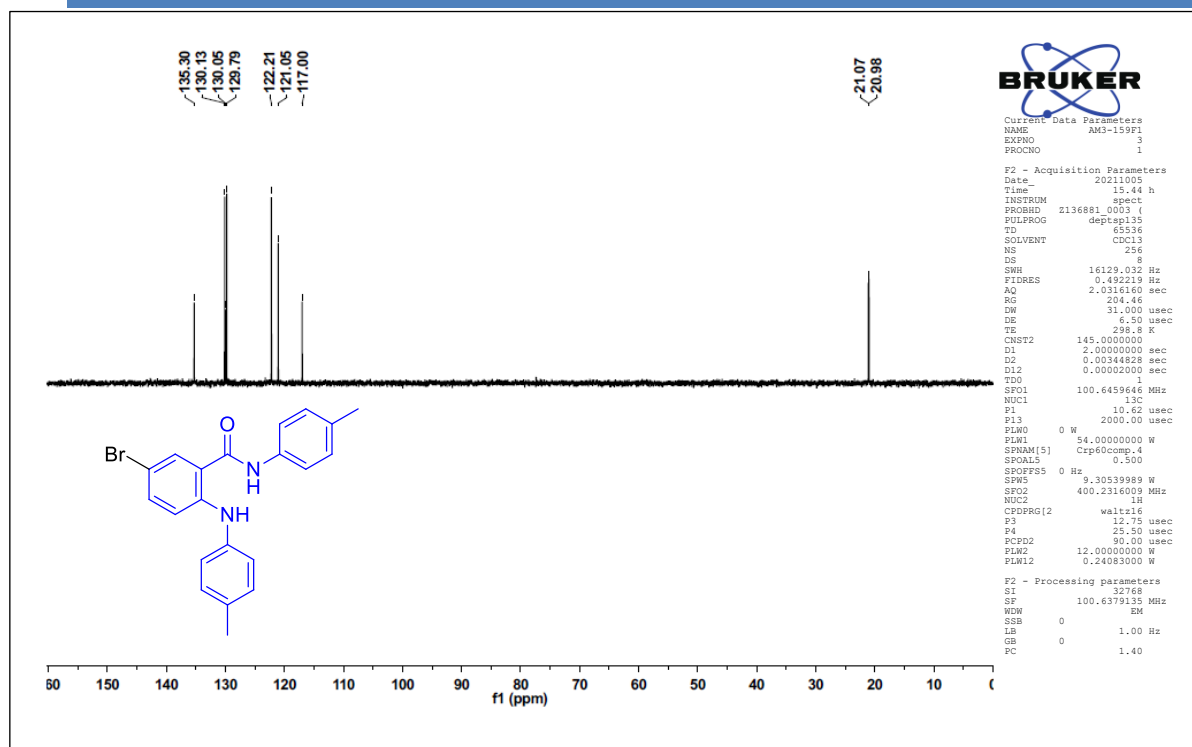


Figure 115 DEPT-135 NMR spectrum of compound **2f**

2. Basic crystallographic data for compound **3i** & **4b**

Table 1. Crystal data and structure refinement for **3i**

Identification code	3i	
Empirical formula	$C_{35} H_{25} Cl_2 I N_2 O$	
Formula weight	687.37	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	$a = 11.086(4)$ Å	$\alpha = 113.666(12)^\circ$.
	$b = 11.540(4)$ Å	$\beta = 91.973(14)^\circ$.
	$c = 12.936(4)$ Å	$\gamma = 94.252(13)^\circ$.
Volume	$1507.8(9)$ Å ³	
Z	2	
Density (calculated)	1.514 Mg/m ³	
Absorption coefficient	1.270 mm ⁻¹	
F(000)	688	

Crystal size	0.200 x 0.150 x 0.150 mm ³
Theta range for data collection	3.070 to 26.499°.
Index ranges	-13<=h<=13, -14<=k<=14, -16<=l<=16
Reflections collected	48643
Independent reflections	6188 [R(int) = 0.0493]
Completeness to theta = 25.242°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6303
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6188 / 0 / 375
Goodness-of-fit on F ²	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0604, wR2 = 0.1315
R indices (all data)	R1 = 0.0836, wR2 = 0.1482
Extinction coefficient	0.0203(13)
Largest diff. peak and hole	2.290 and -1.667 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for am63. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3950(5)	10691(5)	7679(5)	57(1)
C(2)	3606(6)	11822(6)	7663(6)	71(2)
C(3)	4210(7)	12388(6)	7037(6)	76(2)
C(4)	5171(6)	11866(5)	6436(5)	67(2)
C(5)	5539(5)	10748(5)	6462(4)	50(1)
C(6)	4923(5)	10159(4)	7073(4)	46(1)
C(7)	5509(4)	8996(4)	6955(4)	42(1)
C(8)	6532(4)	8946(5)	6227(4)	48(1)
C(9)	6529(5)	10005(5)	5941(4)	52(1)
C(10)	7396(6)	10204(6)	5257(5)	69(2)
C(11)	8254(6)	9348(8)	4860(6)	77(2)
C(12)	8256(6)	8309(7)	5130(5)	75(2)
C(13)	7401(5)	8096(6)	5817(5)	60(1)
C(14)	5120(4)	8274(4)	7495(4)	41(1)
C(15)	5622(4)	7122(4)	7575(4)	38(1)
C(16)	4760(4)	6579(4)	8216(4)	40(1)
C(17)	3655(5)	5933(5)	7692(5)	55(1)

C(18)	2833(6)	5481(6)	8262(7)	75(2)
C(19)	3101(7)	5662(6)	9358(7)	75(2)
C(20)	4187(7)	6304(7)	9896(6)	75(2)
C(21)	5020(5)	6759(5)	9327(4)	56(1)
C(22)	7194(4)	5236(4)	7151(3)	36(1)
C(23)	7492(4)	6426(4)	8057(4)	35(1)
C(24)	8409(4)	6545(4)	8868(4)	42(1)
C(25)	9018(4)	5517(4)	8778(4)	44(1)
C(26)	8713(4)	4344(4)	7881(4)	40(1)
C(27)	7813(4)	4201(4)	7072(4)	39(1)
C(28)	7399(4)	8733(4)	8736(4)	39(1)
C(29)	6798(5)	9636(5)	9556(4)	49(1)
C(30)	7346(6)	10867(5)	10098(5)	60(1)
C(31)	8489(6)	11199(5)	9870(5)	65(2)
C(32)	9092(5)	10296(5)	9074(5)	59(1)
C(33)	8549(5)	9073(4)	8497(4)	46(1)
C(34)	6315(4)	5116(4)	6221(4)	40(1)
C(35)	8839(10)	3245(12)	4131(10)	139(4)
N(1)	6864(3)	7449(3)	8129(3)	38(1)
N(2)	5702(4)	6135(4)	6422(3)	42(1)
O(1)	6213(3)	4179(3)	5305(3)	50(1)
I(1)	9665(1)	2790(1)	7744(1)	75(1)
Cl(1)	8556(4)	1644(4)	3312(4)	195(2)
Cl(2)	9678(4)	3980(4)	3480(3)	173(1)

Table 3. Bond lengths [Å] and angles [°] for am63.

