Supporting Information

A convenient method to construct (*Z*)-form oxazines via 6-*exo-dig* Iodocyclization and synthesis of Indolin-3-one

Jaya Kishore Vandavasi,[a,†] Kung-Kai Kuo,[b,†] Wan-Ping Hu,[c] Ho-Chanu Shen,[a] Wei-Sheng Lo,[a] and Jeh-Jeng Wang*,[a]

[a]Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung city 807, Taiwan.
[b]Department of Surgery, School of Medicine, Kaohsiung Medical University, Taiwan.
[c]Department of Biotechnology, Kaohsiung Medical University, Taiwan.
†Equally contributed

E-mail: jjwang@kmu.edu.tw

Contents:

1. General Information

Melting points are uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded in 400 MHz instrument using $CDCl_3$ as a solvent. ^{1}H NMR chemical shifts are referenced to TMS (0 ppm) or $CDCl_3$ (7.26 ppm). ^{13}C NMR was referenced to $CDCl_3$ (77.0 ppm). Multiplicities were denoted as s, d, t, q. Mass spectra and high resolution mass spectra (HRMS) were measured using the electron-impact (EI, 70 eV). Flash column chromatography was carried out over silica gel 60 (E. Merck, 230-400 mesh).

2. ORTEP Diagrams

4-(iodo(phenyl)methylene)-2-phenyl-4H-benzo[d][1,3]oxazine (2a)

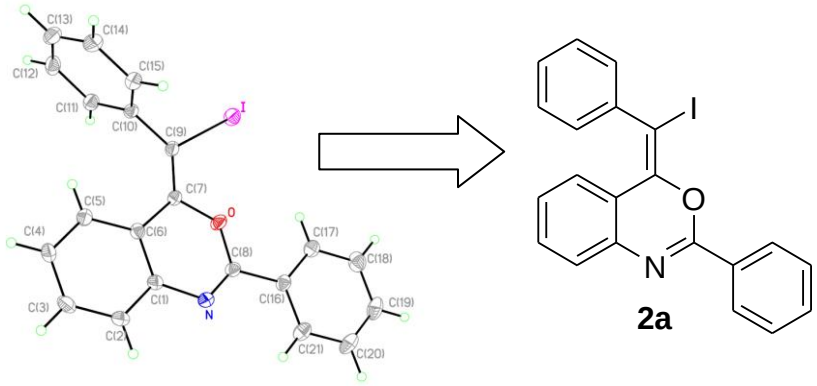


Table 1. Crystal data and structure refinement for 2a.

Identification code	2a	
Empirical formula	C21 H14 I N O	
Formula weight	423.23	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.6684(5) Å	α= 90°.
	b = 20.5140(12) Å	β= 105.7630(10)°.
	c = 9.9755(6) Å	γ = 90°.
Volume	1707.17(17) $Å^3$	
Z	4	
Density (calculated)	1.647 Mg/m^3	
Absorption coefficient	1.882 mm^{-1}	
F(000)	832	
Crystal size	0.69 x 0.58 x 0.21 mm^3	
Theta range for data collection	1.99 to 26.01°.	
Index ranges	-9<=h<=10, -23<=k<=25, -12<=l<=9	
Reflections collected	9397	
Independent reflections	3351 [R(int) = 0.0202]	
Completeness to theta = 26.01°	99.7 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.563	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	3351 / 0 / 227
Goodness-of-fit on F^2	1.138
Final R indices [I>2sigma(I)]	R1 = 0.0227, wR2 = 0.0729
R indices (all data)	R1 = 0.0258, wR2 = 0.0757
Largest diff. peak and hole	0.281 and -0.373 e.Å^{-3}

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

	x	y	z	U(eq)
I	2314(5)	1832(1)	7798(2)	53(1)
I'	2090(19)	1803(3)	7807(5)	57(1)
O	1916(2)	695(1)	9623(2)	51(1)
N	2157(2)	-20(1)	11496(2)	50(1)
C(1)	-256(3)	2751(1)	9765(2)	50(1)
C(2)	-486(3)	3377(1)	10235(3)	60(1)
C(3)	776(3)	3710(1)	11090(3)	62(1)
C(4)	2286(3)	3433(1)	11481(3)	61(1)
C(5)	2517(3)	2816(1)	11005(2)	51(1)
C(6)	1249(2)	2465(1)	10163(2)	41(1)
C(7)	1540(3)	1807(1)	9664(2)	41(1)
C(8)	1521(2)	1239(1)	10301(2)	40(1)
C(9)	1154(2)	1096(1)	11630(2)	40(1)
C(10)	451(3)	1536(1)	12358(2)	50(1)
C(11)	154(3)	1364(1)	13596(2)	53(1)
C(12)	574(3)	754(1)	14161(2)	56(1)
C(13)	1248(3)	309(1)	13465(2)	55(1)
C(14)	1513(2)	470(1)	12179(2)	44(1)
C(15)	2302(2)	116(1)	10295(2)	42(1)
C(16)	2945(2)	-353(1)	9452(2)	45(1)
C(17)	3257(3)	-987(1)	9924(3)	59(1)
C(18)	3891(4)	-1430(1)	9177(3)	70(1)
C(19)	4217(3)	-1244(1)	7964(3)	70(1)
C(20)	3930(4)	-610(1)	7495(3)	70(1)
C(21)	3288(3)	-171(1)	8225(3)	57(1)

Table 3. Bond lengths [Å] and angles [°] for 2a

I-C(7)	2.144(4)
I'-C(7)	2.034(10)
O-C(15)	1.360(2)
O-C(8)	1.394(2)
N-C(15)	1.269(3)
N-C(14)	1.412(3)
C(1)-C(6)	1.386(3)
C(1)-C(2)	1.400(3)
C(1)-H(1A)	0.9300
C(2)-C(3)	1.372(4)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.382(4)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.386(3)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.389(3)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.484(2)
C(7)-C(8)	1.330(3)
C(8)-C(9)	1.474(3)
C(9)-C(14)	1.396(3)
C(9)-C(10)	1.399(3)
C(10)-C(11)	1.374(3)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.380(3)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.370(3)
C(12)-H(12A)	0.9300
C(13)-C(14)	1.403(3)
C(13)-H(13A)	0.9300
C(15)-C(16)	1.482(3)
C(16)-C(21)	1.387(3)
C(16)-C(17)	1.385(3)
C(17)-C(18)	1.381(3)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.369(4)

C(18)-H(18A)	0.9300
C(19)-C(20)	1.383(4)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.368(3)
C(20)-H(20A)	0.9300
C(21)-H(21A)	0.9300

C(15)-O-C(8)	121.30(15)
C(15)-N-C(14)	116.88(17)
C(6)-C(1)-C(2)	120.1(2)
C(6)-C(1)-H(1A)	120.0
C(2)-C(1)-H(1A)	120.0
C(3)-C(2)-C(1)	120.1(2)
C(3)-C(2)-H(2A)	119.9
C(1)-C(2)-H(2A)	119.9
C(2)-C(3)-C(4)	120.4(2)
C(2)-C(3)-H(3A)	119.8
C(4)-C(3)-H(3A)	119.8
C(5)-C(4)-C(3)	119.5(2)
C(5)-C(4)-H(4A)	120.3
C(3)-C(4)-H(4A)	120.3
C(4)-C(5)-C(6)	121.0(2)
C(4)-C(5)-H(5A)	119.5
C(6)-C(5)-H(5A)	119.5
C(1)-C(6)-C(5)	118.88(19)
C(1)-C(6)-C(7)	121.43(19)
C(5)-C(6)-C(7)	119.64(19)
C(8)-C(7)-C(6)	127.7(2)
C(8)-C(7)-I'	117.9(2)
C(6)-C(7)-I'	114.4(2)
C(8)-C(7)-I	118.87(15)
C(6)-C(7)-I	113.06(14)
I'-C(7)-I	4.8(4)
C(7)-C(8)-O	115.66(17)
C(7)-C(8)-C(9)	129.61(18)
O-C(8)-C(9)	114.73(16)
C(14)-C(9)-C(10)	118.16(18)
C(14)-C(9)-C(8)	117.13(17)

C(10)-C(9)-C(8)	124.70(18)
C(11)-C(10)-C(9)	121.0(2)
C(11)-C(10)-H(10A)	119.5
C(9)-C(10)-H(10A)	119.5
C(10)-C(11)-C(12)	120.5(2)
C(10)-C(11)-H(11A)	119.8
C(12)-C(11)-H(11A)	119.8
C(13)-C(12)-C(11)	119.9(2)
C(13)-C(12)-H(12A)	120.0
C(11)-C(12)-H(12A)	120.0
C(12)-C(13)-C(14)	120.3(2)
C(12)-C(13)-H(13A)	119.9
C(14)-C(13)-H(13A)	119.9
C(9)-C(14)-C(13)	120.08(18)
C(9)-C(14)-N	122.70(18)
C(13)-C(14)-N	117.21(18)
N-C(15)-O	125.67(17)
N-C(15)-C(16)	122.78(18)
O-C(15)-C(16)	111.54(17)
C(21)-C(16)-C(17)	118.91(19)
C(21)-C(16)-C(15)	121.99(19)
C(17)-C(16)-C(15)	119.1(2)
C(18)-C(17)-C(16)	120.3(2)
C(18)-C(17)-H(17A)	119.8
C(16)-C(17)-H(17A)	119.8
C(19)-C(18)-C(17)	120.1(2)
C(19)-C(18)-H(18A)	119.9
C(17)-C(18)-H(18A)	119.9
C(18)-C(19)-C(20)	120.0(2)
C(18)-C(19)-H(19A)	120.0
C(20)-C(19)-H(19A)	120.0
C(21)-C(20)-C(19)	120.1(3)
C(21)-C(20)-H(20A)	119.9
C(19)-C(20)-H(20A)	119.9
C(20)-C(21)-C(16)	120.6(2)
C(20)-C(21)-H(21A)	119.7
C(16)-C(21)-H(21A)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2a. 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}
I	75(1)	49(1)	45(1)	3(1)	31(1)	6(1)
I'	76(3)	64(2)	37(1)	12(1)	27(1)	21(2)
O	77(1)	38(1)	45(1)	-3(1)	28(1)	8(1)
N	64(1)	39(1)	54(1)	1(1)	28(1)	3(1)
C(1)	55(1)	51(1)	45(1)	2(1)	16(1)	8(1)
C(2)	71(2)	58(1)	58(2)	11(1)	31(1)	25(1)
C(3)	91(2)	41(1)	62(2)	-1(1)	36(1)	10(1)
C(4)	76(2)	50(1)	62(2)	-10(1)	24(1)	-6(1)
C(5)	54(1)	46(1)	56(1)	-2(1)	20(1)	3(1)
C(6)	54(1)	36(1)	37(1)	4(1)	19(1)	6(1)
C(7)	48(1)	42(1)	35(1)	1(1)	16(1)	5(1)
C(8)	46(1)	37(1)	39(1)	-3(1)	15(1)	4(1)
C(9)	44(1)	40(1)	40(1)	-4(1)	16(1)	-4(1)
C(10)	60(1)	45(1)	49(1)	2(1)	24(1)	7(1)
C(11)	63(1)	54(1)	52(1)	-6(1)	33(1)	0(1)
C(12)	69(1)	57(1)	54(1)	2(1)	36(1)	-11(1)
C(13)	75(2)	42(1)	59(1)	6(1)	34(1)	-6(1)
C(14)	46(1)	40(1)	50(1)	0(1)	21(1)	-5(1)
C(15)	45(1)	33(1)	50(1)	-5(1)	15(1)	-3(1)
C(16)	44(1)	40(1)	51(1)	-13(1)	14(1)	-3(1)
C(17)	70(1)	47(1)	60(1)	-8(1)	18(1)	8(1)
C(18)	81(2)	49(1)	75(2)	-13(1)	13(1)	17(1)
C(19)	70(2)	64(2)	77(2)	-27(1)	20(1)	15(1)
C(20)	76(2)	73(2)	69(2)	-20(1)	34(1)	-2(1)
C(21)	70(1)	46(1)	61(1)	-8(1)	26(1)	0(1)

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

	x	y	z	U(eq)

H(1A)	-1114	2527	9185	59
H(2A)	-1497	3568	9968	72
H(3A)	615	4124	11408	74
H(4A)	3141	3660	12059	74
H(5A)	3538	2633	11254	61
H(10A)	181	1952	12000	60
H(11A)	-332	1661	14056	64
H(12A)	398	645	15012	68
H(13A)	1532	-102	13848	67
H(17A)	3039	-1115	10748	71
H(18A)	4096	-1856	9498	84
H(19A)	4632	-1545	7456	84
H(20A)	4175	-481	6683	84
H(21A)	3079	253	7896	69

2-(4-chlorophenyl)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]oxazine(2c):

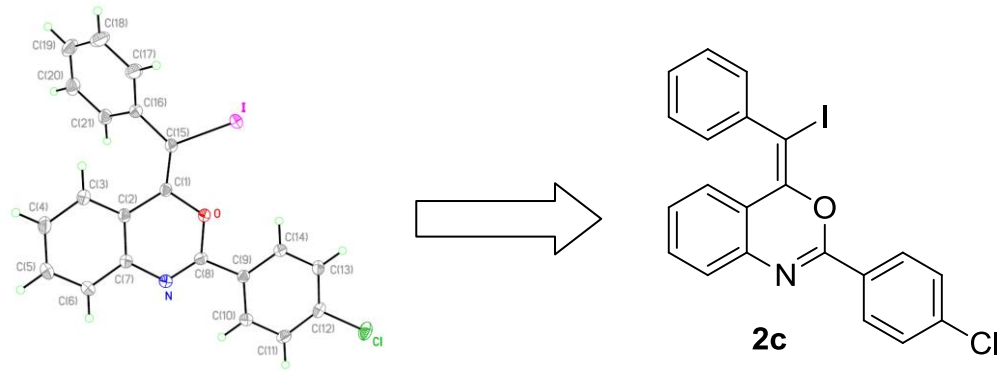


Table 1. Crystal data and structure refinement for 2c

Identification code	2c	
Empirical formula	C21 H13 Cl I N O	
Formula weight	457.67	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 15.6740(11) Å	α= 90°.
	b = 8.2808(6) Å	β= 101.6950(10)°.
	c = 28.5842(19) Å	γ = 90°.
Volume	3633.0(4) Å^3	

Z	8
Density (calculated)	1.674 Mg/m^3
Absorption coefficient	1.918 mm^{-1}
F(000)	1792
Crystal size	0.60 x 0.41 x 0.18 mm^3
Theta range for data collection	2.65 to 26.03°.
Index ranges	-19<=h<=19, -10<=k<=10, -16<=l<=35
Reflections collected	9855
Independent reflections	3551 [R(int) = 0.0239]
Completeness to theta = 26.03°	99.5 %
Absorption correction	Empirical
Max. and min. transmission	1.000000 and 0.650068
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3551 / 0 / 226
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0288, wR2 = 0.0751
R indices (all data)	R1 = 0.0330, wR2 = 0.0778
Largest diff. peak and hole	0.279 and -0.759 $e.Å^{-3}$

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

	x	y	z	U(eq)
I	2464(1)	1261(1)	4445(1)	56(1)
Cl	6336(1)	5467(1)	6269(1)	64(1)
O	4369(1)	1004(2)	4441(1)	41(1)
N	5735(2)	1175(3)	4228(1)	47(1)
C(1)	3960(2)	342(3)	4007(1)	36(1)
C(2)	4551(2)	-347(3)	3720(1)	38(1)
C(3)	4306(2)	-1509(3)	3365(1)	46(1)
C(4)	4915(2)	-2114(4)	3120(1)	57(1)
C(5)	5768(2)	-1602(4)	3229(1)	65(1)
C(6)	6025(2)	-483(4)	3588(1)	59(1)
C(7)	5426(2)	131(3)	3839(1)	42(1)
C(8)	5218(2)	1508(3)	4503(1)	38(1)
C(9)	5475(2)	2471(3)	4942(1)	37(1)

C(10)	6336(2)	2964(3)	5082(1)	46(1)
C(11)	6610(2)	3881(3)	5488(1)	50(1)
C(12)	6001(2)	4299(3)	5754(1)	44(1)
C(13)	5142(2)	3831(3)	5628(1)	47(1)
C(14)	4878(2)	2912(3)	5220(1)	43(1)
C(15)	3087(2)	362(3)	3912(1)	39(1)
C(16)	2494(2)	-78(3)	3456(1)	42(1)
C(17)	1821(2)	-1175(4)	3441(1)	59(1)
C(18)	1276(2)	-1554(5)	3008(2)	75(1)
C(19)	1386(2)	-832(5)	2592(1)	70(1)
C(20)	2051(2)	278(4)	2601(1)	62(1)
C(21)	2593(2)	656(4)	3032(1)	50(1)

Table 3. Bond lengths [Å] and angles [°] for 2c.

I-C(15)	2.105(2)
Cl-C(12)	1.749(3)
O-C(8)	1.372(3)
O-C(1)	1.389(3)
N-C(8)	1.269(4)
N-C(7)	1.414(3)
C(1)-C(15)	1.340(4)
C(1)-C(2)	1.470(3)
C(2)-C(3)	1.395(4)
C(2)-C(7)	1.402(4)
C(3)-C(4)	1.388(4)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.377(5)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.379(5)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.390(4)
C(6)-H(6A)	0.9300
C(8)-C(9)	1.471(3)
C(9)-C(10)	1.390(4)
C(9)-C(14)	1.393(4)
C(10)-C(11)	1.380(4)
C(10)-H(10A)	0.9300

C(11)-C(12)	1.380(4)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.378(4)
C(13)-C(14)	1.385(4)
C(13)-H(13A)	0.9300
C(14)-H(14A)	0.9300
C(15)-C(16)	1.486(3)
C(16)-C(17)	1.386(4)
C(16)-C(21)	1.391(4)
C(17)-C(18)	1.389(5)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.373(6)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.386(5)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.384(4)
C(20)-H(20A)	0.9300
C(21)-H(21A)	0.9300

C(8)-O-C(1)	119.72(19)
C(8)-N-C(7)	117.4(2)
C(15)-C(1)-O	116.3(2)
C(15)-C(1)-C(2)	128.7(2)
O-C(1)-C(2)	115.0(2)
C(3)-C(2)-C(7)	118.9(2)
C(3)-C(2)-C(1)	124.2(2)
C(7)-C(2)-C(1)	116.8(2)
C(4)-C(3)-C(2)	120.0(3)
C(4)-C(3)-H(3A)	120.0
C(2)-C(3)-H(3A)	120.0
C(5)-C(4)-C(3)	120.7(3)
C(5)-C(4)-H(4A)	119.7
C(3)-C(4)-H(4A)	119.7
C(4)-C(5)-C(6)	120.0(3)
C(4)-C(5)-H(5A)	120.0
C(6)-C(5)-H(5A)	120.0
C(5)-C(6)-C(7)	120.3(3)
C(5)-C(6)-H(6A)	119.9

C(7)-C(6)-H(6A)	119.9
C(6)-C(7)-C(2)	120.1(2)
C(6)-C(7)-N	118.1(2)
C(2)-C(7)-N	121.7(2)
N-C(8)-O	125.3(2)
N-C(8)-C(9)	123.2(2)
O-C(8)-C(9)	111.5(2)
C(10)-C(9)-C(14)	119.0(2)
C(10)-C(9)-C(8)	119.1(2)
C(14)-C(9)-C(8)	121.9(2)
C(11)-C(10)-C(9)	121.4(3)
C(11)-C(10)-H(10A)	119.3
C(9)-C(10)-H(10A)	119.3
C(12)-C(11)-C(10)	118.1(3)
C(12)-C(11)-H(11A)	121.0
C(10)-C(11)-H(11A)	121.0
C(13)-C(12)-C(11)	122.2(2)
C(13)-C(12)-Cl	119.1(2)
C(11)-C(12)-Cl	118.7(2)
C(12)-C(13)-C(14)	118.9(3)
C(12)-C(13)-H(13A)	120.5
C(14)-C(13)-H(13A)	120.5
C(13)-C(14)-C(9)	120.3(3)
C(13)-C(14)-H(14A)	119.8
C(9)-C(14)-H(14A)	119.8
C(1)-C(15)-C(16)	127.3(2)
C(1)-C(15)-I	117.58(18)
C(16)-C(15)-I	114.97(17)
C(17)-C(16)-C(21)	118.5(3)
C(17)-C(16)-C(15)	121.7(2)
C(21)-C(16)-C(15)	119.8(2)
C(16)-C(17)-C(18)	120.2(3)
C(16)-C(17)-H(17A)	119.9
C(18)-C(17)-H(17A)	119.9
C(17)-C(18)-C(19)	120.7(3)
C(17)-C(18)-H(18A)	119.7
C(19)-C(18)-H(18A)	119.7
C(20)-C(19)-C(18)	120.0(3)

C(20)-C(19)-H(19A)	120.0
C(18)-C(19)-H(19A)	120.0
C(21)-C(20)-C(19)	119.3(3)
C(21)-C(20)-H(20A)	120.3
C(19)-C(20)-H(20A)	120.3
C(20)-C(21)-C(16)	121.3(3)
C(20)-C(21)-H(21A)	119.3
C(16)-C(21)-H(21A)	119.3

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I	44(1)	83(1)	46(1)	-13(1)	19(1)	-6(1)
Cl	83(1)	63(1)	43(1)	-15(1)	7(1)	-20(1)
O	37(1)	53(1)	34(1)	-8(1)	8(1)	-6(1)
N	37(1)	60(1)	44(1)	-10(1)	9(1)	-2(1)
C(1)	41(1)	39(1)	30(1)	0(1)	8(1)	-5(1)
C(2)	42(1)	40(1)	32(1)	1(1)	8(1)	4(1)
C(3)	49(2)	47(1)	41(1)	-7(1)	8(1)	-1(1)
C(4)	64(2)	59(2)	47(2)	-16(1)	12(1)	8(1)
C(5)	55(2)	82(2)	60(2)	-21(2)	19(2)	15(2)
C(6)	41(2)	83(2)	54(2)	-16(2)	12(1)	7(2)
C(7)	39(1)	51(1)	37(1)	-3(1)	7(1)	3(1)
C(8)	34(1)	41(1)	37(1)	2(1)	3(1)	-1(1)
C(9)	38(1)	39(1)	32(1)	2(1)	5(1)	2(1)
C(10)	37(1)	55(2)	46(2)	-7(1)	8(1)	-1(1)
C(11)	43(2)	58(2)	47(2)	-5(1)	1(1)	-8(1)
C(12)	56(2)	40(1)	33(1)	-1(1)	2(1)	-6(1)
C(13)	52(2)	54(2)	36(1)	-3(1)	11(1)	2(1)
C(14)	37(1)	52(1)	39(1)	-2(1)	6(1)	-3(1)
C(15)	41(1)	44(1)	34(1)	-2(1)	11(1)	-4(1)
C(16)	38(1)	48(1)	37(1)	-2(1)	5(1)	2(1)
C(17)	52(2)	73(2)	51(2)	2(1)	6(1)	-13(1)
C(18)	56(2)	88(2)	73(2)	-10(2)	-6(2)	-20(2)

C(19)	64(2)	85(2)	50(2)	-15(2)	-14(2)	8(2)
C(20)	69(2)	76(2)	36(1)	4(1)	3(1)	16(2)
C(21)	54(2)	56(2)	40(1)	1(1)	10(1)	2(1)

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

	x	y	z	U(eq)
H(3A)	3734	-1878	3292	55
H(4A)	4745	-2873	2879	68
H(5A)	6170	-2010	3062	78
H(6A)	6601	-139	3661	71
H(10A)	6737	2669	4898	55
H(11A)	7187	4209	5578	60
H(13A)	4745	4128	5815	56
H(14A)	4300	2587	5131	52
H(17A)	1734	-1659	3721	71
H(18A)	832	-2304	3000	90
H(19A)	1015	-1088	2305	84
H(20A)	2133	763	2320	74
H(21A)	3032	1416	3039	60

4-(iodo(phenyl)methylene)-2-phenyl-6-(trifluoromethyl)-4H-benzo[d][1,3]oxazine (2e):

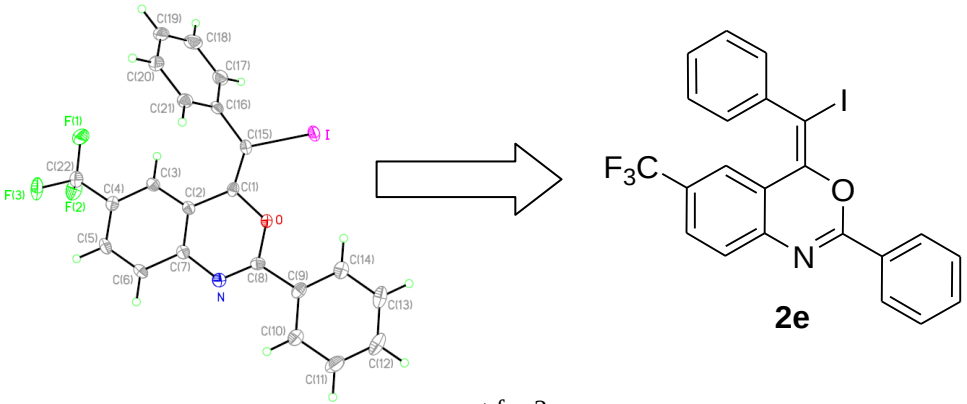


Table 1. Crystal data and structure refinement for 2e.

Identification code	2e

Empirical formula	C22 H13 F3 I N O	
Formula weight	491.23	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.1298(2) Å	α= 80.375(2)°.
	b = 10.6900(3) Å	β= 87.307(2)°.
	c = 11.1738(3) Å	γ = 73.916(2)°.
Volume	919.94(4) $Å^3$	
Z	2	
Density (calculated)	1.773 Mg/m^3	
Absorption coefficient	1.782 mm^{-1}	
F(000)	480	
Crystal size	0.60 x 0.46 x 0.40 mm^3	
Theta range for data collection	2.94 to 29.28°.	
Index ranges	-10<=h<=10, -13<=k<=14, -14<=l<=14	
Reflections collected	8019	
Independent reflections	4233 [R(int) = 0.0202]	
Completeness to theta = 26.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.85697	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4233 / 0 / 253	
Goodness-of-fit on F^2	0.994	
Final R indices [I>2sigma(I)]	R1 = 0.0243, wR2 = 0.0599	
R indices (all data)	R1 = 0.0299, wR2 = 0.0611	
Largest diff. peak and hole	0.621 and -0.634 e.$Å^{-3}$	

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

	x	y	z	U(eq)
I	3733(1)	7123(1)	7268(1)	21(1)
F(1)	1975(2)	7674(2)	819(1)	36(1)
F(2)	3400(2)	5849(2)	283(1)	33(1)
F(3)	669(2)	6447(2)	130(1)	34(1)

O	3282(2)	4755(2)	6340(1)	17(1)
N	1901(2)	3434(2)	5522(2)	18(1)
C(1)	2912(3)	5770(2)	5340(2)	15(1)
C(2)	2431(3)	5380(2)	4233(2)	15(1)
C(3)	2478(3)	6085(2)	3068(2)	17(1)
C(4)	1845(3)	5699(2)	2097(2)	17(1)
C(5)	1175(3)	4620(2)	2266(2)	19(1)
C(6)	1197(3)	3886(2)	3407(2)	19(1)
C(7)	1849(3)	4250(2)	4391(2)	16(1)
C(8)	2622(3)	3702(2)	6392(2)	16(1)
C(9)	2870(3)	2870(2)	7595(2)	20(1)
C(10)	2529(3)	1648(3)	7737(2)	27(1)
C(11)	2720(4)	858(3)	8868(3)	32(1)
C(12)	3235(3)	1277(3)	9852(2)	31(1)
C(13)	3580(3)	2482(3)	9710(2)	30(1)
C(14)	3389(3)	3300(3)	8590(2)	24(1)
C(15)	3041(3)	6945(2)	5528(2)	16(1)
C(16)	2600(3)	8193(2)	4649(2)	17(1)
C(17)	3804(3)	8898(3)	4319(2)	24(1)
C(18)	3373(4)	10054(3)	3480(3)	30(1)
C(19)	1755(4)	10517(3)	2979(2)	27(1)
C(20)	552(3)	9826(2)	3321(2)	24(1)
C(21)	960(3)	8681(2)	4156(2)	20(1)
C(22)	1959(3)	6425(3)	846(2)	22(1)

Table 3. Bond lengths [Å] and angles [°] for 2e.