C(1)-C(6)	1.388(7)
C(1)-C(2)	1.394(8)
C(1)-H(1)	0.9300
C(2)-C(3)	1.389(10)
C(2)-H(2)	0.9300
C(3)-C(4)	1.371(10)
C(3)-H(3)	0.9300
C(4)-C(5)	1.394(7)
C(4)-H(4)	0.9300
C(5)-C(6)	1.398(7)
C(5)-C(9)	1.457(8)

C(6)-C(7)	1.489(6)
C(7)-C(14)	1.342(7)
C(7)-C(8)	1.489(7)
C(8)-C(13)	1.389(7)
C(8)-C(9)	1.412(7)
C(9)-C(10)	1.396(8)
C(10)-C(11)	1.381(10)
C(10)-H(10)	0.9300
C(11)-C(12)	1.377(10)
C(11)-H(11)	0.9300
C(12)-C(13)	1.396(8)
C(12)-H(12)	0.9300
C(13)-H(13)	0.9300
C(14)-C(15)	1.519(6)
C(14)-H(14)	0.9300
C(15)-N(1)	1.479(6)
C(15)-N(2)	1.480(6)
C(15)-C(16)	1.541(6)
C(16)-C(21)	1.384(7)
C(16)-C(17)	1.385(7)
C(17)-C(18)	1.389(8)
C(17)-H(17)	0.9300
C(18)-C(19)	1.366(10)
C(18)-H(18)	0.9300
C(19)-C(20)	1.371(10)
C(19)-H(19)	0.9300
C(20)-C(21)	1.398(8)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(22)-C(27)	1.392(6)
C(22)-C(23)	1.408(6)
C(22)-C(34)	1.476(6)
C(23)-N(1)	1.387(5)
C(23)-C(24)	1.395(6)
C(24)-C(25)	1.374(6)
C(24)-H(24)	0.9300
C(25)-C(26)	1.392(6)
C(25)-H(25)	0.9300

C(26)-C(27)	1.372(6)
C(26)-I(1)	2.098(4)
C(27)-H(27)	0.9300
C(28)-C(29)	1.385(6)
C(28)-C(33)	1.388(7)
C(28)-N(1)	1.439(5)
C(29)-C(30)	1.387(7)
C(29)-H(29)	0.9300
C(30)-C(31)	1.372(8)
C(30)-H(30)	0.9300
C(31)-C(32)	1.372(8)
C(31)-H(31)	0.9300
C(32)-C(33)	1.381(7)
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(34)-O(1)	1.237(5)
C(34)-N(2)	1.341(6)
C(35)-Cl(2)	1.675(10)
C(35)-Cl(1)	1.719(13)
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
N(2)-H(2A)	0.86(6)
C(6)-C(1)-C(2)	118.5(6)
C(6)-C(1)-H(1)	120.8
C(2)-C(1)-H(1)	120.8
C(3)-C(2)-C(1)	120.7(6)
C(3)-C(2)-H(2)	119.7
C(1)-C(2)-H(2)	119.7
C(4)-C(3)-C(2)	121.1(6)
C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
C(3)-C(4)-C(5)	118.8(6)
C(3)-C(4)-H(4)	120.6
C(5)-C(4)-H(4)	120.6
C(4)-C(5)-C(6)	120.5(6)
C(4)-C(5)-C(9)	131.0(5)
C(6)-C(5)-C(9)	108.4(4)

C(1)-C(6)-C(5)	120.4(5)
C(1)-C(6)-C(7)	130.6(5)
C(5)-C(6)-C(7)	109.0(4)
C(14)-C(7)-C(8)	133.3(4)
C(14)-C(7)-C(6)	121.2(4)
C(8)-C(7)-C(6)	105.4(4)
C(13)-C(8)-C(9)	119.6(5)
C(13)-C(8)-C(7)	132.7(5)
C(9)-C(8)-C(7)	107.7(4)
C(10)-C(9)-C(8)	120.4(6)
C(10)-C(9)-C(5)	130.1(5)
C(8)-C(9)-C(5)	109.4(5)
C(11)-C(10)-C(9)	119.1(6)
C(11)-C(10)-H(10)	120.5
C(9)-C(10)-H(10)	120.5
C(12)-C(11)-C(10)	120.8(6)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(11)-C(12)-C(13)	121.0(6)
C(11)-C(12)-H(12)	119.5
C(13)-C(12)-H(12)	119.5
C(8)-C(13)-C(12)	119.1(6)
C(8)-C(13)-H(13)	120.4
C(12)-C(13)-H(13)	120.4
C(7)-C(14)-C(15)	130.6(4)
C(7)-C(14)-H(14)	114.7
C(15)-C(14)-H(14)	114.7
N(1)-C(15)-N(2)	107.0(3)
N(1)-C(15)-C(14)	111.1(4)
N(2)-C(15)-C(14)	109.3(3)
N(1)-C(15)-C(16)	111.3(4)
N(2)-C(15)-C(16)	108.7(4)
C(14)-C(15)-C(16)	109.3(4)
C(21)-C(16)-C(17)	117.8(5)
C(21)-C(16)-C(15)	122.5(4)
C(17)-C(16)-C(15)	119.6(4)
C(16)-C(17)-C(18)	121.1(6)
C(16)-C(17)-H(17)	119.4

C(18)-C(17)-H(17)	119.4
C(19)-C(18)-C(17)	120.5(6)
C(19)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	119.4(6)
C(18)-C(19)-H(19)	120.3
C(20)-C(19)-H(19)	120.3
C(19)-C(20)-C(21)	120.5(6)
C(19)-C(20)-H(20)	119.8
C(21)-C(20)-H(20)	119.8
C(16)-C(21)-C(20)	120.7(6)
C(16)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(27)-C(22)-C(23)	120.1(4)
C(27)-C(22)-C(34)	119.7(4)
C(23)-C(22)-C(34)	120.0(4)
N(1)-C(23)-C(24)	121.5(4)
N(1)-C(23)-C(22)	119.5(4)
C(24)-C(23)-C(22)	119.0(4)
C(25)-C(24)-C(23)	120.3(4)
C(25)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	120.2(4)
C(24)-C(25)-H(25)	119.9
C(26)-C(25)-H(25)	119.9
C(27)-C(26)-C(25)	120.6(4)
C(27)-C(26)-I(1)	119.7(3)
C(25)-C(26)-I(1)	119.7(3)
C(26)-C(27)-C(22)	119.8(4)
C(26)-C(27)-H(27)	120.1
C(22)-C(27)-H(27)	120.1
C(29)-C(28)-C(33)	119.3(4)
C(29)-C(28)-N(1)	121.6(4)
C(33)-C(28)-N(1)	119.1(4)
C(28)-C(29)-C(30)	119.2(5)
C(28)-C(29)-H(29)	120.4
C(30)-C(29)-H(29)	120.4
C(31)-C(30)-C(29)	121.5(5)

C(31)-C(30)-H(30)	119.3
C(29)-C(30)-H(30)	119.3
C(30)-C(31)-C(32)	119.1(5)
C(30)-C(31)-H(31)	120.4
C(32)-C(31)-H(31)	120.4
C(31)-C(32)-C(33)	120.4(5)
C(31)-C(32)-H(32)	119.8
C(33)-C(32)-H(32)	119.8
C(32)-C(33)-C(28)	120.4(5)
C(32)-C(33)-H(33)	119.8
C(28)-C(33)-H(33)	119.8
O(1)-C(34)-N(2)	122.9(4)
O(1)-C(34)-C(22)	122.3(4)
N(2)-C(34)-C(22)	114.7(4)
Cl(2)-C(35)-Cl(1)	111.6(7)
Cl(2)-C(35)-H(35A)	109.3
Cl(1)-C(35)-H(35A)	109.3
Cl(2)-C(35)-H(35B)	109.3
Cl(1)-C(35)-H(35B)	109.3
H(35A)-C(35)-H(35B)	108.0
C(23)-N(1)-C(28)	120.9(4)
C(23)-N(1)-C(15)	115.6(3)
C(28)-N(1)-C(15)	123.5(3)
C(34)-N(2)-C(15)	122.5(4)
C(34)-N(2)-H(2A)	115(4)
C(15)-N(2)-H(2A)	119(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for am63. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	65(3)	48(3)	55(3)	17(2)	-1(3)	17(3)
C(2)	82(4)	51(3)	72(4)	14(3)	-11(3)	25(3)
C(3)	105(5)	40(3)	81(4)	24(3)	-23(4)	8(3)
C(4)	86(4)	41(3)	71(4)	25(3)	-22(3)	-10(3)

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C(5)	59(3)	42(3)	47(3)	18(2)	-16(2)	-7(2)
C(6)	54(3)	41(2)	43(2)	16(2)	-9(2)	5(2)
C(7)	44(3)	45(2)	38(2)	16(2)	-3(2)	8(2)
C(8)	47(3)	57(3)	40(2)	22(2)	-4(2)	4(2)
C(9)	55(3)	57(3)	44(3)	25(2)	-11(2)	-10(2)
C(10)	79(4)	73(4)	57(3)	34(3)	-7(3)	-20(3)
C(11)	67(4)	101(5)	64(4)	37(4)	10(3)	-10(4)
C(12)	60(4)	108(5)	66(4)	43(4)	16(3)	19(4)
C(13)	54(3)	84(4)	56(3)	38(3)	11(3)	19(3)
C(14)	41(2)	40(2)	42(2)	16(2)	2(2)	10(2)
C(15)	41(2)	36(2)	35(2)	12(2)	-1(2)	10(2)
C(16)	41(2)	33(2)	46(2)	14(2)	6(2)	9(2)
C(17)	52(3)	49(3)	60(3)	20(2)	2(2)	1(2)
C(18)	62(4)	60(4)	98(5)	30(4)	13(4)	-7(3)
C(19)	80(5)	64(4)	95(5)	44(4)	34(4)	9(3)
C(20)	92(5)	85(5)	65(4)	46(4)	23(4)	14(4)
C(21)	61(3)	61(3)	48(3)	26(3)	8(2)	7(3)
C(22)	37(2)	34(2)	34(2)	12(2)	-2(2)	3(2)
C(23)	38(2)	33(2)	37(2)	15(2)	3(2)	6(2)
C(24)	50(3)	35(2)	37(2)	11(2)	-8(2)	3(2)
C(25)	47(3)	43(2)	42(2)	19(2)	-8(2)	5(2)
C(26)	47(3)	35(2)	44(2)	20(2)	-2(2)	10(2)
C(27)	42(2)	33(2)	38(2)	12(2)	-1(2)	6(2)
C(28)	46(3)	33(2)	36(2)	13(2)	0(2)	4(2)
C(29)	52(3)	42(3)	48(3)	13(2)	8(2)	7(2)
C(30)	76(4)	39(3)	56(3)	7(2)	11(3)	13(3)
C(31)	70(4)	37(3)	81(4)	18(3)	0(3)	-5(3)
C(32)	52(3)	48(3)	80(4)	29(3)	10(3)	1(2)
C(33)	51(3)	40(2)	51(3)	21(2)	9(2)	7(2)
C(34)	44(2)	38(2)	36(2)	12(2)	-1(2)	9(2)
C(35)	104(7)	189(12)	143(9)	84(9)	38(7)	23(8)
N(1)	38(2)	32(2)	41(2)	10(2)	-4(2)	5(2)
N(2)	47(2)	43(2)	32(2)	11(2)	-4(2)	13(2)
O(1)	57(2)	47(2)	35(2)	3(1)	-9(2)	17(2)
I(1)	92(1)	53(1)	78(1)	22(1)	-19(1)	28(1)
Cl(1)	195(4)	200(4)	178(3)	79(3)	26(3)	-65(3)
Cl(2)	184(3)	170(3)	184(3)	90(3)	71(3)	-4(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for am63.

	x	y	z	U(eq)
H(1)	3536	10302	8086	68
H(2)	2966	12201	8076	85
H(3)	3958	13134	7025	91
H(4)	5571	12251	6018	80
H(10)	7396	10903	5070	83
H(11)	8836	9475	4406	92
H(12)	8837	7739	4849	90
H(13)	7413	7394	5999	72
H(14)	4429	8520	7884	49
H(17)	3460	5800	6945	66
H(18)	2095	5051	7894	90
H(19)	2551	5353	9735	90
H(20)	4371	6437	10644	90
H(21)	5756	7188	9700	67
H(24)	8610	7324	9474	51
H(25)	9635	5606	9317	52
H(27)	7617	3415	6474	46
H(29)	6035	9419	9741	58
H(30)	6930	11481	10627	73
H(31)	8850	12025	10251	78
H(32)	9871	10509	8921	71
H(33)	8957	8474	7945	55
H(35A)	8076	3619	4298	166
H(35B)	9262	3370	4843	166
H(2A)	5160(50)	6060(50)	5900(50)	60(16)

Table 6. Torsion angles [$^\circ$] for am63.

C(6)-C(1)-C(2)-C(3)	1.3(9)
C(1)-C(2)-C(3)-C(4)	-1.2(10)
C(2)-C(3)-C(4)-C(5)	0.0(9)
C(3)-C(4)-C(5)-C(6)	1.1(8)

C(3)-C(4)-C(5)-C(9)	-178.3(5)
C(2)-C(1)-C(6)-C(5)	-0.1(8)
C(2)-C(1)-C(6)-C(7)	178.3(5)
C(4)-C(5)-C(6)-C(1)	-1.1(7)
C(9)-C(5)-C(6)-C(1)	178.5(4)
C(4)-C(5)-C(6)-C(7)	-179.8(4)
C(9)-C(5)-C(6)-C(7)	-0.3(5)
C(1)-C(6)-C(7)-C(14)	-0.9(8)
C(5)-C(6)-C(7)-C(14)	177.6(4)
C(1)-C(6)-C(7)-C(8)	-178.2(5)
C(5)-C(6)-C(7)-C(8)	0.4(5)
C(14)-C(7)-C(8)-C(13)	3.4(9)
C(6)-C(7)-C(8)-C(13)	-179.8(5)
C(14)-C(7)-C(8)-C(9)	-177.1(5)
C(6)-C(7)-C(8)-C(9)	-0.3(5)
C(13)-C(8)-C(9)-C(10)	-0.4(8)
C(7)-C(8)-C(9)-C(10)	-180.0(5)
C(13)-C(8)-C(9)-C(5)	179.7(5)
C(7)-C(8)-C(9)-C(5)	0.1(5)
C(4)-C(5)-C(9)-C(10)	-0.3(9)
C(6)-C(5)-C(9)-C(10)	-179.8(5)
C(4)-C(5)-C(9)-C(8)	179.6(5)
C(6)-C(5)-C(9)-C(8)	0.1(5)
C(8)-C(9)-C(10)-C(11)	0.2(8)
C(5)-C(9)-C(10)-C(11)	-179.9(5)
C(9)-C(10)-C(11)-C(12)	0.2(10)
C(10)-C(11)-C(12)-C(13)	-0.6(10)
C(9)-C(8)-C(13)-C(12)	0.0(8)
C(7)-C(8)-C(13)-C(12)	179.5(5)
C(11)-C(12)-C(13)-C(8)	0.4(10)
C(8)-C(7)-C(14)-C(15)	1.5(9)
C(6)-C(7)-C(14)-C(15)	-174.9(4)
C(7)-C(14)-C(15)-N(1)	61.8(6)
C(7)-C(14)-C(15)-N(2)	-56.1(6)
C(7)-C(14)-C(15)-C(16)	-175.0(5)
N(1)-C(15)-C(16)-C(21)	18.9(6)
N(2)-C(15)-C(16)-C(21)	136.5(4)
C(14)-C(15)-C(16)-C(21)	-104.2(5)