I-C(15)	2.103(2)
F(1)-C(22)	1.334(3)
F(2)-C(22)	1.345(3)
F(3)-C(22)	1.341(3)
O-C(8)	1.367(3)
O-C(1)	1.400(3)
N-C(8)	1.269(3)
N-C(7)	1.405(3)
C(1)-C(15)	1.340(3)
C(1)-C(2)	1.472(3)
C(2)-C(7)	1.397(3)
C(2)-C(3)	1.395(3)
C(3)-C(4)	1.390(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.389(3)
C(4)-C(22)	1.492(3)
C(5)-C(6)	1.379(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.398(3)
C(6)-H(6A)	0.9500
C(8)-C(9)	1.471(3)
C(9)-C(10)	1.392(4)
C(9)-C(14)	1.396(3)
C(10)-C(11)	1.387(4)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.377(4)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.375(4)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.389(4)
C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9500
C(15)-C(16)	1.484(3)
C(16)-C(21)	1.393(3)
C(16)-C(17)	1.394(3)
C(17)-C(18)	1.390(4)

C(17)-H(17A)	0.9500
C(18)-C(19)	1.380(4)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.385(4)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.379(3)
C(20)-H(20A)	0.9500
C(21)-H(21A)	0.9500

C(8)-O-C(1)	119.61(17)
C(8)-N-C(7)	117.4(2)
C(15)-C(1)-O	115.9(2)
C(15)-C(1)-C(2)	129.6(2)
O-C(1)-C(2)	114.51(19)
C(7)-C(2)-C(3)	119.4(2)
C(7)-C(2)-C(1)	116.5(2)
C(3)-C(2)-C(1)	124.1(2)
C(4)-C(3)-C(2)	119.4(2)
C(4)-C(3)-H(3A)	120.3
C(2)-C(3)-H(3A)	120.3
C(5)-C(4)-C(3)	121.1(2)
C(5)-C(4)-C(22)	119.7(2)
C(3)-C(4)-C(22)	119.2(2)
C(4)-C(5)-C(6)	119.6(2)
C(4)-C(5)-H(5A)	120.2
C(6)-C(5)-H(5A)	120.2
C(5)-C(6)-C(7)	120.0(2)
C(5)-C(6)-H(6A)	120.0
C(7)-C(6)-H(6A)	120.0
C(6)-C(7)-C(2)	120.3(2)
C(6)-C(7)-N	117.4(2)
C(2)-C(7)-N	122.3(2)
N-C(8)-O	125.5(2)
N-C(8)-C(9)	122.7(2)
O-C(8)-C(9)	111.78(19)
C(10)-C(9)-C(14)	119.9(2)
C(10)-C(9)-C(8)	118.7(2)
C(14)-C(9)-C(8)	121.4(2)

C(11)-C(10)-C(9)	119.7(3)
C(11)-C(10)-H(10A)	120.1
C(9)-C(10)-H(10A)	120.1
C(12)-C(11)-C(10)	120.5(3)
C(12)-C(11)-H(11A)	119.8
C(10)-C(11)-H(11A)	119.8
C(11)-C(12)-C(13)	119.8(3)
C(11)-C(12)-H(12A)	120.1
C(13)-C(12)-H(12A)	120.1
C(14)-C(13)-C(12)	121.0(3)
C(14)-C(13)-H(13A)	119.5
C(12)-C(13)-H(13A)	119.5
C(13)-C(14)-C(9)	119.0(2)
C(13)-C(14)-H(14A)	120.5
C(9)-C(14)-H(14A)	120.5
C(1)-C(15)-C(16)	126.3(2)
C(1)-C(15)-I	118.31(17)
C(16)-C(15)-I	115.16(15)
C(21)-C(16)-C(17)	119.3(2)
C(21)-C(16)-C(15)	120.0(2)
C(17)-C(16)-C(15)	120.8(2)
C(18)-C(17)-C(16)	119.9(2)
C(18)-C(17)-H(17A)	120.1
C(16)-C(17)-H(17A)	120.1
C(19)-C(18)-C(17)	120.5(2)
C(19)-C(18)-H(18A)	119.8
C(17)-C(18)-H(18A)	119.8
C(18)-C(19)-C(20)	119.6(2)
C(18)-C(19)-H(19A)	120.2
C(20)-C(19)-H(19A)	120.2
C(21)-C(20)-C(19)	120.5(2)
C(21)-C(20)-H(20A)	119.8
C(19)-C(20)-H(20A)	119.8
C(20)-C(21)-C(16)	120.2(2)
C(20)-C(21)-H(21A)	119.9
C(16)-C(21)-H(21A)	119.9
F(1)-C(22)-F(3)	107.0(2)
F(1)-C(22)-F(2)	106.0(2)

F(3)-C(22)-F(2)	105.62(19)
F(1)-C(22)-C(4)	113.7(2)
F(3)-C(22)-C(4)	112.6(2)
F(2)-C(22)-C(4)	111.3(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2e. 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}
I	24(1)	22(1)	17(1)	-6(1)	-5(1)	-5(1)
F(1)	61(1)	26(1)	20(1)	2(1)	-3(1)	-15(1)
F(2)	27(1)	47(1)	20(1)	-3(1)	8(1)	-2(1)
F(3)	30(1)	52(1)	20(1)	2(1)	-11(1)	-14(1)
O	21(1)	17(1)	14(1)	-1(1)	-4(1)	-6(1)
N	18(1)	17(1)	18(1)	-3(1)	-1(1)	-5(1)
C(1)	14(1)	19(1)	13(1)	0(1)	0(1)	-5(1)
C(2)	13(1)	16(1)	16(1)	-5(1)	0(1)	-2(1)
C(3)	17(1)	17(1)	17(1)	-6(1)	1(1)	-4(1)
C(4)	15(1)	18(1)	16(1)	-4(1)	1(1)	0(1)
C(5)	17(1)	22(1)	19(1)	-9(1)	-3(1)	-3(1)
C(6)	19(1)	18(1)	21(1)	-9(1)	0(1)	-7(1)
C(7)	13(1)	16(1)	17(1)	-5(1)	-1(1)	-1(1)
C(8)	14(1)	14(1)	20(1)	-2(1)	0(1)	-3(1)
C(9)	16(1)	21(1)	20(1)	2(1)	0(1)	-3(1)
C(10)	34(1)	24(1)	23(1)	2(1)	-5(1)	-10(1)
C(11)	38(2)	25(2)	31(2)	8(1)	-2(1)	-10(1)
C(12)	27(1)	36(2)	21(1)	9(1)	-1(1)	-1(1)
C(13)	28(1)	41(2)	17(1)	1(1)	-4(1)	-5(1)
C(14)	25(1)	26(1)	20(1)	-2(1)	-1(1)	-5(1)
C(15)	16(1)	21(1)	13(1)	-4(1)	-1(1)	-6(1)
C(16)	22(1)	16(1)	15(1)	-6(1)	1(1)	-6(1)
C(17)	28(1)	25(1)	24(1)	-5(1)	1(1)	-11(1)
C(18)	41(2)	24(1)	31(2)	-4(1)	4(1)	-20(1)
C(19)	46(2)	16(1)	19(1)	-4(1)	1(1)	-7(1)
C(20)	30(1)	19(1)	22(1)	-4(1)	-3(1)	-1(1)

C(21)	22(1)	17(1)	22(1)	-5(1)	1(1)	-4(1)
C(22)	23(1)	26(1)	18(1)	-3(1)	-2(1)	-6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 2e.

	x	y	z	U(eq)
H(3A)	2939	6822	2940	20
H(5A)	705	4389	1600	23
H(6A)	768	3133	3524	22
H(10A)	2167	1356	7063	33
H(11A)	2495	21	8965	39
H(12A)	3350	736	10626	37
H(13A)	3956	2759	10388	36
H(14A)	3608	4138	8504	29
H(17A)	4916	8588	4666	29
H(18A)	4199	10528	3250	36
H(19A)	1468	11305	2403	33
H(20A)	-562	10144	2977	29
H(21A)	120	8223	4396	25

2-(4-chlorophenyl)-4-(iodo(phenyl)methylene)-6-(trifluoromethyl)-4*H*-benzo[*d*][1,3]oxazine (2f).

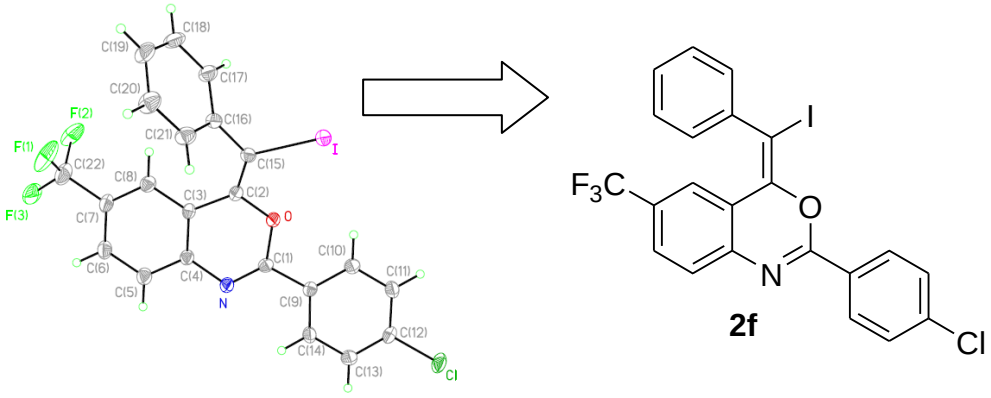


Table 1. Crystal data and structure refinement for 2f.

Identification code	2f	
Empirical formula	C22 H13 F3 I N O	
Formula weight	491.23	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.1298(2) Å	α= 80.375(2)°.
	b = 10.6900(3) Å	β= 87.307(2)°.
	c = 11.1738(3) Å	γ = 73.916(2)°.
Volume	919.94(4) $Å^3$	
Z	2	
Density (calculated)	1.773 Mg/m^3	
Absorption coefficient	1.782 mm^{-1}	
F(000)	480	
Crystal size	0.60 x 0.46 x 0.40 mm^3	
Theta range for data collection	2.94 to 29.28°.	
Index ranges	-10<=h<=10, -13<=k<=14, -14<=l<=14	
Reflections collected	8019	
Independent reflections	4233 [R(int) = 0.0202]	
Completeness to theta = 26.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.85697	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4233 / 0 / 253	
Goodness-of-fit on F^2	0.994	
Final R indices [I>2sigma(I)]	R1 = 0.0243, wR2 = 0.0599	
R indices (all data)	R1 = 0.0299, wR2 = 0.0611	
Largest diff. peak and hole	0.621 and -0.634 $e.Å^{-3}$	

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

	x	y	z	U(eq)
I	3733(1)	7123(1)	7268(1)	21(1)
F(1)	1975(2)	7674(2)	819(1)	36(1)
F(2)	3400(2)	5849(2)	283(1)	33(1)
F(3)	669(2)	6447(2)	130(1)	34(1)
O	3282(2)	4755(2)	6340(1)	17(1)
N	1901(2)	3434(2)	5522(2)	18(1)
C(1)	2912(3)	5770(2)	5340(2)	15(1)
C(2)	2431(3)	5380(2)	4233(2)	15(1)
C(3)	2478(3)	6085(2)	3068(2)	17(1)
C(4)	1845(3)	5699(2)	2097(2)	17(1)
C(5)	1175(3)	4620(2)	2266(2)	19(1)
C(6)	1197(3)	3886(2)	3407(2)	19(1)
C(7)	1849(3)	4250(2)	4391(2)	16(1)
C(8)	2622(3)	3702(2)	6392(2)	16(1)
C(9)	2870(3)	2870(2)	7595(2)	20(1)
C(10)	2529(3)	1648(3)	7737(2)	27(1)
C(11)	2720(4)	858(3)	8868(3)	32(1)
C(12)	3235(3)	1277(3)	9852(2)	31(1)
C(13)	3580(3)	2482(3)	9710(2)	30(1)
C(14)	3389(3)	3300(3)	8590(2)	24(1)
C(15)	3041(3)	6945(2)	5528(2)	16(1)
C(16)	2600(3)	8193(2)	4649(2)	17(1)
C(17)	3804(3)	8898(3)	4319(2)	24(1)
C(18)	3373(4)	10054(3)	3480(3)	30(1)
C(19)	1755(4)	10517(3)	2979(2)	27(1)
C(20)	552(3)	9826(2)	3321(2)	24(1)
C(21)	960(3)	8681(2)	4156(2)	20(1)
C(22)	1959(3)	6425(3)	846(2)	22(1)

Table 3. Bond lengths [Å] and angles [°] for 2f.

I-C(15)	2.103(2)
F(1)-C(22)	1.334(3)
F(2)-C(22)	1.345(3)
F(3)-C(22)	1.341(3)
O-C(8)	1.367(3)
O-C(1)	1.400(3)
N-C(8)	1.269(3)
N-C(7)	1.405(3)
C(1)-C(15)	1.340(3)
C(1)-C(2)	1.472(3)
C(2)-C(7)	1.397(3)
C(2)-C(3)	1.395(3)
C(3)-C(4)	1.390(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.389(3)
C(4)-C(22)	1.492(3)
C(5)-C(6)	1.379(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.398(3)
C(6)-H(6A)	0.9500
C(8)-C(9)	1.471(3)
C(9)-C(10)	1.392(4)
C(9)-C(14)	1.396(3)
C(10)-C(11)	1.387(4)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.377(4)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.375(4)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.389(4)
C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9500
C(15)-C(16)	1.484(3)
C(16)-C(21)	1.393(3)
C(16)-C(17)	1.394(3)
C(17)-C(18)	1.390(4)

C(17)-H(17A)	0.9500
C(18)-C(19)	1.380(4)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.385(4)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.379(3)
C(20)-H(20A)	0.9500
C(21)-H(21A)	0.9500

C(8)-O-C(1)	119.61(17)
C(8)-N-C(7)	117.4(2)
C(15)-C(1)-O	115.9(2)
C(15)-C(1)-C(2)	129.6(2)
O-C(1)-C(2)	114.51(19)
C(7)-C(2)-C(3)	119.4(2)
C(7)-C(2)-C(1)	116.5(2)
C(3)-C(2)-C(1)	124.1(2)
C(4)-C(3)-C(2)	119.4(2)
C(4)-C(3)-H(3A)	120.3
C(2)-C(3)-H(3A)	120.3
C(5)-C(4)-C(3)	121.1(2)
C(5)-C(4)-C(22)	119.7(2)
C(3)-C(4)-C(22)	119.2(2)
C(4)-C(5)-C(6)	119.6(2)
C(4)-C(5)-H(5A)	120.2
C(6)-C(5)-H(5A)	120.2
C(5)-C(6)-C(7)	120.0(2)
C(5)-C(6)-H(6A)	120.0
C(7)-C(6)-H(6A)	120.0
C(6)-C(7)-C(2)	120.3(2)
C(6)-C(7)-N	117.4(2)
C(2)-C(7)-N	122.3(2)
N-C(8)-O	125.5(2)
N-C(8)-C(9)	122.7(2)
O-C(8)-C(9)	111.78(19)
C(10)-C(9)-C(14)	119.9(2)
C(10)-C(9)-C(8)	118.7(2)
C(14)-C(9)-C(8)	121.4(2)

C(11)-C(10)-C(9)	119.7(3)
C(11)-C(10)-H(10A)	120.1
C(9)-C(10)-H(10A)	120.1
C(12)-C(11)-C(10)	120.5(3)
C(12)-C(11)-H(11A)	119.8
C(10)-C(11)-H(11A)	119.8
C(11)-C(12)-C(13)	119.8(3)
C(11)-C(12)-H(12A)	120.1
C(13)-C(12)-H(12A)	120.1
C(14)-C(13)-C(12)	121.0(3)
C(14)-C(13)-H(13A)	119.5
C(12)-C(13)-H(13A)	119.5
C(13)-C(14)-C(9)	119.0(2)
C(13)-C(14)-H(14A)	120.5
C(9)-C(14)-H(14A)	120.5
C(1)-C(15)-C(16)	126.3(2)
C(1)-C(15)-I	118.31(17)
C(16)-C(15)-I	115.16(15)
C(21)-C(16)-C(17)	119.3(2)
C(21)-C(16)-C(15)	120.0(2)
C(17)-C(16)-C(15)	120.8(2)
C(18)-C(17)-C(16)	119.9(2)
C(18)-C(17)-H(17A)	120.1
C(16)-C(17)-H(17A)	120.1
C(19)-C(18)-C(17)	120.5(2)
C(19)-C(18)-H(18A)	119.8
C(17)-C(18)-H(18A)	119.8
C(18)-C(19)-C(20)	119.6(2)
C(18)-C(19)-H(19A)	120.2
C(20)-C(19)-H(19A)	120.2
C(21)-C(20)-C(19)	120.5(2)
C(21)-C(20)-H(20A)	119.8
C(19)-C(20)-H(20A)	119.8
C(20)-C(21)-C(16)	120.2(2)
C(20)-C(21)-H(21A)	119.9
C(16)-C(21)-H(21A)	119.9
F(1)-C(22)-F(3)	107.0(2)
F(1)-C(22)-F(2)	106.0(2)

F(3)-C(22)-F(2)	105.62(19)
F(1)-C(22)-C(4)	113.7(2)
F(3)-C(22)-C(4)	112.6(2)
F(2)-C(22)-C(4)	111.3(2)

Symmetry transformations used to generate equivalent atoms:

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

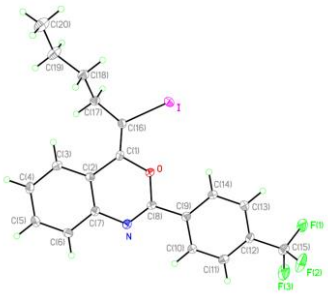
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I	24(1)	22(1)	17(1)	-6(1)	-5(1)	-5(1)
F(1)	61(1)	26(1)	20(1)	2(1)	-3(1)	-15(1)
F(2)	27(1)	47(1)	20(1)	-3(1)	8(1)	-2(1)
F(3)	30(1)	52(1)	20(1)	2(1)	-11(1)	-14(1)
O	21(1)	17(1)	14(1)	-1(1)	-4(1)	-6(1)
N	18(1)	17(1)	18(1)	-3(1)	-1(1)	-5(1)
C(1)	14(1)	19(1)	13(1)	0(1)	0(1)	-5(1)
C(2)	13(1)	16(1)	16(1)	-5(1)	0(1)	-2(1)
C(3)	17(1)	17(1)	17(1)	-6(1)	1(1)	-4(1)
C(4)	15(1)	18(1)	16(1)	-4(1)	1(1)	0(1)
C(5)	17(1)	22(1)	19(1)	-9(1)	-3(1)	-3(1)
C(6)	19(1)	18(1)	21(1)	-9(1)	0(1)	-7(1)
C(7)	13(1)	16(1)	17(1)	-5(1)	-1(1)	-1(1)
C(8)	14(1)	14(1)	20(1)	-2(1)	0(1)	-3(1)
C(9)	16(1)	21(1)	20(1)	2(1)	0(1)	-3(1)
C(10)	34(1)	24(1)	23(1)	2(1)	-5(1)	-10(1)
C(11)	38(2)	25(2)	31(2)	8(1)	-2(1)	-10(1)
C(12)	27(1)	36(2)	21(1)	9(1)	-1(1)	-1(1)
C(13)	28(1)	41(2)	17(1)	1(1)	-4(1)	-5(1)
C(14)	25(1)	26(1)	20(1)	-2(1)	-1(1)	-5(1)
C(15)	16(1)	21(1)	13(1)	-4(1)	-1(1)	-6(1)
C(16)	22(1)	16(1)	15(1)	-6(1)	1(1)	-6(1)
C(17)	28(1)	25(1)	24(1)	-5(1)	1(1)	-11(1)
C(18)	41(2)	24(1)	31(2)	-4(1)	4(1)	-20(1)
C(19)	46(2)	16(1)	19(1)	-4(1)	1(1)	-7(1)
C(20)	30(1)	19(1)	22(1)	-4(1)	-3(1)	-1(1)

C(21)	22(1)	17(1)	22(1)	-5(1)	1(1)	-4(1)
C(22)	23(1)	26(1)	18(1)	-3(1)	-2(1)	-6(1)

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

	x	y	z	U(eq)
H(3A)	2939	6822	2940	20
H(5A)	705	4389	1600	23
H(6A)	768	3133	3524	22
H(10A)	2167	1356	7063	33
H(11A)	2495	21	8965	39
H(12A)	3350	736	10626	37
H(13A)	3956	2759	10388	36
H(14A)	3608	4138	8504	29
H(17A)	4916	8588	4666	29
H(18A)	4199	10528	3250	36
H(19A)	1468	11305	2403	33
H(20A)	-562	10144	2977	29
H(21A)	120	8223	4396	25

4-(1-iodopentylidene)-2-(4-(trifluoromethyl)phenyl)-4H-benzo[d][1,3]oxazine (2j)



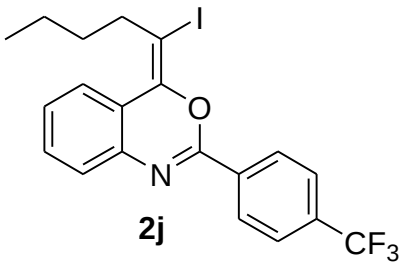


Table 1. Crystal data and structure refinement for 2j.

Identification code	2j
Empirical formula	C20 H17 F3 I N O
Formula weight	471.25
Temperature	100(2) K

Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 5.3560(2) Å	α= 107.043(6)°.
	b = 11.4646(7) Å	β= 96.345(4)°.
	c = 15.8424(10) Å	γ = 98.308(4)°.
Volume	908.22(9) $Å^3$	
Z	2	
Density (calculated)	1.723 Mg/m^3	
Absorption coefficient	1.801 mm^{-1}	
F(000)	464	
Crystal size	0.72 x 0.32 x 0.26 mm^3	
Theta range for data collection	3.60 to 29.17°.	
Index ranges	-7<=h<=6, -14<=k<=15, -20<=l<=21	
Reflections collected	7973	
Independent reflections	4162 [R(int) = 0.0178]	
Completeness to theta = 26.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.88597	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4162 / 0 / 235	
Goodness-of-fit on F^2	1.013	
Final R indices [I>2sigma(I)]	R1 = 0.0201, wR2 = 0.0480	
R indices (all data)	R1 = 0.0237, wR2 = 0.0486	
Largest diff. peak and hole	0.383 and -0.330 e.$Å^{-3}$	

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

	x	y	z	U(eq)
I	10801(1)	4090(1)	3872(1)	20(1)
F(1)	13480(3)	5226(1)	8850(1)	33(1)
F(2)	12767(3)	3398(1)	8962(1)	37(1)
F(3)	16596(2)	4424(1)	9250(1)	39(1)
O	13496(2)	2244(1)	4442(1)	15(1)
N	17081(3)	1396(1)	4779(1)	15(1)
C(1)	13860(3)	2080(2)	3558(1)	13(1)

C(2)	15359(3)	1114(2)	3215(1)	13(1)
C(3)	15211(3)	452(2)	2313(1)	16(1)
C(4)	16812(3)	-389(2)	2051(1)	18(1)
C(5)	18553(3)	-593(2)	2687(1)	17(1)
C(6)	18636(3)	5(2)	3587(1)	16(1)
C(7)	17016(3)	849(2)	3860(1)	14(1)
C(8)	15324(3)	2009(2)	5012(1)	13(1)
C(9)	15035(3)	2557(2)	5952(1)	13(1)
C(10)	16711(3)	2386(2)	6628(1)	17(1)
C(11)	16537(3)	2921(2)	7515(1)	19(1)
C(12)	14666(3)	3626(2)	7738(1)	15(1)
C(13)	12975(3)	3790(2)	7069(1)	17(1)
C(14)	13154(3)	3259(2)	6181(1)	16(1)
C(15)	14392(4)	4172(2)	8695(1)	21(1)
C(16)	12882(3)	2820(2)	3152(1)	14(1)
C(17)	13077(3)	2882(2)	2228(1)	16(1)
C(18)	10678(3)	2229(2)	1538(1)	19(1)
C(19)	10983(4)	2258(2)	596(1)	27(1)
C(20)	8572(4)	1641(2)	-79(2)	34(1)

Table 3. Bond lengths [Å] and angles [°] for 2j.