N(1)-C(15)-C(16)-C(17)	-164.1(4)
N(2)-C(15)-C(16)-C(17)	-46.5(5)
C(14)-C(15)-C(16)-C(17)	72.8(5)
C(21)-C(16)-C(17)-C(18)	0.0(8)
C(15)-C(16)-C(17)-C(18)	-177.1(5)
C(16)-C(17)-C(18)-C(19)	-0.2(9)
C(17)-C(18)-C(19)-C(20)	0.4(10)
C(18)-C(19)-C(20)-C(21)	-0.6(10)
C(17)-C(16)-C(21)-C(20)	-0.1(8)
C(15)-C(16)-C(21)-C(20)	176.9(5)
C(19)-C(20)-C(21)-C(16)	0.4(9)
C(27)-C(22)-C(23)-N(1)	-179.6(4)
C(34)-C(22)-C(23)-N(1)	6.7(6)
C(27)-C(22)-C(23)-C(24)	-0.1(7)
C(34)-C(22)-C(23)-C(24)	-173.8(4)
N(1)-C(23)-C(24)-C(25)	180.0(4)
C(22)-C(23)-C(24)-C(25)	0.5(7)
C(23)-C(24)-C(25)-C(26)	-0.8(7)
C(24)-C(25)-C(26)-C(27)	0.7(7)
C(24)-C(25)-C(26)-I(1)	179.3(4)
C(25)-C(26)-C(27)-C(22)	-0.3(7)
I(1)-C(26)-C(27)-C(22)	-178.9(3)
C(23)-C(22)-C(27)-C(26)	0.0(7)
C(34)-C(22)-C(27)-C(26)	173.7(4)
C(33)-C(28)-C(29)-C(30)	1.7(7)
N(1)-C(28)-C(29)-C(30)	-178.6(5)
C(28)-C(29)-C(30)-C(31)	-2.5(9)
C(29)-C(30)-C(31)-C(32)	1.2(9)
C(30)-C(31)-C(32)-C(33)	0.9(9)
C(31)-C(32)-C(33)-C(28)	-1.7(8)
C(29)-C(28)-C(33)-C(32)	0.4(7)
N(1)-C(28)-C(33)-C(32)	-179.4(4)
C(27)-C(22)-C(34)-O(1)	-9.4(7)
C(23)-C(22)-C(34)-O(1)	164.3(5)
C(27)-C(22)-C(34)-N(2)	175.0(4)
C(23)-C(22)-C(34)-N(2)	-11.3(6)
C(24)-C(23)-N(1)-C(28)	24.7(6)
C(22)-C(23)-N(1)-C(28)	-155.8(4)

C(24)-C(23)-N(1)-C(15)	-153.7(4)
C(22)-C(23)-N(1)-C(15)	25.8(6)
C(29)-C(28)-N(1)-C(23)	-128.5(5)
C(33)-C(28)-N(1)-C(23)	51.2(6)
C(29)-C(28)-N(1)-C(15)	49.8(6)
C(33)-C(28)-N(1)-C(15)	-130.5(5)
N(2)-C(15)-N(1)-C(23)	-49.1(5)
C(14)-C(15)-N(1)-C(23)	-168.4(4)
C(16)-C(15)-N(1)-C(23)	69.6(5)
N(2)-C(15)-N(1)-C(28)	132.5(4)
C(14)-C(15)-N(1)-C(28)	13.3(6)
C(16)-C(15)-N(1)-C(28)	-108.8(4)
O(1)-C(34)-N(2)-C(15)	166.6(5)
C(22)-C(34)-N(2)-C(15)	-17.8(6)
N(1)-C(15)-N(2)-C(34)	47.0(6)
C(14)-C(15)-N(2)-C(34)	167.4(4)
C(16)-C(15)-N(2)-C(34)	-73.3(5)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for am63 [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
C(35)-H(35A)...O(1)	0.97	2.47	3.376(11)	156.0
N(2)-H(2A)...O(1)#1	0.86(6)	2.06(6)	2.922(5)	176(5)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1, -y+1, -z+1$

Basic crystallographic data for compound 4b

Table 1. Crystal data and structure refinement for 4b.

	shelx	
Empirical formula	$\text{C}_{43}\text{H}_{33}\text{BrN}_2\text{O}$	
Formula weight	672.177	
Temperature	296(2) K	
Wavelength	1.54178 \AA	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	$a = 13.7423(4) \text{\AA}$ $b = 18.5947(6) \text{\AA}$ $c = 15.4410(5) \text{\AA}$	$\alpha = 90^\circ$ $\beta = 108.1530(10)^\circ$ $\gamma = 90^\circ$
Volume	3749.3(2) \AA^3	
Z	4	
Density (calculated)	1.269 Mg/m^3	
Absorption coefficient	2.414 mm^{-1}	
F(000)	1476	
Crystal size	0.150 x 0.120 x 0.100 mm^3	
Theta range for data collection	3.765 to 65.997 $^\circ$.	
Index ranges	$-16 \leq h \leq 16, -22 \leq k \leq 21, -18 \leq l \leq 18$	
Reflections collected	72176	
Independent reflections	6524 [R(int) = 0.0692]	
Completeness to theta = 65.997 $^\circ$	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7531 and 0.3833	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6524 / 345 / 548	
Goodness-of-fit on F^2	1.044	

Final R indices [$I > 2\sigma(I)$] R1 = 0.0700, wR2 = 0.2117

R indices (all data) R1 = 0.0890, wR2 = 0.2428

Extinction coefficient 0.0023(4)

Largest diff. peak and hole 0.456 and -0.557 e. \AA^{-3} Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for am3142. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2556(3)	6237(2)	4103(2)	82(1)
C(2)	3508(3)	6344(2)	4002(2)	87(1)
C(3)	3623(4)	6331(2)	3141(3)	101(1)
C(4)	2788(5)	6192(3)	2377(3)	117(2)
C(5)	1834(4)	6067(2)	2467(3)	111(2)
C(6)	1716(3)	6083(2)	3318(3)	93(1)
C(7)	807(3)	5977(2)	3605(3)	102(1)
C(8)	-208(5)	5805(3)	3101(5)	138(2)
C(9)	-909(4)	5725(3)	3586(7)	160(3)
C(10)	-640(4)	5836(3)	4512(6)	144(2)
C(11)	346(4)	6005(3)	4997(4)	118(2)
C(12)	1071(3)	6078(2)	4543(3)	94(1)
C(13)	2174(3)	6255(2)	4900(2)	81(1)
C(14)	2618(3)	6421(2)	5776(2)	85(1)
C(15)	4118(3)	5281(2)	6343(2)	75(1)
C(16)	3728(3)	4848(2)	5603(2)	88(1)
C(17)	3479(3)	4139(2)	5714(3)	103(1)
C(18)	3633(3)	3846(2)	6567(4)	104(1)
C(19)	4042(3)	4294(2)	7309(3)	102(1)
C(20)	4283(3)	5001(2)	7199(2)	90(1)
C(21)	3377(6)	3071(3)	6699(5)	157(2)
C(22)	3860(20)	6759(13)	7327(8)	85(3)
C(23)	3310(19)	6399(13)	7819(13)	103(4)
C(24)	3527(18)	6470(11)	8762(13)	106(4)
C(25)	4272(17)	6901(10)	9245(10)	100(3)
C(26)	4885(18)	7227(11)	8788(12)	100(3)
C(27)	4681(17)	7154(14)	7850(13)	92(3)
C(28)	4480(20)	6972(11)	10266(10)	129(5)
C(22')	3830(40)	6670(20)	7337(13)	89(5)

C(23')	3130(30)	6300(19)	7664(17)	91(4)
C(24')	3220(20)	6377(16)	8580(17)	99(4)
C(25')	3980(30)	6766(17)	9182(17)	101(5)
C(26')	4570(30)	7207(18)	8830(20)	104(5)
C(27')	4470(30)	7170(20)	7900(20)	95(5)
C(28')	4030(30)	6810(20)	10172(19)	144(8)
C(29)	5446(3)	6154(2)	6421(2)	78(1)
C(30)	6202(3)	5623(2)	6691(2)	86(1)
C(31)	7223(3)	5790(2)	6871(3)	97(1)
C(32)	7518(3)	6491(2)	6778(3)	96(1)
C(33)	6797(3)	7018(2)	6492(3)	93(1)
C(34)	5772(3)	6858(2)	6310(2)	82(1)
C(35)	5005(3)	7425(2)	5976(2)	89(1)
C(36)	3272(3)	7835(2)	5581(2)	84(1)
C(37)	2911(4)	8221(2)	6173(3)	108(1)
C(38)	2254(4)	8793(3)	5856(3)	119(2)
C(39)	1935(4)	8991(2)	4957(3)	107(1)
C(40)	2313(4)	8605(2)	4380(3)	111(1)
C(41)	2974(4)	8032(2)	4674(3)	100(1)
C(42)	1226(5)	9623(3)	4635(4)	147(2)
N(1)	4410(2)	6011(1)	6209(2)	78(1)
C(43)	3718(3)	6608(2)	6310(2)	81(1)
N(2)	4016(2)	7267(1)	5900(2)	81(1)
O(1)	5247(2)	8021(2)	5740(2)	112(1)
Br(1)	8933(1)	6707(1)	7043(1)	145(1)
C(44)	5372(19)	9152(11)	4440(20)	176(10)
Cl(1)	6045(15)	9871(9)	4660(16)	309(8)
Cl(2)	6132(17)	8534(11)	4327(15)	324(9)
C(44')	5950(30)	9340(30)	3993(18)	237(14)
Cl(1')	5080(20)	9767(15)	4270(20)	455(16)
Cl(2')	6608(9)	8926(12)	4981(7)	272(8)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for 4b.

C(1)-C(2)	1.380(6)
C(1)-C(6)	1.418(5)
C(1)-C(13)	1.481(5)
C(2)-C(3)	1.386(5)
C(2)-H(2)	0.9300

C(3)-C(4)	1.390(7)
C(3)-H(3)	0.9300
C(4)-C(5)	1.380(7)
C(4)-H(4)	0.9300
C(5)-C(6)	1.375(6)
C(5)-H(5)	0.9300
C(6)-C(7)	1.462(6)
C(7)-C(12)	1.393(6)
C(7)-C(8)	1.406(7)
C(8)-C(9)	1.400(10)
C(8)-H(8)	0.9300
C(9)-C(10)	1.377(10)
C(9)-H(9)	0.9300
C(10)-C(11)	1.366(8)
C(10)-H(10)	0.9300
C(11)-C(12)	1.392(6)
C(11)-H(11)	0.9300
C(12)-C(13)	1.479(5)
C(13)-C(14)	1.336(5)
C(14)-C(43)	1.519(5)
C(14)-H(14)	0.9300
C(15)-C(16)	1.364(5)
C(15)-C(20)	1.374(5)
C(15)-N(1)	1.447(4)
C(16)-C(17)	1.387(5)
C(16)-H(16)	0.9300
C(17)-C(18)	1.379(7)
C(17)-H(17)	0.9300
C(18)-C(19)	1.386(7)
C(18)-C(21)	1.513(6)
C(19)-C(20)	1.379(6)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-C(27)	1.380(14)
C(22)-C(23)	1.394(13)

C(22)-C(43)	1.548(10)
C(23)-C(24)	1.399(13)
C(23)-H(23)	0.9300
C(24)-C(25)	1.331(13)
C(24)-H(24)	0.9300
C(25)-C(26)	1.395(13)
C(25)-C(28)	1.518(12)
C(26)-C(27)	1.393(13)
C(26)-H(26)	0.9300
C(27)-H(27)	0.9300
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(22')-C(27')	1.384(18)
C(22')-C(23')	1.401(18)
C(22')-C(43)	1.549(14)
C(23')-C(24')	1.389(17)
C(23')-H(23')	0.9300
C(24')-C(25')	1.374(16)
C(24')-H(24')	0.9300
C(25')-C(26')	1.380(18)
C(25')-C(28')	1.510(18)
C(26')-C(27')	1.392(18)
C(26')-H(26')	0.9300
C(27')-H(27')	0.9300
C(28')-H(28D)	0.9600
C(28')-H(28E)	0.9600
C(28')-H(28F)	0.9600
C(29)-N(1)	1.383(5)
C(29)-C(30)	1.399(5)
C(29)-C(34)	1.412(5)
C(30)-C(31)	1.378(6)
C(30)-H(30)	0.9300
C(31)-C(32)	1.386(6)
C(31)-H(31)	0.9300
C(32)-C(33)	1.366(6)
C(32)-Br(1)	1.901(4)
C(33)-C(34)	1.380(6)

C(33)-H(33)	0.9300
C(34)-C(35)	1.466(5)
C(35)-O(1)	1.243(4)
C(35)-N(2)	1.360(5)
C(36)-C(37)	1.371(6)
C(36)-C(41)	1.380(5)
C(36)-N(2)	1.446(5)
C(37)-C(38)	1.383(6)
C(37)-H(37)	0.9300
C(38)-C(39)	1.369(6)
C(38)-H(38)	0.9300
C(39)-C(40)	1.367(7)
C(39)-C(42)	1.508(6)
C(40)-C(41)	1.382(6)
C(40)-H(40)	0.9300
C(41)-H(41)	0.9300
C(42)-H(42A)	0.9600
C(42)-H(42B)	0.9600
C(42)-H(42C)	0.9600
N(1)-C(43)	1.502(5)
C(43)-N(2)	1.493(4)
C(44)-Cl(2)	1.597(19)
C(44)-Cl(1)	1.600(18)
C(44)-H(44A)	0.9700
C(44)-H(44B)	0.9700
C(44')-Cl(1')	1.60(2)
C(44')-Cl(2')	1.69(2)
C(44')-H(44C)	0.9700
C(44')-H(44D)	0.9700
C(2)-C(1)-C(6)	118.8(4)
C(2)-C(1)-C(13)	133.2(3)
C(6)-C(1)-C(13)	108.0(4)
C(1)-C(2)-C(3)	120.0(4)
C(1)-C(2)-H(2)	120.0
C(3)-C(2)-H(2)	120.0
C(2)-C(3)-C(4)	120.5(5)
C(2)-C(3)-H(3)	119.7

C(4)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	120.3(4)
C(5)-C(4)-H(4)	119.9
C(3)-C(4)-H(4)	119.9
C(6)-C(5)-C(4)	119.5(4)
C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3
C(5)-C(6)-C(1)	120.9(4)
C(5)-C(6)-C(7)	130.8(4)
C(1)-C(6)-C(7)	108.2(4)
C(12)-C(7)-C(8)	119.9(5)
C(12)-C(7)-C(6)	109.1(3)
C(8)-C(7)-C(6)	131.1(5)
C(9)-C(8)-C(7)	117.3(6)
C(9)-C(8)-H(8)	121.4
C(7)-C(8)-H(8)	121.4
C(10)-C(9)-C(8)	122.2(5)
C(10)-C(9)-H(9)	118.9
C(8)-C(9)-H(9)	118.9
C(11)-C(10)-C(9)	120.2(7)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	119.4(6)
C(10)-C(11)-H(11)	120.3
C(12)-C(11)-H(11)	120.3
C(11)-C(12)-C(7)	121.0(4)
C(11)-C(12)-C(13)	130.2(4)
C(7)-C(12)-C(13)	108.8(4)
C(14)-C(13)-C(12)	121.3(4)
C(14)-C(13)-C(1)	132.8(3)
C(12)-C(13)-C(1)	105.8(3)
C(13)-C(14)-C(43)	131.7(4)
C(13)-C(14)-H(14)	114.2
C(43)-C(14)-H(14)	114.2
C(16)-C(15)-C(20)	119.1(3)
C(16)-C(15)-N(1)	119.2(3)
C(20)-C(15)-N(1)	121.6(3)
C(15)-C(16)-C(17)	120.4(4)