I-C(16)	2.1070(17)
F(1)-C(15)	1.335(2)
F(2)-C(15)	1.343(2)
F(3)-C(15)	1.332(2)
O-C(8)	1.368(2)
O-C(1)	1.396(2)
N-C(8)	1.277(2)
N-C(7)	1.402(2)
C(1)-C(16)	1.335(2)
C(1)-C(2)	1.471(2)
C(2)-C(3)	1.396(3)
C(2)-C(7)	1.408(2)
C(3)-C(4)	1.386(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.391(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.382(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.399(2)
C(6)-H(6A)	0.9500
C(8)-C(9)	1.472(3)
C(9)-C(14)	1.392(2)
C(9)-C(10)	1.396(2)
C(10)-C(11)	1.379(3)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.389(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.390(3)
C(12)-C(15)	1.493(3)
C(13)-C(14)	1.380(3)
C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9500
C(16)-C(17)	1.500(2)
C(17)-C(18)	1.529(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900

C(18)-C(19)	1.528(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.516(3)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(8)-O-C(1)	118.69(13)
C(8)-N-C(7)	116.86(16)
C(16)-C(1)-O	116.96(16)
C(16)-C(1)-C(2)	129.16(17)
O-C(1)-C(2)	113.86(15)
C(3)-C(2)-C(7)	119.12(16)
C(3)-C(2)-C(1)	124.59(16)
C(7)-C(2)-C(1)	116.28(16)
C(2)-C(3)-C(4)	120.30(17)
C(2)-C(3)-H(3A)	119.8
C(4)-C(3)-H(3A)	119.8
C(5)-C(4)-C(3)	120.18(18)
C(5)-C(4)-H(4A)	119.9
C(3)-C(4)-H(4A)	119.9
C(4)-C(5)-C(6)	120.37(17)
C(4)-C(5)-H(5A)	119.8
C(6)-C(5)-H(5A)	119.8
C(5)-C(6)-C(7)	119.90(17)
C(5)-C(6)-H(6A)	120.1
C(7)-C(6)-H(6A)	120.1
C(6)-C(7)-C(2)	119.90(17)
C(6)-C(7)-N	118.13(16)
C(2)-C(7)-N	121.96(16)
N-C(8)-O	125.58(17)
N-C(8)-C(9)	122.98(16)
O-C(8)-C(9)	111.43(14)
C(14)-C(9)-C(10)	119.45(17)
C(14)-C(9)-C(8)	121.28(16)
C(10)-C(9)-C(8)	119.26(16)

C(11)-C(10)-C(9)	120.52(17)
C(11)-C(10)-H(10A)	119.7
C(9)-C(10)-H(10A)	119.7
C(10)-C(11)-C(12)	119.72(17)
C(10)-C(11)-H(11A)	120.1
C(12)-C(11)-H(11A)	120.1
C(11)-C(12)-C(13)	120.05(17)
C(11)-C(12)-C(15)	120.32(17)
C(13)-C(12)-C(15)	119.59(16)
C(12)-C(13)-C(14)	120.27(17)
C(12)-C(13)-H(13A)	119.9
C(14)-C(13)-H(13A)	119.9
C(9)-C(14)-C(13)	119.99(17)
C(9)-C(14)-H(14A)	120.0
C(13)-C(14)-H(14A)	120.0
F(3)-C(15)-F(1)	106.79(16)
F(3)-C(15)-F(2)	106.24(17)
F(1)-C(15)-F(2)	105.93(16)
F(3)-C(15)-C(12)	112.70(16)
F(1)-C(15)-C(12)	112.90(16)
F(2)-C(15)-C(12)	111.78(15)
C(1)-C(16)-C(17)	128.23(16)
C(1)-C(16)-I	117.75(14)
C(17)-C(16)-I	114.02(12)
C(16)-C(17)-C(18)	114.34(15)
C(16)-C(17)-H(17A)	108.7
C(18)-C(17)-H(17A)	108.7
C(16)-C(17)-H(17B)	108.7
C(18)-C(17)-H(17B)	108.7
H(17A)-C(17)-H(17B)	107.6
C(17)-C(18)-C(19)	112.99(15)
C(17)-C(18)-H(18A)	109.0
C(19)-C(18)-H(18A)	109.0
C(17)-C(18)-H(18B)	109.0
C(19)-C(18)-H(18B)	109.0
H(18A)-C(18)-H(18B)	107.8
C(20)-C(19)-C(18)	112.62(17)
C(20)-C(19)-H(19A)	109.1

C(18)-C(19)-H(19A)	109.1
C(20)-C(19)-H(19B)	109.1
C(18)-C(19)-H(19B)	109.1
H(19A)-C(19)-H(19B)	107.8
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2j. 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}
I	25(1)	19(1)	20(1)	7(1)	6(1)	12(1)
F(1)	57(1)	26(1)	18(1)	3(1)	13(1)	20(1)
F(2)	58(1)	27(1)	22(1)	4(1)	20(1)	-5(1)
F(3)	35(1)	57(1)	13(1)	-4(1)	-4(1)	11(1)
O	17(1)	20(1)	11(1)	6(1)	2(1)	7(1)
N	17(1)	16(1)	12(1)	3(1)	1(1)	4(1)
C(1)	13(1)	15(1)	11(1)	3(1)	3(1)	1(1)
C(2)	13(1)	13(1)	14(1)	5(1)	2(1)	2(1)
C(3)	17(1)	18(1)	14(1)	6(1)	1(1)	3(1)
C(4)	22(1)	16(1)	14(1)	2(1)	6(1)	3(1)
C(5)	19(1)	15(1)	19(1)	4(1)	6(1)	5(1)
C(6)	15(1)	15(1)	18(1)	5(1)	1(1)	4(1)
C(7)	15(1)	13(1)	13(1)	4(1)	2(1)	2(1)
C(8)	14(1)	13(1)	12(1)	5(1)	1(1)	2(1)
C(9)	14(1)	13(1)	13(1)	4(1)	1(1)	1(1)
C(10)	19(1)	19(1)	14(1)	6(1)	3(1)	7(1)
C(11)	19(1)	23(1)	14(1)	6(1)	-1(1)	6(1)
C(12)	18(1)	14(1)	11(1)	3(1)	4(1)	1(1)
C(13)	20(1)	17(1)	17(1)	5(1)	5(1)	7(1)
C(14)	17(1)	20(1)	13(1)	6(1)	1(1)	6(1)

C(15)	28(1)	19(1)	15(1)	5(1)	4(1)	3(1)
C(16)	14(1)	14(1)	14(1)	3(1)	3(1)	4(1)
C(17)	17(1)	17(1)	16(1)	9(1)	3(1)	3(1)
C(18)	19(1)	23(1)	16(1)	9(1)	3(1)	3(1)
C(19)	28(1)	35(1)	17(1)	11(1)	1(1)	-1(1)
C(20)	34(1)	41(1)	22(1)	9(1)	-2(1)	2(1)

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

	x	y	z	U(eq)
H(3A)	14007	578	1876	19
H(4A)	16719	-828	1435	21
H(5A)	19692	-1146	2502	21
H(6A)	19791	-157	4020	19
H(10A)	17981	1897	6474	20
H(11A)	17692	2807	7971	23
H(13A)	11691	4269	7224	21
H(14A)	11994	3372	5726	20
H(17A)	14540	2503	2024	19
H(17B)	13444	3765	2256	19
H(18A)	9227	2633	1724	23
H(18B)	10260	1354	1526	23
H(19A)	11449	3132	610	32
H(19B)	12400	1831	402	32
H(20A)	8867	1680	-670	50
H(20B)	7172	2072	101	50
H(20C)	8119	770	-104	50

4-(iodo(trimethylsilyl)methylene)-2-(4-nitrophenyl)-4H-benzo[d][1,3]oxazine (2k)

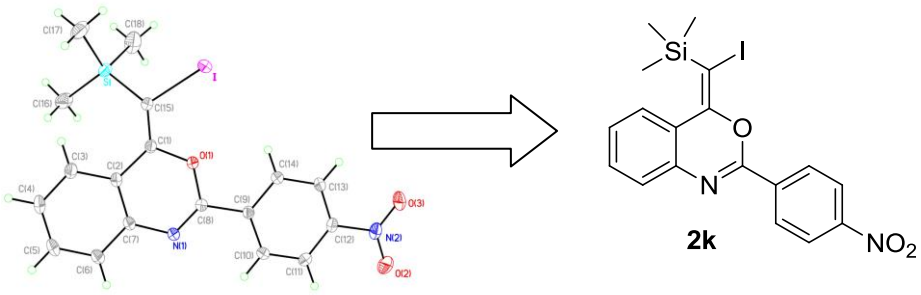


Table 1. Crystal data and structure refinement for 2k.

Identification code	2k	
Empirical formula	C18 H17 I N2 O3 Si	
Formula weight	464.33	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 6.6498(4) Å	α= 90°.
	b = 20.2549(11) Å	β= 98.4040(10)°.
	c = 14.0362(8) Å	γ = 90°.
Volume	1870.25(19) $Å^3$	
Z	4	
Density (calculated)	1.649 Mg/m^3	
Absorption coefficient	1.795 mm^{-1}	
F(000)	920	
Crystal size	0.56 x 0.40 x 0.21 mm^3	
Theta range for data collection	1.78 to 26.02°.	
Index ranges	-8<=h<=8, -23<=k<=25, -15<=l<=17	
Reflections collected	10400	
Independent reflections	3668 [R(int) = 0.0255]	
Completeness to theta = 26.02°	99.6 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000000 and 0.778417	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3668 / 0 / 226	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0276, wR2 = 0.0746	
R indices (all data)	R1 = 0.0338, wR2 = 0.0786	
Largest diff. peak and hole	0.638 and -0.646 $e.Å^{-3}$	

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

	x	y	z	U(eq)
I	2496(1)	5116(1)	9241(1)	58(1)
Si	-967(1)	5392(1)	7342(1)	50(1)
O(1)	889(3)	3743(1)	9070(1)	43(1)
O(2)	9003(4)	1456(1)	10539(2)	87(1)
O(3)	9950(3)	2432(1)	10993(2)	73(1)
N(1)	-280(3)	2722(1)	8420(2)	39(1)
N(2)	8685(4)	2043(1)	10607(2)	54(1)
C(1)	-464(3)	4109(1)	8415(2)	38(1)
C(2)	-2251(3)	3729(1)	8005(2)	38(1)
C(3)	-4135(4)	4015(2)	7661(2)	49(1)
C(4)	-5741(4)	3627(2)	7271(2)	54(1)
C(5)	-5531(4)	2949(2)	7229(2)	53(1)
C(6)	-3719(4)	2654(1)	7600(2)	46(1)
C(7)	-2079(3)	3039(1)	8003(2)	38(1)
C(8)	1032(4)	3077(1)	8928(2)	36(1)
C(9)	2973(4)	2807(1)	9423(2)	36(1)
C(10)	3307(4)	2131(1)	9430(2)	43(1)
C(11)	5181(4)	1875(1)	9814(2)	47(1)
C(12)	6685(4)	2304(1)	10199(2)	41(1)
C(13)	6381(4)	2974(1)	10230(2)	45(1)
C(14)	4510(4)	3230(1)	9839(2)	42(1)
C(15)	-10(4)	4743(1)	8266(2)	43(1)
C(16)	-2605(7)	5067(2)	6243(3)	76(1)
C(17)	-2359(6)	6022(2)	7951(3)	81(1)
C(18)	1313(6)	5766(3)	6920(4)	104(2)

Table 3. Bond lengths [Å] and angles [°] for 2k.

I-C(15)	2.134(3)
Si-C(17)	1.855(4)
Si-C(16)	1.873(4)
Si-C(18)	1.867(4)
Si-C(15)	1.892(3)
O(1)-C(8)	1.368(3)
O(1)-C(1)	1.400(3)
O(2)-N(2)	1.214(4)
O(3)-N(2)	1.219(3)
N(1)-C(8)	1.267(3)
N(1)-C(7)	1.407(3)
N(2)-C(12)	1.467(3)
C(1)-C(15)	1.342(4)
C(1)-C(2)	1.461(3)
C(2)-C(3)	1.401(3)
C(2)-C(7)	1.403(4)
C(3)-C(4)	1.373(4)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.382(5)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.378(4)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.392(3)
C(6)-H(6A)	0.9300
C(8)-C(9)	1.479(3)
C(9)-C(10)	1.386(4)
C(9)-C(14)	1.394(3)
C(10)-C(11)	1.385(4)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.374(4)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.374(4)
C(13)-C(14)	1.385(4)
C(13)-H(13A)	0.9300
C(14)-H(14A)	0.9300
C(16)-H(16A)	0.9600

C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600

C(17)-Si-C(16)	110.6(2)
C(17)-Si-C(18)	110.5(2)
C(16)-Si-C(18)	106.4(2)
C(17)-Si-C(15)	107.63(15)
C(16)-Si-C(15)	114.61(14)
C(18)-Si-C(15)	106.98(16)
C(8)-O(1)-C(1)	118.47(19)
C(8)-N(1)-C(7)	116.6(2)
O(3)-N(2)-O(2)	123.4(3)
O(3)-N(2)-C(12)	117.9(3)
O(2)-N(2)-C(12)	118.7(3)
C(15)-C(1)-O(1)	118.1(2)
C(15)-C(1)-C(2)	129.1(2)
O(1)-C(1)-C(2)	112.8(2)
C(3)-C(2)-C(7)	118.7(2)
C(3)-C(2)-C(1)	123.7(2)
C(7)-C(2)-C(1)	117.6(2)
C(4)-C(3)-C(2)	120.4(3)
C(4)-C(3)-H(3A)	119.8
C(2)-C(3)-H(3A)	119.8
C(3)-C(4)-C(5)	120.5(3)
C(3)-C(4)-H(4A)	119.7
C(5)-C(4)-H(4A)	119.7
C(6)-C(5)-C(4)	120.2(3)
C(6)-C(5)-H(5A)	119.9
C(4)-C(5)-H(5A)	119.9
C(5)-C(6)-C(7)	120.0(3)
C(5)-C(6)-H(6A)	120.0
C(7)-C(6)-H(6A)	120.0

C(6)-C(7)-N(1)	118.8(2)
C(6)-C(7)-C(2)	120.0(2)
N(1)-C(7)-C(2)	121.2(2)
N(1)-C(8)-O(1)	125.8(2)
N(1)-C(8)-C(9)	122.4(2)
O(1)-C(8)-C(9)	111.8(2)
C(10)-C(9)-C(14)	119.7(2)
C(10)-C(9)-C(8)	119.8(2)
C(14)-C(9)-C(8)	120.4(2)
C(9)-C(10)-C(11)	120.5(2)
C(9)-C(10)-H(10A)	119.8
C(11)-C(10)-H(10A)	119.8
C(12)-C(11)-C(10)	118.6(2)
C(12)-C(11)-H(11A)	120.7
C(10)-C(11)-H(11A)	120.7
C(11)-C(12)-C(13)	122.3(2)
C(11)-C(12)-N(2)	119.5(2)
C(13)-C(12)-N(2)	118.1(2)
C(12)-C(13)-C(14)	119.0(2)
C(12)-C(13)-H(13A)	120.5
C(14)-C(13)-H(13A)	120.5
C(9)-C(14)-C(13)	119.9(2)
C(9)-C(14)-H(14A)	120.1
C(13)-C(14)-H(14A)	120.1
C(1)-C(15)-Si	135.4(2)
C(1)-C(15)-I	114.28(19)
Si-C(15)-I	110.25(12)
Si-C(16)-H(16A)	109.5
Si-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
Si-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
Si-C(17)-H(17A)	109.5
Si-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
Si-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5

H(17B)-C(17)-H(17C)	109.5
Si-C(18)-H(18A)	109.5
Si-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
Si-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

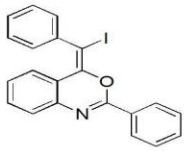
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I	49(1)	41(1)	79(1)	-6(1)	-11(1)	-6(1)
Si	47(1)	41(1)	61(1)	9(1)	4(1)	6(1)
O(1)	40(1)	34(1)	49(1)	-1(1)	-11(1)	1(1)
O(2)	65(2)	65(2)	125(2)	15(2)	-9(2)	25(1)
O(3)	41(1)	90(2)	81(2)	2(1)	-14(1)	6(1)
N(1)	36(1)	38(1)	42(1)	-1(1)	-2(1)	-2(1)
N(2)	41(1)	68(2)	53(1)	14(1)	3(1)	10(1)
C(1)	33(1)	40(1)	40(1)	1(1)	1(1)	5(1)
C(2)	32(1)	45(1)	38(1)	2(1)	2(1)	1(1)
C(3)	38(1)	55(2)	52(2)	7(1)	3(1)	6(1)
C(4)	31(1)	80(2)	49(2)	9(1)	-2(1)	4(1)
C(5)	36(1)	74(2)	46(2)	-4(1)	-3(1)	-10(1)
C(6)	42(1)	53(2)	42(1)	-3(1)	0(1)	-8(1)
C(7)	34(1)	45(1)	34(1)	0(1)	3(1)	-4(1)
C(8)	35(1)	35(1)	37(1)	1(1)	3(1)	0(1)
C(9)	35(1)	40(1)	33(1)	2(1)	0(1)	0(1)
C(10)	42(1)	37(1)	49(1)	-3(1)	-2(1)	-4(1)
C(11)	48(2)	38(1)	53(2)	4(1)	3(1)	5(1)
C(12)	36(1)	50(1)	37(1)	7(1)	1(1)	5(1)
C(13)	38(1)	48(2)	45(1)	0(1)	-6(1)	-5(1)
C(14)	42(1)	36(1)	46(1)	0(1)	-3(1)	0(1)
C(15)	36(1)	37(1)	52(2)	0(1)	-1(1)	4(1)
C(16)	110(3)	58(2)	52(2)	13(2)	-10(2)	6(2)

C(17)	94(3)	62(2)	86(3)	0(2)	6(2)	30(2)
C(18)	68(2)	118(4)	125(4)	65(3)	16(2)	-6(2)

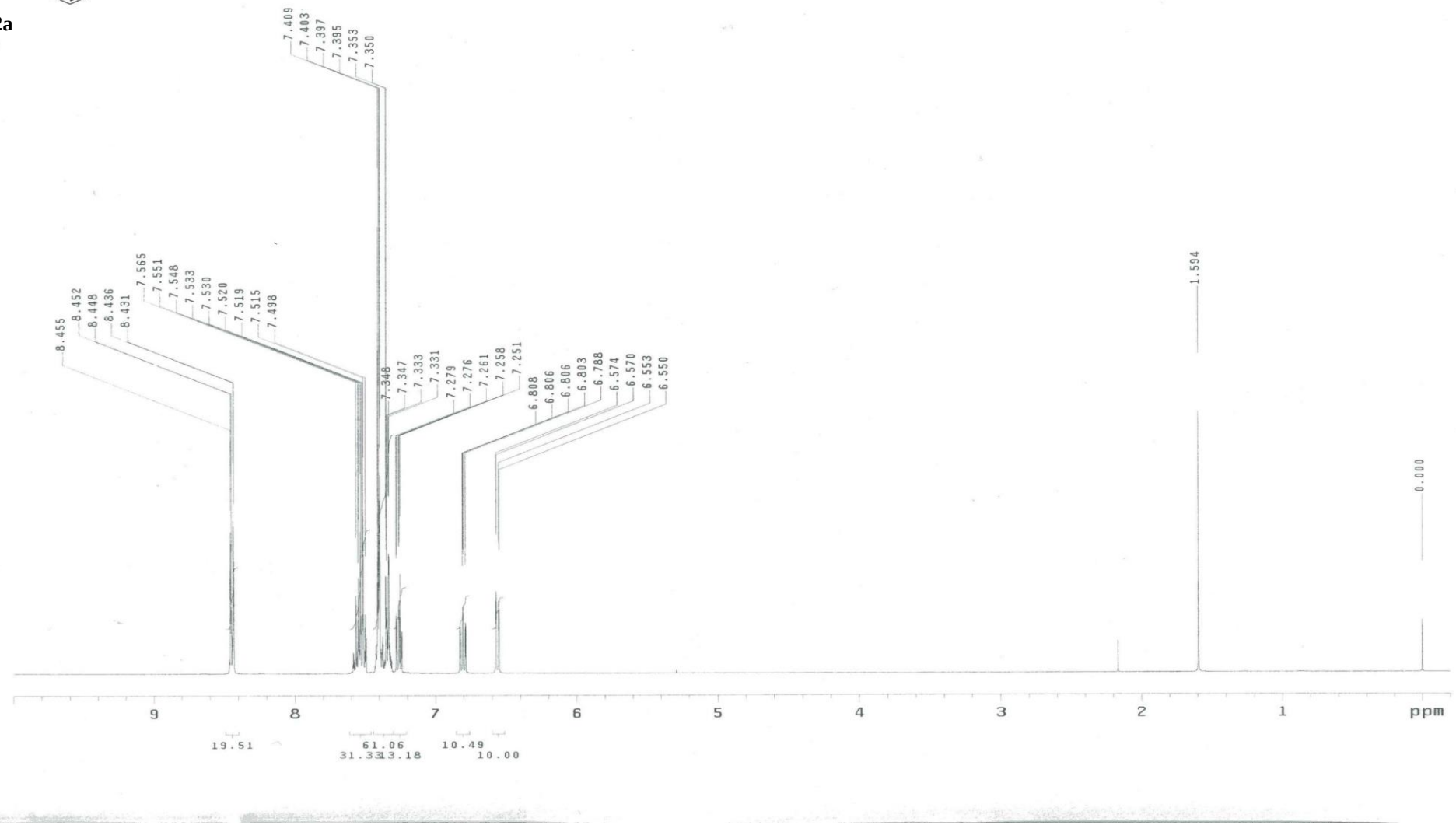
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2k.

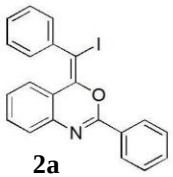
	x	y	z	U(eq)
H(3A)	-4301	4470	7697	58
H(4A)	-6979	3822	7033	65
H(5A)	-6618	2692	6950	63
H(6A)	-3590	2197	7581	55
H(10A)	2264	1848	9175	52
H(11A)	5417	1423	9812	56
H(13A)	7416	3252	10510	54
H(14A)	4280	3682	9853	51
H(16A)	-3030	5426	5814	113
H(16B)	-3779	4854	6428	113
H(16C)	-1846	4754	5925	113
H(17A)	-2867	6358	7497	122
H(17B)	-1455	6217	8471	122
H(17C)	-3475	5816	8200	122
H(18A)	888	6100	6448	155
H(18B)	2056	5430	6638	155
H(18C)	2169	5961	7457	155