C(15)-C(16)-H(16)	119.8
C(17)-C(16)-H(16)	119.8
C(18)-C(17)-C(16)	121.6(4)
C(18)-C(17)-H(17)	119.2
C(16)-C(17)-H(17)	119.2
C(17)-C(18)-C(19)	117.1(4)
C(17)-C(18)-C(21)	122.1(5)
C(19)-C(18)-C(21)	120.8(5)
C(20)-C(19)-C(18)	121.4(4)
C(20)-C(19)-H(19)	119.3
C(18)-C(19)-H(19)	119.3
C(15)-C(20)-C(19)	120.5(4)
C(15)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(27)-C(22)-C(23)	114.8(14)
C(27)-C(22)-C(43)	120.7(16)
C(23)-C(22)-C(43)	123.3(14)
C(22)-C(23)-C(24)	123.1(12)
C(22)-C(23)-H(23)	118.5
C(24)-C(23)-H(23)	118.5
C(25)-C(24)-C(23)	121.2(13)
C(25)-C(24)-H(24)	119.4
C(23)-C(24)-H(24)	119.4
C(24)-C(25)-C(26)	117.3(13)
C(24)-C(25)-C(28)	119.8(12)
C(26)-C(25)-C(28)	122.8(12)
C(27)-C(26)-C(25)	121.7(15)
C(27)-C(26)-H(26)	119.1
C(25)-C(26)-H(26)	119.1
C(22)-C(27)-C(26)	121.5(17)
C(22)-C(27)-H(27)	119.2
C(26)-C(27)-H(27)	119.2

C(25)-C(28)-H(28A)	109.5
C(25)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(25)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27')-C(22')-C(23')	118(2)
C(27')-C(22')-C(43)	123(2)
C(23')-C(22')-C(43)	118(2)
C(24')-C(23')-C(22')	118(2)
C(24')-C(23')-H(23')	121.1
C(22')-C(23')-H(23')	121.1
C(25')-C(24')-C(23')	123(2)
C(25')-C(24')-H(24')	118.4
C(23')-C(24')-H(24')	118.4
C(24')-C(25')-C(26')	118(2)
C(24')-C(25')-C(28')	120(2)
C(26')-C(25')-C(28')	122(2)
C(25')-C(26')-C(27')	119(3)
C(25')-C(26')-H(26')	120.4
C(27')-C(26')-H(26')	120.4
C(22')-C(27')-C(26')	122(3)
C(22')-C(27')-H(27')	119.1
C(26')-C(27')-H(27')	119.1
C(25')-C(28')-H(28D)	109.5
C(25')-C(28')-H(28E)	109.5
H(28D)-C(28')-H(28E)	109.5
C(25')-C(28')-H(28F)	109.5
H(28D)-C(28')-H(28F)	109.5
H(28E)-C(28')-H(28F)	109.5
N(1)-C(29)-C(30)	123.3(3)
N(1)-C(29)-C(34)	119.4(3)
C(30)-C(29)-C(34)	117.1(4)
C(31)-C(30)-C(29)	121.1(4)
C(31)-C(30)-H(30)	119.4
C(29)-C(30)-H(30)	119.4
C(30)-C(31)-C(32)	120.2(4)
C(30)-C(31)-H(31)	119.9

C(32)-C(31)-H(31)	119.9
C(33)-C(32)-C(31)	120.1(4)
C(33)-C(32)-Br(1)	120.6(3)
C(31)-C(32)-Br(1)	119.3(3)
C(32)-C(33)-C(34)	120.2(4)
C(32)-C(33)-H(33)	119.9
C(34)-C(33)-H(33)	119.9
C(33)-C(34)-C(29)	121.2(4)
C(33)-C(34)-C(35)	119.5(3)
C(29)-C(34)-C(35)	119.3(4)
O(1)-C(35)-N(2)	121.3(4)
O(1)-C(35)-C(34)	121.0(4)
N(2)-C(35)-C(34)	117.6(3)
C(37)-C(36)-C(41)	118.9(4)
C(37)-C(36)-N(2)	121.3(3)
C(41)-C(36)-N(2)	119.6(3)
C(36)-C(37)-C(38)	119.8(4)
C(36)-C(37)-H(37)	120.1
C(38)-C(37)-H(37)	120.1
C(39)-C(38)-C(37)	122.3(4)
C(39)-C(38)-H(38)	118.8
C(37)-C(38)-H(38)	118.8
C(40)-C(39)-C(38)	116.8(4)
C(40)-C(39)-C(42)	122.2(4)
C(38)-C(39)-C(42)	121.0(5)
C(39)-C(40)-C(41)	122.4(4)
C(39)-C(40)-H(40)	118.8
C(41)-C(40)-H(40)	118.8
C(36)-C(41)-C(40)	119.6(4)
C(36)-C(41)-H(41)	120.2
C(40)-C(41)-H(41)	120.2
C(39)-C(42)-H(42A)	109.5
C(39)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(39)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(29)-N(1)-C(15)	117.2(3)

C(29)-N(1)-C(43)	118.1(3)
C(15)-N(1)-C(43)	117.7(3)
N(2)-C(43)-N(1)	107.2(3)
N(2)-C(43)-C(14)	108.4(3)
N(1)-C(43)-C(14)	109.3(3)
N(2)-C(43)-C(22)	108.6(8)
N(1)-C(43)-C(22)	110.9(12)
C(14)-C(43)-C(22)	112.3(11)
N(2)-C(43)-C(22')	114.9(14)
N(1)-C(43)-C(22')	107(2)
C(14)-C(43)-C(22')	109.8(17)
C(35)-N(2)-C(36)	116.9(3)
C(35)-N(2)-C(43)	122.7(3)
C(36)-N(2)-C(43)	119.0(3)
Cl(2)-C(44)-Cl(1)	105.7(15)
Cl(2)-C(44)-H(44A)	110.6
Cl(1)-C(44)-H(44A)	110.6
Cl(2)-C(44)-H(44B)	110.6
Cl(1)-C(44)-H(44B)	110.6
H(44A)-C(44)-H(44B)	108.7
Cl(1')-C(44')-Cl(2')	102.4(15)
Cl(1')-C(44')-H(44C)	111.3
Cl(2')-C(44')-H(44C)	111.3
Cl(1')-C(44')-H(44D)	111.3
Cl(2')-C(44')-H(44D)	111.3
H(44C)-C(44')-H(44D)	109.2

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for am3142. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^* U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	90(2)	64(2)	79(2)	-1(1)	8(2)	5(2)
C(2)	96(2)	78(2)	81(2)	-2(2)	18(2)	10(2)
C(3)	120(3)	89(3)	94(3)	7(2)	34(2)	23(2)
C(4)	153(5)	106(3)	82(3)	11(2)	23(3)	41(3)

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C(5)	128(4)	94(3)	85(3)	-2(2)	-6(2)	26(3)
C(6)	102(3)	71(2)	85(2)	-1(2)	0(2)	16(2)
C(7)	88(3)	74(2)	122(3)	-3(2)	-1(2)	7(2)
C(8)	103(4)	113(4)	158(5)	-17(3)	-18(3)	8(3)
C(9)	79(3)	121(4)	247(9)	-13(5)	2(4)	-11(3)
C(10)	91(3)	120(4)	207(7)	17(4)	27(4)	-12(3)
C(11)	93(3)	105(3)	152(4)	18(3)	32(3)	1(2)
C(12)	83(2)	74(2)	113(3)	4(2)	12(2)	2(2)
C(13)	83(2)	66(2)	86(2)	2(2)	15(2)	3(2)
C(14)	92(2)	76(2)	86(2)	1(2)	28(2)	6(2)
C(15)	84(2)	63(2)	72(2)	-1(1)	16(2)	0(1)
C(16)	103(2)	71(2)	79(2)	-6(2)	12(2)	3(2)
C(17)	103(3)	73(2)	115(3)	-14(2)	6(2)	-7(2)
C(18)	92(3)	76(2)	144(4)	8(2)	36(3)	-5(2)
C(19)	115(3)	90(3)	107(3)	23(2)	43(2)	7(2)
C(20)	108(3)	80(2)	78(2)	2(2)	21(2)	6(2)
C(21)	166(6)	79(3)	230(7)	25(4)	67(5)	-14(3)
C(22)	116(5)	60(6)	75(5)	5(4)	23(4)	11(5)
C(23)	136(8)	84(6)	84(7)	-10(5)	27(6)	-2(5)
C(24)	145(9)	94(6)	76(6)	7(5)	29(6)	-2(7)
C(25)	143(9)	80(6)	74(5)	0(4)	31(5)	4(6)
C(26)	137(9)	83(4)	76(4)	-2(3)	25(5)	7(6)
C(27)	124(8)	77(5)	72(4)	-7(4)	24(4)	12(6)
C(28)	182(14)	132(10)	69(5)	-9(5)	35(7)	-11(9)
C(22')	123(8)	65(8)	73(7)	-7(6)	23(7)	4(7)
C(23')	129(9)	77(8)	68(7)	-2(6)	35(7)	-4(7)
C(24')	140(10)	86(7)	70(8)	-4(6)	32(7)	-6(7)
C(25')	138(11)	79(8)	77(7)	-2(6)	19(7)	-6(8)
C(26')	141(10)	83(6)	81(6)	-14(6)	23(8)	8(8)
C(27')	128(10)	71(6)	79(7)	4(6)	23(7)	13(8)
C(28')	190(20)	131(16)	106(11)	-18(10)	32(13)	6(15)
C(29)	96(2)	65(2)	68(2)	-4(1)	18(2)	-2(2)
C(30)	98(2)	66(2)	90(2)	-3(2)	21(2)	0(2)
C(31)	104(3)	84(2)	100(3)	1(2)	28(2)	13(2)
C(32)	93(2)	88(2)	102(3)	-3(2)	24(2)	-5(2)
C(33)	102(3)	74(2)	96(2)	-3(2)	21(2)	-8(2)
C(34)	95(2)	67(2)	78(2)	-2(2)	16(2)	-3(2)
C(35)	108(3)	68(2)	79(2)	0(2)	13(2)	-2(2)

C(36)	99(2)	66(2)	78(2)	2(2)	13(2)	5(2)
C(37)	144(4)	98(3)	80(2)	12(2)	35(2)	29(3)
C(38)	138(4)	109(3)	112(3)	7(3)	42(3)	36(3)
C(39)	115(3)	86(3)	106(3)	9(2)	14(2)	17(2)
C(40)	141(4)	89(3)	82(2)	11(2)	6(2)	18(3)
C(41)	135(3)	79(2)	77(2)	2(2)	20(2)	18(2)
C(42)	153(5)	116(4)	146(4)	17(3)	11(4)	47(4)
N(1)	89(2)	62(1)	76(2)	-3(1)	16(1)	0(1)
C(43)	99(2)	66(2)	75(2)	4(1)	21(2)	5(2)
N(2)	95(2)	65(2)	75(2)	2(1)	15(1)	3(1)
O(1)	113(2)	75(2)	130(2)	18(2)	13(2)	-11(2)
Br(1)	99(1)	129(1)	200(1)	13(1)	37(1)	-7(1)
C(44)	151(17)	165(19)	204(19)	63(16)	44(16)	-14(16)
Cl(1)	270(16)	244(13)	410(20)	6(14)	101(15)	-123(13)
Cl(2)	280(17)	450(20)	289(17)	-2(18)	158(15)	-59(18)
C(44')	148(19)	240(20)	290(20)	-20(20)	30(19)	-40(20)
Cl(1')	410(30)	340(30)	510(30)	90(30)	0(30)	-60(20)
Cl(2')	199(9)	480(20)	139(6)	32(10)	52(6)	-87(12)

Table 5.

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for am3142.

	x	y	z	U(eq)
H(2)	4074	6426	4511	104
H(3)	4263	6416	3074	121
H(4)	2873	6183	1802	141
H(5)	1277	5972	1955	134
H(8)	-405	5746	2472	166
H(9)	-1579	5594	3271	192
H(10)	-1132	5795	4809	173
H(11)	532	6070	5625	141
H(14)	2173	6422	6123	102
H(16)	3629	5030	5021	106
H(17)	3201	3854	5202	124
H(19)	4156	4113	7894	122
H(20)	4558	5289	7709	109

H(21A)	3780	2912	7294	235
H(21B)	3526	2776	6245	235
H(21C)	2663	3032	6641	235
H(23)	2775	6099	7505	123
H(24)	3144	6211	9056	128
H(26)	5444	7501	9118	121
H(27)	5111	7376	7570	111
H(28A)	3847	7067	10389	193
H(28B)	4947	7361	10495	193
H(28C)	4770	6532	10561	193
H(23')	2621	6013	7281	109
H(24')	2732	6154	8796	119
H(26')	5038	7525	9205	125
H(27')	4831	7488	7660	114
H(28D)	4418	6404	10495	217
H(28E)	3353	6794	10217	217
H(28F)	4364	7246	10432	217
H(30)	6013	5150	6750	104
H(31)	7715	5431	7055	116
H(33)	6997	7486	6419	111
H(37)	3109	8098	6787	129
H(38)	2021	9052	6267	143
H(40)	2119	8732	3768	133
H(41)	3217	7780	4263	120
H(42A)	1536	9962	4333	220
H(42B)	1100	9850	5149	220
H(42C)	589	9459	4218	220
H(44A)	5096	9039	4926	211
H(44B)	4807	9208	3876	211
H(44C)	6388	9662	3790	284
H(44D)	5654	8989	3516	284

Table 6.

Torsion angles [°] for am3142.

C(6)-C(1)-C(2)-C(3)	2.6(5)
C(13)-C(1)-C(2)-C(3)	-176.3(4)
C(1)-C(2)-C(3)-C(4)	-1.6(6)
C(2)-C(3)-C(4)-C(5)	0.1(7)

C(3)-C(4)-C(5)-C(6)	0.2(7)
C(4)-C(5)-C(6)-C(1)	0.9(6)
C(4)-C(5)-C(6)-C(7)	179.5(4)
C(2)-C(1)-C(6)-C(5)	-2.3(5)
C(13)-C(1)-C(6)-C(5)	176.9(3)
C(2)-C(1)-C(6)-C(7)	178.8(3)
C(13)-C(1)-C(6)-C(7)	-2.0(4)
C(5)-C(6)-C(7)-C(12)	-177.5(4)
C(1)-C(6)-C(7)-C(12)	1.3(4)
C(5)-C(6)-C(7)-C(8)	2.3(8)
C(1)-C(6)-C(7)-C(8)	-178.9(4)
C(12)-C(7)-C(8)-C(9)	-1.5(7)
C(6)-C(7)-C(8)-C(9)	178.8(5)
C(7)-C(8)-C(9)-C(10)	2.4(9)
C(8)-C(9)-C(10)-C(11)	-2.3(10)
C(9)-C(10)-C(11)-C(12)	1.3(9)
C(10)-C(11)-C(12)-C(7)	-0.5(7)
C(10)-C(11)-C(12)-C(13)	-180.0(4)
C(8)-C(7)-C(12)-C(11)	0.6(6)
C(6)-C(7)-C(12)-C(11)	-179.6(4)
C(8)-C(7)-C(12)-C(13)	-179.8(4)
C(6)-C(7)-C(12)-C(13)	0.0(4)
C(11)-C(12)-C(13)-C(14)	-4.4(6)
C(7)-C(12)-C(13)-C(14)	176.0(3)
C(11)-C(12)-C(13)-C(1)	178.3(4)
C(7)-C(12)-C(13)-C(1)	-1.2(4)
C(2)-C(1)-C(13)-C(14)	4.2(7)
C(6)-C(1)-C(13)-C(14)	-174.8(4)
C(2)-C(1)-C(13)-C(12)	-179.0(4)
C(6)-C(1)-C(13)-C(12)	2.0(4)
C(12)-C(13)-C(14)-C(43)	178.9(3)
C(1)-C(13)-C(14)-C(43)	-4.8(7)
C(20)-C(15)-C(16)-C(17)	1.5(6)
N(1)-C(15)-C(16)-C(17)	177.5(4)
C(15)-C(16)-C(17)-C(18)	-1.3(7)
C(16)-C(17)-C(18)-C(19)	0.5(7)
C(16)-C(17)-C(18)-C(21)	-179.2(5)
C(17)-C(18)-C(19)-C(20)	0.0(7)