3. ^{1}H NMR and **^{13}C NMR** spectra of compounds 2**a**-2**o.**

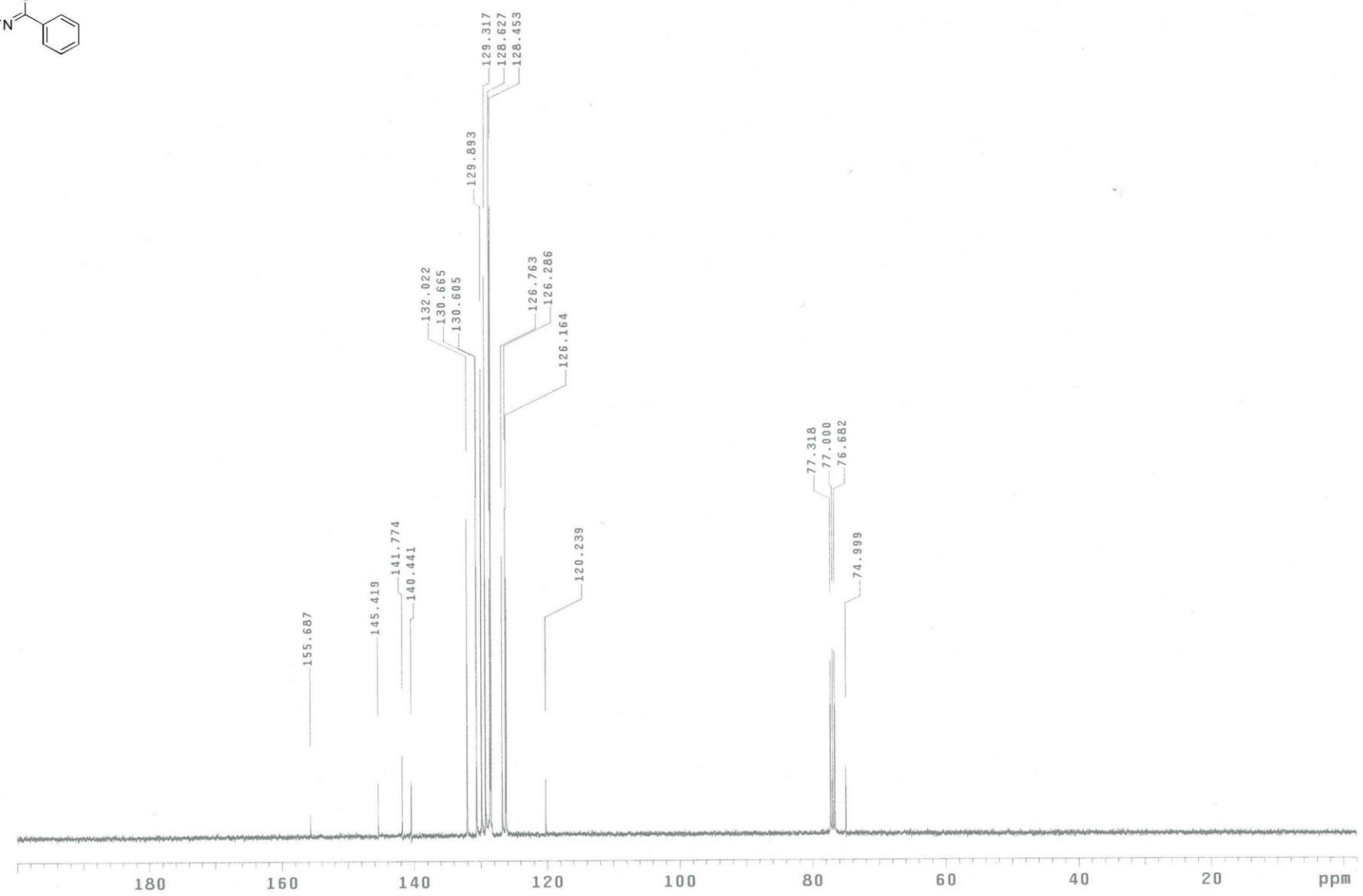


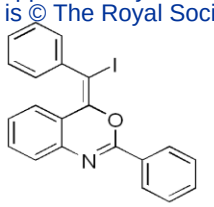
2a



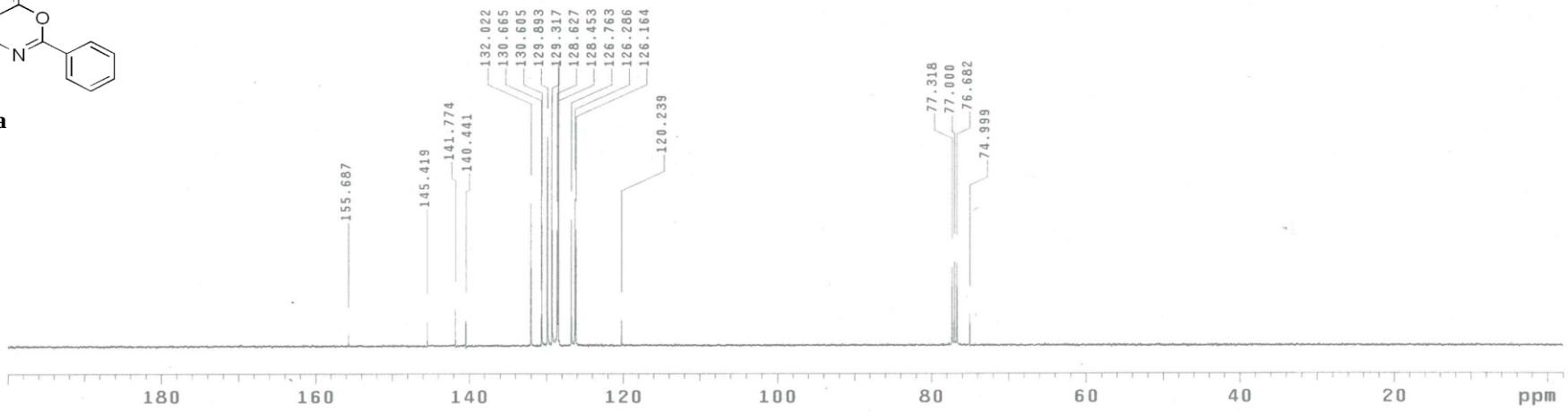


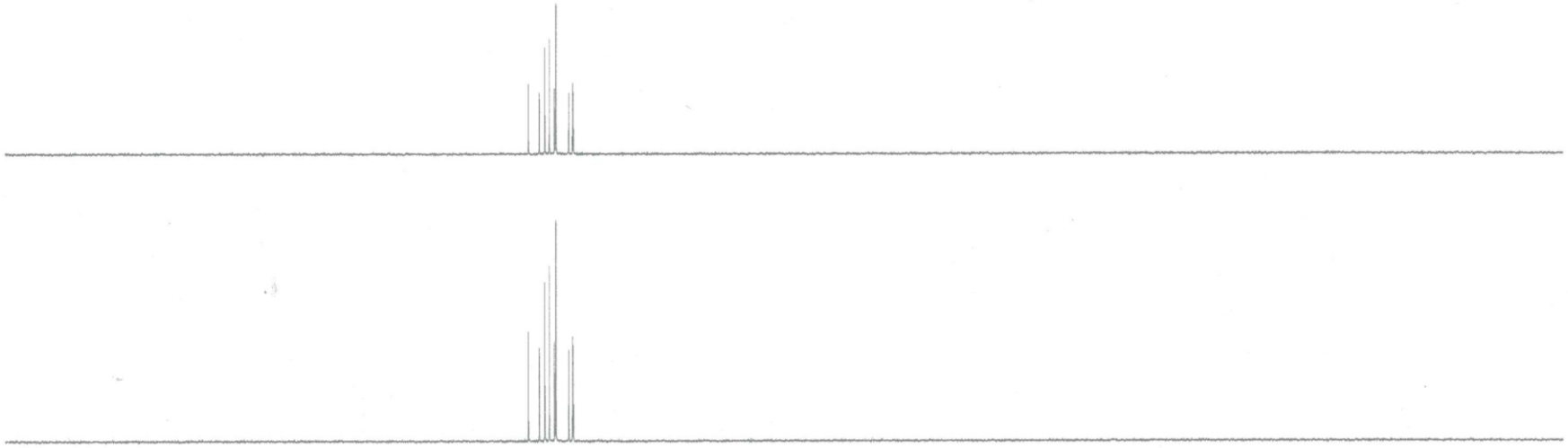
2a

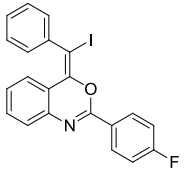




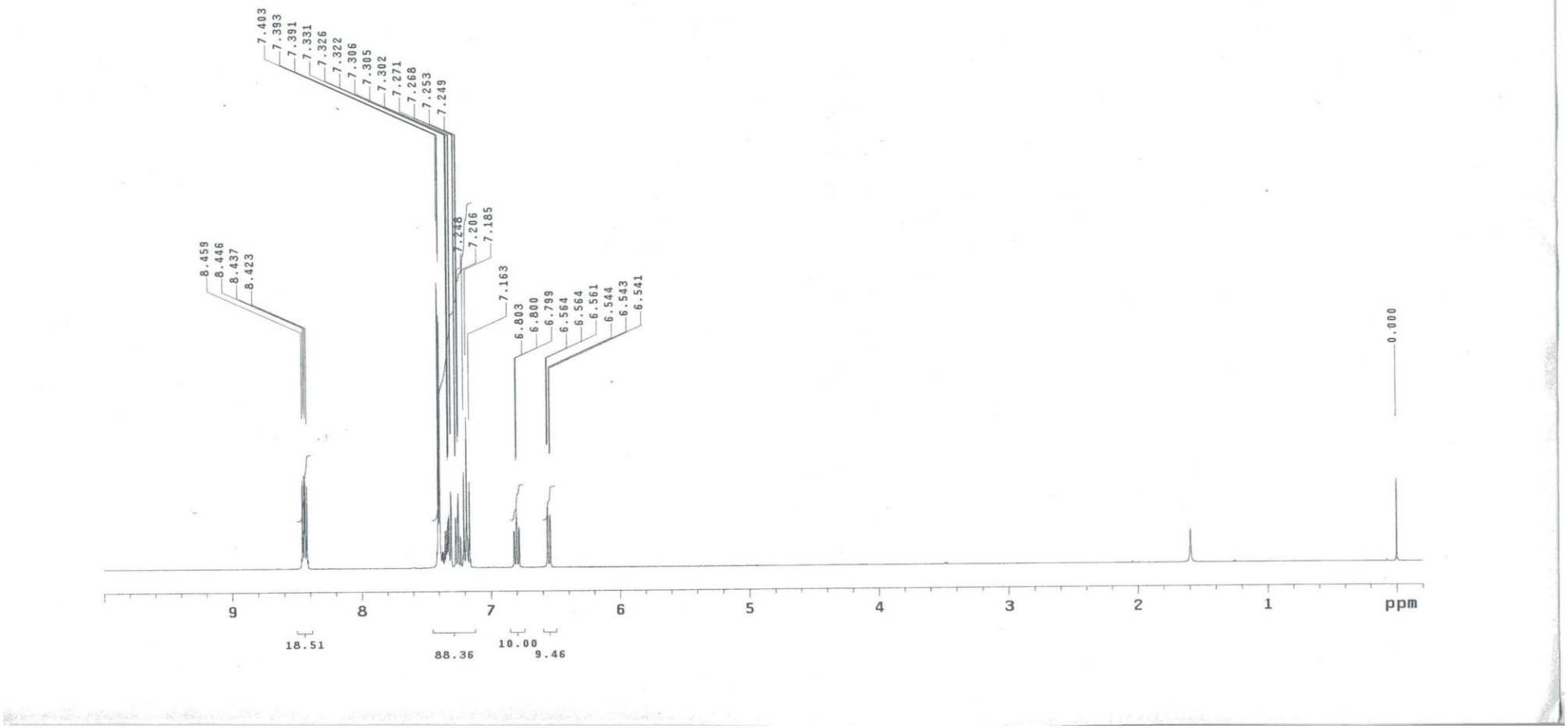
2a

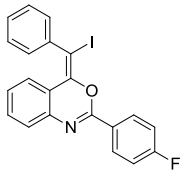




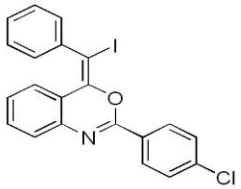


2b

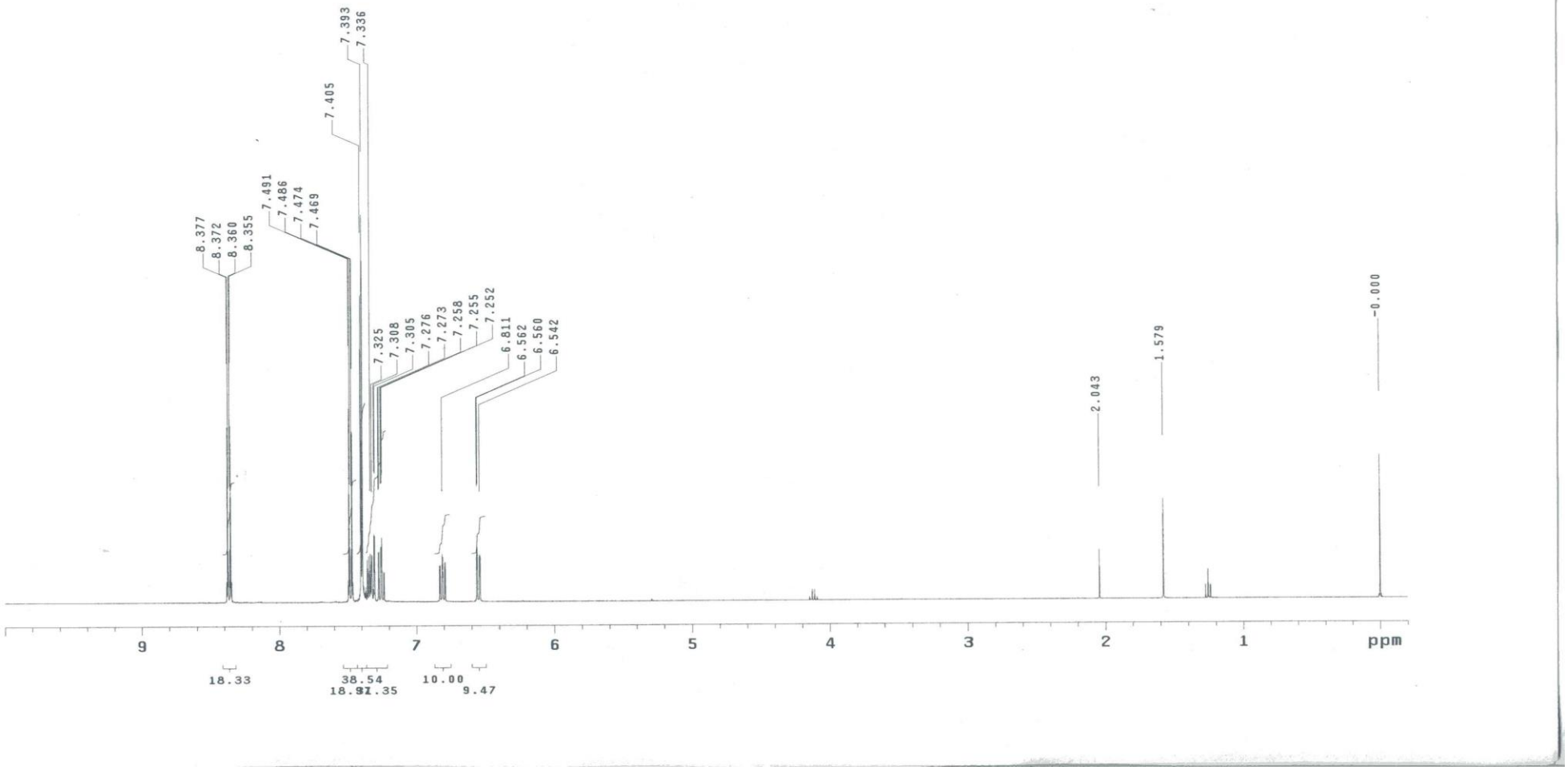


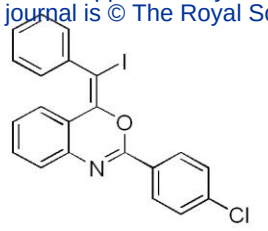


2b

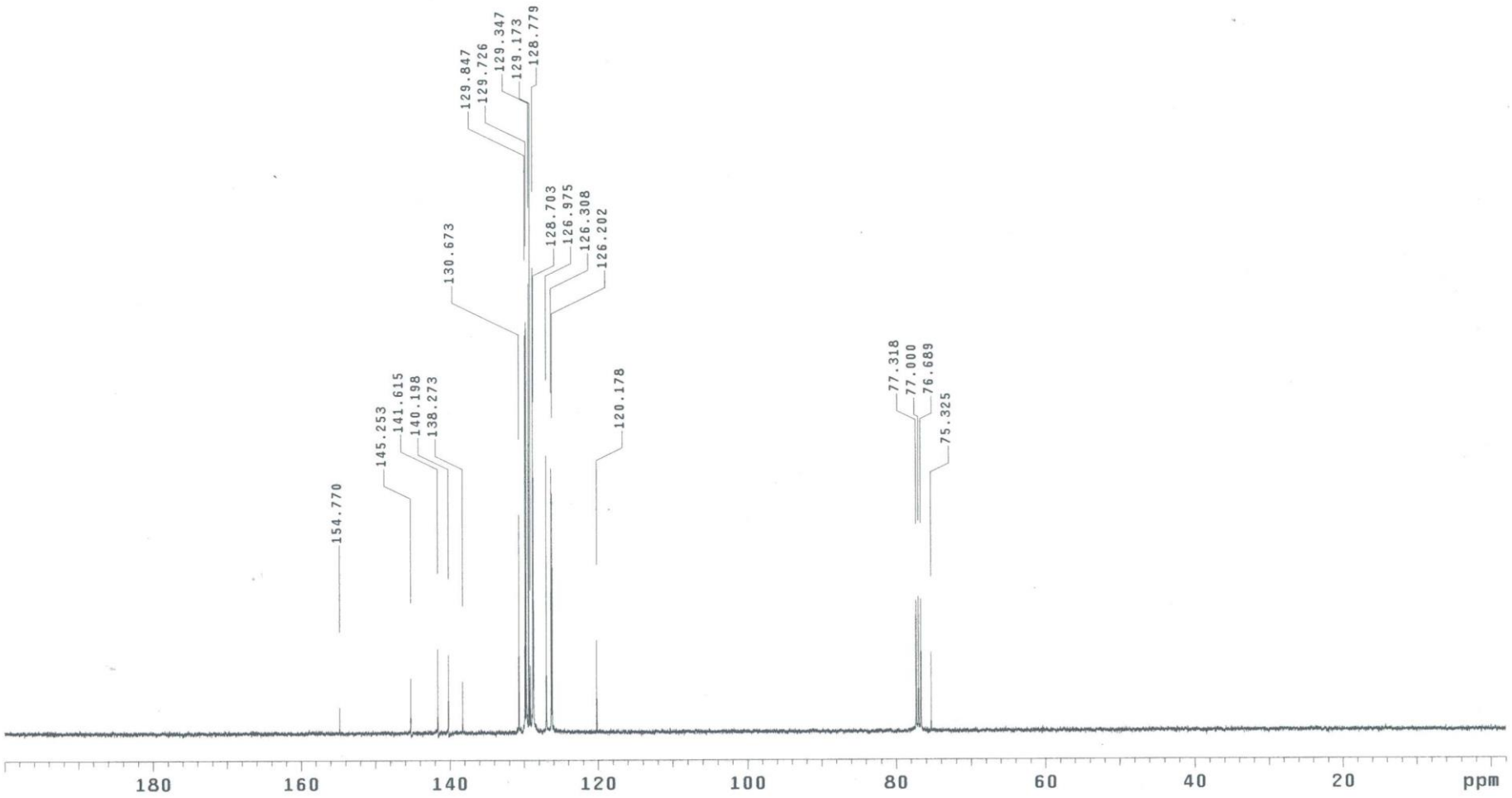


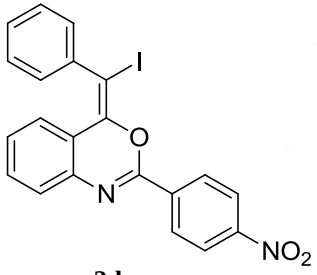
2c



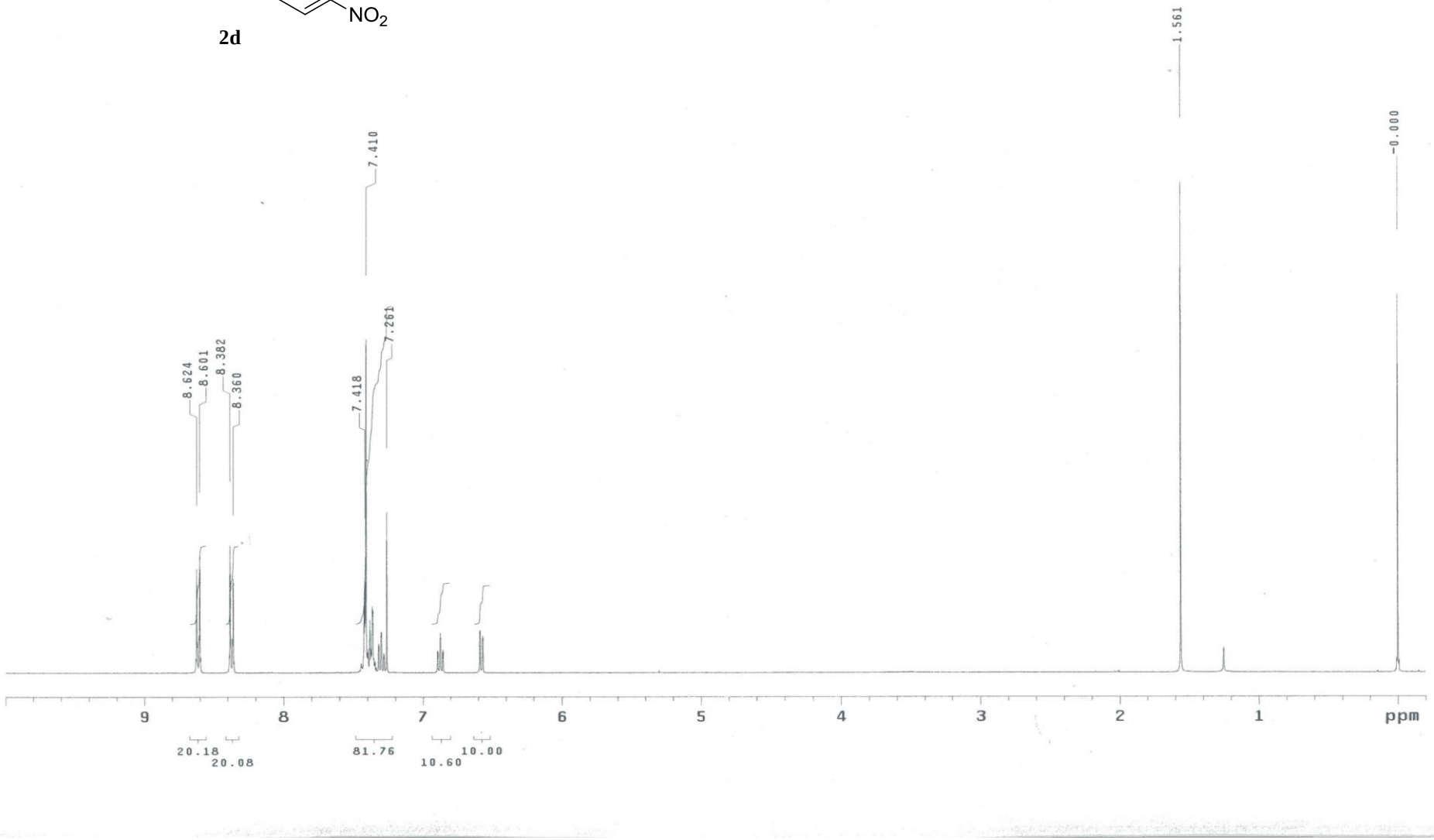


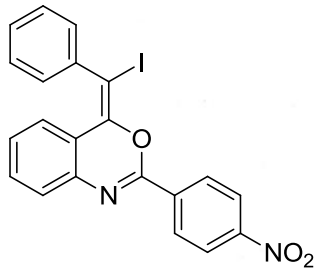
2c





2d





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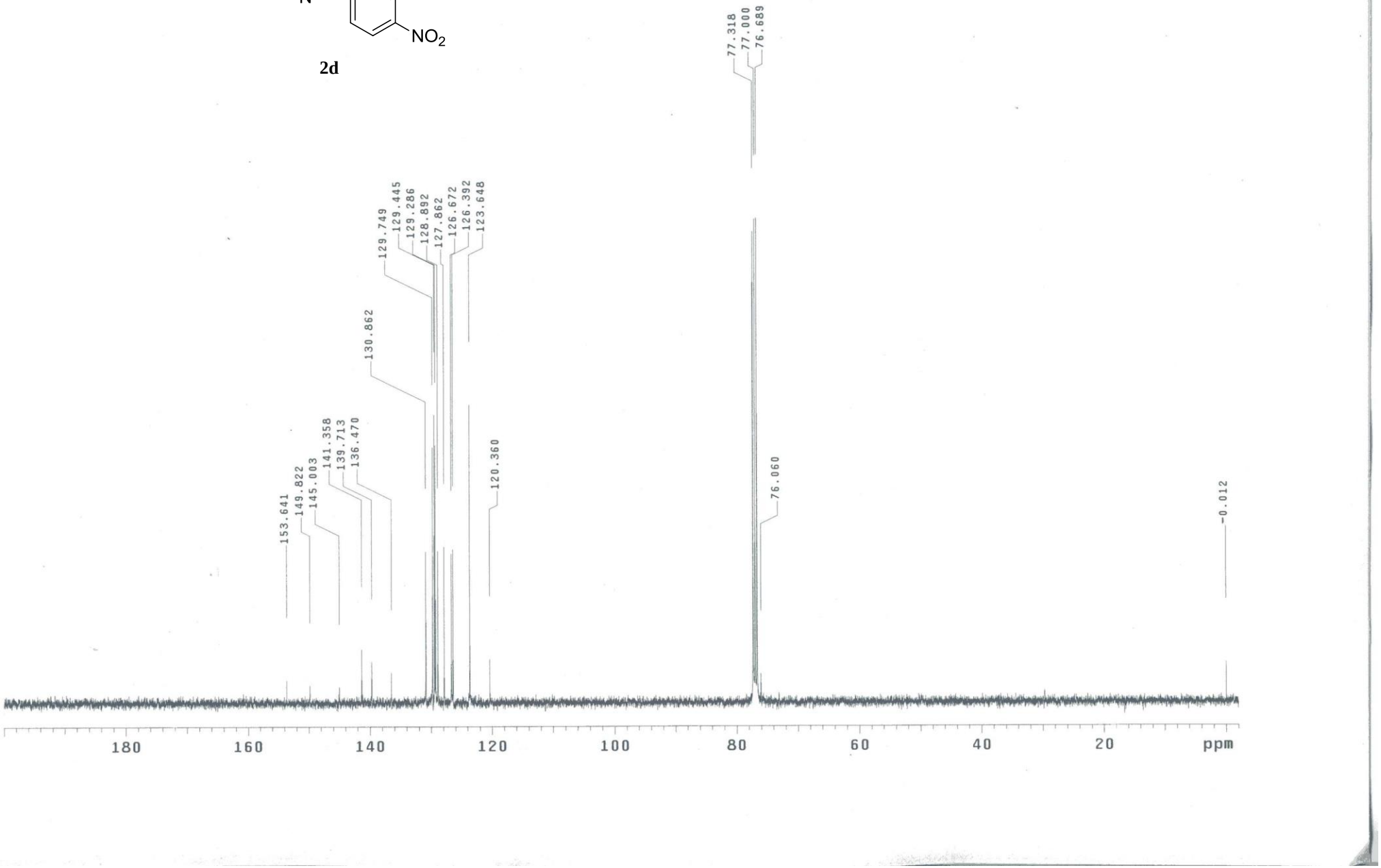

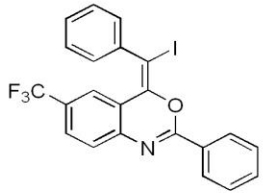

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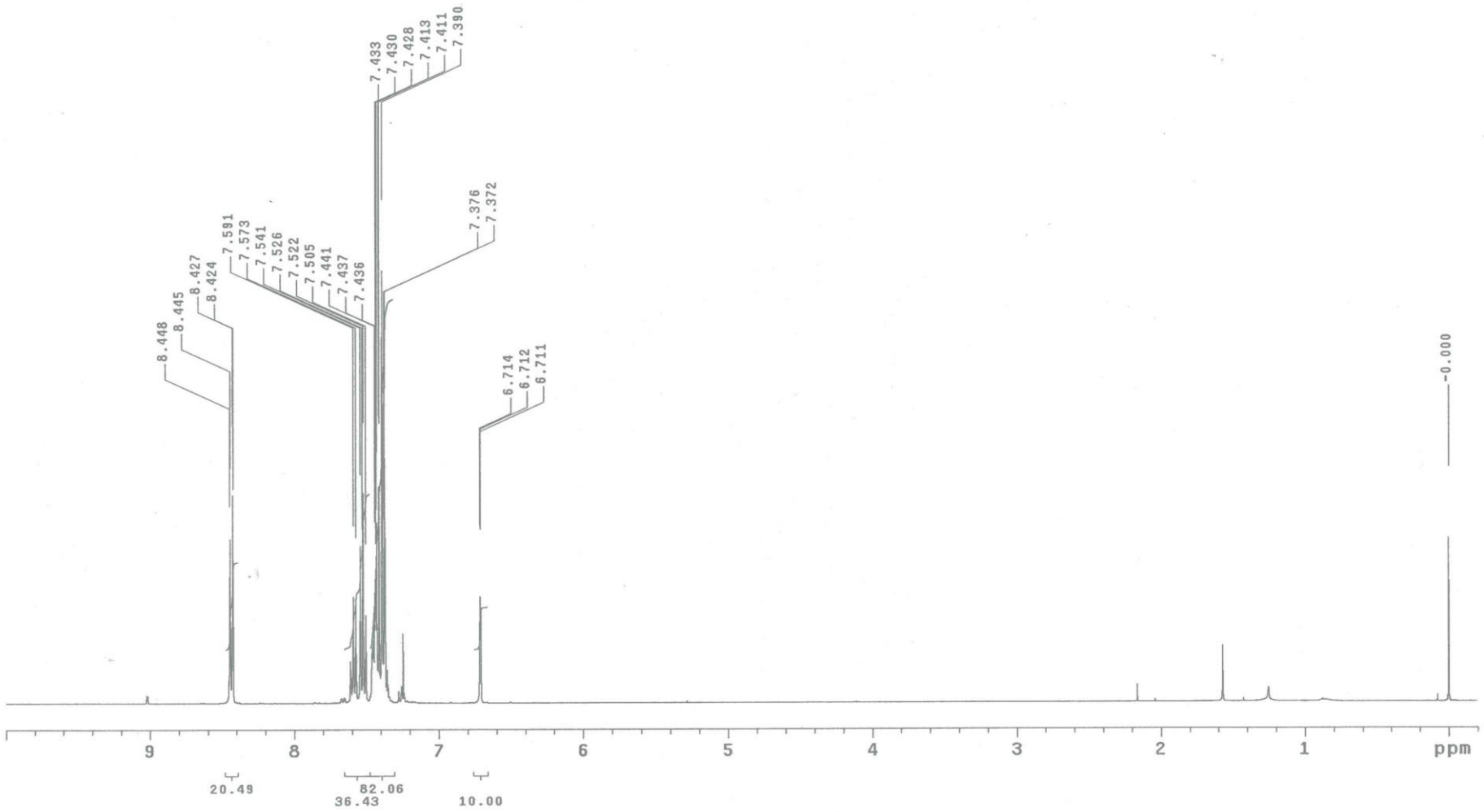

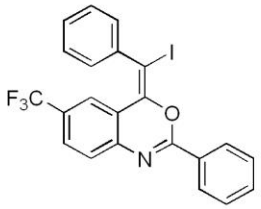

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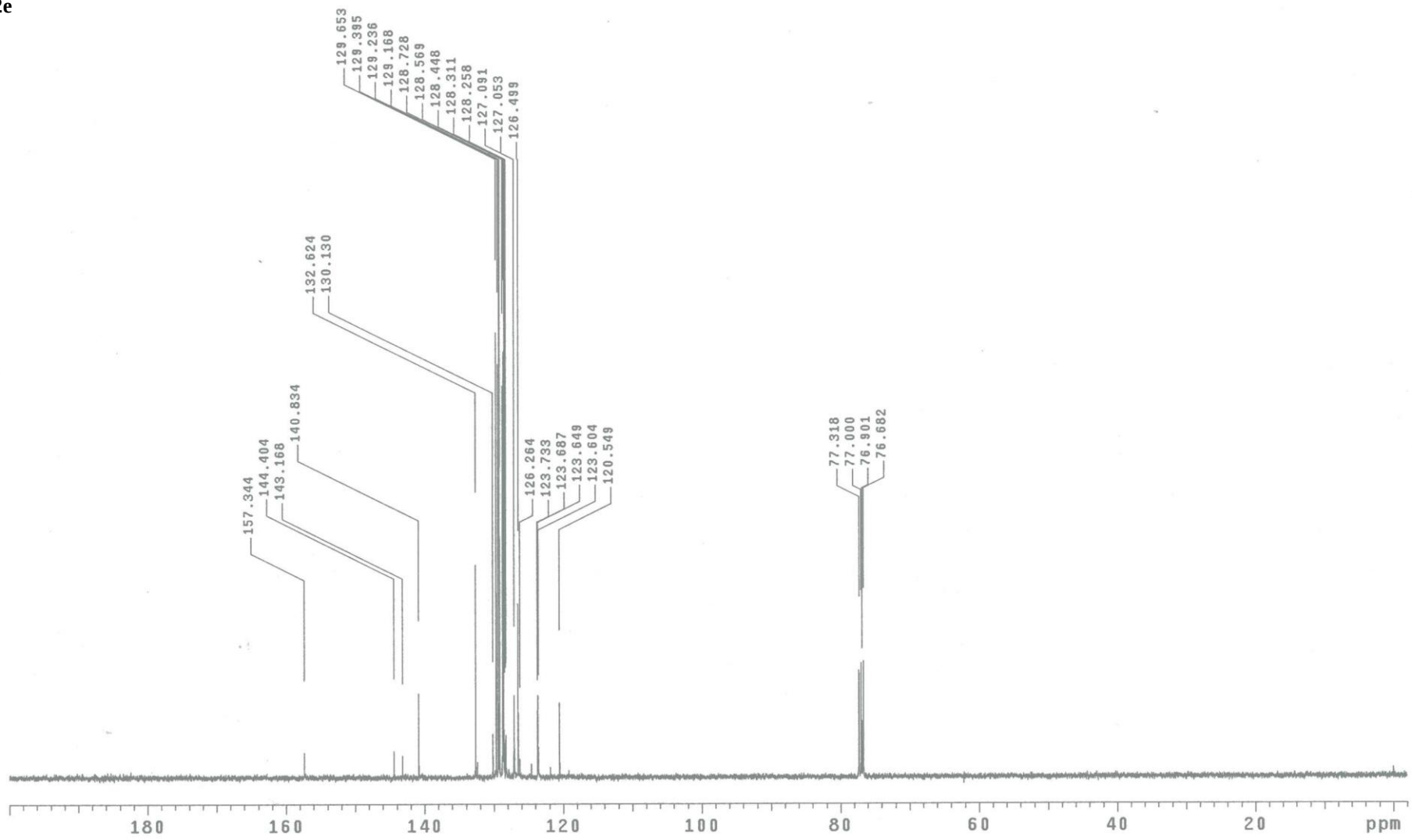

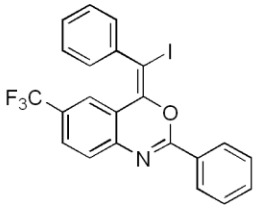

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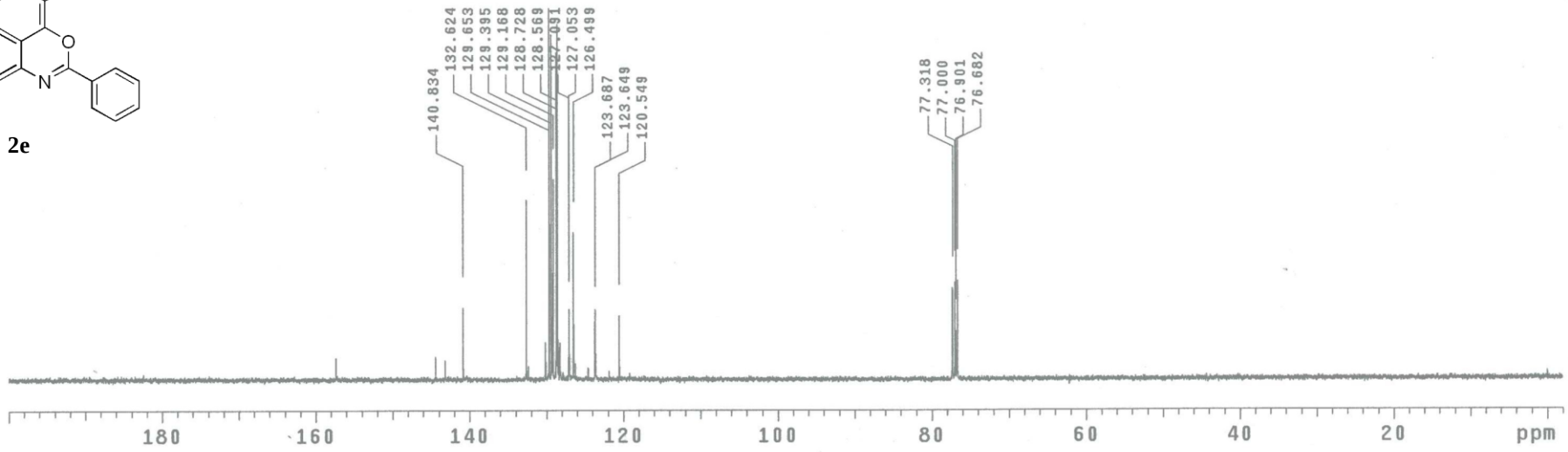

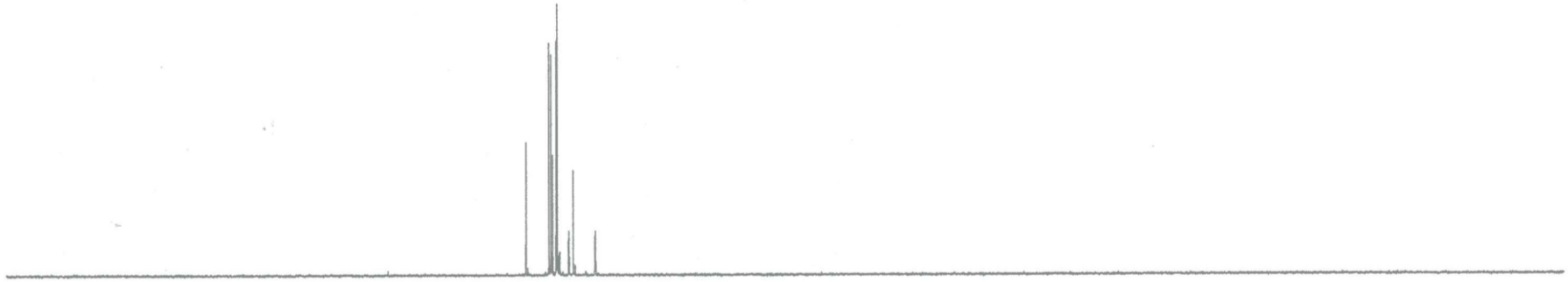

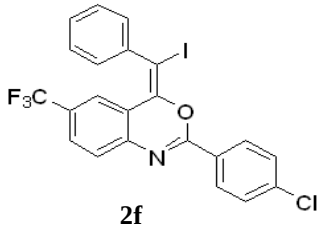

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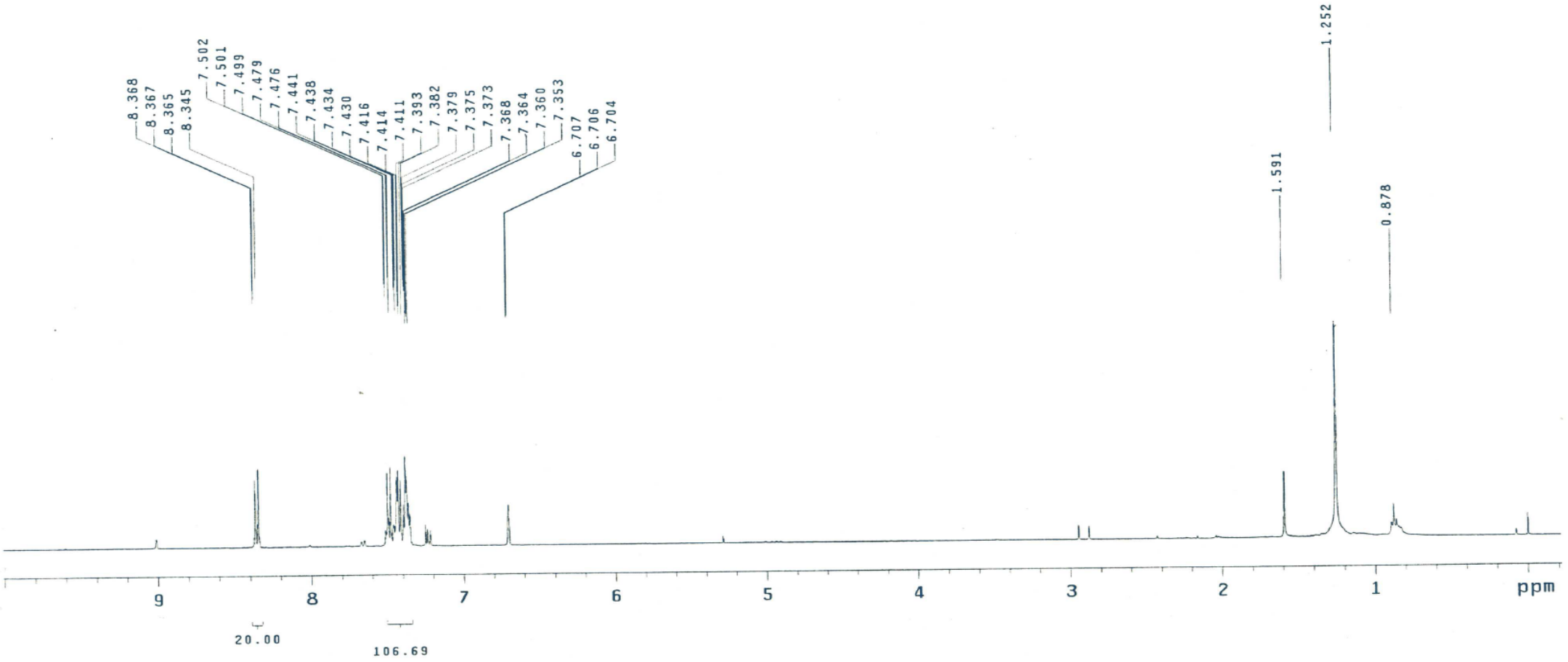

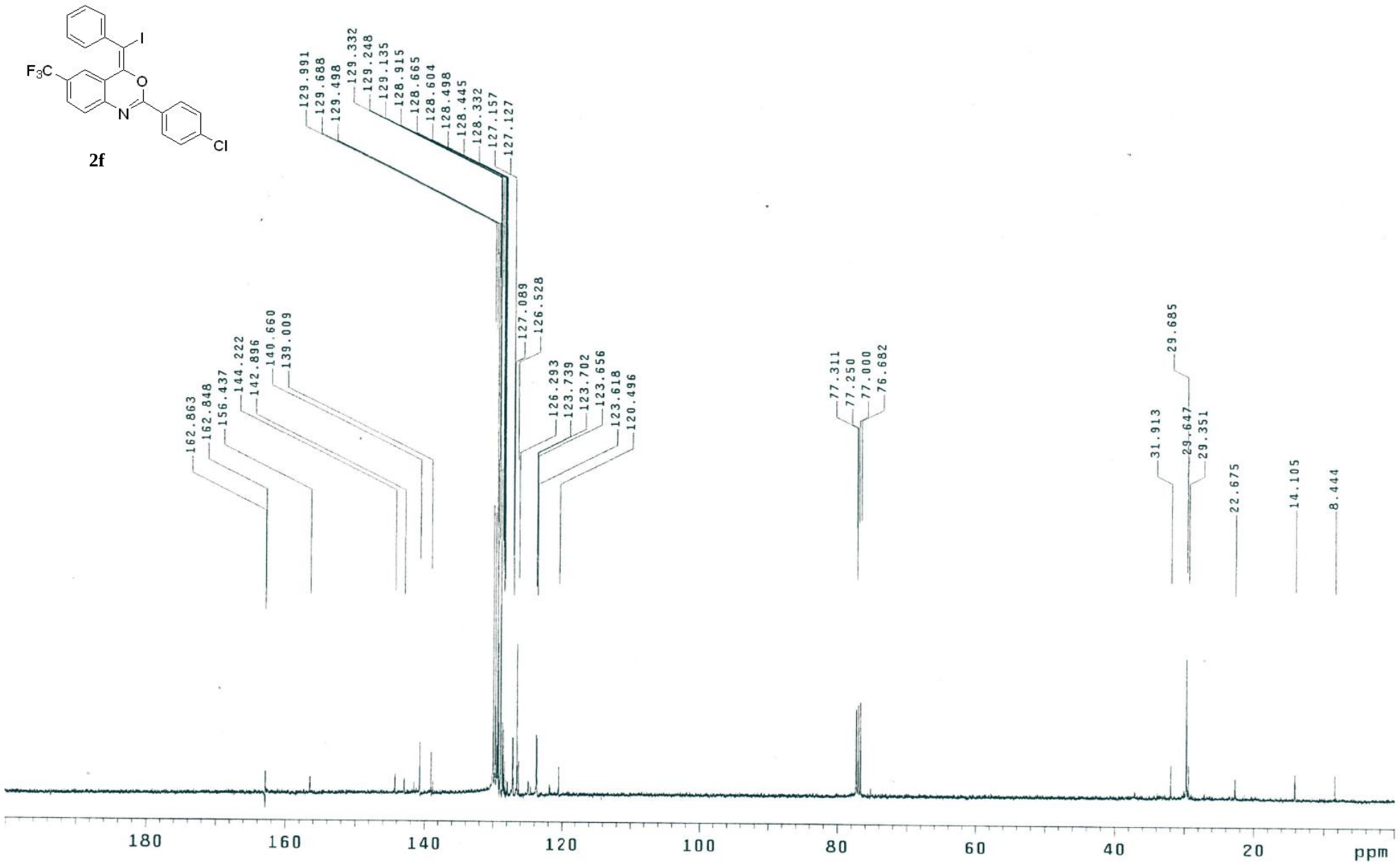

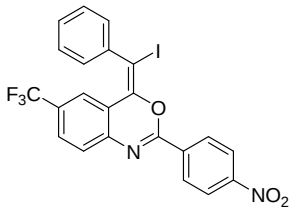

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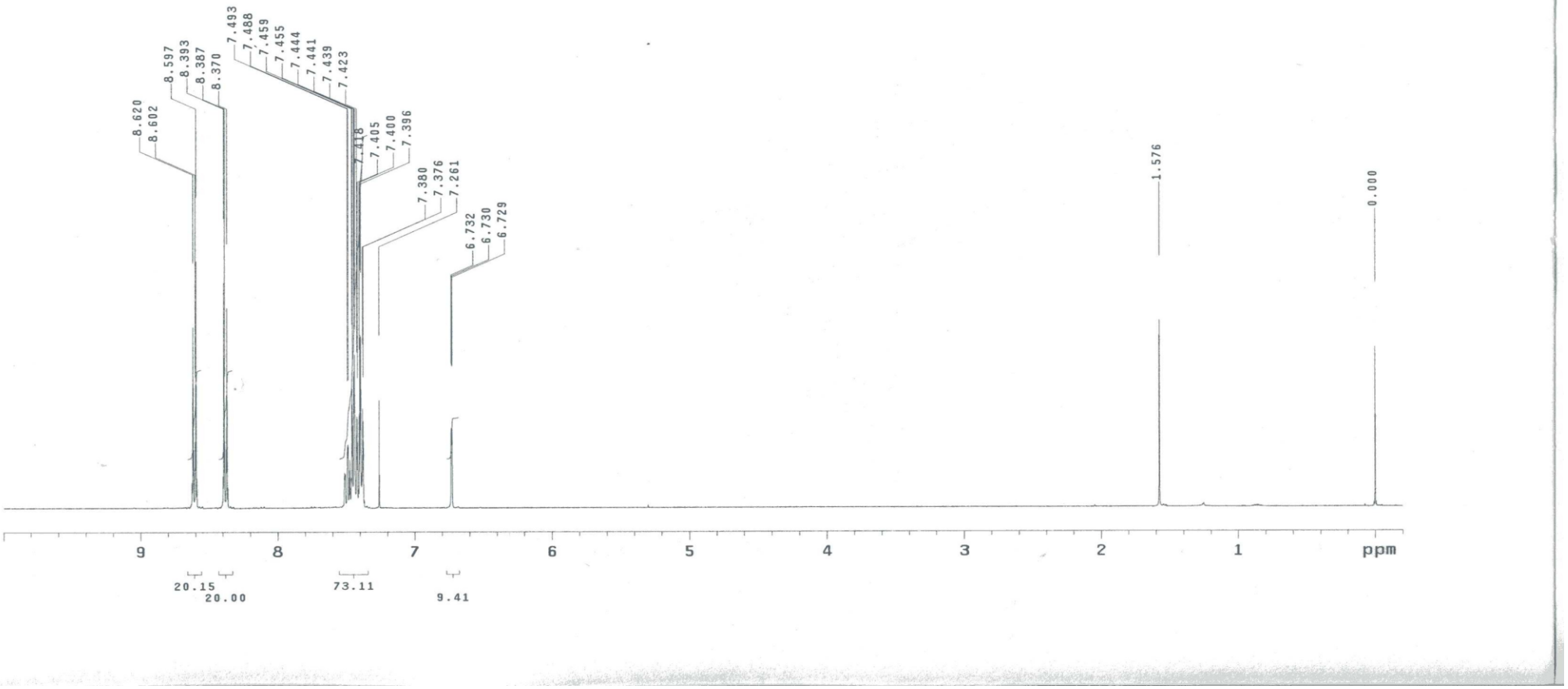

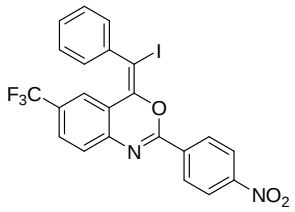

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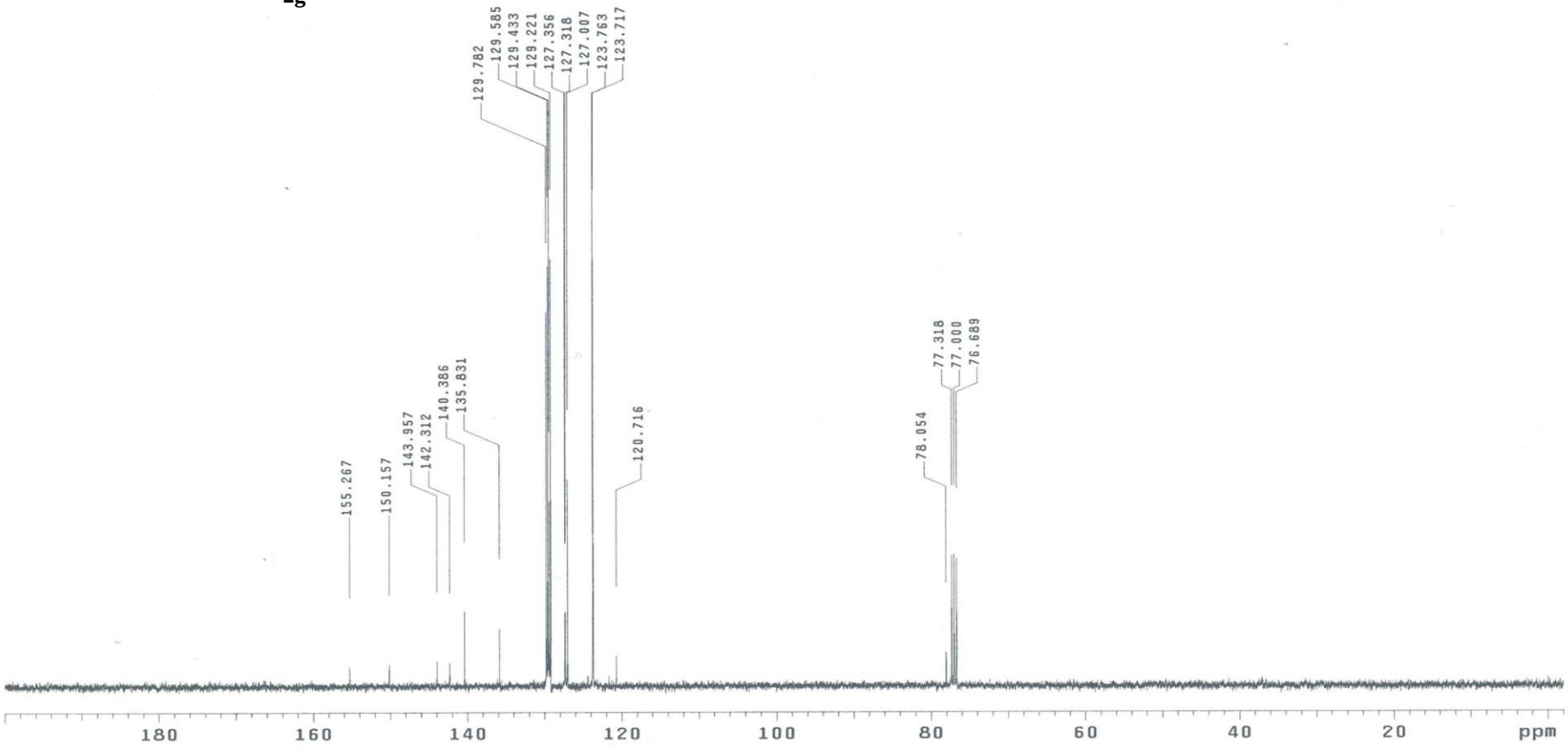

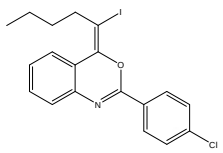

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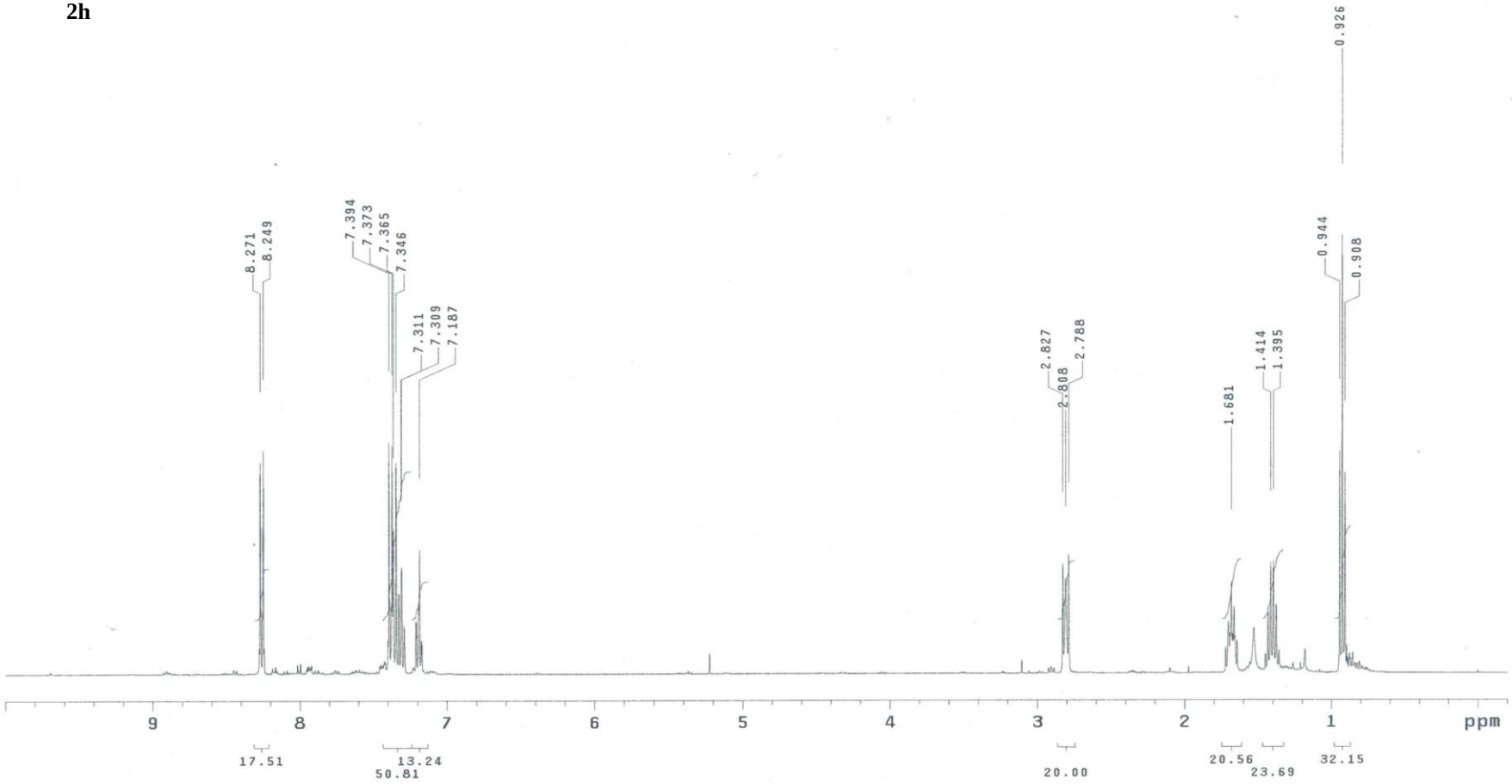

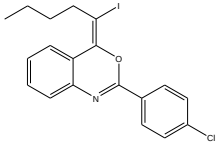

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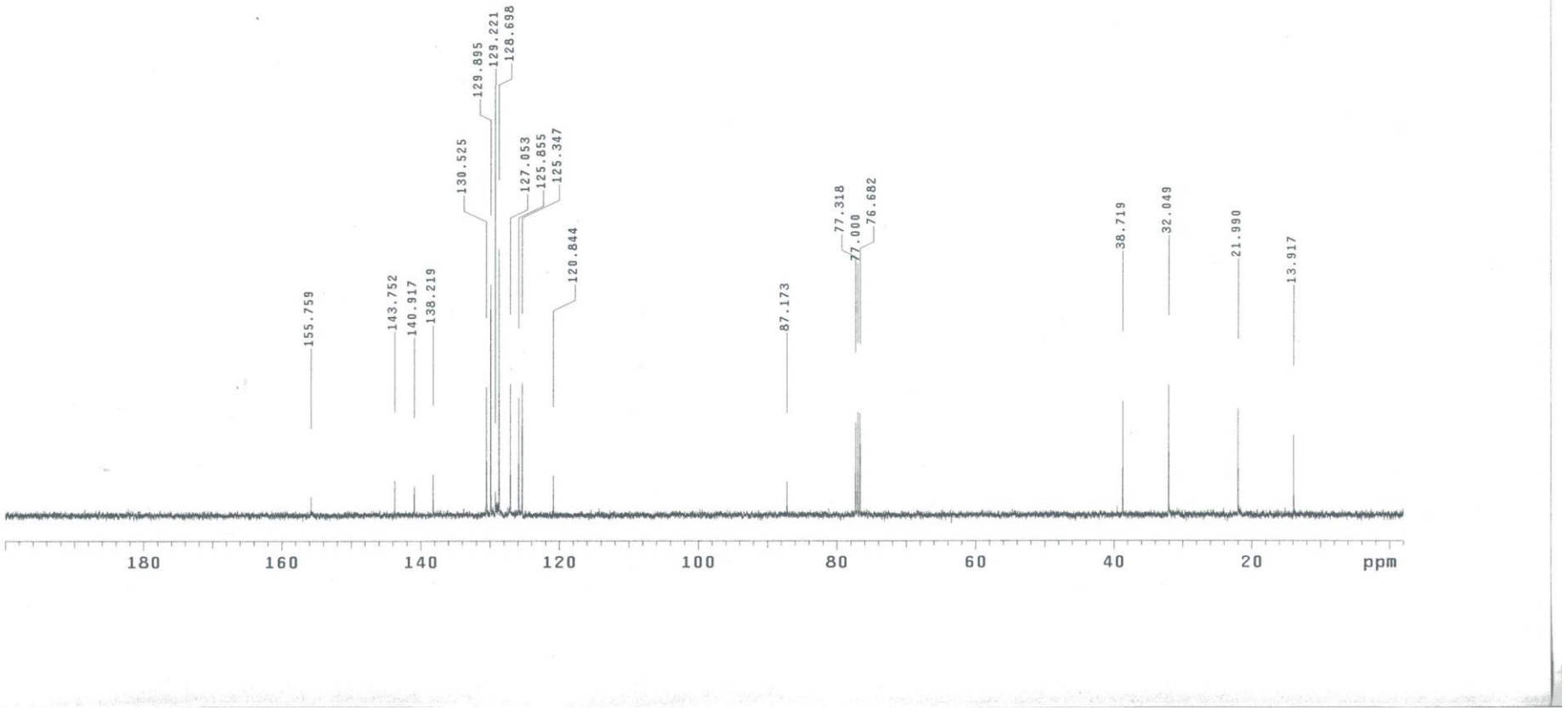

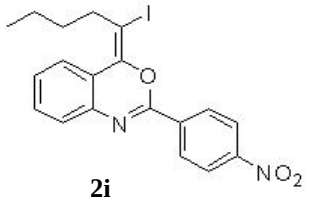
I
O
N
NO2

2i

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8.305
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7.438
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7.412
7.262
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8
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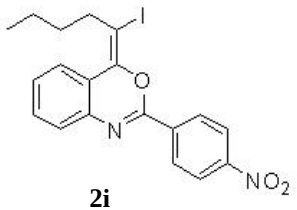

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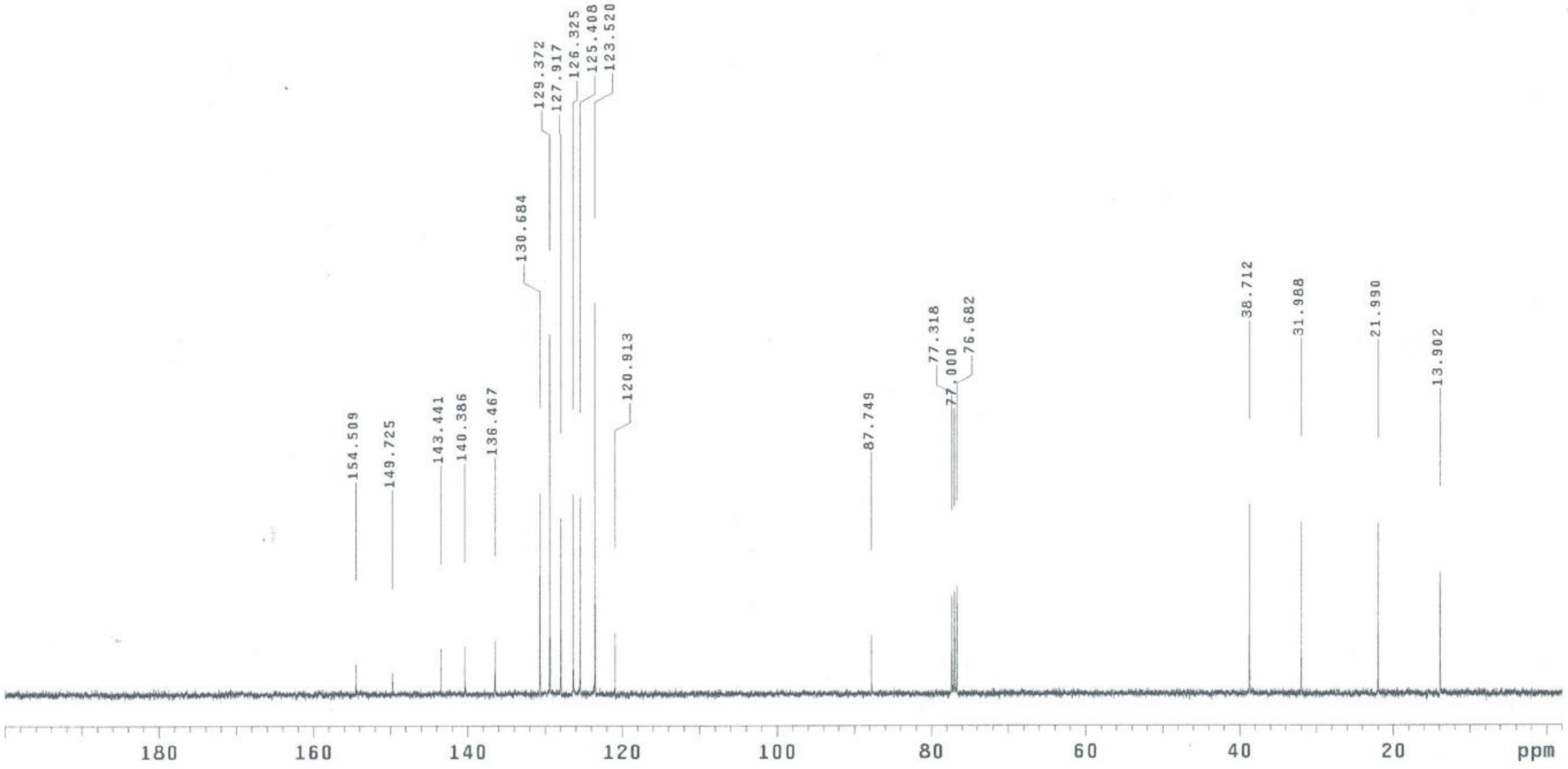

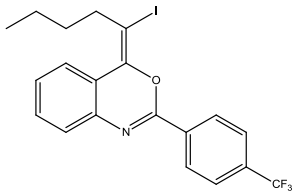

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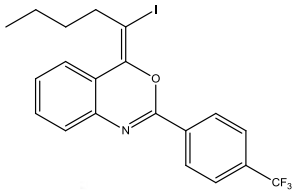

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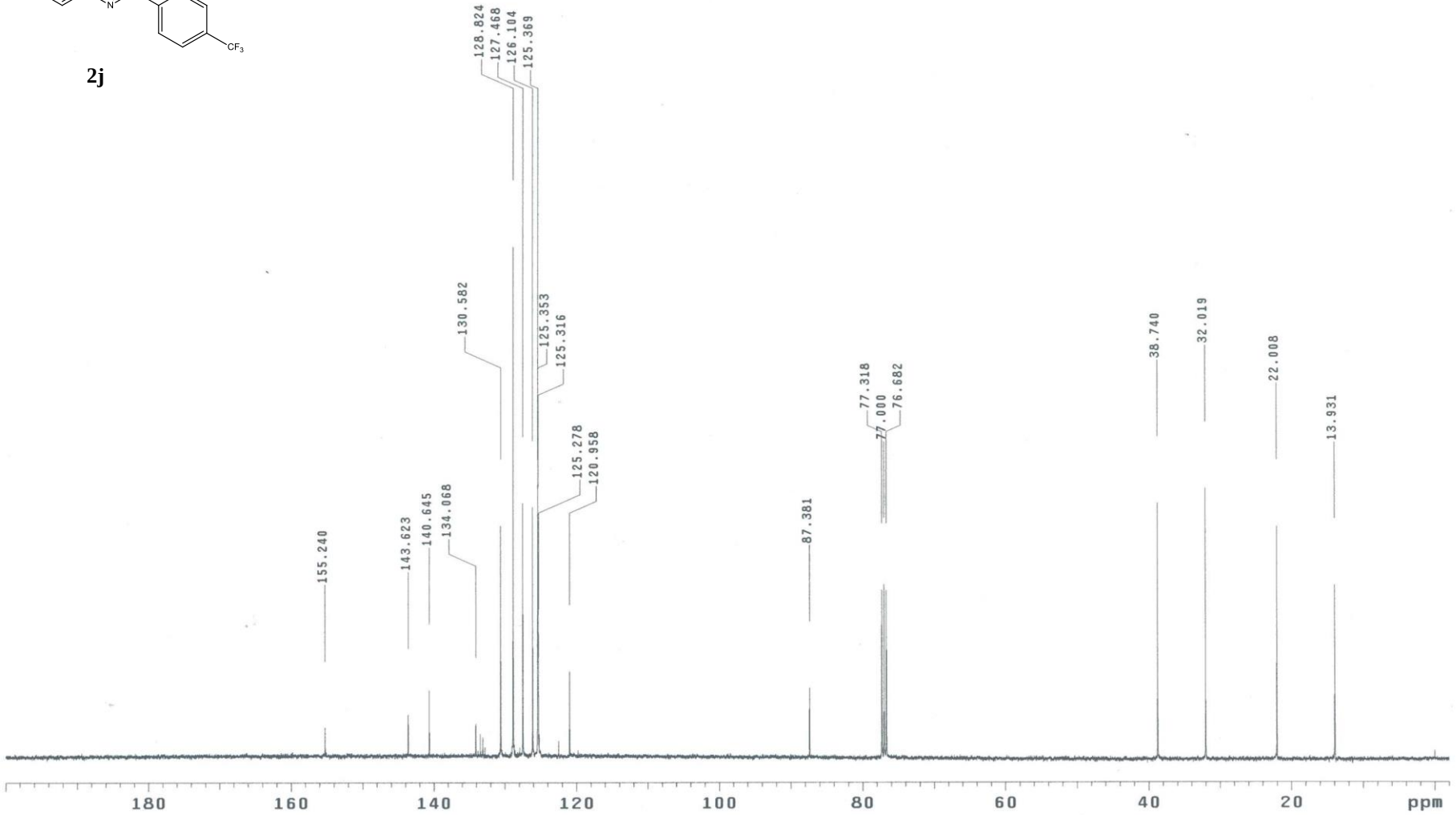

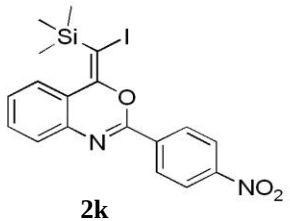

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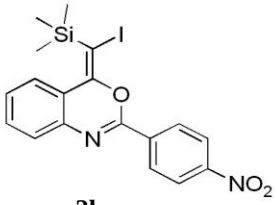

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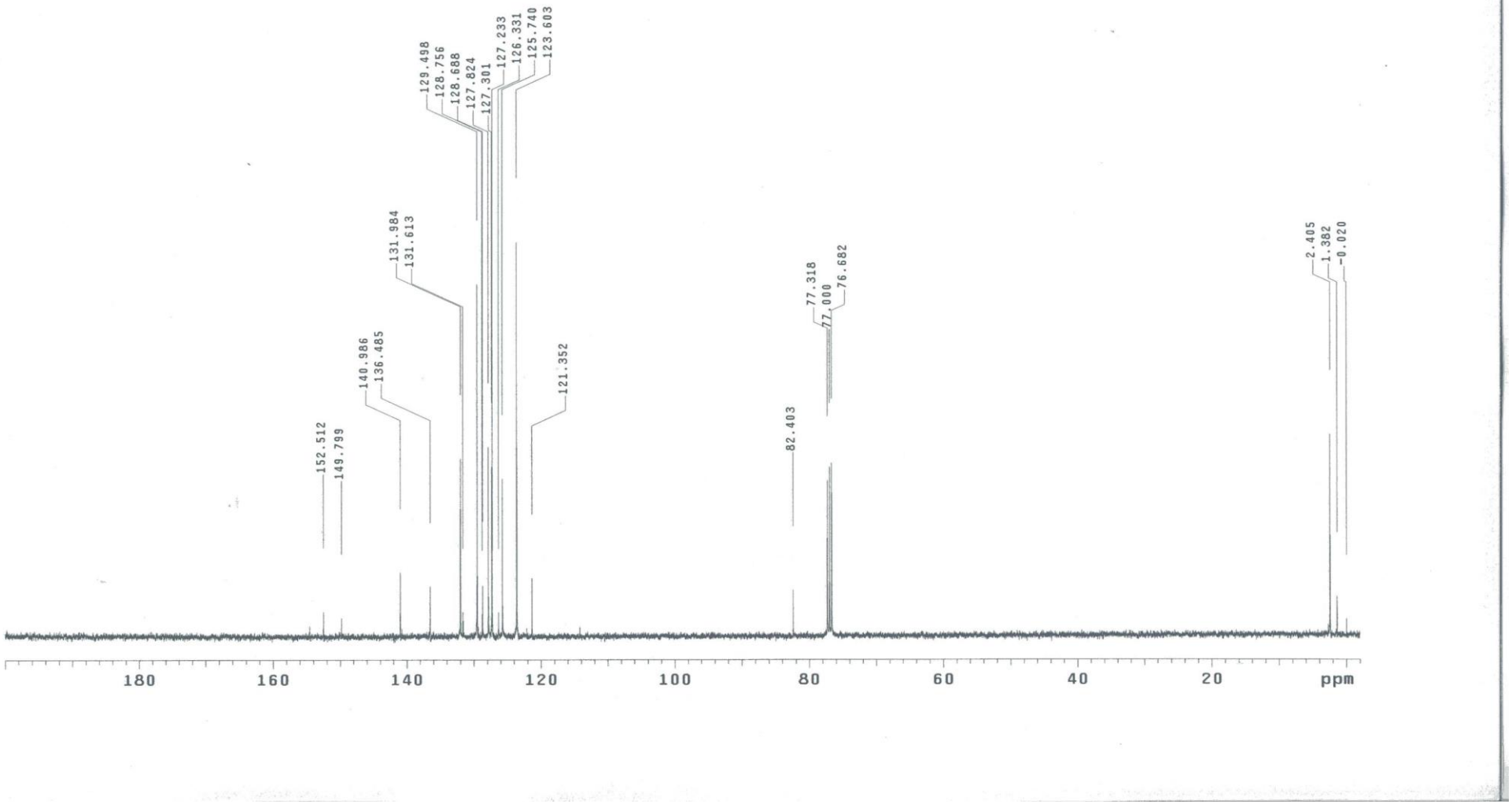

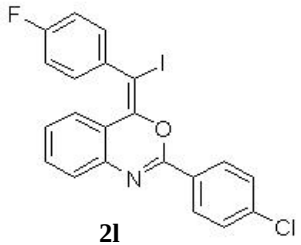

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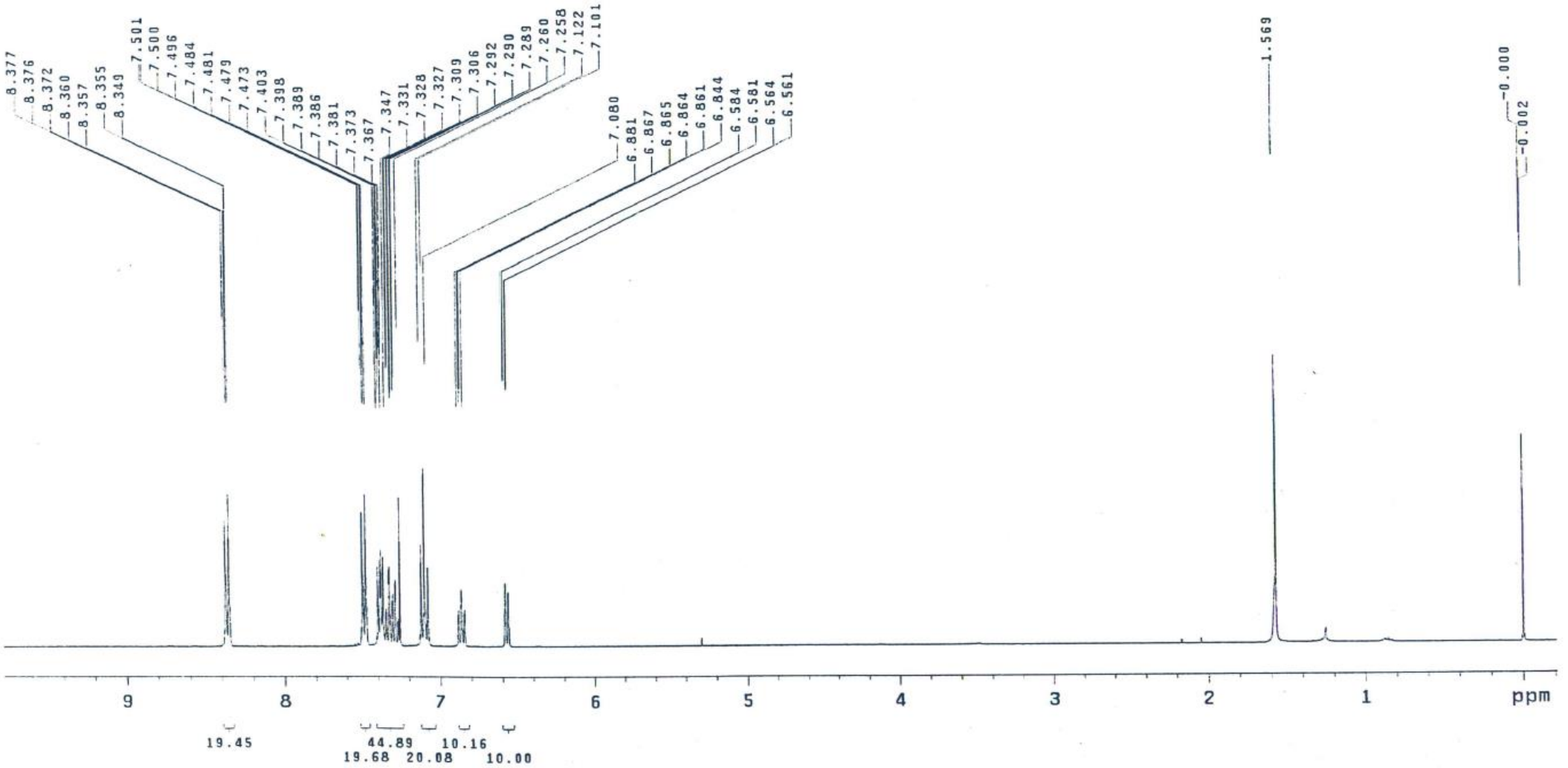

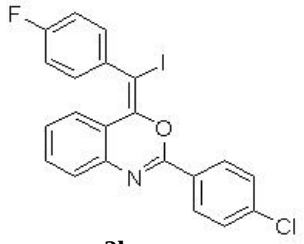

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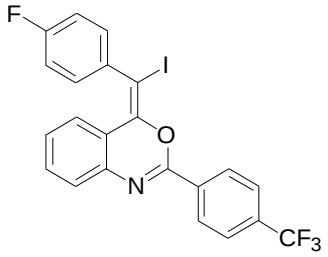

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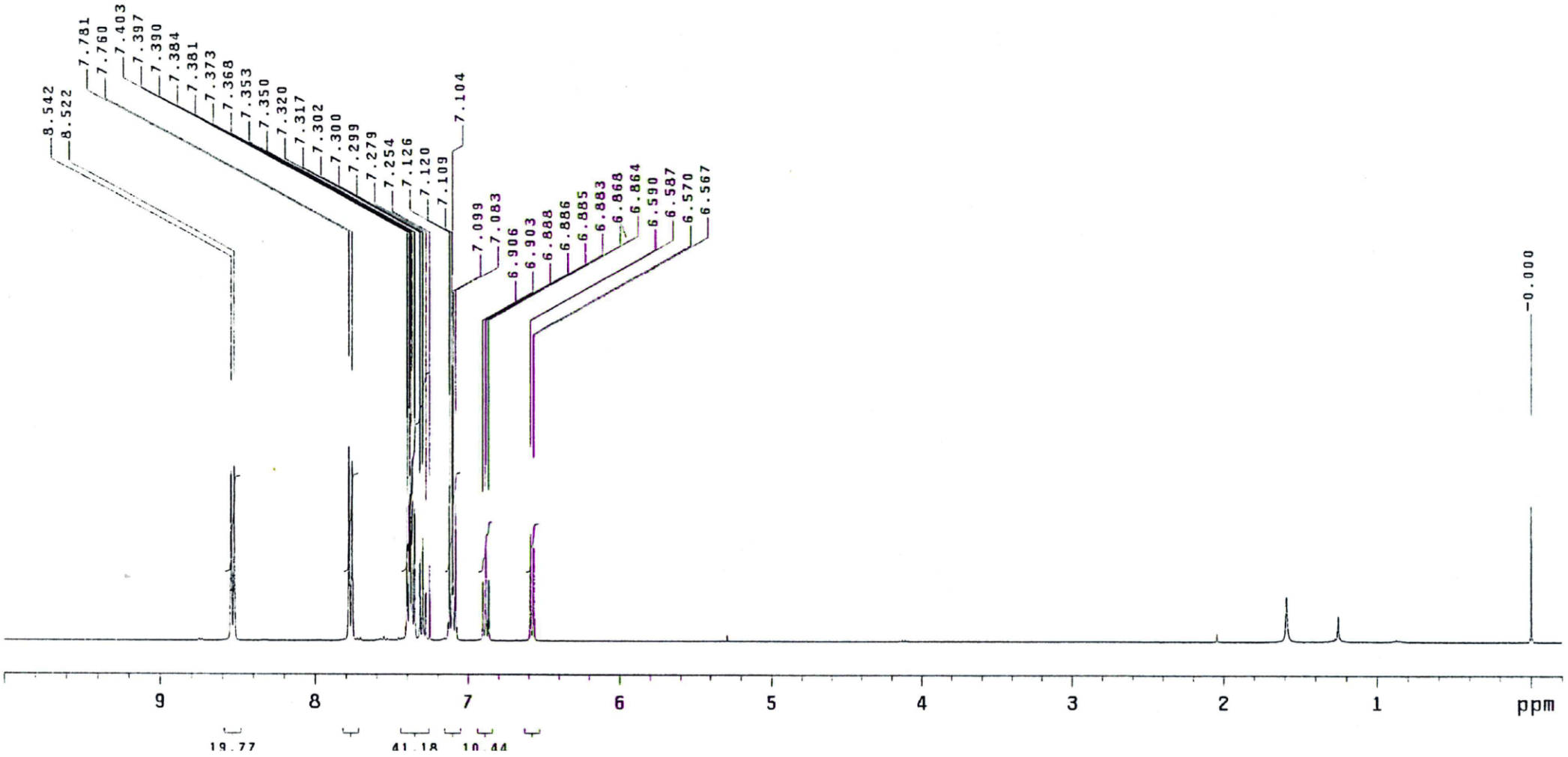

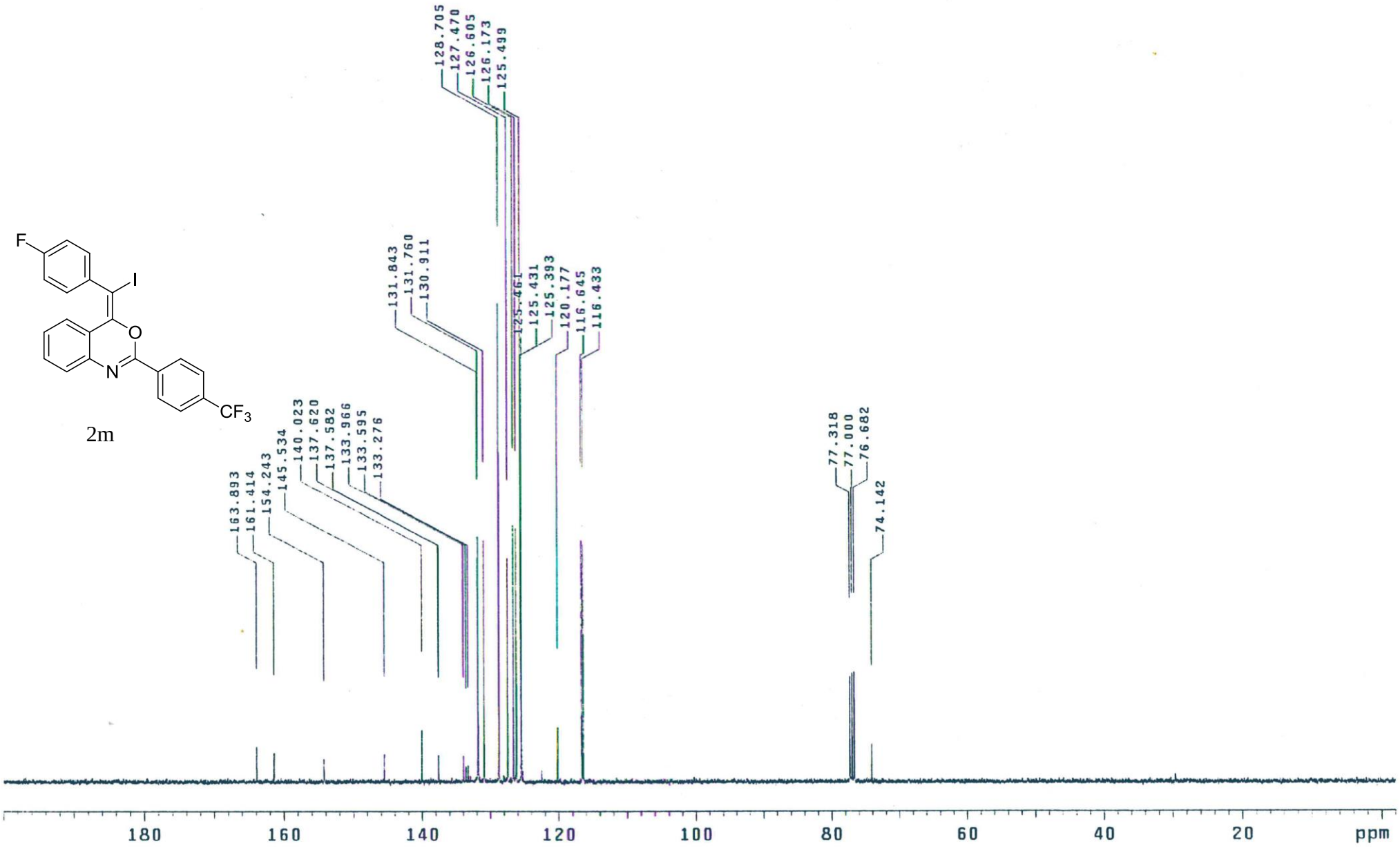

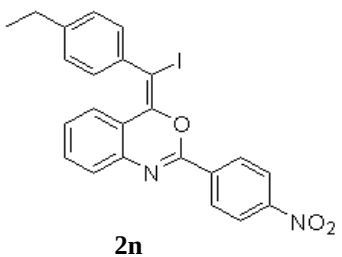

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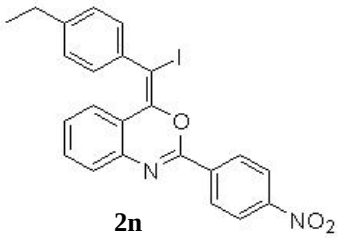

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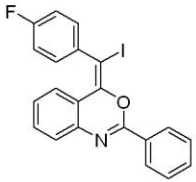

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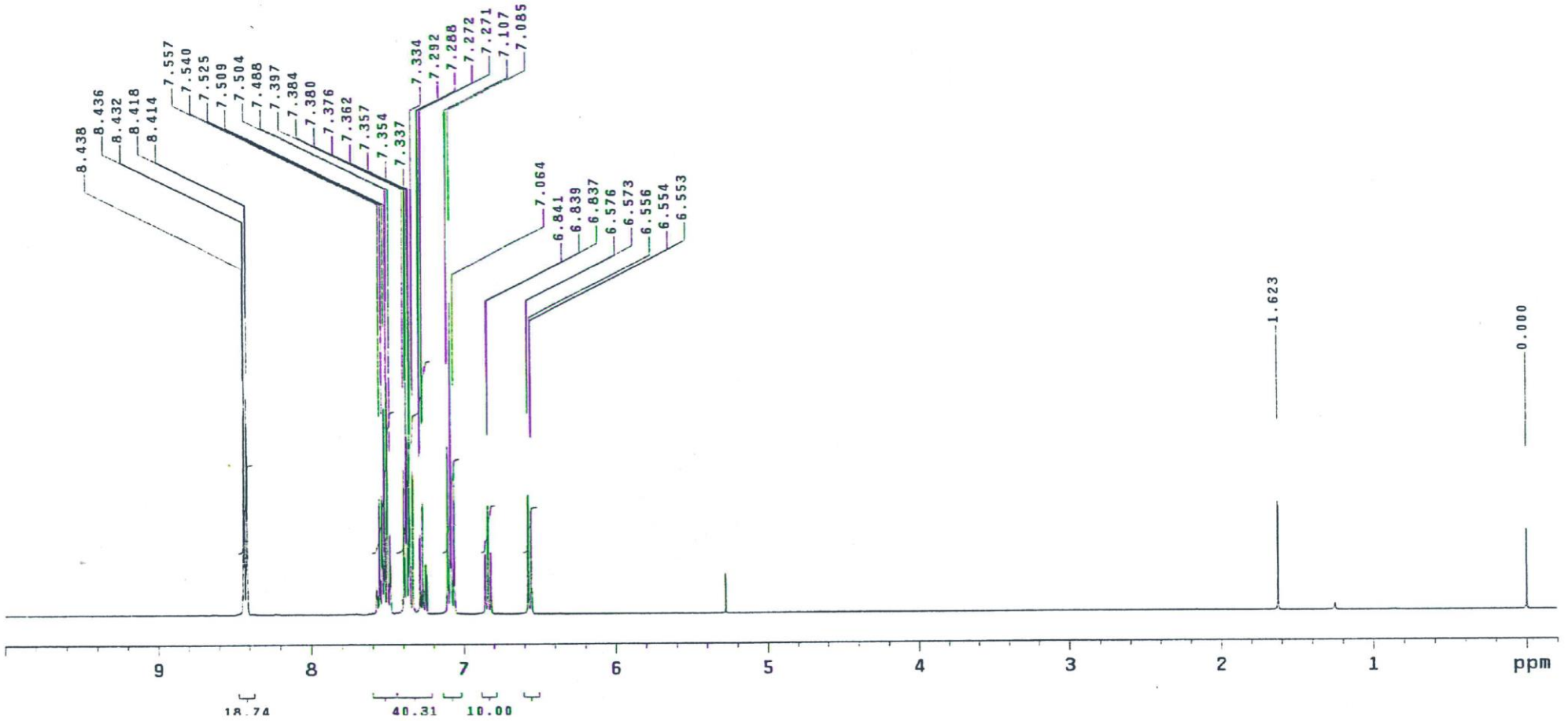
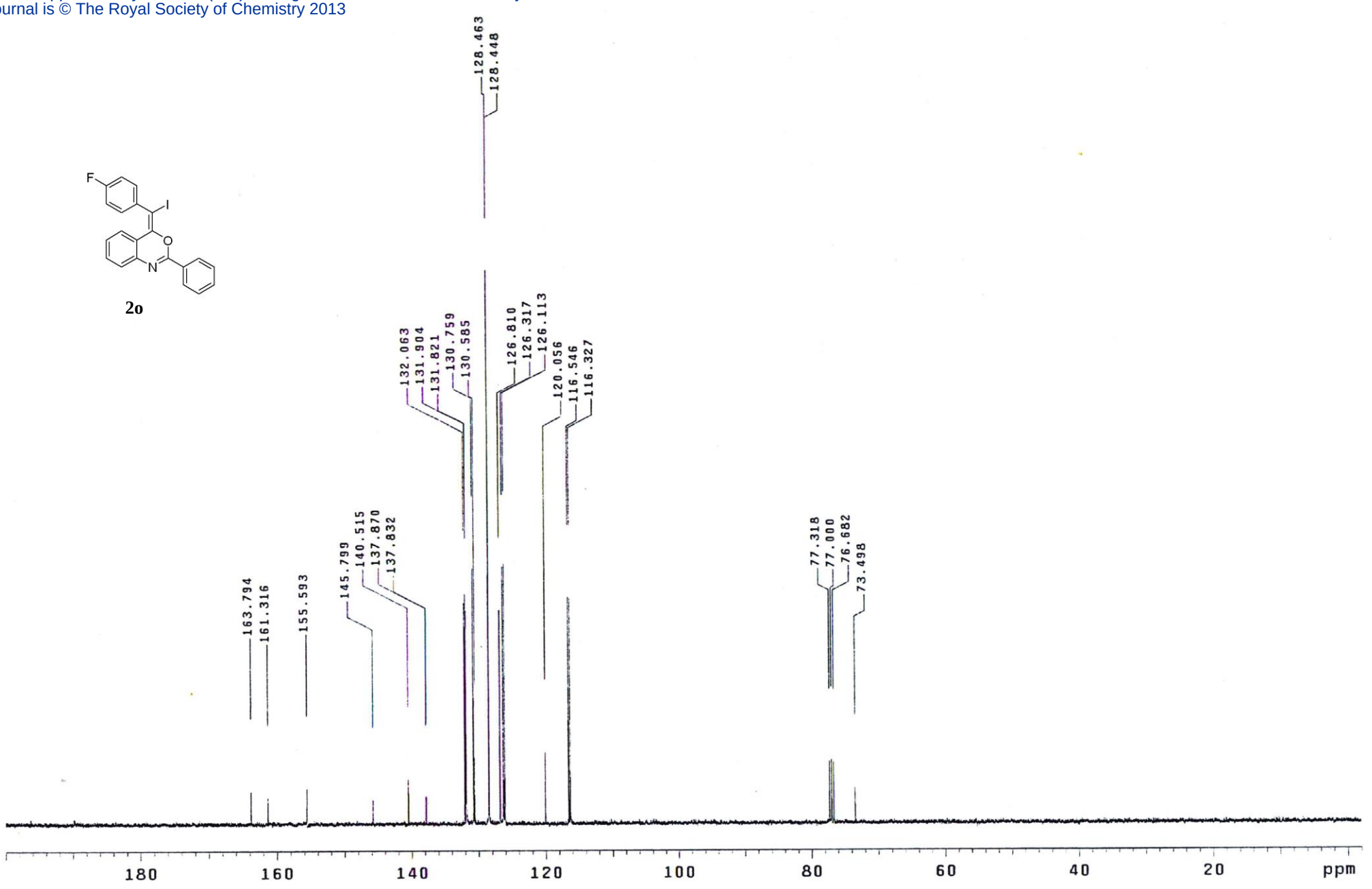
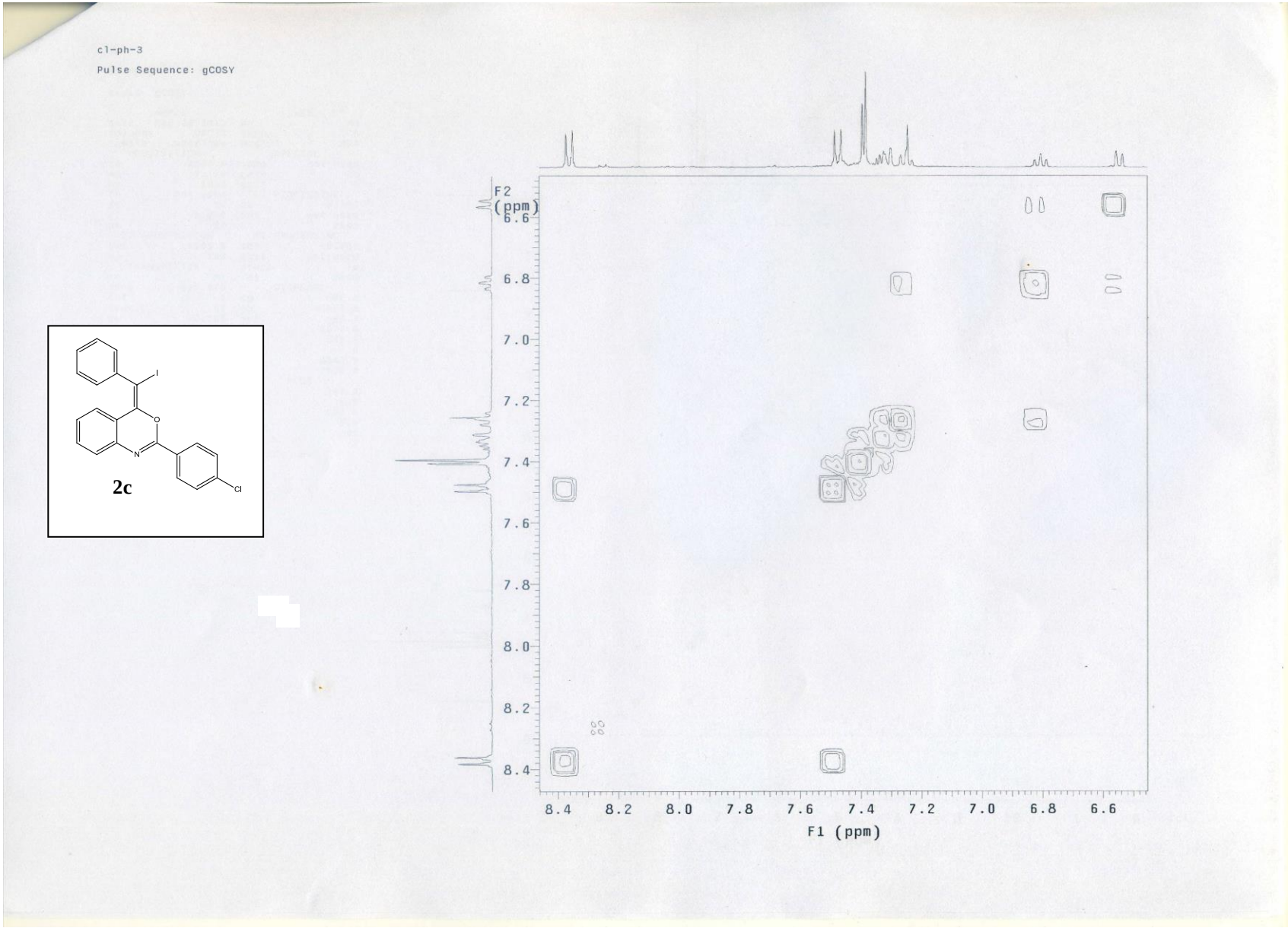


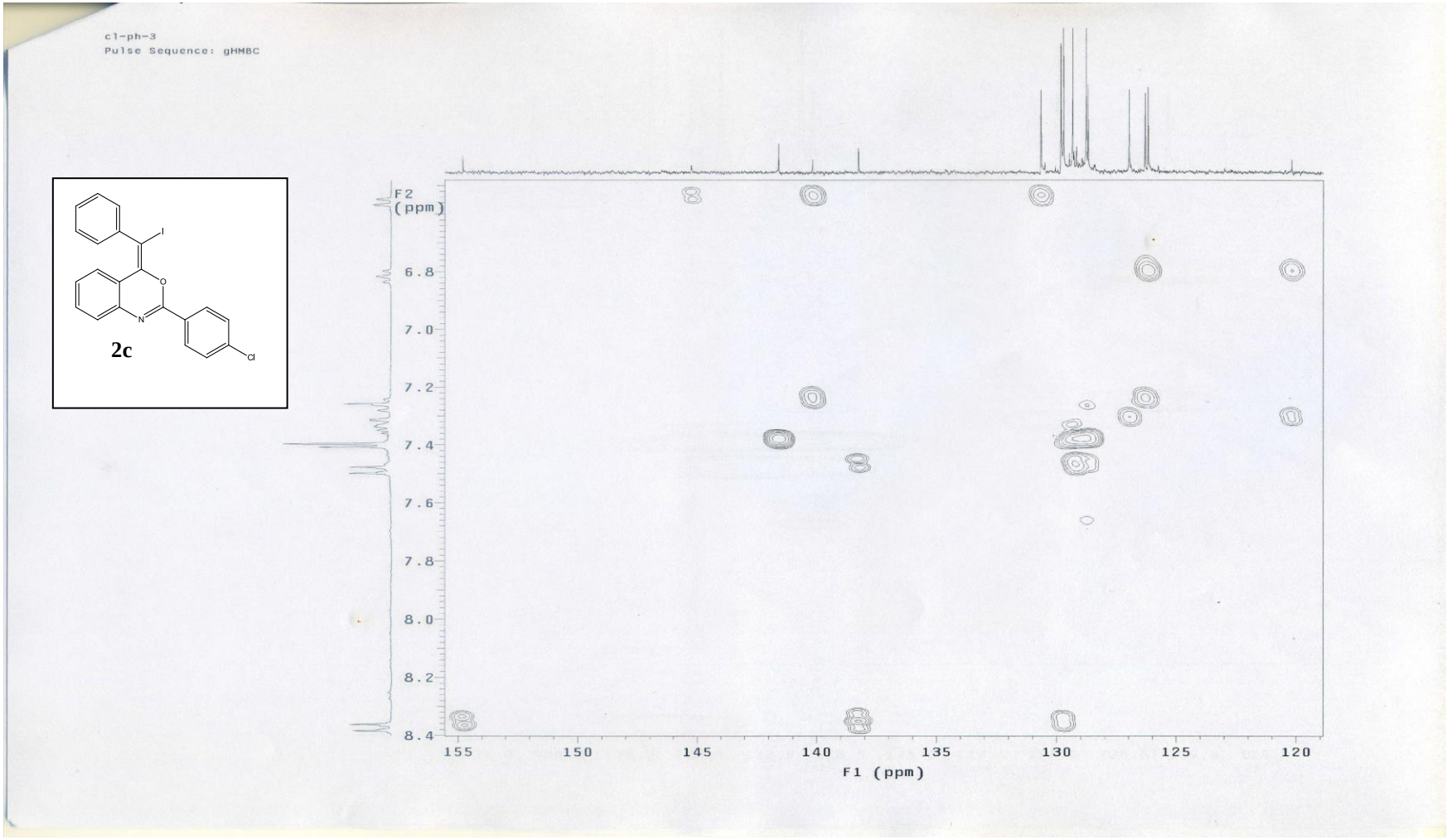


COSY, HMBC and NOESY data for compound 2c.

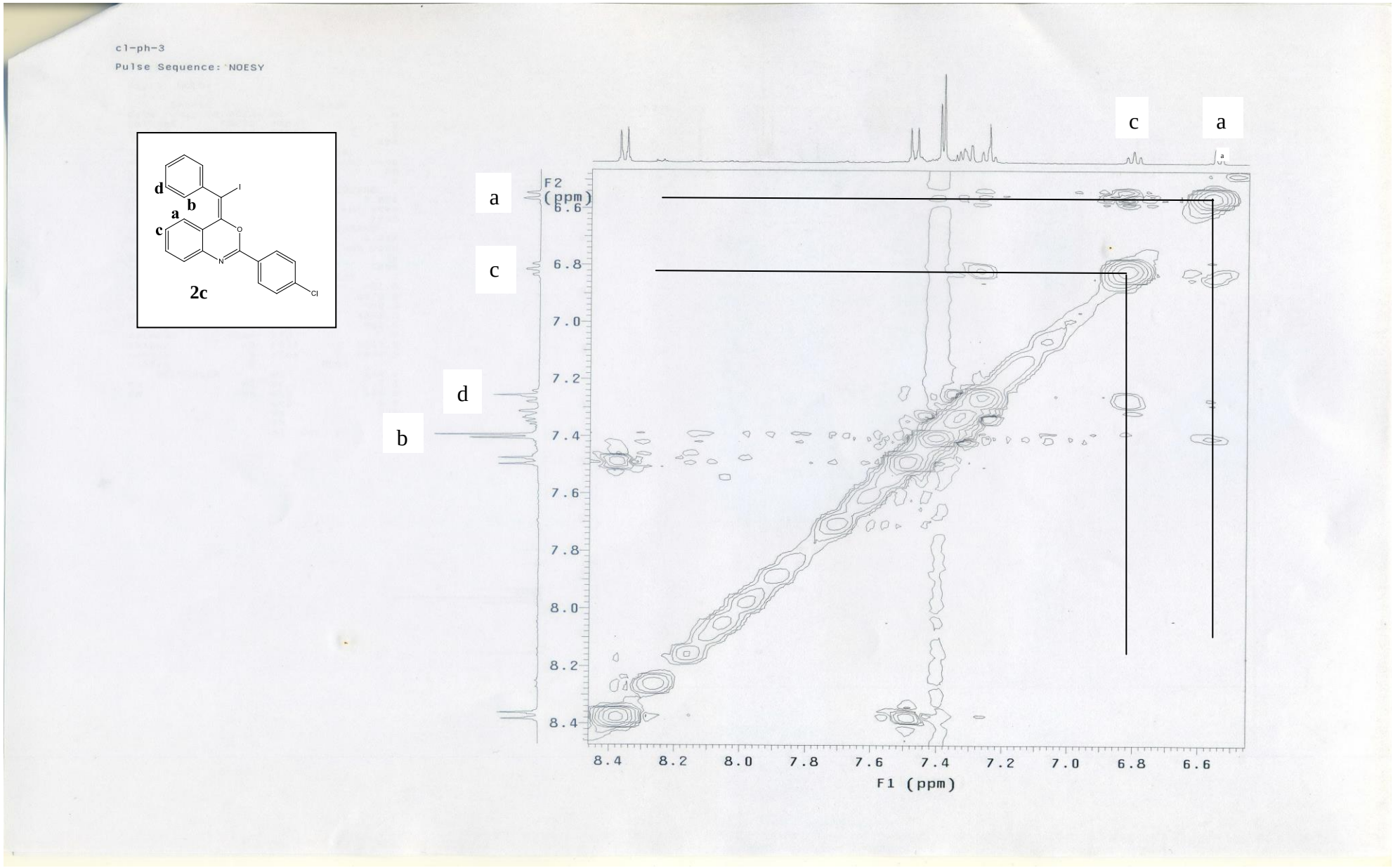
COSY for 2c



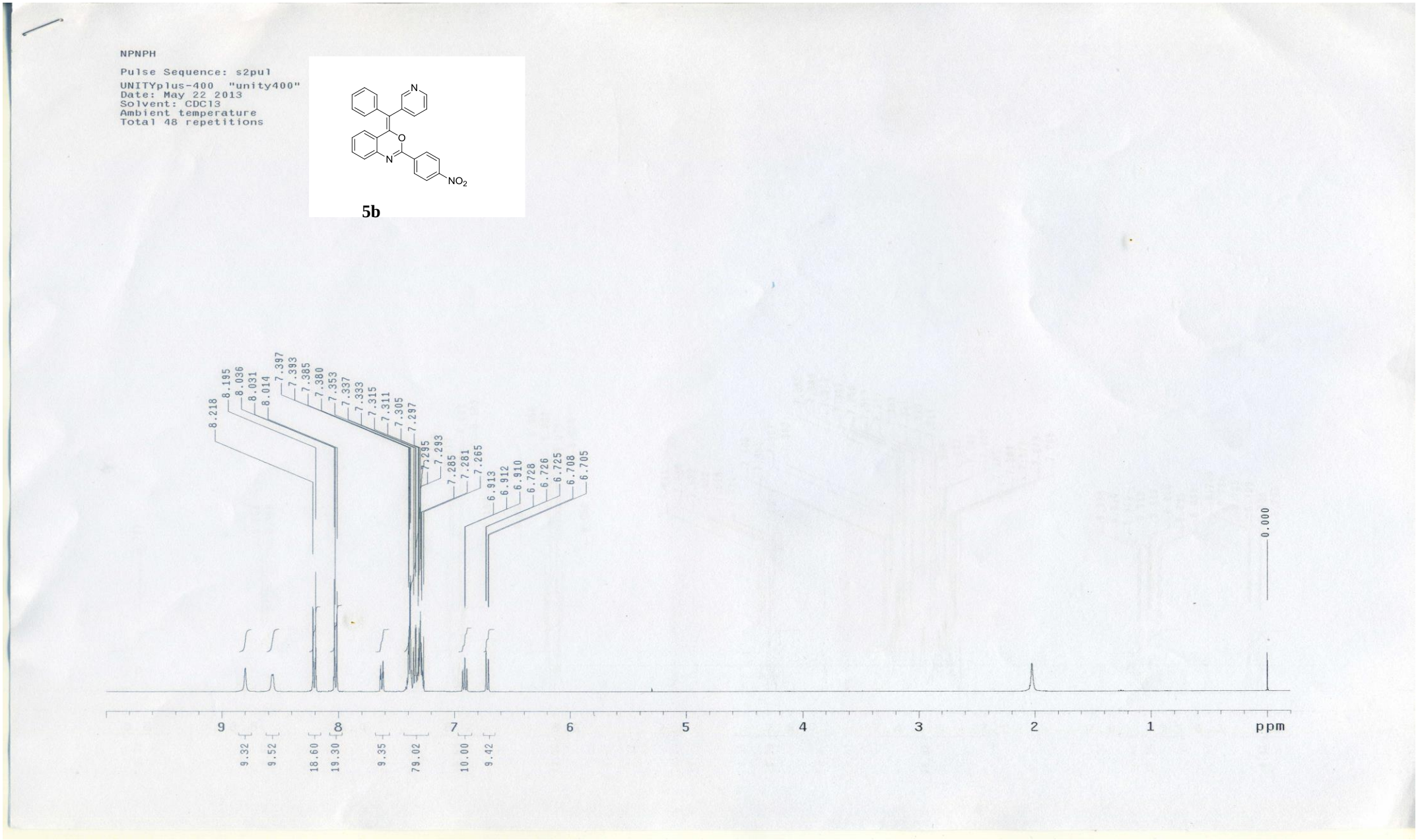
HMBC for 2c



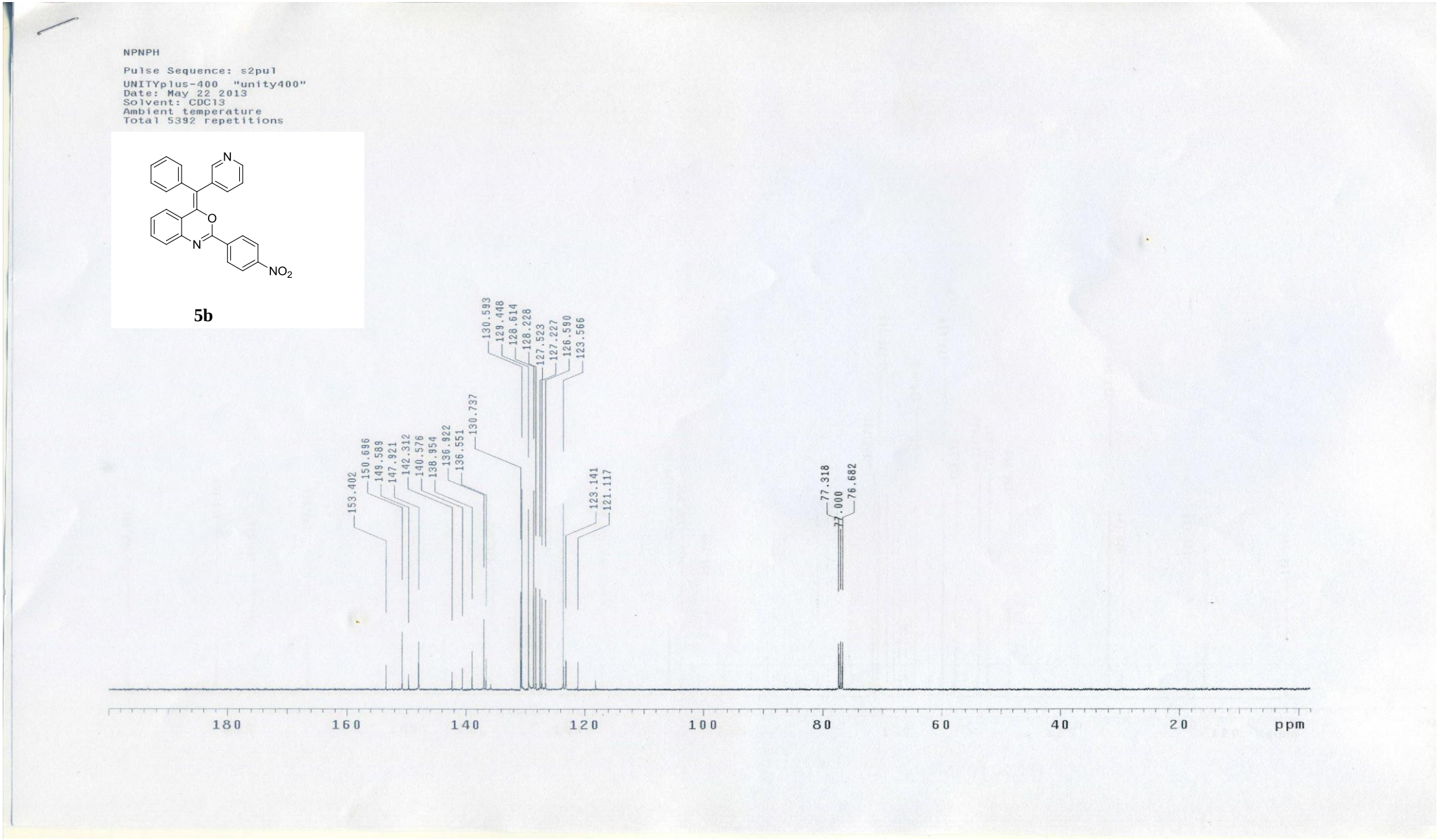
NOESY for 2c

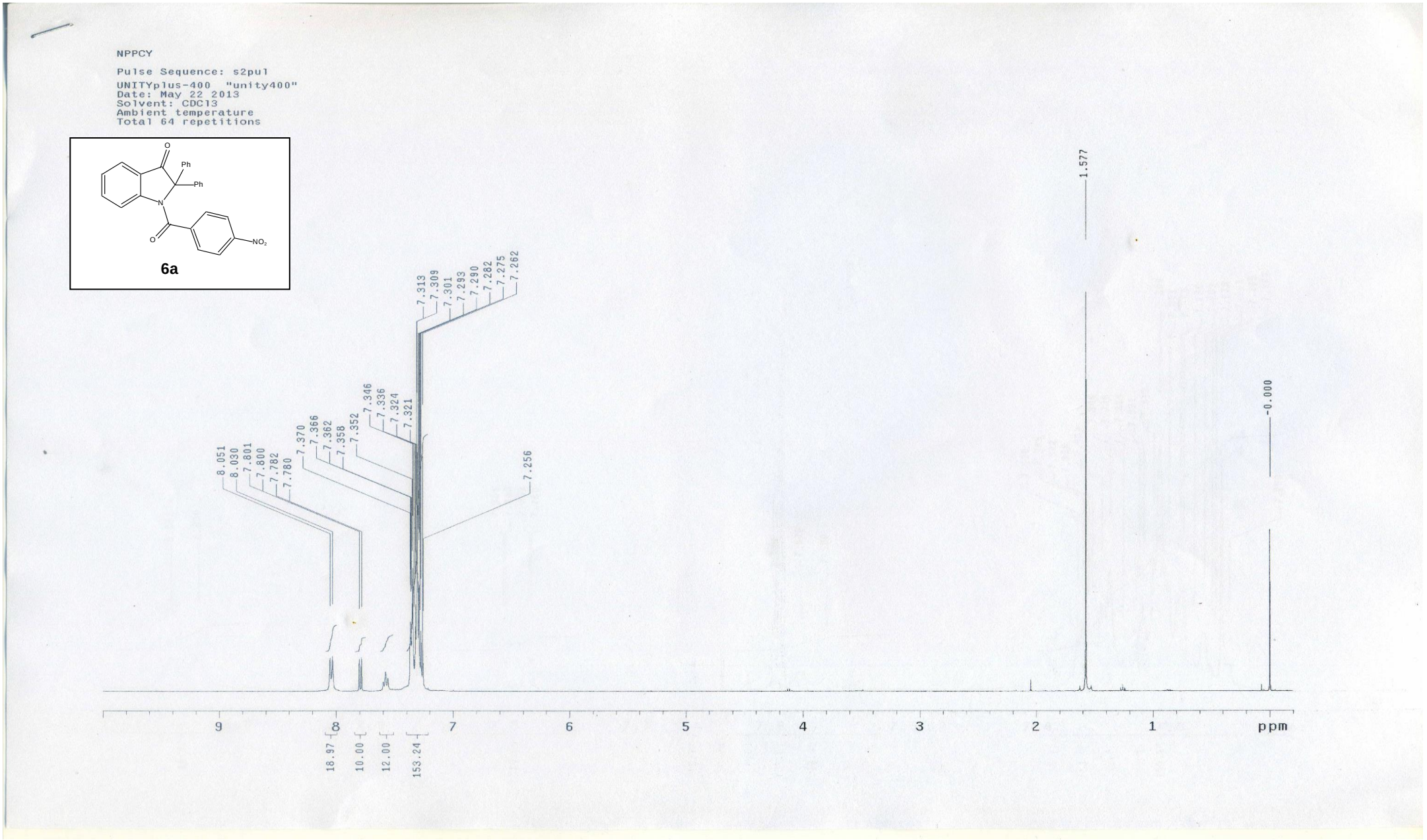


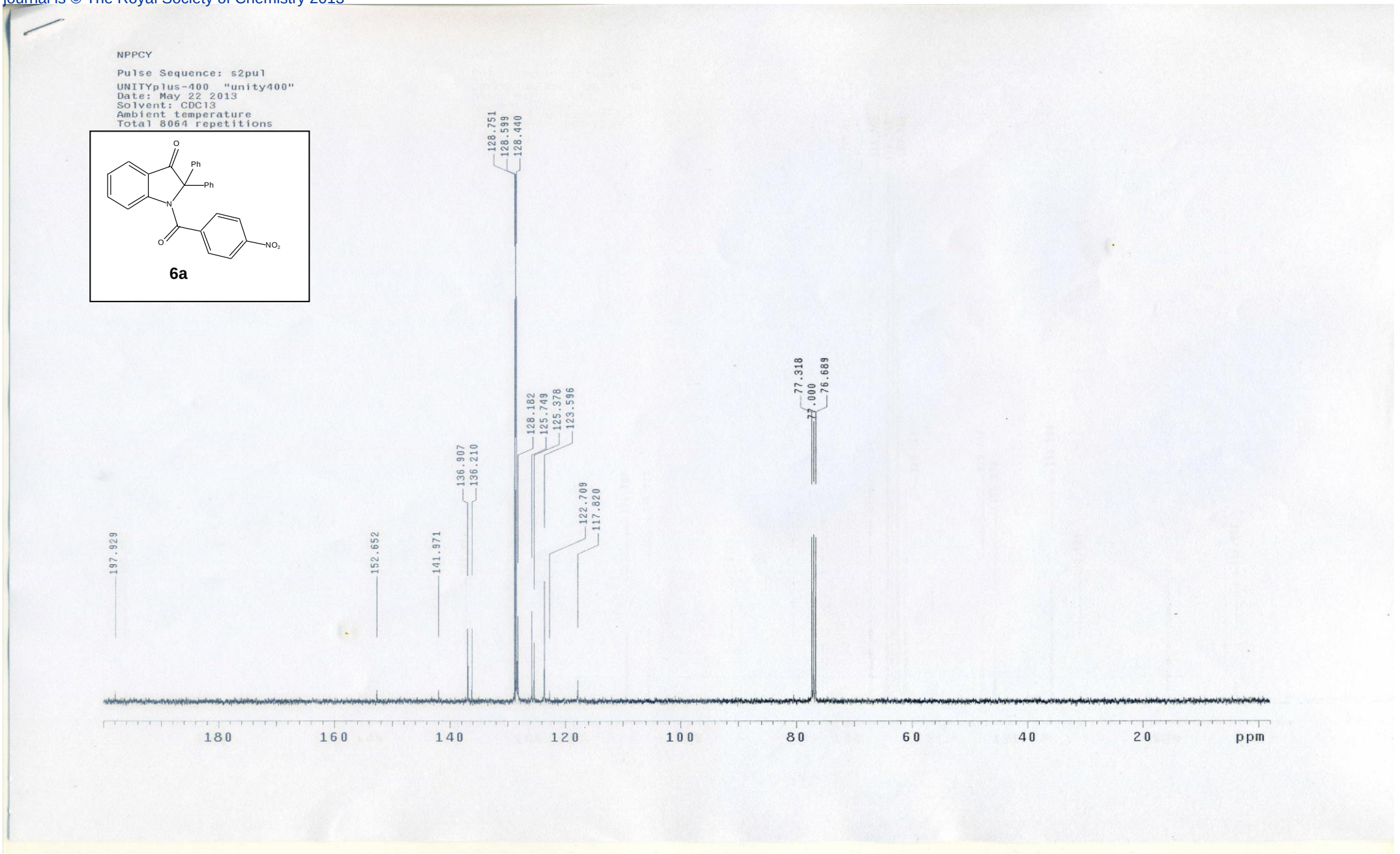
4. 1HNMR and 13CNMR for compound 5b and 6a.



5b

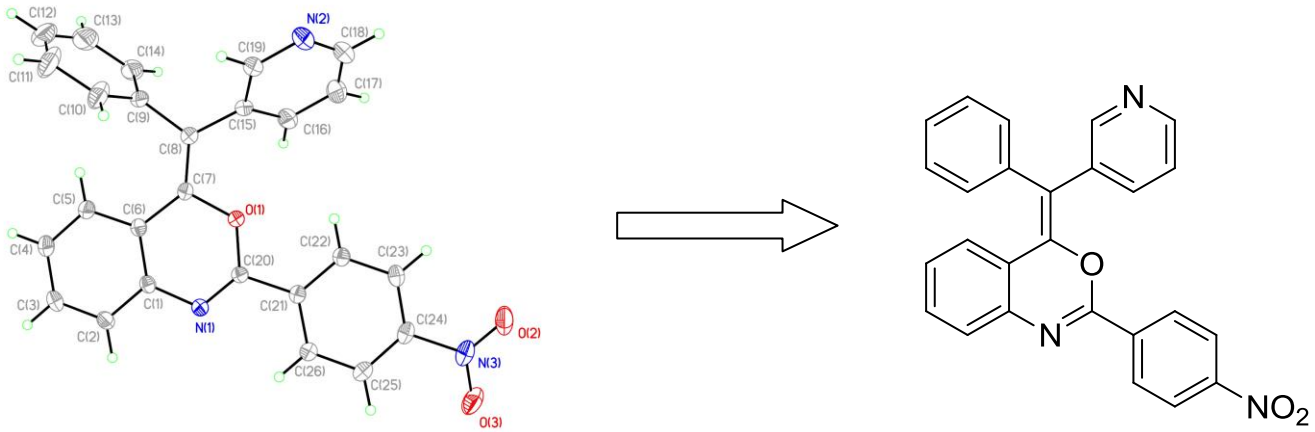






5. ORTEP diagram for compound 5b and 6a.

i) ORTEP diagram of comp 5b.



Compound 5b

Table 1. Crystal data and structure refinement for 5b.

Identification code	nhnphm	
Empirical formula	C26 H17 N3 O3	
Formula weight	419.43	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 31.297(3) Å	α= 90°.
	b = 8.1567(7) Å	β= 119.988(2)°.
	c = 18.7872(16) Å	γ = 90°.
Volume	4153.9(6) $Å^3$	
Z	8	
Density (calculated)	1.341 Mg/m^3	

Absorption coefficient	0.090 mm^{-1}
F(000)	1744
Crystal size	0.65 x 0.50 x 0.12 mm^3
Theta range for data collection	2.18 to 26.04°.
Index ranges	-38<=h<=32, -10<=k<=9, -18<=l<=23
Reflections collected	11428
Independent reflections	4083 [R(int) = 0.0293]
Completeness to theta = 26.04°	99.6 %
Absorption correction	Empirical
Max. and min. transmission	1.000000 and 0.788340
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4083 / 0 / 289
Goodness-of-fit on F^2	1.009
Final R indices [I>2sigma(I)]	R1 = 0.0431, wR2 = 0.1128
R indices (all data)	R1 = 0.0748, wR2 = 0.1319
Largest diff. peak and hole	0.231 and -0.229 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1878(1)	4013(2)	4763(1)	51(1)
O(2)	3409(1)	8654(2)	4007(1)	86(1)
O(3)	4039(1)	7742(2)	5113(1)	91(1)
N(1)	2496(1)	3501(2)	6107(1)	44(1)
N(2)	562(1)	6363(3)	2409(1)	95(1)
N(3)	3595(1)	7841(2)	4639(1)	64(1)
C(1)	2158(1)	2578(2)	6230(1)	40(1)
C(2)	2338(1)	1833(2)	6995(1)	49(1)
C(3)	2036(1)	879(2)	7157(1)	55(1)
C(4)	1555(1)	627(2)	6550(1)	57(1)
C(5)	1371(1)	1343(2)	5788(1)	51(1)
C(6)	1666(1)	2362(2)	5612(1)	40(1)
C(7)	1501(1)	3197(2)	4825(1)	40(1)
C(8)	1055(1)	3347(2)	4146(1)	47(1)
C(9)	598(1)	2682(3)	4106(1)	59(1)
C(10)	402(1)	3399(3)	4548(2)	85(1)
C(11)	-2(1)	2736(5)	4547(2)	121(1)
C(12)	-217(1)	1355(6)	4097(3)	138(2)
C(13)	-37(1)	621(5)	3633(2)	133(2)
C(14)	376(1)	1300(4)	3634(2)	96(1)
C(15)	989(1)	4226(2)	3404(1)	52(1)
C(16)	1265(1)	3889(3)	3029(1)	68(1)
C(17)	1180(1)	4792(4)	2346(1)	89(1)

C(18)	830(1)	6009(4)	2070(2)	97(1)
C(19)	640(1)	5460(3)	3054(1)	71(1)
C(20)	2341(1)	4134(2)	5406(1)	37(1)
C(21)	2661(1)	5117(2)	5204(1)	39(1)
C(22)	2487(1)	5746(2)	4420(1)	44(1)
C(23)	2790(1)	6663(2)	4239(1)	49(1)
C(24)	3268(1)	6923(2)	4849(1)	49(1)
C(25)	3453(1)	6332(2)	5635(1)	53(1)
C(26)	3146(1)	5433(2)	5812(1)	47(1)

Table 3. Bond lengths [Å] and angles [°] for 5b.

O(1)-C(20)	1.3482(19)
O(1)-C(7)	1.4076(19)
O(2)-N(3)	1.224(2)
O(3)-N(3)	1.222(2)
N(1)-C(20)	1.264(2)
N(1)-C(1)	1.409(2)
N(2)-C(18)	1.315(3)
N(2)-C(19)	1.332(3)
N(3)-C(24)	1.471(2)
C(1)-C(2)	1.393(2)
C(1)-C(6)	1.402(2)
C(2)-C(3)	1.371(2)
C(2)-H(2B)	0.9300
C(3)-C(4)	1.376(3)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.378(2)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.398(2)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.467(2)
C(7)-C(8)	1.347(2)
C(8)-C(15)	1.488(2)
C(8)-C(9)	1.494(2)
C(9)-C(14)	1.387(3)
C(9)-C(10)	1.385(3)
C(10)-C(11)	1.375(3)

C(10)-H(10A)	0.9300
C(11)-C(12)	1.367(5)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.389(5)
C(12)-H(12A)	0.9300
C(13)-C(14)	1.404(4)
C(13)-H(13A)	0.9300
C(14)-H(14A)	0.9300
C(15)-C(19)	1.385(3)
C(15)-C(16)	1.387(3)
C(16)-C(17)	1.386(3)
C(16)-H(16A)	0.9300
C(17)-C(18)	1.373(4)
C(17)-H(17A)	0.9300
C(18)-H(18A)	0.9300
C(19)-H(19A)	0.9300
C(20)-C(21)	1.474(2)
C(21)-C(22)	1.388(2)
C(21)-C(26)	1.394(2)
C(22)-C(23)	1.379(2)
C(22)-H(22A)	0.9300
C(23)-C(24)	1.372(2)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.376(3)
C(25)-C(26)	1.373(2)
C(25)-H(25A)	0.9300
C(26)-H(26A)	0.9300

C(20)-O(1)-C(7)	121.97(12)
C(20)-N(1)-C(1)	117.41(14)
C(18)-N(2)-C(19)	116.5(2)
O(3)-N(3)-O(2)	124.03(18)
O(3)-N(3)-C(24)	117.44(19)
O(2)-N(3)-C(24)	118.53(19)
C(2)-C(1)-C(6)	120.77(16)
C(2)-C(1)-N(1)	116.85(15)
C(6)-C(1)-N(1)	122.35(14)
C(3)-C(2)-C(1)	120.44(17)
C(3)-C(2)-H(2B)	119.8
C(1)-C(2)-H(2B)	119.8
C(2)-C(3)-C(4)	119.49(17)
C(2)-C(3)-H(3A)	120.3
C(4)-C(3)-H(3A)	120.3
C(3)-C(4)-C(5)	120.83(18)
C(3)-C(4)-H(4A)	119.6
C(5)-C(4)-H(4A)	119.6
C(4)-C(5)-C(6)	121.08(17)
C(4)-C(5)-H(5A)	119.5
C(6)-C(5)-H(5A)	119.5
C(1)-C(6)-C(5)	117.35(15)
C(1)-C(6)-C(7)	117.61(14)
C(5)-C(6)-C(7)	125.03(15)
C(8)-C(7)-O(1)	113.18(14)
C(8)-C(7)-C(6)	132.19(15)
O(1)-C(7)-C(6)	114.62(13)
C(7)-C(8)-C(15)	121.59(15)

C(7)-C(8)-C(9)	121.92(15)
C(15)-C(8)-C(9)	116.47(14)
C(14)-C(9)-C(10)	119.7(2)
C(14)-C(9)-C(8)	119.3(2)
C(10)-C(9)-C(8)	121.0(2)
C(11)-C(10)-C(9)	121.1(3)
C(11)-C(10)-H(10A)	119.5
C(9)-C(10)-H(10A)	119.5
C(12)-C(11)-C(10)	119.6(3)
C(12)-C(11)-H(11A)	120.2
C(10)-C(11)-H(11A)	120.2
C(11)-C(12)-C(13)	120.9(3)
C(11)-C(12)-H(12A)	119.5
C(13)-C(12)-H(12A)	119.5
C(12)-C(13)-C(14)	119.4(3)
C(12)-C(13)-H(13A)	120.3
C(14)-C(13)-H(13A)	120.3
C(9)-C(14)-C(13)	119.3(3)
C(9)-C(14)-H(14A)	120.4
C(13)-C(14)-H(14A)	120.4
C(19)-C(15)-C(16)	116.41(18)
C(19)-C(15)-C(8)	120.19(17)
C(16)-C(15)-C(8)	123.40(17)
C(15)-C(16)-C(17)	119.1(2)
C(15)-C(16)-H(16A)	120.5
C(17)-C(16)-H(16A)	120.5
C(18)-C(17)-C(16)	118.7(2)
C(18)-C(17)-H(17A)	120.6

C(16)-C(17)-H(17A)	120.6
N(2)-C(18)-C(17)	124.0(2)
N(2)-C(18)-H(18A)	118.0
C(17)-C(18)-H(18A)	118.0
N(2)-C(19)-C(15)	125.3(2)
N(2)-C(19)-H(19A)	117.4
C(15)-C(19)-H(19A)	117.4
N(1)-C(20)-O(1)	125.77(15)
N(1)-C(20)-C(21)	122.25(14)
O(1)-C(20)-C(21)	111.98(13)
C(22)-C(21)-C(26)	119.37(16)
C(22)-C(21)-C(20)	121.12(14)
C(26)-C(21)-C(20)	119.51(15)
C(23)-C(22)-C(21)	120.55(16)
C(23)-C(22)-H(22A)	119.7
C(21)-C(22)-H(22A)	119.7
C(24)-C(23)-C(22)	118.41(16)
C(24)-C(23)-H(23A)	120.8
C(22)-C(23)-H(23A)	120.8
C(23)-C(24)-C(25)	122.66(17)
C(23)-C(24)-N(3)	117.94(18)
C(25)-C(24)-N(3)	119.38(17)
C(26)-C(25)-C(24)	118.51(17)
C(26)-C(25)-H(25A)	120.7
C(24)-C(25)-H(25A)	120.7
C(25)-C(26)-C(21)	120.47(17)
C(25)-C(26)-H(26A)	119.8
C(21)-C(26)-H(26A)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 5b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

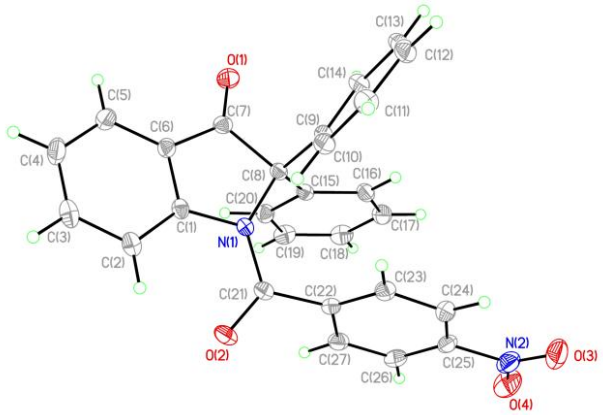
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	38(1)	69(1)	41(1)	10(1)	16(1)	-7(1)
O(2)	112(1)	79(1)	92(1)	12(1)	69(1)	-18(1)
O(3)	69(1)	98(1)	125(1)	6(1)	61(1)	-18(1)
N(1)	44(1)	50(1)	39(1)	-1(1)	21(1)	-5(1)
N(2)	72(1)	127(2)	78(1)	50(1)	31(1)	13(1)
N(3)	73(1)	52(1)	89(1)	-10(1)	59(1)	-12(1)
C(1)	48(1)	37(1)	38(1)	-2(1)	25(1)	1(1)
C(2)	54(1)	53(1)	40(1)	1(1)	22(1)	-1(1)
C(3)	71(1)	54(1)	45(1)	8(1)	34(1)	3(1)
C(4)	65(1)	56(1)	59(1)	8(1)	38(1)	-5(1)
C(5)	48(1)	53(1)	53(1)	6(1)	27(1)	-4(1)
C(6)	44(1)	38(1)	41(1)	-1(1)	24(1)	2(1)
C(7)	41(1)	40(1)	43(1)	-1(1)	25(1)	-2(1)
C(8)	41(1)	52(1)	46(1)	3(1)	21(1)	-2(1)
C(9)	38(1)	76(1)	55(1)	22(1)	16(1)	-2(1)
C(10)	69(2)	82(2)	129(2)	28(2)	67(2)	12(1)
C(11)	79(2)	133(3)	187(3)	64(3)	93(2)	23(2)
C(12)	57(2)	195(4)	139(3)	62(3)	33(2)	-27(2)
C(13)	92(2)	169(4)	91(2)	20(2)	10(2)	-74(2)
C(14)	75(2)	124(2)	62(1)	2(1)	15(1)	-46(2)
C(15)	39(1)	66(1)	42(1)	4(1)	14(1)	-7(1)

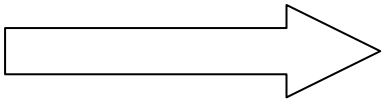
C(16)	67(1)	90(2)	49(1)	2(1)	29(1)	-1(1)
C(17)	84(2)	137(2)	56(1)	4(2)	42(1)	-12(2)
C(18)	75(2)	143(3)	59(2)	36(2)	23(1)	-8(2)
C(19)	50(1)	97(2)	61(1)	28(1)	23(1)	6(1)
C(20)	39(1)	38(1)	37(1)	-6(1)	20(1)	0(1)
C(21)	43(1)	36(1)	43(1)	-4(1)	26(1)	2(1)
C(22)	47(1)	44(1)	46(1)	-2(1)	26(1)	0(1)
C(23)	63(1)	45(1)	52(1)	3(1)	38(1)	3(1)
C(24)	57(1)	38(1)	68(1)	-6(1)	43(1)	-5(1)
C(25)	44(1)	53(1)	62(1)	-5(1)	27(1)	-6(1)
C(26)	45(1)	50(1)	47(1)	0(1)	24(1)	-3(1)

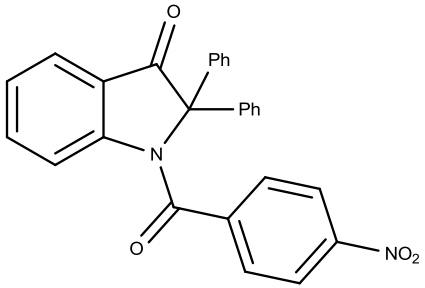
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 5b.

	x	y	z	U(eq)
H(2B)	2666	1983	7398	59
H(3A)	2155	406	7672	65
H(4A)	1351	-34	6656	68
H(5A)	1046	1145	5384	61
H(10A)	546	4344	4851	102
H(11A)	-128	3224	4851	146
H(12A)	-489	901	4101	165
H(13A)	-188	-312	3324	160
H(14A)	499	828	3323	115
H(16A)	1503	3070	3234	82
H(17A)	1356	4577	2078	107
H(18A)	781	6621	1617	117
H(19A)	446	5677	3289	85
H(22A)	2162	5548	4014	53
H(23A)	2674	7094	3716	59
H(25A)	3778	6536	6037	64
H(26A)	3263	5033	6341	57

ii) ORTEP diagram of comp 6a.







Comp 6a

Table 1. Crystal data and structure refinement for 6a.

Identification code	6a	
Empirical formula	C27 H18 N2 O4	
Formula weight	434.43	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.0042(3) Å	α= 90°.
	b = 14.4363(3) Å	β= 106.177(3)°.
	c = 12.4330(4) Å	γ = 90°.
Volume	2069.28(9) $Å^3$	
Z	4	
Density (calculated)	1.394 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	904	

Crystal size	0.60 x 0.50 x 0.34 mm^3
Theta range for data collection	2.52 to 29.20°.
Index ranges	-14<=h<=15, -18<=k<=18, -13<=l<=15
Reflections collected	17616
Independent reflections	4858 [R(int) = 0.0221]
Completeness to theta = 26.00°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.98997
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4858 / 0 / 298
Goodness-of-fit on F^2	1.182
Final R indices [I>2sigma(I)]	R1 = 0.0364, wR2 = 0.0674
R indices (all data)	R1 = 0.0660, wR2 = 0.0698
Largest diff. peak and hole	0.154 and -0.166 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 6a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2126(1)	834(1)	1367(1)	54(1)
O(2)	6679(1)	2108(1)	1793(1)	63(1)
O(3)	5622(1)	6275(1)	4281(1)	93(1)
O(4)	5356(1)	6667(1)	2546(1)	89(1)
N(1)	5017(1)	1655(1)	2150(1)	34(1)
N(2)	5519(1)	6094(1)	3298(1)	64(1)
C(1)	5129(1)	717(1)	1864(1)	36(1)
C(2)	6130(1)	225(1)	1888(1)	47(1)
C(3)	6007(1)	-697(1)	1601(1)	58(1)
C(4)	4943(1)	-1131(1)	1279(1)	62(1)
C(5)	3951(1)	-645(1)	1240(1)	52(1)
C(6)	4058(1)	279(1)	1551(1)	39(1)
C(7)	3165(1)	940(1)	1619(1)	38(1)
C(8)	3790(1)	1846(1)	2162(1)	34(1)
C(9)	3653(1)	1819(1)	3346(1)	34(1)
C(10)	4531(1)	1499(1)	4250(1)	42(1)
C(11)	4354(1)	1420(1)	5296(1)	50(1)
C(12)	3309(1)	1654(1)	5457(1)	51(1)
C(13)	2425(1)	1941(1)	4565(1)	50(1)
C(14)	2582(1)	2017(1)	3513(1)	43(1)
C(15)	3311(1)	2683(1)	1433(1)	34(1)
C(16)	2978(1)	3502(1)	1833(1)	42(1)
C(17)	2629(1)	4253(1)	1120(1)	52(1)

C(18)	2612(1)	4193(1)	16(1)	55(1)
C(19)	2931(1)	3379(1)	-395(1)	52(1)
C(20)	3269(1)	2632(1)	310(1)	43(1)
C(21)	5833(1)	2312(1)	2096(1)	39(1)
C(22)	5695(1)	3287(1)	2433(1)	37(1)
C(23)	5695(1)	3529(1)	3511(1)	43(1)
C(24)	5660(1)	4451(1)	3800(1)	47(1)
C(25)	5594(1)	5111(1)	2994(1)	45(1)
C(26)	5599(1)	4896(1)	1922(1)	49(1)
C(27)	5676(1)	3978(1)	1648(1)	45(1)

Table 3. Bond lengths [Å] and angles [°] for 6a.

O(1)-C(7)	1.2082(12)
O(2)-C(21)	1.2142(12)
O(3)-N(2)	1.2228(15)
O(4)-N(2)	1.2219(15)
N(1)-C(21)	1.3778(13)
N(1)-C(1)	1.4157(13)
N(1)-C(8)	1.5024(12)
N(2)-C(25)	1.4777(16)
C(1)-C(6)	1.3883(14)
C(1)-C(2)	1.3886(14)
C(2)-C(3)	1.3751(17)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.3784(17)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.3719(17)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.3843(16)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.4546(15)
C(7)-C(8)	1.5643(15)
C(8)-C(9)	1.5260(15)
C(8)-C(15)	1.5244(14)
C(9)-C(14)	1.3876(14)
C(9)-C(10)	1.3881(14)
C(10)-C(11)	1.3802(16)
C(10)-H(10A)	0.9300

C(11)-C(12)	1.3658(16)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.3686(17)
C(12)-H(12A)	0.9300
C(13)-C(14)	1.3771(16)
C(13)-H(13A)	0.9300
C(14)-H(14A)	0.9300
C(15)-C(20)	1.3859(15)
C(15)-C(16)	1.3836(15)
C(16)-C(17)	1.3886(16)
C(16)-H(16A)	0.9300
C(17)-C(18)	1.3703(17)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.3779(18)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.3773(16)
C(19)-H(19A)	0.9300
C(20)-H(20A)	0.9300
C(21)-C(22)	1.4912(16)
C(22)-C(23)	1.3855(15)
C(22)-C(27)	1.3916(16)
C(23)-C(24)	1.3817(16)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.3691(17)
C(24)-H(24A)	0.9300
C(25)-C(26)	1.3702(16)
C(26)-C(27)	1.3768(16)
C(26)-H(26A)	0.9300

C(27)-H(27A)	0.9300

C(21)-N(1)-C(1)	121.78(9)
C(21)-N(1)-C(8)	125.93(9)
C(1)-N(1)-C(8)	109.87(8)
O(4)-N(2)-O(3)	124.75(14)
O(4)-N(2)-C(25)	117.57(14)
O(3)-N(2)-C(25)	117.68(13)
C(6)-C(1)-C(2)	120.09(11)
C(6)-C(1)-N(1)	111.14(9)
C(2)-C(1)-N(1)	128.76(10)
C(3)-C(2)-C(1)	117.35(11)
C(3)-C(2)-H(2A)	121.3
C(1)-C(2)-H(2A)	121.3
C(2)-C(3)-C(4)	122.69(12)
C(2)-C(3)-H(3A)	118.7
C(4)-C(3)-H(3A)	118.7
C(5)-C(4)-C(3)	120.13(13)
C(5)-C(4)-H(4A)	119.9
C(3)-C(4)-H(4A)	119.9
C(4)-C(5)-C(6)	118.12(12)
C(4)-C(5)-H(5A)	120.9
C(6)-C(5)-H(5A)	120.9
C(1)-C(6)-C(5)	121.60(10)
C(1)-C(6)-C(7)	108.96(10)
C(5)-C(6)-C(7)	129.44(10)
O(1)-C(7)-C(6)	128.77(11)
O(1)-C(7)-C(8)	123.64(10)

C(6)-C(7)-C(8)	107.50(9)
N(1)-C(8)-C(9)	112.01(8)
N(1)-C(8)-C(15)	110.36(8)
C(9)-C(8)-C(15)	117.99(9)
N(1)-C(8)-C(7)	101.31(8)
C(9)-C(8)-C(7)	103.16(8)
C(15)-C(8)-C(7)	110.46(8)
C(14)-C(9)-C(10)	118.25(10)
C(14)-C(9)-C(8)	119.49(9)
C(10)-C(9)-C(8)	121.85(9)
C(11)-C(10)-C(9)	120.62(11)
C(11)-C(10)-H(10A)	119.7
C(9)-C(10)-H(10A)	119.7
C(12)-C(11)-C(10)	120.42(11)
C(12)-C(11)-H(11A)	119.8
C(10)-C(11)-H(11A)	119.8
C(11)-C(12)-C(13)	119.50(12)
C(11)-C(12)-H(12A)	120.3
C(13)-C(12)-H(12A)	120.3
C(14)-C(13)-C(12)	120.91(11)
C(14)-C(13)-H(13A)	119.5
C(12)-C(13)-H(13A)	119.5
C(13)-C(14)-C(9)	120.22(11)
C(13)-C(14)-H(14A)	119.9
C(9)-C(14)-H(14A)	119.9
C(20)-C(15)-C(16)	118.31(11)
C(20)-C(15)-C(8)	117.31(10)
C(16)-C(15)-C(8)	124.27(10)

C(15)-C(16)-C(17)	120.29(11)
C(15)-C(16)-H(16A)	119.9
C(17)-C(16)-H(16A)	119.9
C(16)-C(17)-C(18)	120.46(12)
C(16)-C(17)-H(17A)	119.8
C(18)-C(17)-H(17A)	119.8
C(19)-C(18)-C(17)	119.87(12)
C(19)-C(18)-H(18A)	120.1
C(17)-C(18)-H(18A)	120.1
C(18)-C(19)-C(20)	119.64(12)
C(18)-C(19)-H(19A)	120.2
C(20)-C(19)-H(19A)	120.2
C(19)-C(20)-C(15)	121.42(12)
C(19)-C(20)-H(20A)	119.3
C(15)-C(20)-H(20A)	119.3
O(2)-C(21)-N(1)	121.12(11)
O(2)-C(21)-C(22)	118.88(10)
N(1)-C(21)-C(22)	119.99(9)
C(23)-C(22)-C(27)	119.53(11)
C(23)-C(22)-C(21)	122.66(11)
C(27)-C(22)-C(21)	117.53(11)
C(24)-C(23)-C(22)	120.20(12)
C(24)-C(23)-H(23A)	119.9
C(22)-C(23)-H(23A)	119.9
C(25)-C(24)-C(23)	118.65(12)
C(25)-C(24)-H(24A)	120.7
C(23)-C(24)-H(24A)	120.7
C(24)-C(25)-C(26)	122.61(11)

C(24)-C(25)-N(2)	118.49(13)
C(26)-C(25)-N(2)	118.90(12)
C(27)-C(26)-C(25)	118.54(12)
C(27)-C(26)-H(26A)	120.7
C(25)-C(26)-H(26A)	120.7
C(26)-C(27)-C(22)	120.36(12)
C(26)-C(27)-H(27A)	119.8
C(22)-C(27)-H(27A)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 6a. 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}
O(1)	39(1)	59(1)	63(1)	-9(1)	11(1)	-8(1)
O(2)	55(1)	60(1)	90(1)	-3(1)	47(1)	-1(1)
O(3)	127(1)	59(1)	100(1)	-28(1)	46(1)	-19(1)
O(4)	101(1)	47(1)	113(1)	11(1)	19(1)	0(1)
N(1)	33(1)	35(1)	37(1)	-3(1)	14(1)	1(1)
N(2)	59(1)	45(1)	87(1)	-6(1)	19(1)	-10(1)
C(1)	43(1)	35(1)	31(1)	0(1)	14(1)	5(1)
C(2)	48(1)	49(1)	46(1)	-5(1)	15(1)	10(1)
C(3)	66(1)	54(1)	58(1)	-5(1)	22(1)	19(1)
C(4)	80(1)	39(1)	71(1)	-11(1)	29(1)	5(1)
C(5)	62(1)	44(1)	54(1)	-6(1)	22(1)	-8(1)
C(6)	47(1)	36(1)	36(1)	-1(1)	16(1)	0(1)
C(7)	40(1)	42(1)	34(1)	0(1)	12(1)	-4(1)
C(8)	30(1)	37(1)	35(1)	-1(1)	11(1)	1(1)
C(9)	36(1)	33(1)	35(1)	-1(1)	13(1)	-1(1)
C(10)	40(1)	44(1)	41(1)	2(1)	11(1)	1(1)
C(11)	57(1)	55(1)	36(1)	5(1)	10(1)	-1(1)
C(12)	71(1)	49(1)	41(1)	1(1)	28(1)	-2(1)
C(13)	54(1)	51(1)	56(1)	4(1)	32(1)	5(1)
C(14)	41(1)	46(1)	44(1)	5(1)	18(1)	4(1)
C(15)	30(1)	39(1)	34(1)	0(1)	10(1)	-1(1)
C(16)	42(1)	42(1)	45(1)	0(1)	19(1)	4(1)
C(17)	49(1)	41(1)	67(1)	5(1)	21(1)	8(1)

C(18)	53(1)	52(1)	57(1)	18(1)	9(1)	3(1)
C(19)	55(1)	60(1)	38(1)	7(1)	6(1)	-8(1)
C(20)	46(1)	43(1)	39(1)	-3(1)	11(1)	-2(1)
C(21)	37(1)	45(1)	37(1)	2(1)	15(1)	0(1)
C(22)	31(1)	40(1)	42(1)	-2(1)	11(1)	-5(1)
C(23)	43(1)	43(1)	42(1)	2(1)	11(1)	-3(1)
C(24)	46(1)	49(1)	44(1)	-8(1)	11(1)	-5(1)
C(25)	39(1)	37(1)	58(1)	-6(1)	12(1)	-7(1)
C(26)	46(1)	45(1)	56(1)	9(1)	14(1)	-9(1)
C(27)	44(1)	51(1)	44(1)	1(1)	16(1)	-8(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 6a.

	x	y	z	U(eq)
H(2A)	6855	508	2090	57
H(3A)	6668	-1041	1626	70
H(4A)	4898	-1756	1088	74
H(5A)	3227	-927	1011	63
H(10A)	5245	1336	4149	50
H(11A)	4950	1207	5896	60
H(12A)	3200	1618	6168	62
H(13A)	1708	2086	4670	60
H(14A)	1969	2202	2912	51
H(16A)	2989	3550	2581	50
H(17A)	2404	4800	1395	62
H(18A)	2386	4700	-455	66
H(19A)	2918	3334	-1145	62
H(20A)	3475	2082	26	51
H(23A)	5719	3070	4042	51
H(24A)	5681	4619	4528	56
H(26A)	5551	5359	1391	59
H(27A)	5715	3820	934	54