C(21)-C(18)-C(19)-C(20)	179.8(5)
C(16)-C(15)-C(20)-C(19)	-1.0(6)
N(1)-C(15)-C(20)-C(19)	-176.9(4)
C(18)-C(19)-C(20)-C(15)	0.2(7)
C(27)-C(22)-C(23)-C(24)	4(4)
C(43)-C(22)-C(23)-C(24)	172(2)
C(22)-C(23)-C(24)-C(25)	1(3)
C(23)-C(24)-C(25)-C(26)	-6(2)
C(23)-C(24)-C(25)-C(28)	179.2(18)
C(24)-C(25)-C(26)-C(27)	5(2)
C(28)-C(25)-C(26)-C(27)	179.9(18)
C(23)-C(22)-C(27)-C(26)	-5(4)
C(43)-C(22)-C(27)-C(26)	-172.7(18)
C(25)-C(26)-C(27)-C(22)	0(3)
C(27)-C(22)-C(23)-C(24)	-10(6)
C(43)-C(22)-C(23)-C(24)	-178(3)
C(22)-C(23)-C(24)-C(25)	-3(4)
C(23)-C(24)-C(25)-C(26)	12(4)
C(23)-C(24)-C(25)-C(28)	-178(3)
C(24)-C(25)-C(26)-C(27)	-9(4)
C(28)-C(25)-C(26)-C(27)	-177(3)
C(23)-C(22)-C(27)-C(26)	14(6)
C(43)-C(22)-C(27)-C(26)	-179(3)
C(25)-C(26)-C(27)-C(22)	-4(5)
N(1)-C(29)-C(30)-C(31)	178.1(3)
C(34)-C(29)-C(30)-C(31)	2.3(5)
C(29)-C(30)-C(31)-C(32)	-0.6(6)
C(30)-C(31)-C(32)-C(33)	-1.2(6)
C(30)-C(31)-C(32)-Br(1)	179.3(3)
C(31)-C(32)-C(33)-C(34)	1.2(6)
Br(1)-C(32)-C(33)-C(34)	-179.3(3)
C(32)-C(33)-C(34)-C(29)	0.5(6)
C(32)-C(33)-C(34)-C(35)	-178.1(4)
N(1)-C(29)-C(34)-C(33)	-178.3(3)
C(30)-C(29)-C(34)-C(33)	-2.2(5)
N(1)-C(29)-C(34)-C(35)	0.3(5)
C(30)-C(29)-C(34)-C(35)	176.4(3)
C(33)-C(34)-C(35)-O(1)	9.5(6)

C(29)-C(34)-C(35)-O(1)	-169.1(4)
C(33)-C(34)-C(35)-N(2)	-173.0(3)
C(29)-C(34)-C(35)-N(2)	8.4(5)
C(41)-C(36)-C(37)-C(38)	0.5(7)
N(2)-C(36)-C(37)-C(38)	175.6(5)
C(36)-C(37)-C(38)-C(39)	0.5(9)
C(37)-C(38)-C(39)-C(40)	-1.3(8)
C(37)-C(38)-C(39)-C(42)	-179.4(6)
C(38)-C(39)-C(40)-C(41)	1.1(8)
C(42)-C(39)-C(40)-C(41)	179.1(5)
C(37)-C(36)-C(41)-C(40)	-0.7(7)
N(2)-C(36)-C(41)-C(40)	-175.9(4)
C(39)-C(40)-C(41)-C(36)	-0.1(8)
C(30)-C(29)-N(1)-C(15)	4.7(5)
C(34)-C(29)-N(1)-C(15)	-179.5(3)
C(30)-C(29)-N(1)-C(43)	154.9(3)
C(34)-C(29)-N(1)-C(43)	-29.3(4)
C(16)-C(15)-N(1)-C(29)	-104.6(4)
C(20)-C(15)-N(1)-C(29)	71.3(4)
C(16)-C(15)-N(1)-C(43)	105.0(4)
C(20)-C(15)-N(1)-C(43)	-79.1(4)
C(29)-N(1)-C(43)-N(2)	45.1(4)
C(15)-N(1)-C(43)-N(2)	-164.9(3)
C(29)-N(1)-C(43)-C(14)	162.4(3)
C(15)-N(1)-C(43)-C(14)	-47.5(4)
C(29)-N(1)-C(43)-C(22)	-73.3(10)
C(15)-N(1)-C(43)-C(22)	76.8(10)
C(29)-N(1)-C(43)-C(22')	-78.8(14)
C(15)-N(1)-C(43)-C(22')	71.3(14)
C(13)-C(14)-C(43)-N(2)	60.2(5)
C(13)-C(14)-C(43)-N(1)	-56.3(5)
C(13)-C(14)-C(43)-C(22)	-179.8(11)
C(13)-C(14)-C(43)-C(22')	-173.5(19)
C(27)-C(22)-C(43)-N(2)	-39(3)
C(23)-C(22)-C(43)-N(2)	154(2)
C(27)-C(22)-C(43)-N(1)	79(3)
C(23)-C(22)-C(43)-N(1)	-88(3)
C(27)-C(22)-C(43)-C(14)	-159(2)

C(23)-C(22)-C(43)-C(14)	35(3)
C(27')-C(22')-C(43)-N(2)	-21(6)
C(23')-C(22')-C(43)-N(2)	146(3)
C(27')-C(22')-C(43)-N(1)	98(5)
C(23')-C(22')-C(43)-N(1)	-95(4)
C(27')-C(22')-C(43)-C(14)	-144(4)
C(23')-C(22')-C(43)-C(14)	24(4)
O(1)-C(35)-N(2)-C(36)	-3.3(5)
C(34)-C(35)-N(2)-C(36)	179.2(3)
O(1)-C(35)-N(2)-C(43)	-169.9(3)
C(34)-C(35)-N(2)-C(43)	12.6(5)
C(37)-C(36)-N(2)-C(35)	-101.6(5)
C(41)-C(36)-N(2)-C(35)	73.4(5)
C(37)-C(36)-N(2)-C(43)	65.5(5)
C(41)-C(36)-N(2)-C(43)	-119.5(4)
N(1)-C(43)-N(2)-C(35)	-37.3(4)
C(14)-C(43)-N(2)-C(35)	-155.2(3)
C(22)-C(43)-N(2)-C(35)	82.6(13)
C(22')-C(43)-N(2)-C(35)	82(2)
N(1)-C(43)-N(2)-C(36)	156.4(3)
C(14)-C(43)-N(2)-C(36)	38.5(4)
C(22)-C(43)-N(2)-C(36)	-83.8(13)
C(22')-C(43)-N(2)-C(36)	-85(2)

Symmetry transformations used to generate equivalent atoms: