Supporting Information

Regioselective, Molecular Iodine-mediated C3 Iodination of Quinolines

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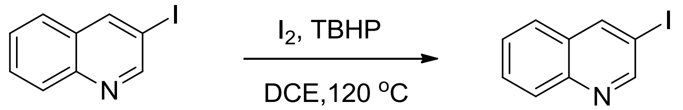
I. General Remarks:

Unless otherwise stated, all commercial reagents and solvents were used without additional purification. All the reactions were carried out under air atmosphere. ^{1}H NMR spectra of compounds **2** were recorded at 25ºC on a Bruker Ascend™ 400 spectrometer. Chemical shifts (in ppm) were referenced TMS in $CDCl_3$ (0 ppm). ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.00 ppm). Melting points were obtained with a micro melting point XT4A Beijing Keyi electrooptic apparatus and are uncorrected. HRMS data were obtained on a Waters LCT Premierxe™ (USA). All reactions were monitored by TLC with Taizhou GF254 silica gel coated plates. Flash column chromatography was carried out using 200-300 mesh silica gel at increased pressure.

II. Synthesis procedure for compounds 2 (1a as an example).



1a **2a**

Quinoline **1a** (64.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol), and DCE (2.0 mL). The mixture was stirred at 120 °C for 24.0 h (monitored by TLC), quenched with water, extracted with dichloromethane (5×3 ml), and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by a shot flash silica gel column chromatography (EtOAc/petro ether = 1:8) to give compound **2a** as a white solid (113.5 mg, 89%).

III. Crystallographic data for 2j

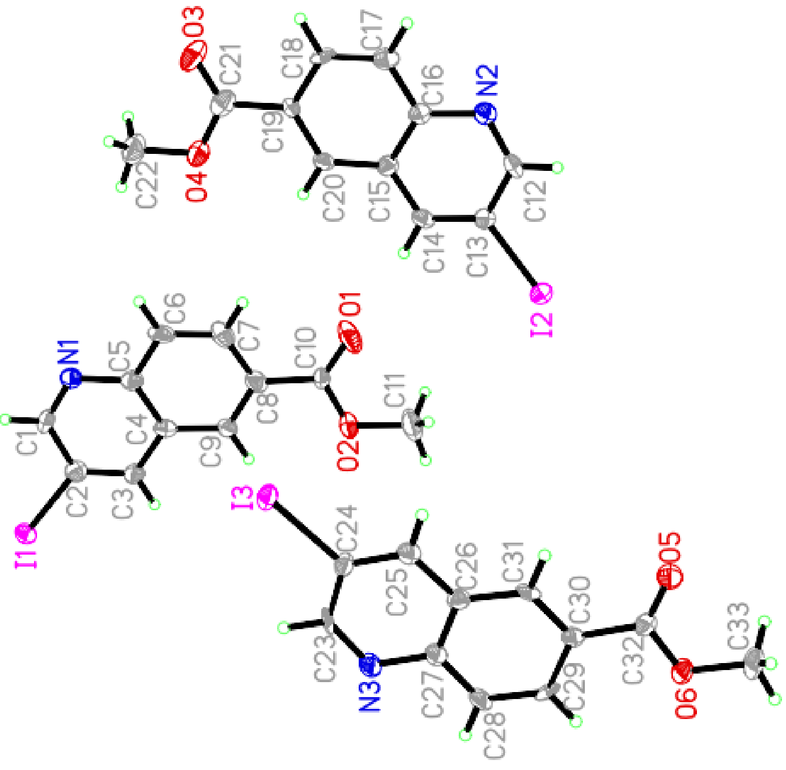


Table 1. Crystal data and structure refinement for **2j**.

Identification code	**2j**
Empirical formula	$C_{11}H_8INO_2$
Formula weight	313.08
Temperature	293(2) K
Wavelength	0.71073Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 12.355(3) Å alpha = 90 deg.
	b = 12.786(3) Å beta = 94.35(3) deg.
	c = 20.330(4) Å gamma = 90 deg.
Volume	3202.3(11) Å 3
Z	12
Calculated density	1.948 Mg/m^3
Absorption coefficient	2.978 mm^{-1}
F(000)	1800
Crystal size	0.20 x 0.20 x 0.20 mm
Theta range for data collection	1.87 to 25.01 deg.
Limiting indices	-14<=h<=14, -15<=k<=15, -23<=l<=24
Reflections collected / unique	31088 / 5639 [R(int) = 0.0699]
Completeness to theta = 25.01	99.9 %
Absorption correction	NONE
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5639 / 0 / 407
Goodness-of-fit on F^2	1.209
Final R indices [I>2sigma (I)]	R1 = 0.0674, wR2 = 0.1600
R indices (all data)	R1 = 0.0752, wR2 = 0.1640
Extinction coefficient	0.00079 (14)
Largest diff. peak and hole	1.646 and -1.663 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(1)	2537(1)	5375(1)	5754(1)	44(1)
I(2)	12080(1)	366(1)	5755(1)	44(1)
I(3)	7392(1)	1789(1)	2472(1)	42(1)
O(6)	14139(5)	4616(5)	2477(4)	48(2)
O(2)	8653(6)	3118(7)	5937(5)	64(2)
C(27)	10126(8)	4504(7)	2494(5)	39(2)
C(20)	8228(7)	-1816(7)	5936(5)	35(2)

C(15)	9353(8)	-1804(8)	5872(5)	37(2)
O(5)	13839(6)	2901(5)	2447(4)	49(2)
O(4)	6006(6)	-1862(7)	6015(4)	56(2)
C(31)	11596(7)	3265(6)	2439(5)	35(2)
C(30)	12339(7)	4055(7)	2459(5)	34(2)
O(1)	8679(7)	1381(7)	5905(5)	73(3)
C(9)	6411(8)	3162(8)	5826(5)	41(2)
C(4)	5272(8)	3179(8)	5782(5)	38(2)
N(3)	9043(7)	4760(6)	2511(5)	44(2)
C(23)	8348(7)	3986(8)	2508(6)	46(3)
C(29)	11962(8)	5105(7)	2492(5)	41(2)
O(3)	5981(7)	-3605(7)	5974(5)	67(2)
C(14)	9978(8)	-877(8)	5857(5)	41(2)
C(24)	8619(7)	2928(7)	2478(5)	34(2)
N(2)	11020(7)	-2824(6)	5750(5)	43(2)
C(8)	6968(8)	2242(8)	5827(5)	44(3)
C(1)	3065(7)	3055(8)	5701(5)	41(2)
C(26)	10480(7)	3468(7)	2469(5)	34(2)
C(28)	10872(8)	5305(7)	2499(6)	43(2)
N(1)	3587(7)	2180(6)	5682(4)	40(2)
C(3)	4652(8)	4118(7)	5799(5)	40(2)
C(13)	11057(8)	-941(8)	5801(5)	38(2)
C(32)	13502(8)	3781(8)	2458(5)	39(2)
C(19)	7664(7)	-2759(7)	5923(5)	32(2)
C(18)	8224(8)	-3689(7)	5867(5)	40(2)
C(25)	9667(8)	2666(8)	2453(5)	39(2)
C(33)	15283(8)	4417(11)	2476(8)	67(4)
C(12)	11531(8)	-1926(8)	5741(6)	44(2)
C(2)	3567(8)	4064(8)	5747(5)	43(2)
C(10)	8160(7)	2187(8)	5894(5)	37(2)
C(21)	6473(9)	-2789(10)	5967(6)	51(3)
C(11)	9824(9)	3122(13)	6009(8)	78(4)
C(16)	9905(8)	-2764(8)	5811(5)	39(2)
C(17)	9314(9)	-3700(8)	5804(6)	47(3)
C(6)	5276(9)	1294(8)	5700(6)	48(3)
C(7)	6383(9)	1305(9)	5747(6)	51(3)
C(22)	4851(9)	-1873(12)	6081(7)	72(4)
C(5)	4702(8)	2223(7)	5727(5)	37(2)

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

I(1)-C(2)	2.106(10)
I(2)-C(13)	2.102(10)

I(3)-C(24)	2.101(9)
O(6)-C(32)	1.326(11)
O(6)-C(33)	1.436(13)
O(2)-C(10)	1.336(13)
O(2)-C(11)	1.444(13)
C(27)-C(28)	1.376(14)
C(27)-N(3)	1.381(12)
C(27)-C(26)	1.397(13)
C(20)-C(19)	1.392(13)
C(20)-C(15)	1.406(13)
C(20)-H(20A)	0.9300
C(15)-C(16)	1.414(14)
C(15)-C(14)	1.415(14)
O(5)-C(32)	1.200(12)
O(4)-C(21)	1.326(15)
O(4)-C(22)	1.444(13)
C(31)-C(30)	1.364(13)
C(31)-C(26)	1.409(13)
C(31)-H(31A)	0.9300
C(30)-C(29)	1.425(13)
C(30)-C(32)	1.479(13)
O(1)-C(10)	1.212(12)
C(9)-C(8)	1.363(14)
C(9)-C(4)	1.404(14)
C(9)-H(9A)	0.9300
C(4)-C(5)	1.411(14)
C(4)-C(3)	1.425(14)
N(3)-C(23)	1.310(13)
C(23)-C(24)	1.396(14)
C(23)-H(23A)	0.9300
C(29)-C(28)	1.372(14)
C(29)-H(29A)	0.9300
O(3)-C(21)	1.208(13)
C(14)-C(13)	1.349(13)
C(14)-H(14A)	0.9300
C(24)-C(25)	1.343(13)
N(2)-C(12)	1.311(13)
N(2)-C(16)	1.395(12)
C(8)-C(7)	1.403(16)
C(8)-C(10)	1.470(13)
C(1)-N(1)	1.293(13)
C(1)-C(2)	1.431(14)
C(1)-H(1A)	0.9300
C(26)-C(25)	1.433(13)

C(28)-H(28A)	0.9300
N(1)-C(5)	1.376(13)
C(3)-C(2)	1.338(14)
C(3)-H(3A)	0.9300
C(13)-C(12)	1.397(14)
C(19)-C(18)	1.385(13)
C(19)-C(21)	1.481(14)
C(18)-C(17)	1.362(14)
C(18)-H(18A)	0.9300
C(25)-H(25A)	0.9300
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(12)-H(12A)	0.9300
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(16)-C(17)	1.402(14)
C(17)-H(17A)	0.9300
C(6)-C(7)	1.363(15)
C(6)-C(5)	1.387(14)
C(6)-H(6A)	0.9300
C(7)-H(7A)	0.9300
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600

C(32)-O(6)-C(33)	116.1(8)
C(10)-O(2)-C(11)	117.3(10)
C(28)-C(27)-N(3)	118.2(8)
C(28)-C(27)-C(26)	119.6(9)
N(3)-C(27)-C(26)	122.1(9)
C(19)-C(20)-C(15)	120.4(8)
C(19)-C(20)-H(20A)	119.8
C(15)-C(20)-H(20A)	119.8
C(20)-C(15)-C(16)	119.0(9)
C(20)-C(15)-C(14)	123.8(9)
C(16)-C(15)-C(14)	117.2(8)
C(21)-O(4)-C(22)	115.9(10)
C(30)-C(31)-C(26)	121.4(8)
C(30)-C(31)-H(31A)	119.3
C(26)-C(31)-H(31A)	119.3
C(31)-C(30)-C(29)	118.5(8)
C(31)-C(30)-C(32)	118.5(8)

C(29)-C(30)-C(32)	123.0(8)
C(8)-C(9)-C(4)	121.2(10)
C(8)-C(9)-H(9A)	119.4
C(4)-C(9)-H(9A)	119.4
C(9)-C(4)-C(5)	118.9(9)
C(9)-C(4)-C(3)	123.4(9)
C(5)-C(4)-C(3)	117.8(9)
C(23)-N(3)-C(27)	117.2(8)
N(3)-C(23)-C(24)	125.0(8)
N(3)-C(23)-H(23A)	117.5
C(24)-C(23)-H(23A)	117.5
C(28)-C(29)-C(30)	120.1(8)
C(28)-C(29)-H(29A)	120.0
C(30)-C(29)-H(29A)	120.0
C(13)-C(14)-C(15)	119.7(9)
C(13)-C(14)-H(14A)	120.2
C(15)-C(14)-H(14A)	120.2
C(25)-C(24)-C(23)	118.5(8)
C(25)-C(24)-I(3)	121.7(7)
C(23)-C(24)-I(3)	119.8(6)
C(12)-N(2)-C(16)	115.6(8)
C(9)-C(8)-C(7)	118.7(10)
C(9)-C(8)-C(10)	123.0(10)
C(7)-C(8)-C(10)	118.3(9)
N(1)-C(1)-C(2)	124.6(9)
N(1)-C(1)-H(1A)	117.7
C(2)-C(1)-H(1A)	117.7
C(27)-C(26)-C(31)	119.1(8)
C(27)-C(26)-C(25)	117.3(8)
C(31)-C(26)-C(25)	123.6(8)
C(29)-C(28)-C(27)	121.2(9)
C(29)-C(28)-H(28A)	119.4
C(27)-C(28)-H(28A)	119.4
C(1)-N(1)-C(5)	117.5(8)
C(2)-C(3)-C(4)	119.4(9)
C(2)-C(3)-H(3A)	120.3
C(4)-C(3)-H(3A)	120.3
C(14)-C(13)-C(12)	119.0(9)
C(14)-C(13)-I(2)	123.8(7)
C(12)-C(13)-I(2)	117.1(7)
O(5)-C(32)-O(6)	123.3(9)
O(5)-C(32)-C(30)	124.1(9)
O(6)-C(32)-C(30)	112.6(8)
C(18)-C(19)-C(20)	119.5(8)

C(18)-C(19)-C(21)	119.1(9)
C(20)-C(19)-C(21)	121.3(9)
C(17)-C(18)-C(19)	121.3(8)
C(17)-C(18)-H(18A)	119.4
C(19)-C(18)-H(18A)	119.4
C(24)-C(25)-C(26)	119.8(9)
C(24)-C(25)-H(25A)	120.1
C(26)-C(25)-H(25A)	120.1
O(6)-C(33)-H(33A)	109.5
O(6)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
O(6)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
N(2)-C(12)-C(13)	125.6(9)
N(2)-C(12)-H(12A)	117.2
C(13)-C(12)-H(12A)	117.2
C(3)-C(2)-C(1)	118.6(9)
C(3)-C(2)-I(1)	124.1(8)
C(1)-C(2)-I(1)	117.3(7)
O(1)-C(10)-O(2)	121.2(9)
O(1)-C(10)-C(8)	124.5(10)
O(2)-C(10)-C(8)	114.3(8)
O(3)-C(21)-O(4)	123.3(11)
O(3)-C(21)-C(19)	121.8(11)
O(4)-C(21)-C(19)	114.9(9)
O(2)-C(11)-H(11A)	109.5
O(2)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(2)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(2)-C(16)-C(17)	118.0(9)
N(2)-C(16)-C(15)	122.8(9)
C(17)-C(16)-C(15)	119.2(9)
C(18)-C(17)-C(16)	120.6(9)
C(18)-C(17)-H(17A)	119.7
C(16)-C(17)-H(17A)	119.7
C(7)-C(6)-C(5)	120.1(10)
C(7)-C(6)-H(6A)	120.0
C(5)-C(6)-H(6A)	120.0
C(6)-C(7)-C(8)	121.5(10)
C(6)-C(7)-H(7A)	119.2
C(8)-C(7)-H(7A)	119.2

O(4)-C(22)-H(22A)	109.5
O(4)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
O(4)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(1)-C(5)-C(6)	118.4(9)
N(1)-C(5)-C(4)	122.1(9)
C(6)-C(5)-C(4)	119.5(9)

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}]

	U11	U22	U33	U23	U13	U12
I(1)	40(1)	32(1)	60(1)	-1(1)	3(1)	8(1)
I(2)	38(1)	33(1)	59(1)	1(1)	0(1)	-6(1)
I(3)	27(1)	41(1)	58(1)	-1(1)	2(1)	-7(1)
O(6)	28(3)	34(4)	80(6)	2(4)	0(3)	-8(3)
O(2)	29(4)	72(6)	91(7)	24(5)	7(4)	10(4)
C(27)	35(5)	28(5)	53(6)	1(4)	3(4)	4(4)
C(20)	37(5)	23(4)	44(6)	1(4)	-4(4)	3(4)
C(15)	37(5)	33(5)	42(6)	2(4)	-2(4)	-3(4)
O(5)	43(4)	24(4)	80(6)	-7(3)	7(4)	0(3)
O(4)	38(4)	61(5)	69(6)	12(4)	5(4)	-10(4)
C(31)	42(5)	11(4)	51(6)	3(4)	2(4)	8(4)
C(30)	34(5)	21(5)	45(6)	1(4)	0(4)	0(4)
O(1)	48(5)	70(6)	100(7)	-17(5)	-5(5)	30(4)
C(9)	36(5)	37(5)	52(6)	13(5)	11(4)	7(4)
C(4)	46(5)	27(5)	42(6)	4(4)	4(4)	2(4)
N(3)	34(4)	24(4)	73(6)	-2(4)	0(4)	6(3)
C(23)	11(4)	48(6)	79(8)	6(6)	1(4)	13(4)
C(29)	42(5)	19(5)	62(7)	7(4)	7(5)	-20(4)
O(3)	56(5)	65(6)	80(6)	-14(5)	9(4)	-29(4)
C(14)	40(5)	27(5)	56(7)	0(5)	1(5)	8(4)
C(24)	25(4)	32(5)	46(6)	-6(4)	4(4)	-4(4)
N(2)	39(5)	35(5)	54(6)	-1(4)	0(4)	2(4)
C(8)	42(6)	43(6)	49(7)	5(5)	13(5)	14(5)
C(1)	26(5)	48(6)	50(6)	0(5)	5(4)	-9(4)
C(26)	37(5)	26(5)	38(5)	1(4)	5(4)	-1(4)
C(28)	38(5)	25(5)	65(7)	2(5)	-2(5)	11(4)
N(1)	39(4)	29(4)	51(5)	-2(4)	3(4)	2(3)
C(3)	37(5)	26(5)	56(7)	-7(4)	4(4)	-1(4)

C(13)	36(5)	34(5)	43(6)	4(4)	0(4)	-1(4)
C(32)	32(5)	37(6)	47(6)	5(5)	1(4)	-7(4)
C(19)	25(4)	30(5)	41(6)	5(4)	2(4)	7(4)
C(18)	47(6)	12(4)	60(7)	-10(4)	1(5)	-13(4)
C(25)	39(5)	30(5)	46(6)	2(4)	1(4)	2(4)
C(33)	26(5)	70(9)	105(11)	3(8)	2(6)	-12(5)
C(12)	30(5)	44(6)	58(7)	3(5)	1(4)	14(4)
C(2)	44(6)	38(6)	47(6)	-2(5)	10(5)	3(4)
C(10)	22(4)	39(5)	49(6)	1(4)	4(4)	1(4)
C(21)	50(6)	59(8)	44(7)	-1(5)	1(5)	-15(6)
C(11)	38(6)	107(12)	88(11)	11(9)	-1(6)	20(7)
C(16)	38(5)	33(5)	47(6)	-1(4)	1(4)	-2(4)
C(17)	54(6)	28(5)	58(7)	-10(5)	3(5)	-1(4)
C(6)	65(7)	20(5)	56(7)	-1(5)	-4(5)	3(5)
C(7)	48(6)	50(7)	55(7)	-9(5)	1(5)	19(5)
C(22)	45(7)	92(10)	81(10)	15(8)	11(6)	-14(7)
C(5)	44(5)	31(5)	37(6)	-2(4)	1(4)	-1(4)

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

	x	y	z	U(eq)
H(20A)	7859	-1191	5988	42
H(31A)	11831	2577	2405	42
H(9A)	6792	3789	5856	49
H(23A)	7619	4154	2528	55
H(29A)	12455	5656	2510	49
H(14A)	9646	-228	5885	49
H(1A)	2311	3027	5684	49
H(28A)	10632	5994	2507	52
H(3A)	4999	4762	5847	48
H(18A)	7849	-4319	5873	48
H(25A)	9866	1967	2425	46
H(33A)	15669	5070	2487	101
H(33B)	15426	4041	2083	101
H(33C)	15519	4009	2856	101
H(12A)	12272	-1946	5690	53
H(11A)	10081	3831	6031	117
H(11B)	10102	2778	5638	117
H(11C)	10070	2761	6407	117
H(17A)	9669	-4333	5755	56

H(6A)	4906	662	5649	57
H(7A)	6758	677	5725	61
H(22A)	4592	-1168	6113	108
H(22B)	4702	-2252	6471	108
H(22C)	4489	-2205	5702	108

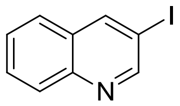
Table 6. Torsion angles [deg] for **2j**.

C(19)-C(20)-C(15)-C(16)	-1.6(15)
C(19)-C(20)-C(15)-C(14)	177.7(10)
C(26)-C(31)-C(30)-C(29)	-1.8(15)
C(26)-C(31)-C(30)-C(32)	177.1(9)
C(8)-C(9)-C(4)-C(5)	-1.0(16)
C(8)-C(9)-C(4)-C(3)	178.0(11)
C(28)-C(27)-N(3)-C(23)	-179.7(11)
C(26)-C(27)-N(3)-C(23)	0.5(16)
C(27)-N(3)-C(23)-C(24)	-1.1(18)
C(31)-C(30)-C(29)-C(28)	-0.5(16)
C(32)-C(30)-C(29)-C(28)	-179.3(10)
C(20)-C(15)-C(14)-C(13)	179.2(10)
C(16)-C(15)-C(14)-C(13)	-1.5(15)
N(3)-C(23)-C(24)-C(25)	0.3(18)
N(3)-C(23)-C(24)-I(3)	-179.5(9)
C(4)-C(9)-C(8)-C(7)	3.3(16)
C(4)-C(9)-C(8)-C(10)	-177.9(10)
C(28)-C(27)-C(26)-C(31)	-1.1(16)
N(3)-C(27)-C(26)-C(31)	178.7(10)
C(28)-C(27)-C(26)-C(25)	-178.9(10)
N(3)-C(27)-C(26)-C(25)	0.9(16)
C(30)-C(31)-C(26)-C(27)	2.5(15)
C(30)-C(31)-C(26)-C(25)	-179.7(10)
C(30)-C(29)-C(28)-C(27)	2.0(17)
N(3)-C(27)-C(28)-C(29)	179.0(10)
C(26)-C(27)-C(28)-C(29)	-1.2(17)
C(2)-C(1)-N(1)-C(5)	1.8(16)
C(9)-C(4)-C(3)-C(2)	179.3(10)
C(5)-C(4)-C(3)-C(2)	-1.7(16)
C(15)-C(14)-C(13)-C(12)	1.8(16)
C(15)-C(14)-C(13)-I(2)	178.8(8)
C(33)-O(6)-C(32)-O(5)	0.7(16)
C(33)-O(6)-C(32)-C(30)	-179.8(10)
C(31)-C(30)-C(32)-O(5)	-0.7(16)
C(29)-C(30)-C(32)-O(5)	178.1(11)

C(31)-C(30)-C(32)-O(6)	179.9(9)
C(29)-C(30)-C(32)-O(6)	-1.4(15)
C(15)-C(20)-C(19)-C(18)	2.1(15)
C(15)-C(20)-C(19)-C(21)	-178.0(9)
C(20)-C(19)-C(18)-C(17)	-2.1(16)
C(21)-C(19)-C(18)-C(17)	177.9(10)
C(23)-C(24)-C(25)-C(26)	1.1(15)
I(3)-C(24)-C(25)-C(26)	-179.0(7)
C(27)-C(26)-C(25)-C(24)	-1.7(15)
C(31)-C(26)-C(25)-C(24)	-179.4(10)
C(16)-N(2)-C(12)-C(13)	1.5(16)
C(14)-C(13)-C(12)-N(2)	-1.9(17)
I(2)-C(13)-C(12)-N(2)	-179.1(9)
C(4)-C(3)-C(2)-C(1)	2.4(16)
C(4)-C(3)-C(2)-I(1)	-179.3(8)
N(1)-C(1)-C(2)-C(3)	-2.7(17)
N(1)-C(1)-C(2)-I(1)	179.0(9)
C(11)-O(2)-C(10)-O(1)	-1.2(17)
C(11)-O(2)-C(10)-C(8)	179.6(10)
C(9)-C(8)-C(10)-O(1)	179.1(12)
C(7)-C(8)-C(10)-O(1)	-2.2(17)
C(9)-C(8)-C(10)-O(2)	-1.8(16)
C(7)-C(8)-C(10)-O(2)	177.0(10)
C(22)-O(4)-C(21)-O(3)	0.3(17)
C(22)-O(4)-C(21)-C(19)	-178.1(10)
C(18)-C(19)-C(21)-O(3)	2.0(17)
C(20)-C(19)-C(21)-O(3)	-177.9(11)
C(18)-C(19)-C(21)-O(4)	-179.6(10)
C(20)-C(19)-C(21)-O(4)	0.4(15)
C(12)-N(2)-C(16)-C(17)	178.2(10)
C(12)-N(2)-C(16)-C(15)	-1.1(15)
C(20)-C(15)-C(16)-N(2)	-179.5(10)
C(14)-C(15)-C(16)-N(2)	1.1(15)
C(20)-C(15)-C(16)-C(17)	1.2(15)
C(14)-C(15)-C(16)-C(17)	-178.2(10)
C(19)-C(18)-C(17)-C(16)	1.7(17)
N(2)-C(16)-C(17)-C(18)	179.5(10)
C(15)-C(16)-C(17)-C(18)	-1.2(17)
C(5)-C(6)-C(7)-C(8)	0.4(18)
C(9)-C(8)-C(7)-C(6)	-3.1(17)
C(10)-C(8)-C(7)-C(6)	178.1(11)
C(1)-N(1)-C(5)-C(6)	-179.2(10)
C(1)-N(1)-C(5)-C(4)	-0.9(15)
C(7)-C(6)-C(5)-N(1)	-179.6(10)

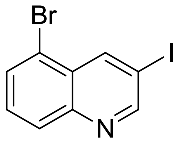
C(7)-C(6)-C(5)-C(4)	2.0(17)
C(9)-C(4)-C(5)-N(1)	179.9(9)
C(3)-C(4)-C(5)-N(1)	0.8(15)
C(9)-C(4)-C(5)-C(6)	-1.7(15)
C(3)-C(4)-C(5)-C(6)	179.2(10)

IV. Analytical data of products obtained in this study



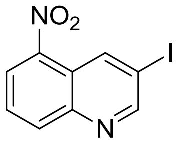
3-iodoquinoline 2a

The reaction of quinoline **1a** (64.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 113.5 mg (89%) of **2a** as white solid. Mp: 133-134 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): *δ* = 7.58 (t, *J* = 6.8 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 2H), 8.07 (d, *J* = 8.8 Hz, 1H), 8.54 (d, *J* = 2.0 Hz, 1H), 9.05 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): *δ* = 126.8, 127.4, 129.5, 129.9, 130.0, 143.7, 146.3, 155.6. HRMS (ESI-TOF) Calcd for C_9H_7NI, $[M+H]^+$ 255.9621; Found 255.9627.



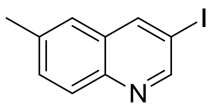
5-bromo-3-iodoquinoline 2b

The reaction of 5-bromoquinoline **1b** (103.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 121.5 mg (73%) of **2b** as white solid. Mp: 100-101 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): *δ* = 7.59 (t, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 8.92 (t, *J* = 1.2 Hz, 1H), 9.07 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): *δ* = 91.5, 120.5, 129.2, 129.5, 130.2, 131.1, 143.2, 147.1, 156.4. HRMS (ESI-TOF) Calcd for C_9H_6NIBr, $[M+H]^+$ 333.8728; Found 333.8724.



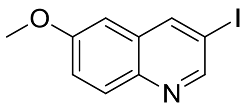
3-iodo-5-nitroquinoline 2c

The reaction of 5-nitroquinoline **1c** (87.0 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 106.5 mg (71%) of **2c** as white solid. Mp: 107-109 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): *δ* = 7.84 (t, *J* = 8.0 Hz, 1H), 8.41 (q, *J* = 7.6 Hz, 2H), 9.18 (d, *J* = 2.0 Hz, 1H), 9.46 (d, *J* = 1.6 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): *δ* = 94.3, 122.4, 125.4, 127.9, 136.8, 139.7, 144.2, 146.4, 157.2. HRMS (ESI-TOF) Calcd for $C_9H_6N_2IO_2$, $[M+H]^+$ 300.9471; Found 300.9474.



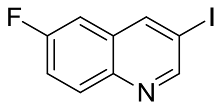
3-iodo-6-methylquinoline 2d

The reaction of 6-methylquinoline **1d** (71.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 122.4 mg (91%) of **2d** as white solid. Mp: 112-113 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.54 (s, 3H), 7.45 (s, 1H), 7.56 (d, J = 8.8 Hz, 1H), 7.95 (d, J = 8.4 Hz, 1H), 8.43 (s, 1H), 8.96 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.6, 89.8, 125.6, 129.1, 129.9, 132.3, 137.5, 143.0, 144.9, 154.6. HRMS (ESI-TOF) Calcd for $C_{10}H_9NI$, $[M+H]^+$ 269.9784; Found 269.9778.



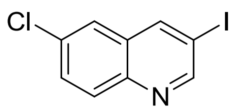
3-iodo-6-methoxyquinoline 2e

The reaction of 6-methoxyquinoline **1e** (79.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 119.7 mg (84%) of **2e** as white solid. Mp: 116-117 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.93 (s, 3H), 6.95 (s, 1H), 7.36 (t, J = 7.2 Hz, 1H), 7.95 (d, J = 9.2 Hz, 1H), 8.43 (s, 1H), 8.88 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 55.6, 90.5, 104.1, 122.9, 130.9, 142.3, 142.5, 153.0, 158.3. HRMS (ESI-TOF) Calcd for $C_{10}H_9NIO$, $[M+H]^+$ 285.9724; Found 285.9728.



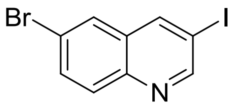
6-fluoro-3-iodoquinoline 2f

The reaction of 6-fluoroquinoline **1f** (73.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 114.7 mg (84%) of **2f** as white solid. Mp: 76-77 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 7.32 (dd, J_1 = 2.8 Hz, J_2 = 8.8 Hz, 1H), 7.50 (dd, J_1 = 2.8 Hz, J_2 = 8.4 Hz, 1H), 8.04 (t, J = 5.2 Hz, 1H), 8.47 (d, J = 1.6 Hz, 1H), 8.98 (d, J = 1.6 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 91.2, 109.7, 109.9, 120.2, 120.4, 130.5, 130.6, 132.1, 132.2, 142.9, 143.5, 154.9, 159.4, 161.9. HRMS (ESI-TOF) Calcd for C_9H_6NIF, $[M+H]^+$ 273.9529; Found 273.9524.



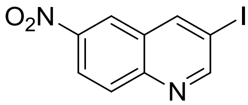
6-chloro-3-iodoquinoline 2g

The reaction of 6-chloroquinoline **1g** (81.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 125.9 mg (87%) of **2g** as white solid. Mp: 118-119 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 7.32 (m, 2H), 8.01 (d, J = 8.8 Hz, 1H), 8.45 (s, 1H), 9.02 (d, J = 1.6 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 91.1, 125.4, 130.3, 130.9, 131.2, 142.7, 155.9. HRMS (ESI-TOF) Calcd for C_9H_6NICl, $[M+H]^+$ 289.9233; Found 289.9227.



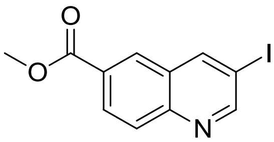
6-bromo-3-iodoquinoline 2h

The reaction of 6-bromoquinoline **1h** (103.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 °C for 24.0 h, affords 133.2 mg (80%) of **2h** as white solid. Mp: 130-132 °C; ^{1}H NMR (400 MHz; CDCl$_3$): δ = 7.77 (d, J = 8.8 Hz, 1H), 7.85 (s, 1H), 7.90 (d, J = 8.8 Hz, 1H), 8.42 (s, 1H), 9.03 (s, 1H). ^{13}C NMR (100 MHz; CDCl$_3$): δ = 91.0, 121.4, 128.7, 130.7, 131.2, 133.5, 142.6, 144.9, 155.9. HRMS (ESI-TOF) Calcd for C_9H_9NIBr, $[M+H]^+$ 333.8728; Found 333.8722.



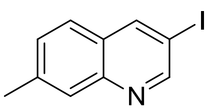
3-iodo-6-nitroquinoline 2i

The reaction of 6-nitroquinoline **1i** (87.0 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 °C for 24.0 h, affords 103.5 mg (69%) of **2i** as white solid. Mp: 120-121 °C; ^{1}H NMR (400 MHz; CDCl$_3$): δ = 8.21 (d, J = 9.2 Hz, 1H), 8.50 (dd, J_1 = 2.4 Hz, J_2 = 9.2 Hz, 1H), 8.69 (d, J = 2.0 Hz, 1H), 8.74 (s, 1H), 9.21 (d, J = 1.6 Hz, 1H). ^{13}C NMR (100 MHz; CDCl$_3$): δ = 92.1, 123.4, 128.6, 131.6, 145.2, 145.9, 148.2, 159.1. HRMS (ESI-TOF) Calcd for $C_9H_6N_2IO_2$, $[M+H]^+$ 300.9471; Found 300.9478.



methyl 3-iodoquinoline-6-carboxylate 2j

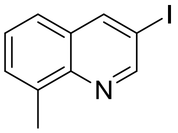
The reaction of methyl quinoline-6-carboxylate **1j** (93.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 °C for 24.0 h, affords 120.5 mg (77%) of **2j** as white solid. Mp: 154-155 °C; ^{1}H NMR (400 MHz; CDCl$_3$): δ = 3.99 (s, 3H), 8.08 (d, J = 8.8 Hz, 1H), 8.30 (dd, J_1 = 1.6 Hz, J_2 = 8.8 Hz, 1H), 8.44 (s, 1H), 8.60 (s, 1H), 9.09 (d, J = 1.6 Hz, 1H). ^{13}C NMR (100 MHz; CDCl$_3$): δ = 52.6, 90.6, 128.9, 129.5, 129.8, 144.8, 148.0, 157.7, 166.2. HRMS (ESI-TOF) Calcd for $C_{11}H_9NIO_2$, $[M+H]^+$ 313.9674; Found 313.9678.



3-iodo-7-methylquinoline 2k

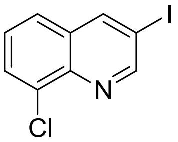
The reaction of 7-methylquinoline **1k** (71.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 °C for 24.0 h, affords 115.7 mg (86%) of **2k** as white solid. Mp: 116-117 °C; ^{1}H NMR (400 MHz;

$CDCl_3$): δ = 2.57 (s, 3H), 7.40 (d, J = 8.0 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.84 (s, 1H), 8.49 (s, 1H), 8.99 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.9, 88.6, 126.4, 128.1, 128.5, 129.6, 140.5, 143.3, 146.6, 155.5. HRMS (ESI-TOF) Calcd for $C_{10}H_9NI$, $[M+H]^+$ 269.9784; Found 269.9781.



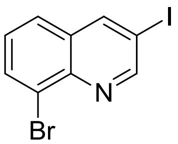
3-iodo-8-methylquinoline 2l

The reaction of 8-methylquinoline **1l** (71.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 °C for 24.0 h, affords 117.0 mg (87%) of **2l** as white solid. Mp: 75-76 °C; ^1H NMR (400 MHz; $CDCl_3$): δ = 2.79 (s, 3H), 7.45 (d, J = 7.2 Hz, 1H), 7.57 (t, J = 8.0 Hz, 2H), 8.51 (d, J = 2.0 Hz, 1H), 9.06 (d, J = 2.0 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 17.8, 89.9, 124.9, 127.3, 130.0, 130.2, 137.5, 143.8, 145.5, 154.4. HRMS (ESI-TOF) Calcd for $C_{10}H_9NI$, $[M+H]^+$ 269.9784; Found 269.9780.



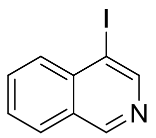
8-chloro-3-iodoquinoline 2m

The reaction of 8-chloroquinoline **1m** (81.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 °C for 24.0 h, affords 133.2 mg (92%) of **2m** as white solid. Mp: 106-107 °C; ^1H NMR (400 MHz; $CDCl_3$): δ = 7.49 (t, J = 7.6 Hz, 1H), 7.65 (dd, J_1 = 1.2 Hz, J_2 = 8.4 Hz, 1H), 7.86 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 1H), 8.57 (d, J = 2.0 Hz, 1H), 9.15 (d, J = 2.0 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 91.1, 125.9, 127.5, 130.2, 131.1, 133.8, 142.8, 144.1, 156.2. HRMS (ESI-TOF) Calcd for C_9H_6NICl, $[M+H]^+$ 289.9233; Found 289.9238.



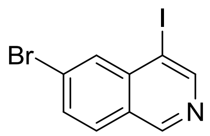
8-bromo-3-iodoquinoline 2n

The reaction of 8-bromoquinoline **1n** (103.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 °C for 24.0 h, affords 133.2 mg (80%) of **2n** as white solid. Mp: 89-90 °C; ^1H NMR (400 MHz; $CDCl_3$): δ = 7.44 (t, J = 8.0 Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 8.08 (dd, J_1 = 0.8 Hz, J_2 = 7.6 Hz, 1H), 8.57 (d, J = 2.0 Hz, 1H), 9.16 (d, J = 2.0 Hz, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 91.0, 124.9, 126.7, 127.9, 131.0, 133.7, 143.7, 144.1, 156.5. HRMS (ESI-TOF) Calcd for C_9H_6NIBr, $[M+H]^+$ 333.8728; Found 333.8723.



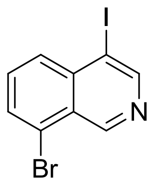
4-iodoisoquinoline 2o

The reaction of isoquinoline **1o** (64.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 94.4 mg (74%) of **2o** as white solid. Mp: 94-95 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 7.68 (s, 1H), 7.80 (s, 1H), 7.90 (d, J = 5.6 Hz, 1H), 8.01 (d, J = 6.0 Hz, 1H), 8.96 (s, 1H), 9.16 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 96.8, 128.2, 128.3, 129.7, 130.7, 131.9, 137.1, 150.9, 152.6. HRMS (ESI-TOF) Calcd for C_9H_7NI, $[M+H]^+$ 255.9621; Found 255.9626.



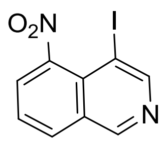
6-bromo-4-iodoisoquinoline 2p

The reaction of 6-bromoisoquinoline **1p** (103.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 139.9 mg (84%) of **2p** as white solid. Mp: 123-124 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 7.73-7.79 (m, 2H), 8.19 (s, 1H), 8.96 (s, 1H), 9.10 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 94.9, 127.3, 128.0, 129.7, 132.1, 133.1, 138.2, 151.9, 152.3. HRMS (ESI-TOF) Calcd for C_9H_6NIBr, $[M+H]^+$ 333.8728; Found 333.8721.



8-bromo-4-iodoisoquinoline 2q

The reaction of 8-bromoisoquinoline **1q** (103.5 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 131.5 mg (79%) of **2q** as white solid. Mp: 114-116 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 7.61 (q, J = 7.6 Hz, 1H), 7.91 (d, J = 7.6 Hz, 1H), 8.00 (d, J = 8.4 Hz, 1H), 9.02 (s, 1H), 9.53 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 96.1, 122.7, 127.8, 131.0, 131.9, 132.4, 138.4, 152.1, 152.2. HRMS (ESI-TOF) Calcd for C_9H_6NIBr, $[M+H]^+$ 333.8728; Found 333.8723.

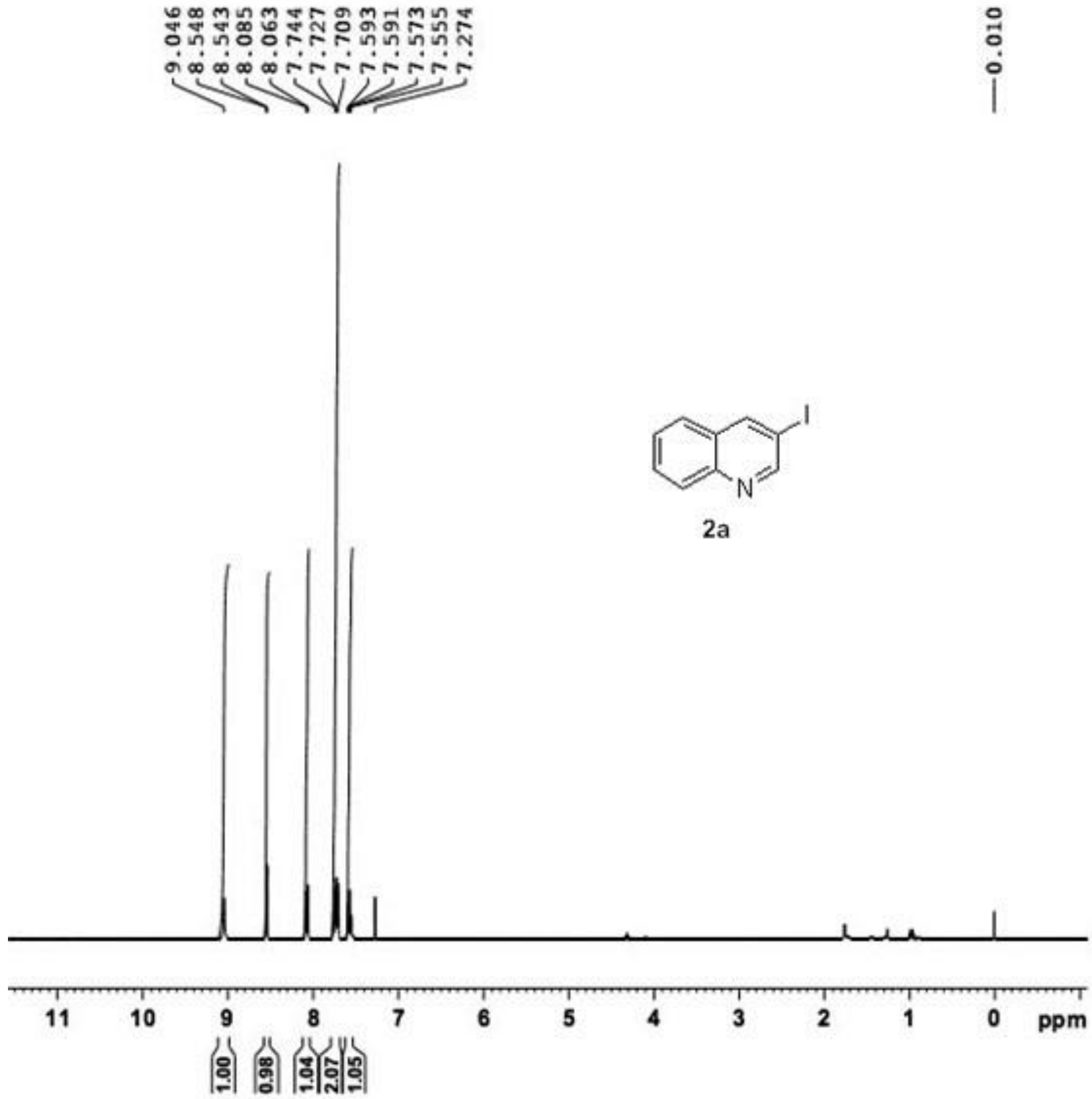


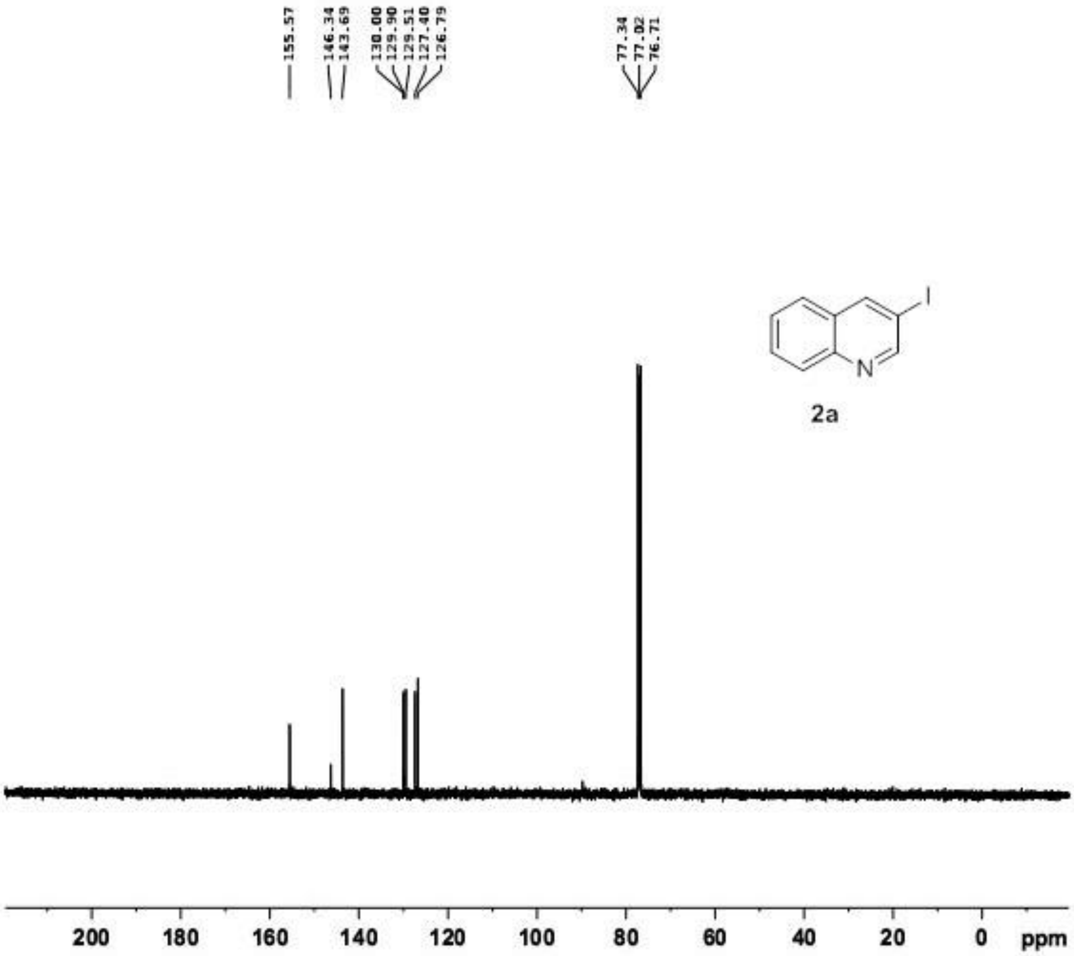
4-iodo-5-nitroisoquinoline 2r

The reaction of 5-nitroisoquinoline **1r** (82.0 mg, 0.5 mmol), molecular iodine (253.8 mg, 1.0 mmol), TBHP (143.6μL, 1.5 mmol) in DCE (2.0 mL) at 120 ^{o}C for 24.0 h, affords 109.5 mg (73%) of **2r** as white solid. Mp: 93-93 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 7.73 (t, J = 8.0 Hz, 1H), 8.04 (dd, J_1 = 0.8 Hz, J_2 = 7.6 Hz, 1H), 8.19 (dd, J_1 = 0.8 Hz, J_2 = 8.0 Hz, 1H), 9.17 (s, 1H), 9.26 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 85.7, 126.7, 127.4, 130.4, 132.7, 148.9, 152.7, 156.7. HRMS (ESI-TOF) Calcd for $C_9H_6N_2O_2I$, $[M+H]^+$ 300.9471; Found 300.9477.

V. ^{1}H NMR and ^{13}C NMR spectra copies of compounds 2

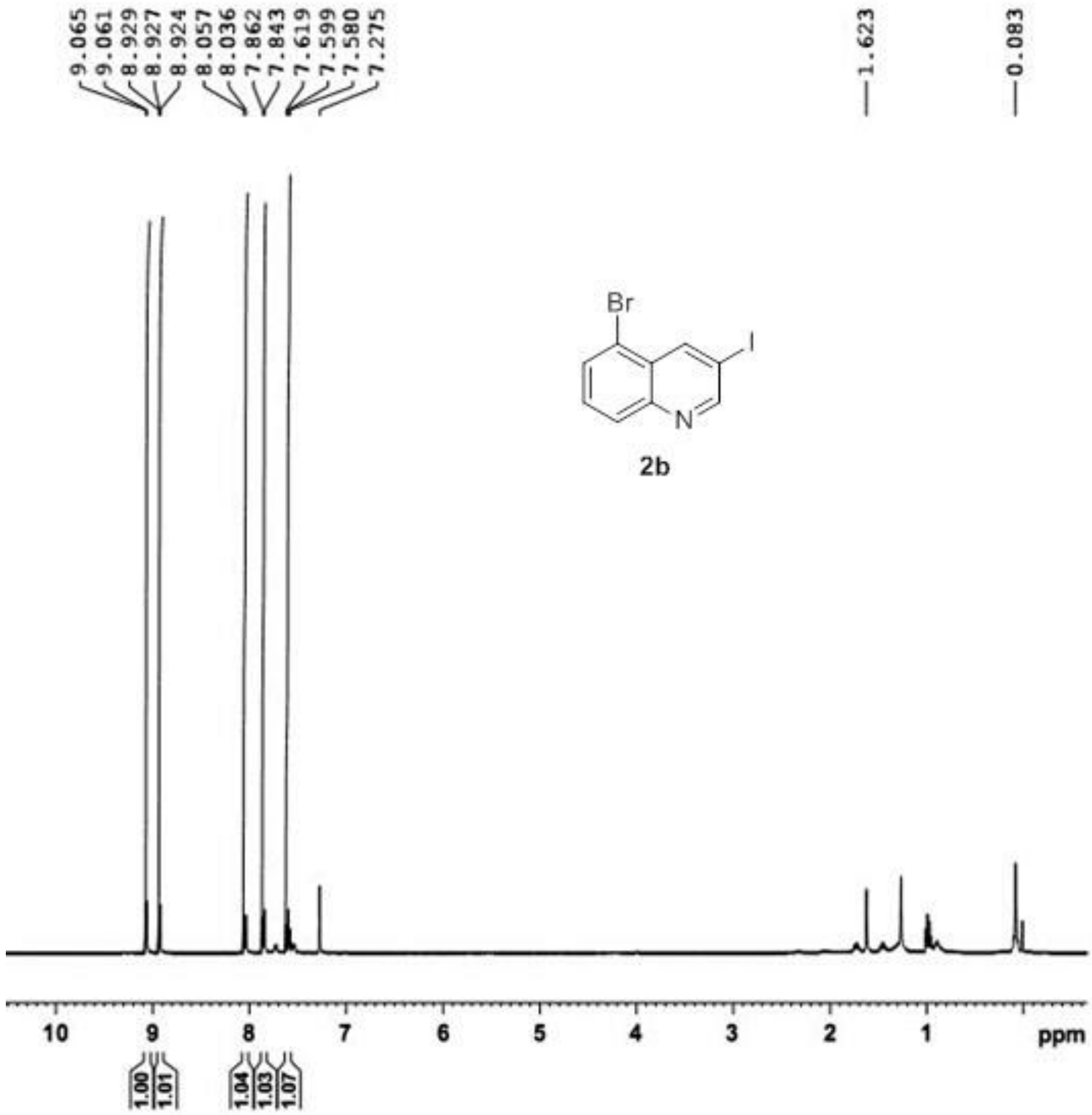
Compound 2a





155.57
146.34
143.69
130.00
129.90
129.51
127.40
126.79
77.34
77.02
76.71
N
I
2a
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 2b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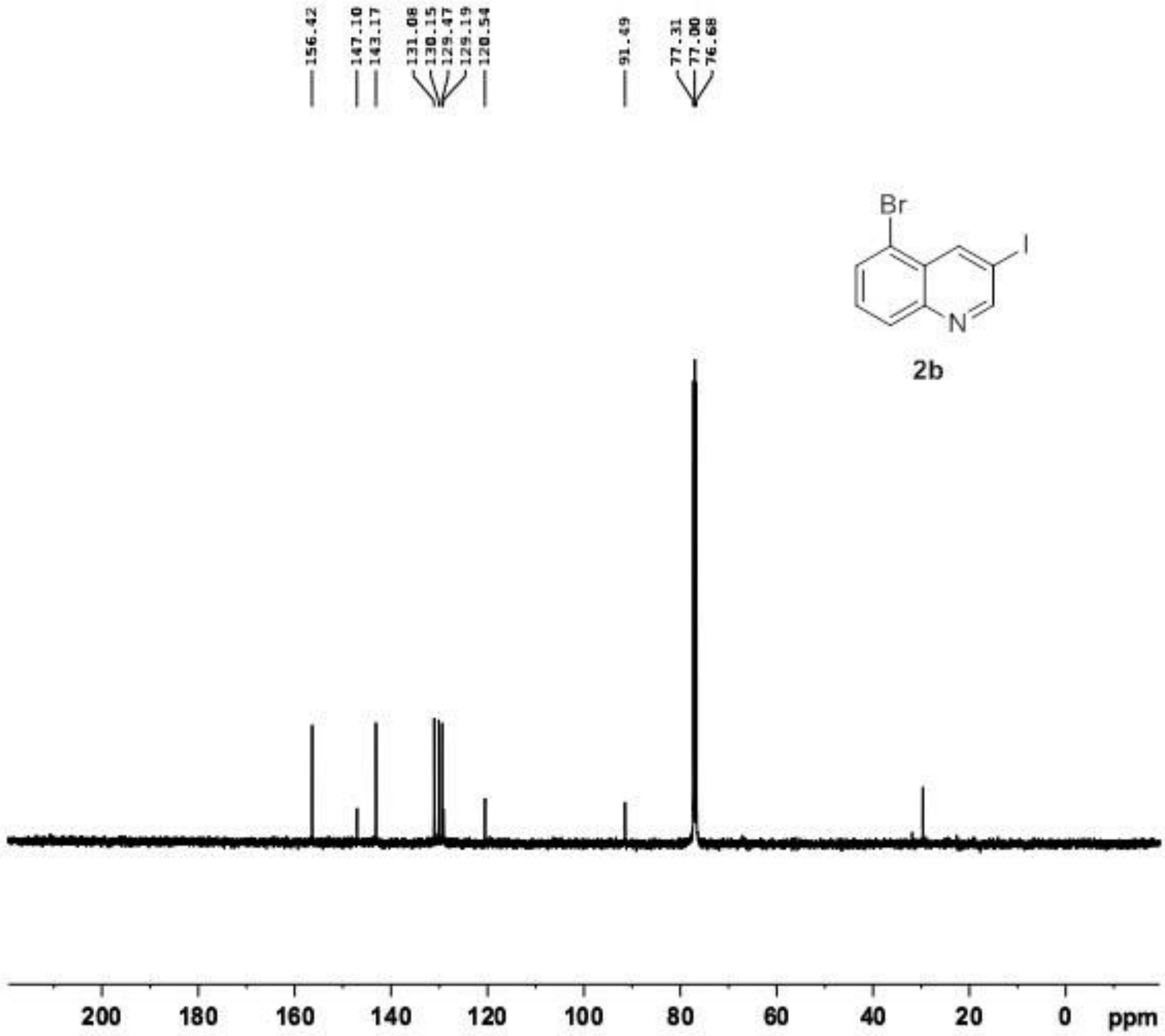
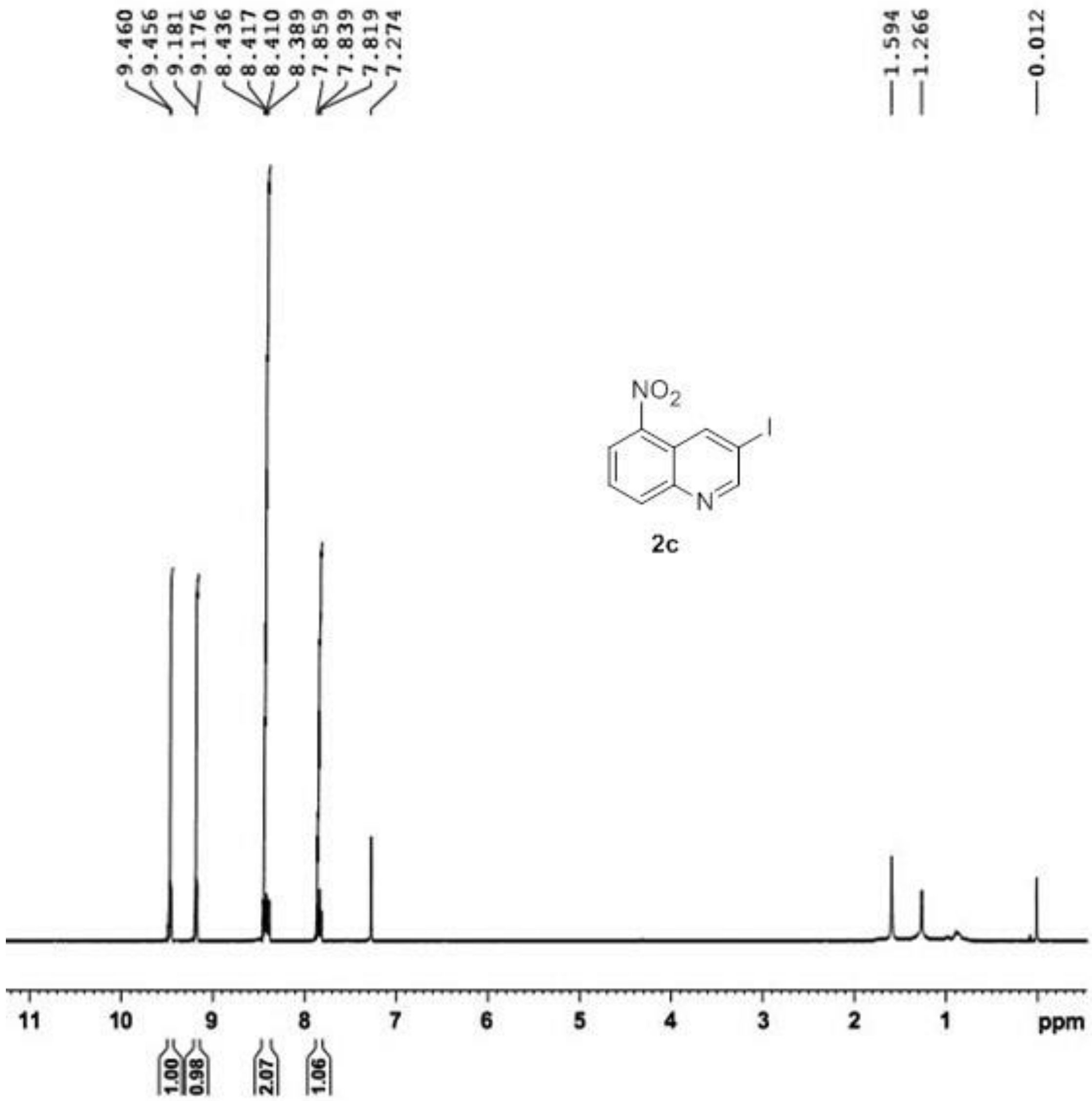
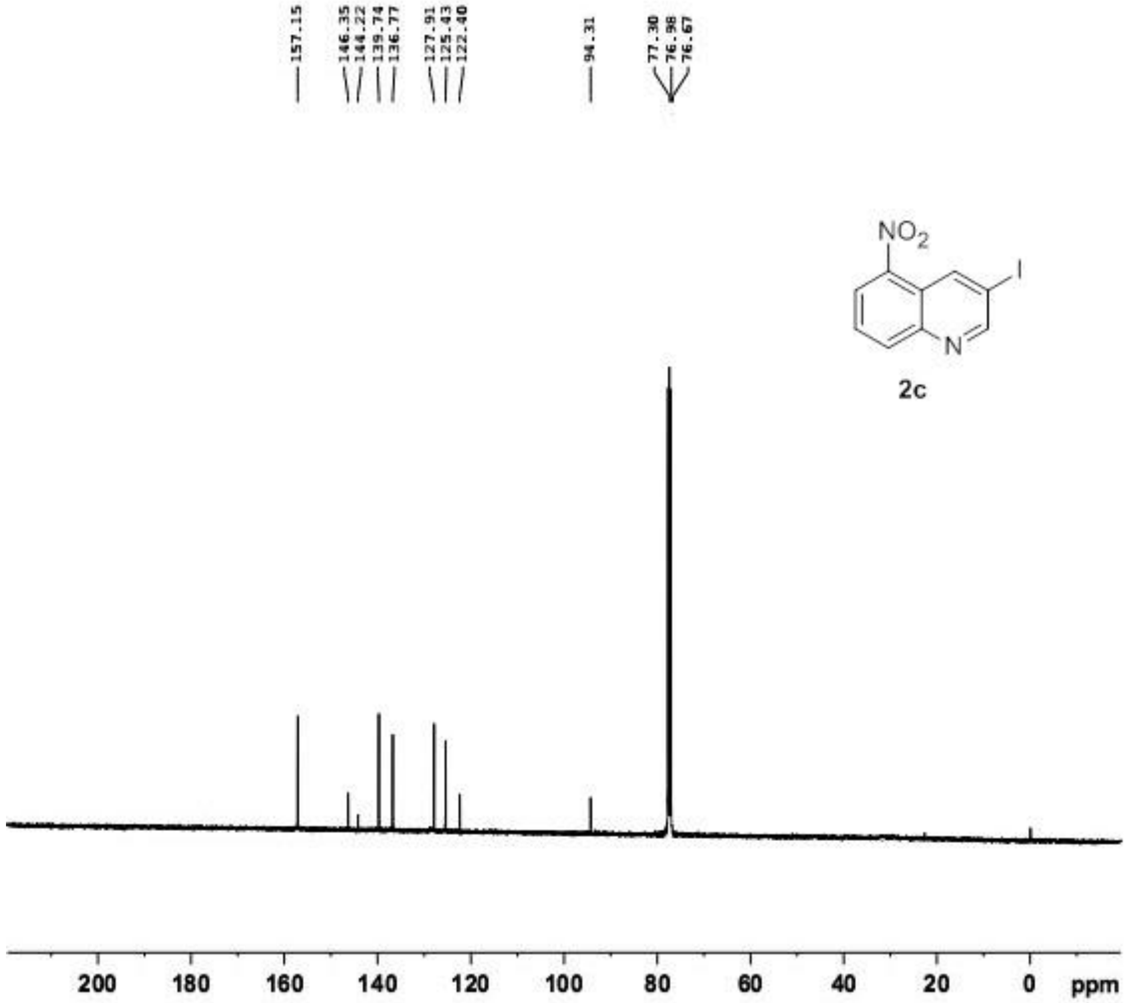
9.061
8.929
8.927
8.924
8.057
8.036
7.862
7.843
7.619
7.599
7.580
7.275
1.623
0.083
Br
I
N
2b
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
1.04
1.03
1.07

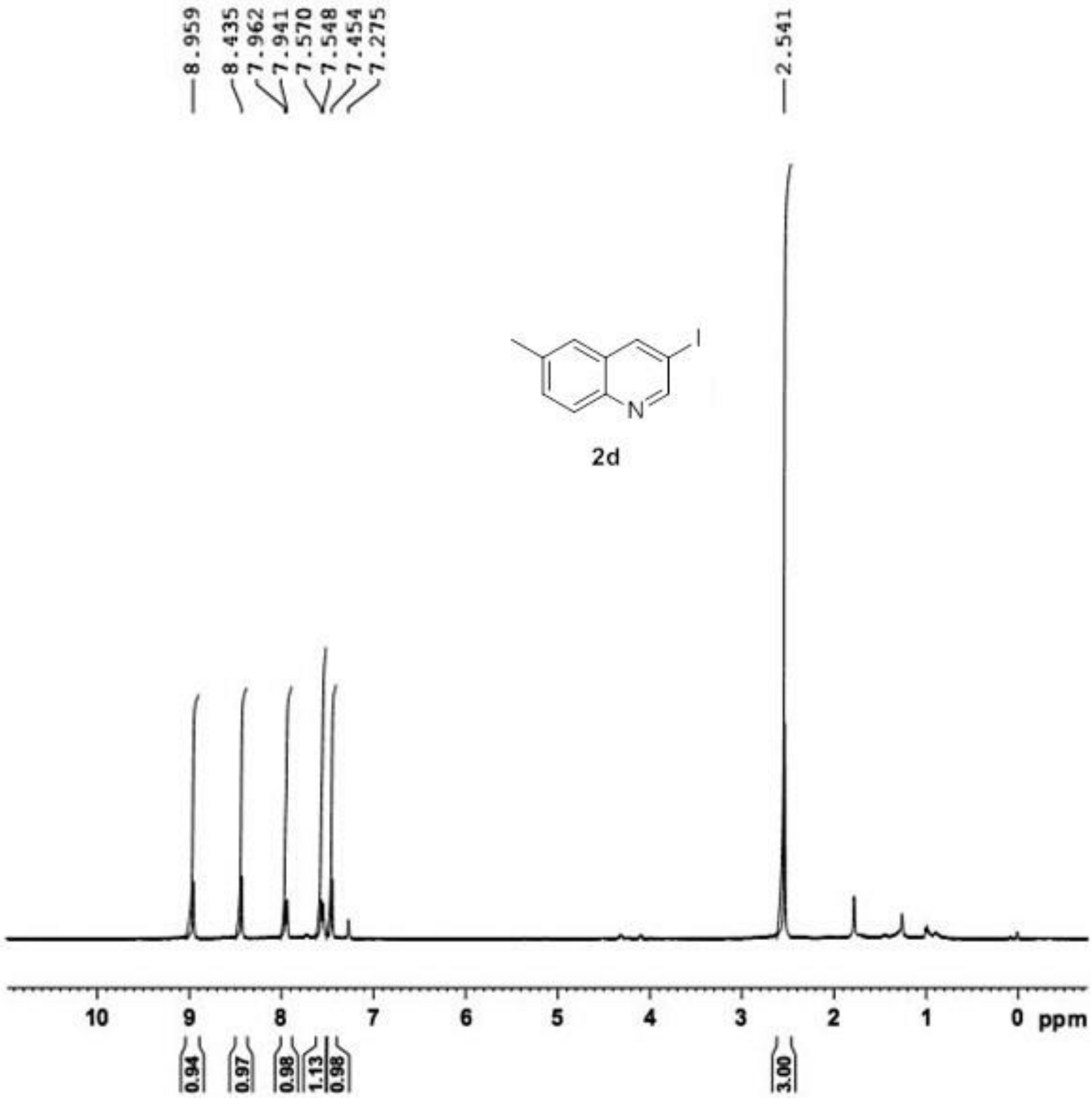

156.42
147.10
143.17
131.08
130.15
129.47
129.19
120.54
91.49
77.31
77.00
76.68
Br
I
N
2b
200
180
160
140
120
100
80
60
40
20
0
ppm

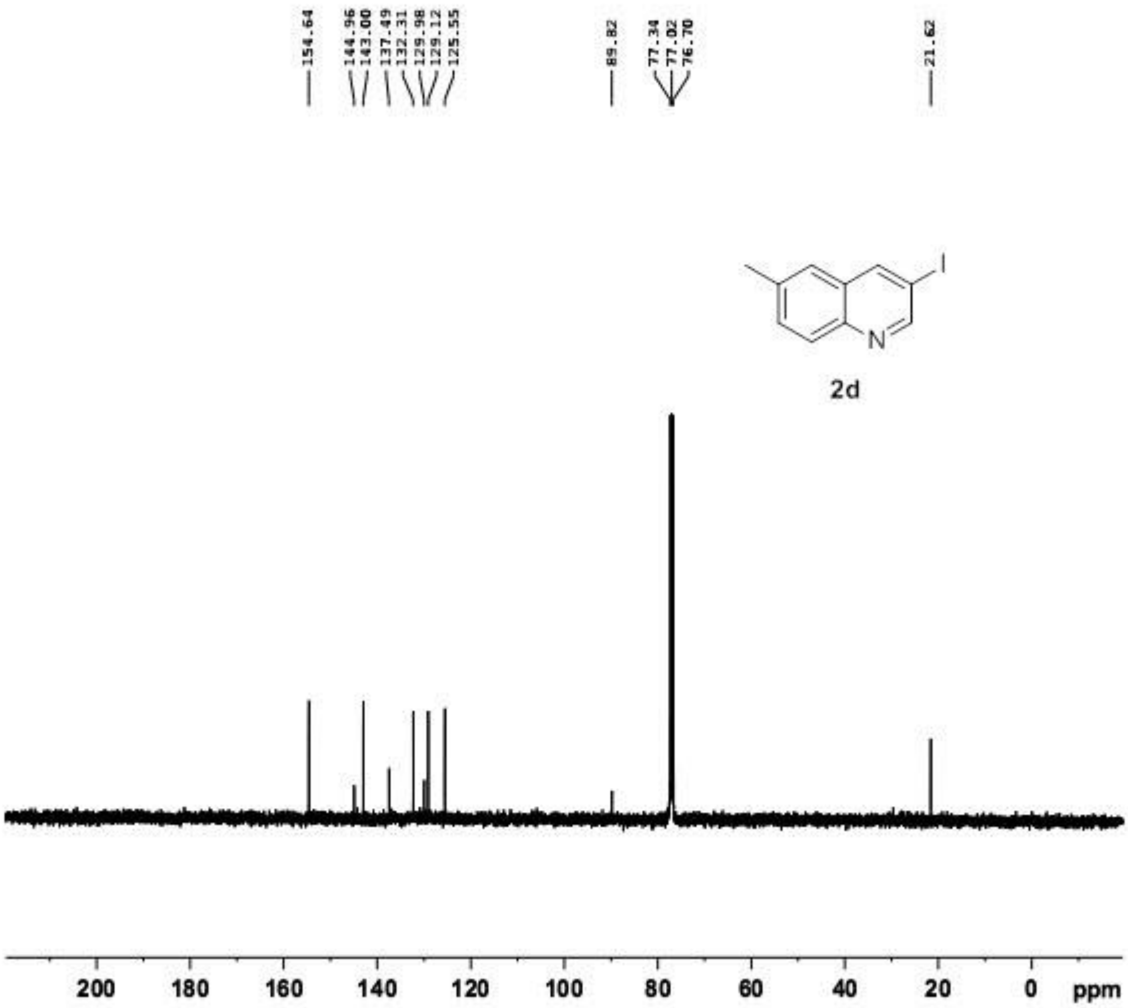
Compound 2c


9.460
9.456
9.181
9.176
8.436
8.417
8.410
8.389
7.859
7.839
7.819
7.274
1.594
1.266
0.012
NO_2
I
N
2c
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.98
2.07
1.06

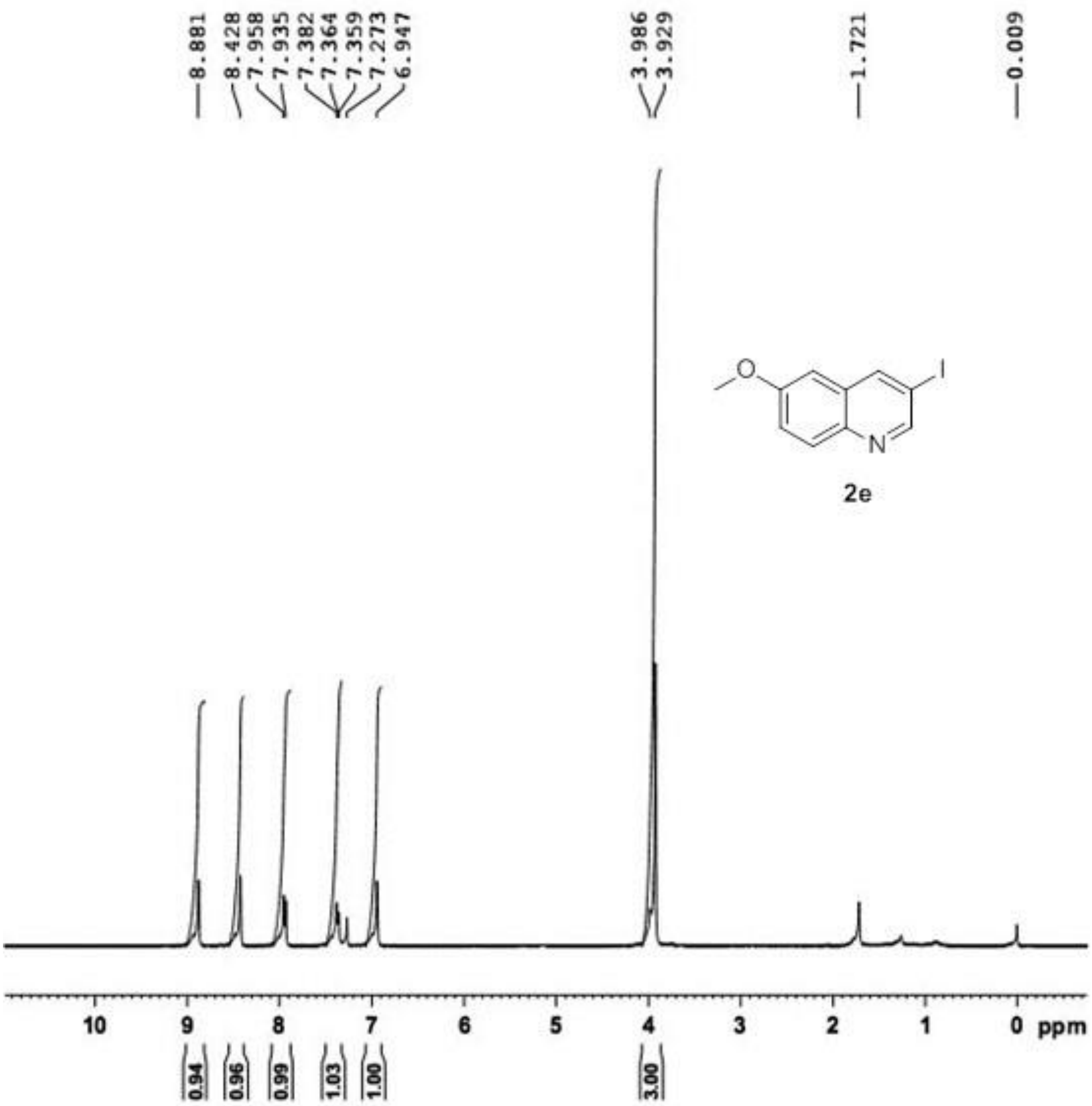

157.15
146.35
144.22
139.74
136.77
127.91
125.43
122.40
94.31
77.30
76.98
76.67
NO2
I
N
2c
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 2d

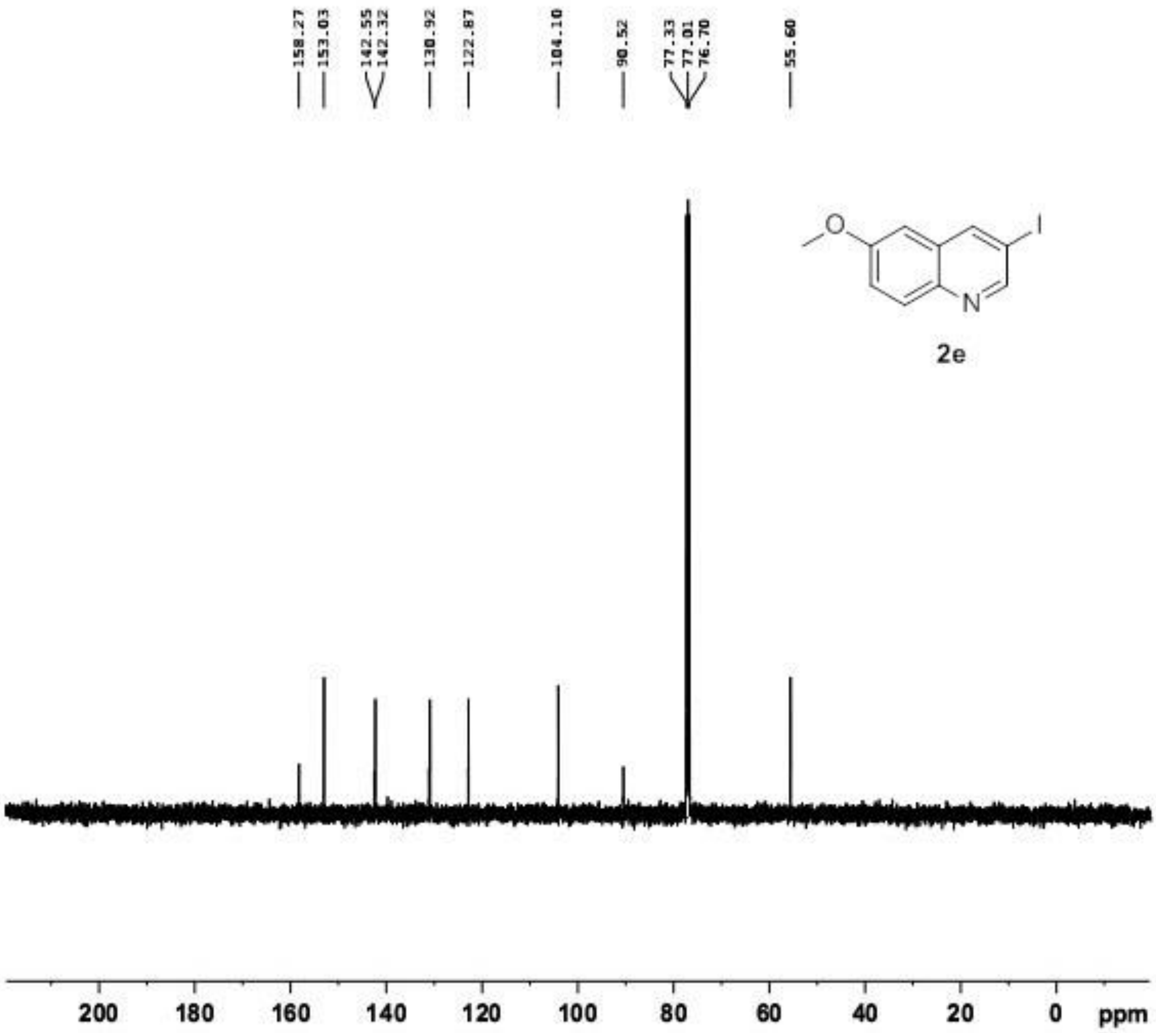

8.959
8.435
7.962
7.941
7.570
7.548
7.454
7.275
2.541
2d
N
I
10
9
8
7
6
5
4
3
2
1
0
ppm
0.94
0.97
0.98
1.13
0.98
3.00


154.64
144.96
143.00
137.49
132.31
129.98
129.12
125.55
89.82
77.34
77.02
76.70
21.62
N
I
2d
200
180
160
140
120
100
80
60
40
20
0
ppm

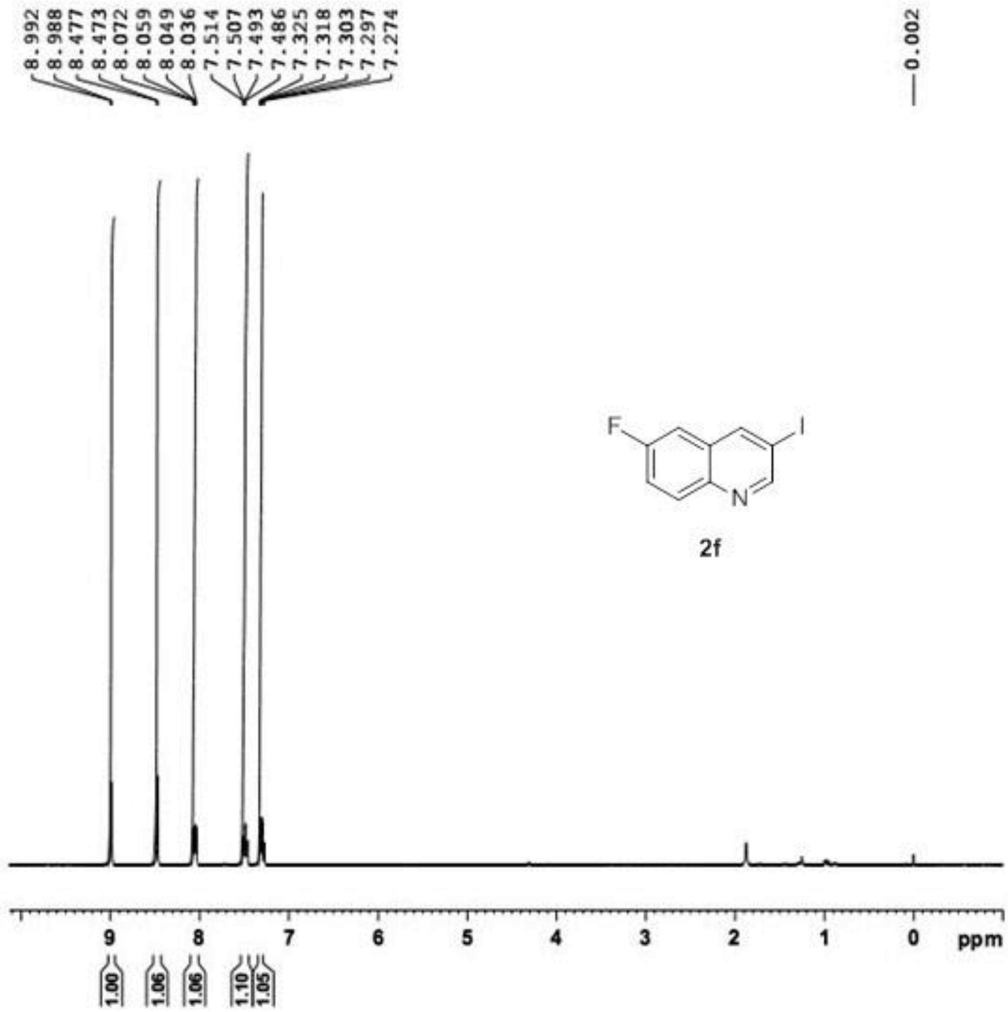
Compound 2e



8.881
8.428
7.958
7.935
7.382
7.364
7.359
7.273
6.947
3.986
3.929
1.721
0.009
2e
10
9
8
7
6
5
4
3
2
1
0 ppm
0.94
0.96
0.99
1.03
1.00
3.00


158.27
153.03
142.55
142.32
130.92
122.87
104.10
90.52
77.33
77.01
76.70
55.60
2e
200 180 160 140 120 100 80 60 40 20 0 ppm

Compound 2f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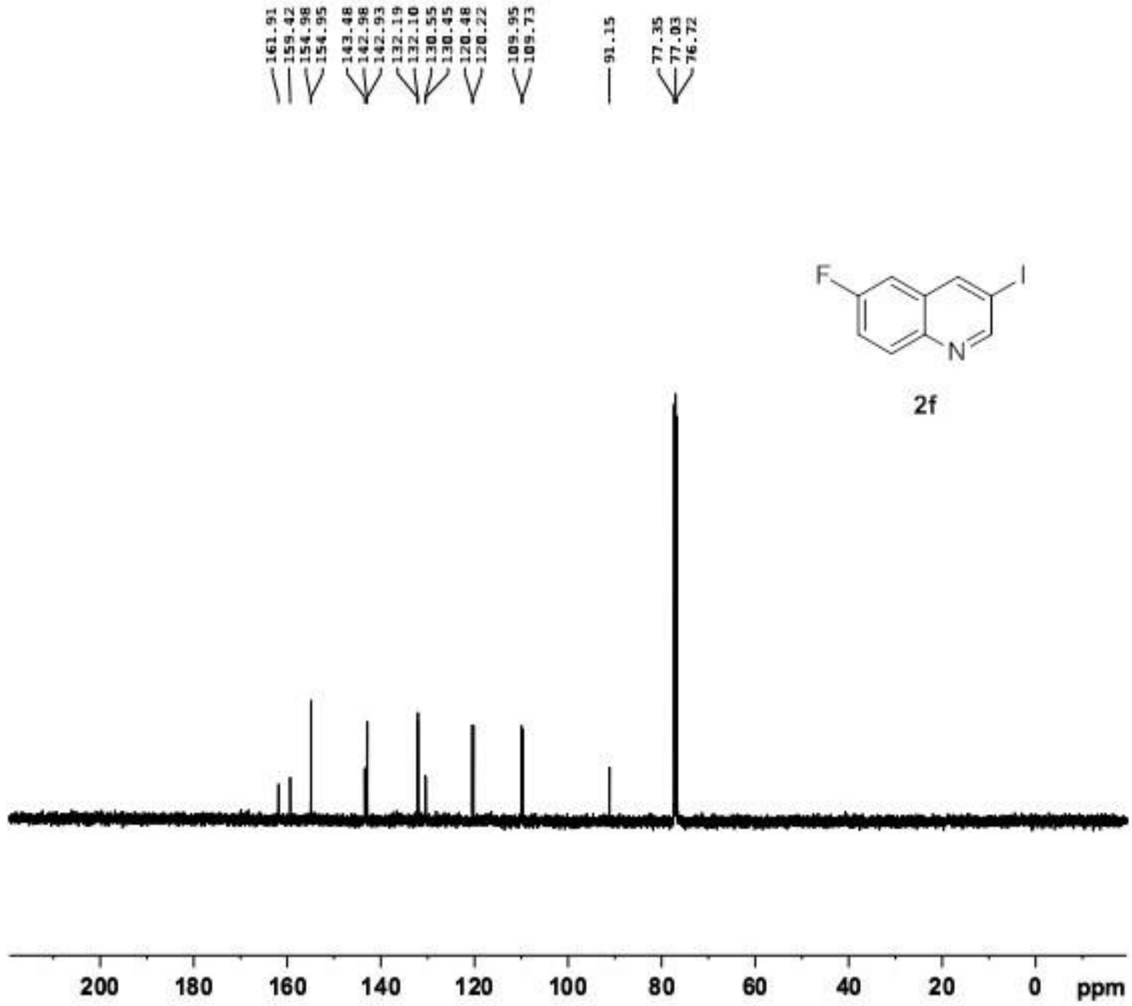
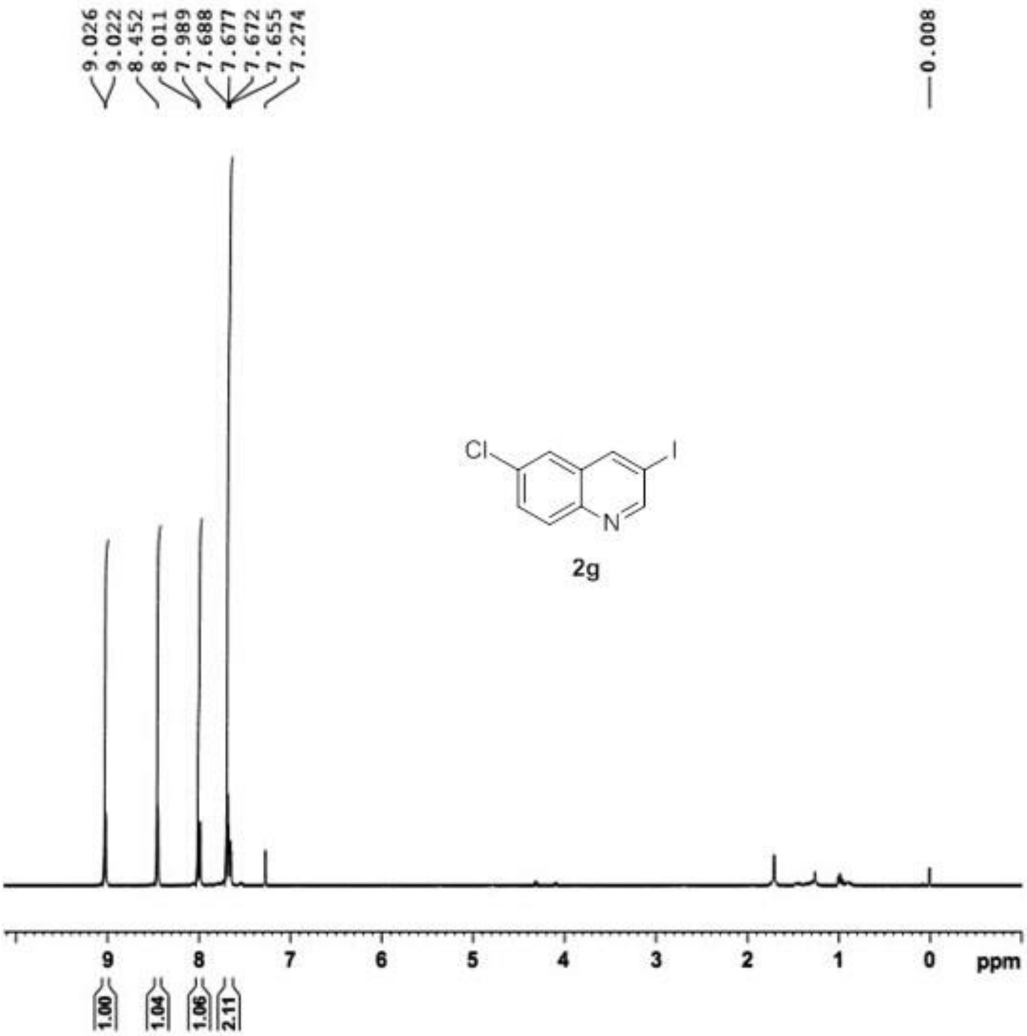
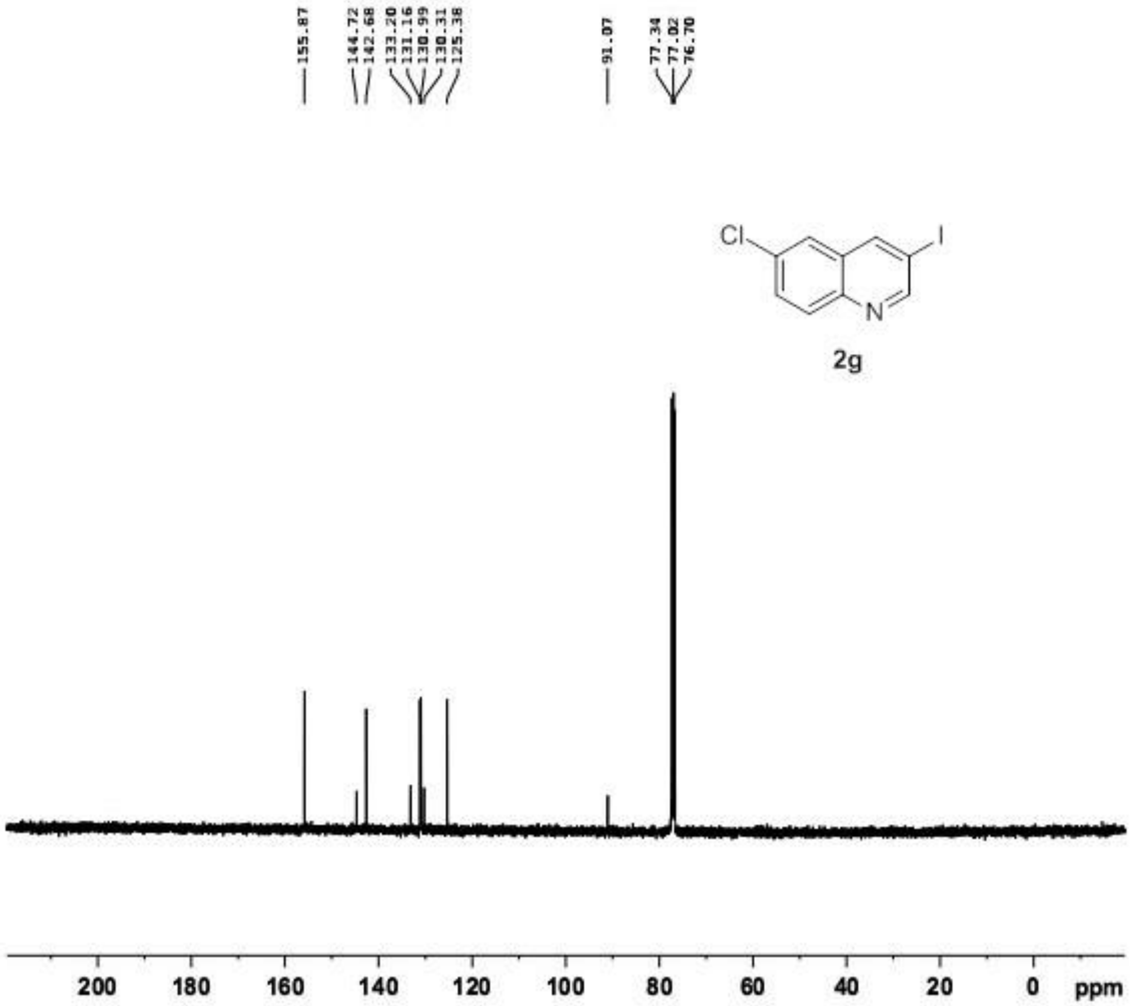
8.988
8.477
8.473
8.072
8.059
8.049
8.036
7.514
7.507
7.493
7.486
7.325
7.318
7.303
7.297
7.274
0.002
F
I
N
2f
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.06
1.06
1.10
1.05


161.91
159.42
154.98
154.95
143.48
142.98
142.93
132.19
132.10
130.55
130.45
120.48
120.22
109.95
109.73
91.15
77.35
77.03
76.72
F
I
N
2f
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 2g



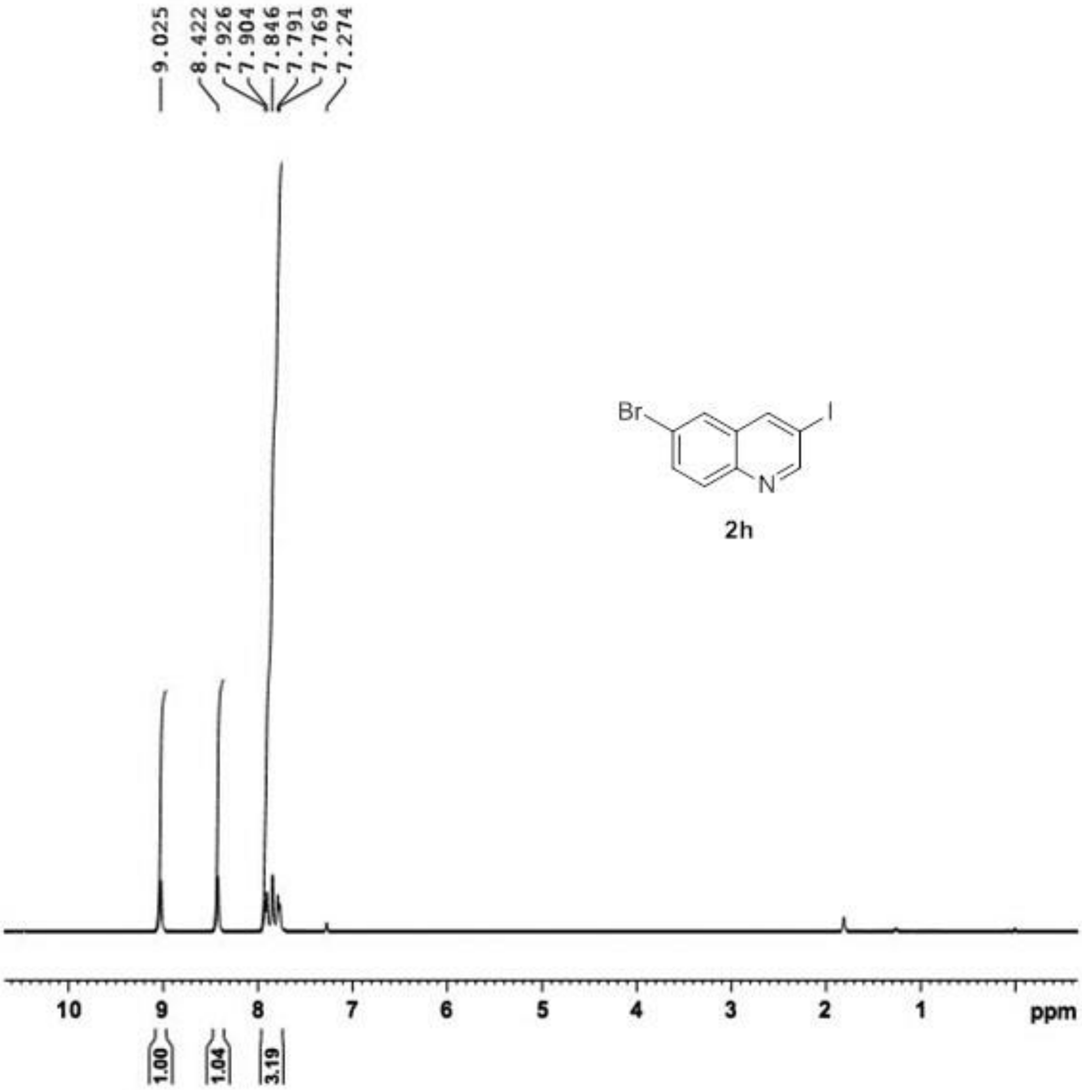
9.026
9.022
8.452
8.011
7.989
7.688
7.677
7.672
7.655
7.274
0.008
Cl
I
N
2g
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.04
1.06
2.11

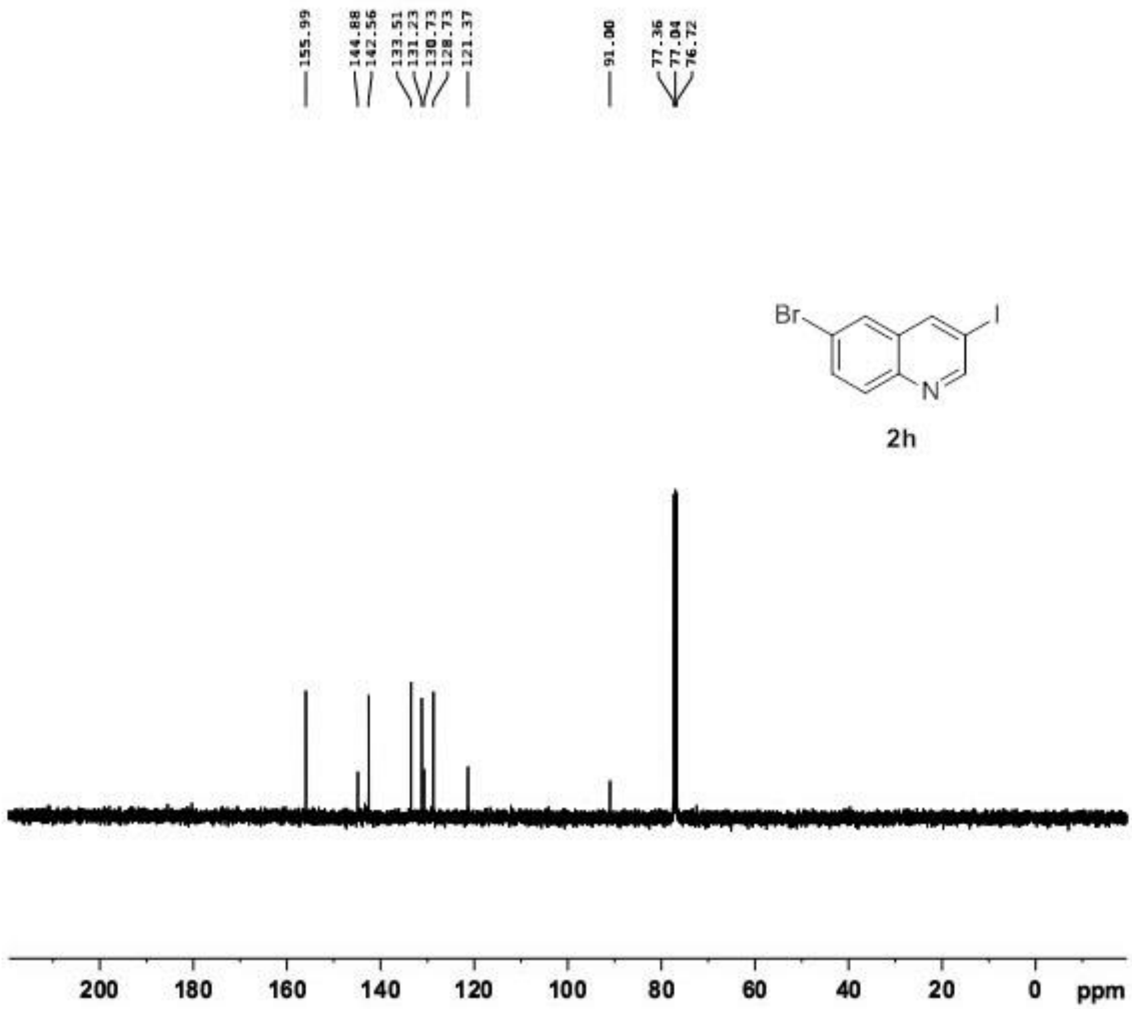


155.87
144.72
142.68
133.20
131.16
130.99
130.31
125.38
91.07
77.34
77.02
76.70
Cl
I
N
200
180
160
140
120
100
80
60
40
20
0
ppm

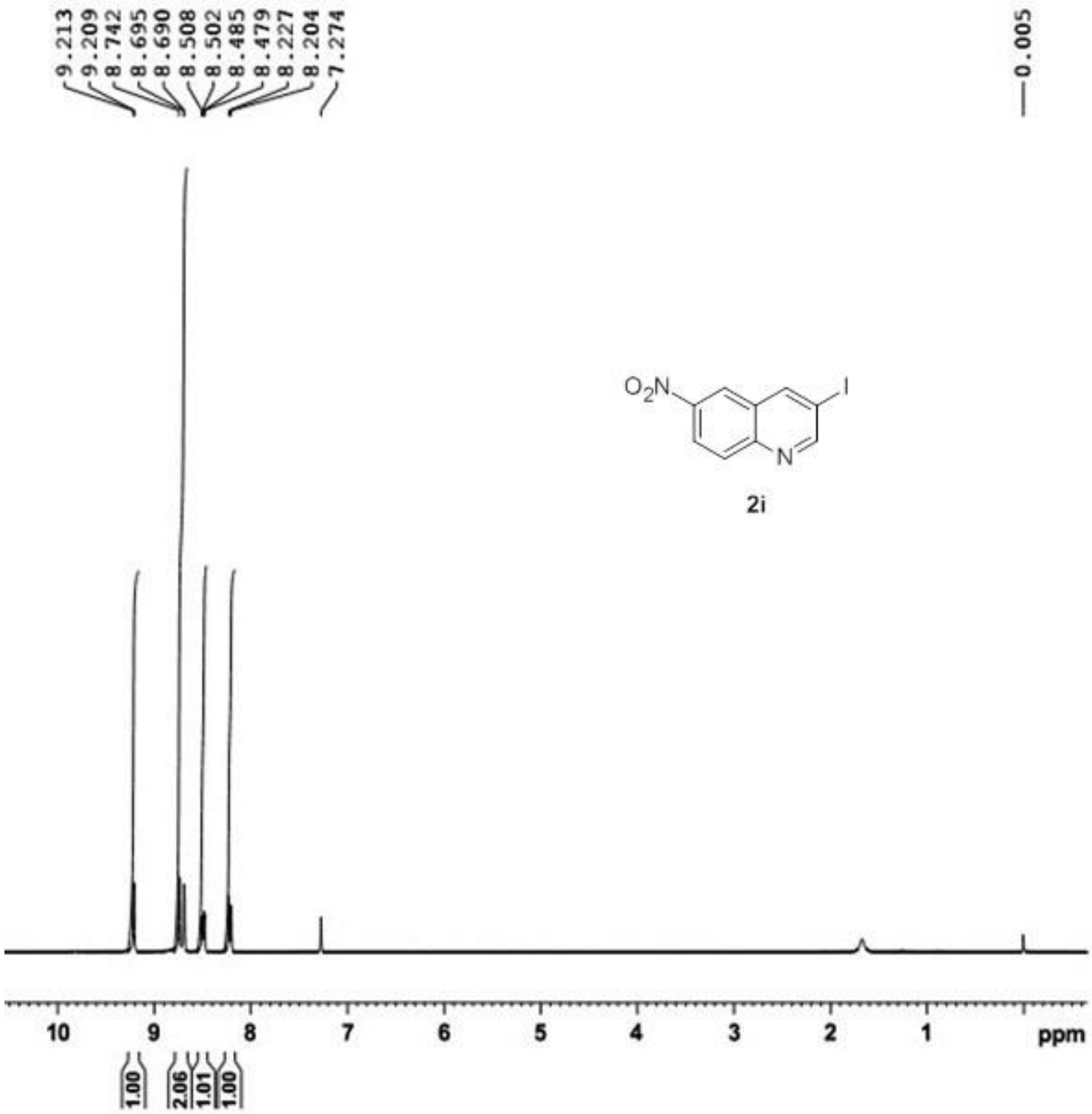
2g

Compound 2h

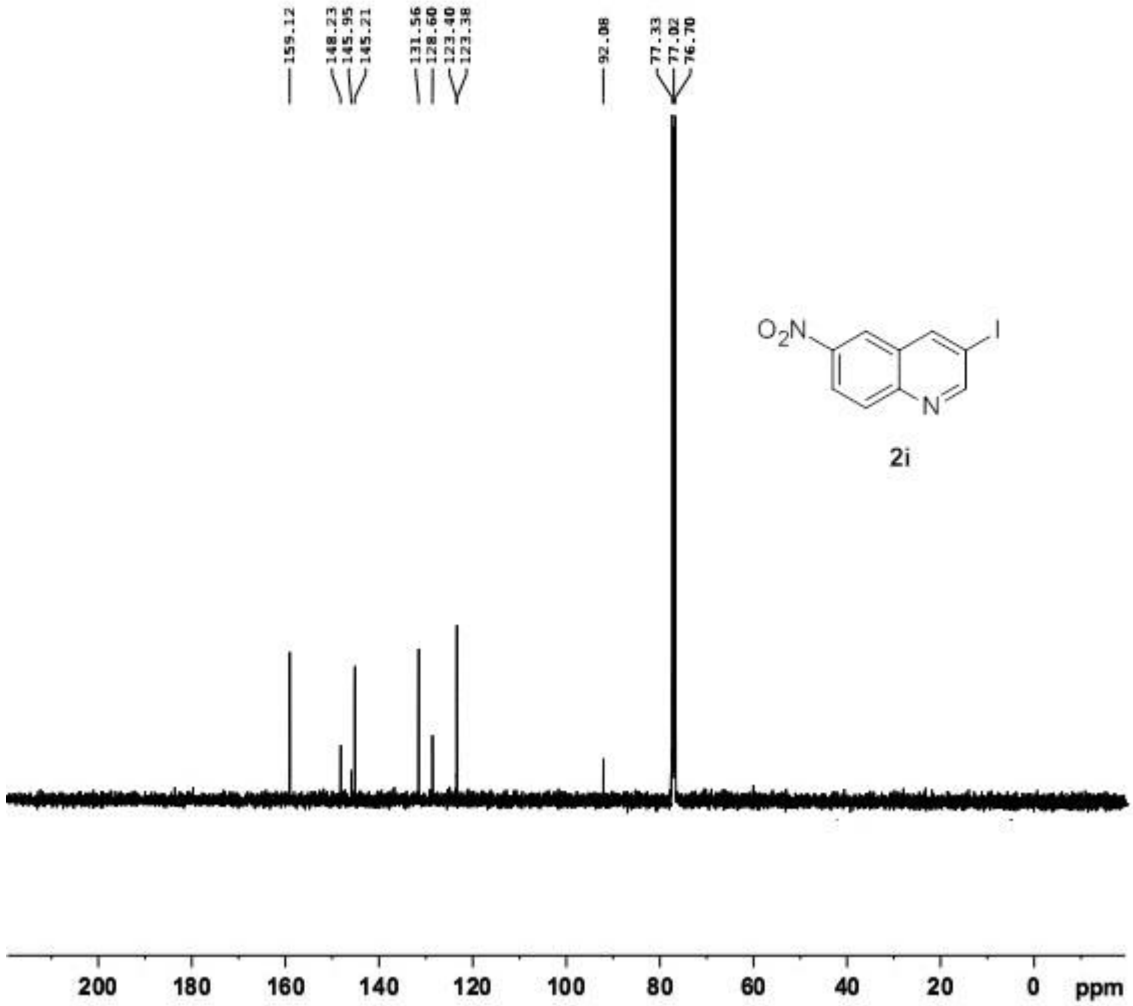

9.025
8.422
7.926
7.904
7.846
7.791
7.769
7.274
Br
I
N
2h
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.04
3.19


155.99
144.88
142.56
133.51
131.23
130.73
128.73
121.37
91.00
77.36
77.04
76.72
Br
I
N
200
180
160
140
120
100
80
60
40
20
0
ppm
2h

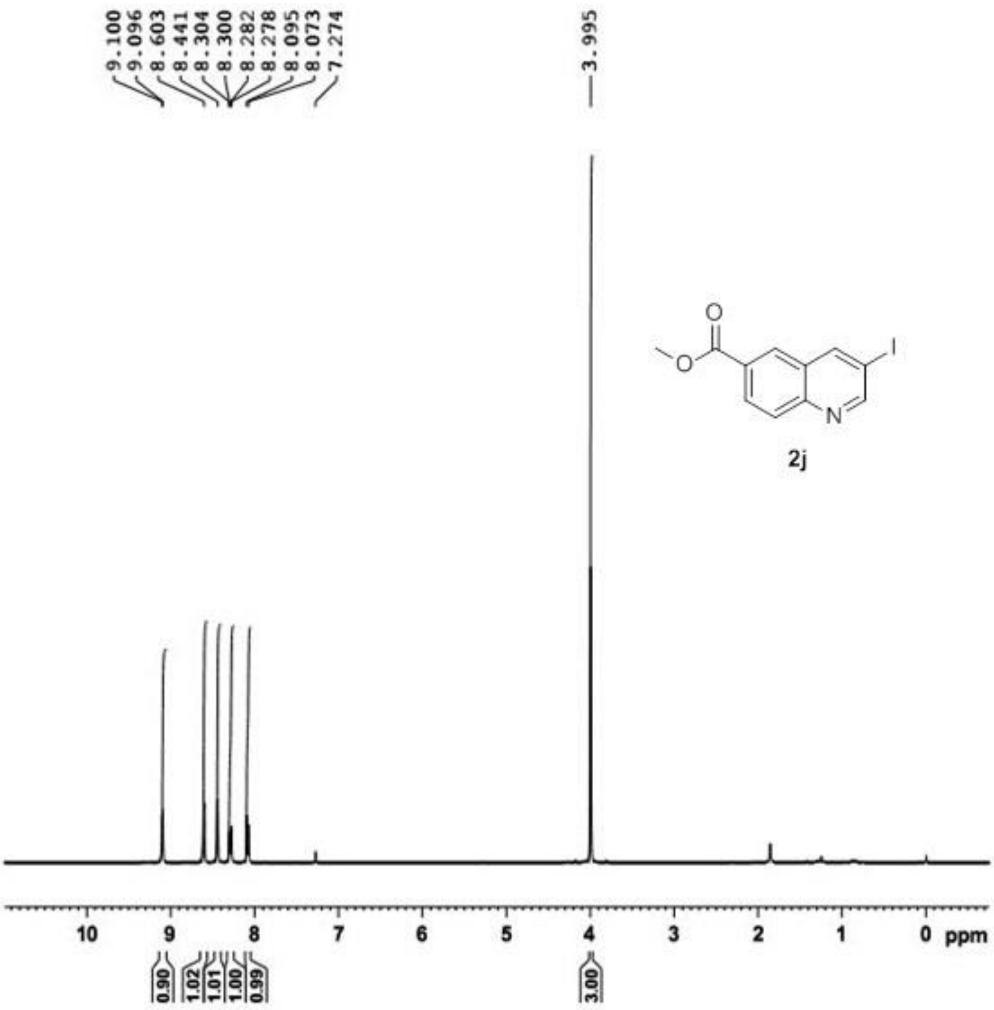
Compound 2i



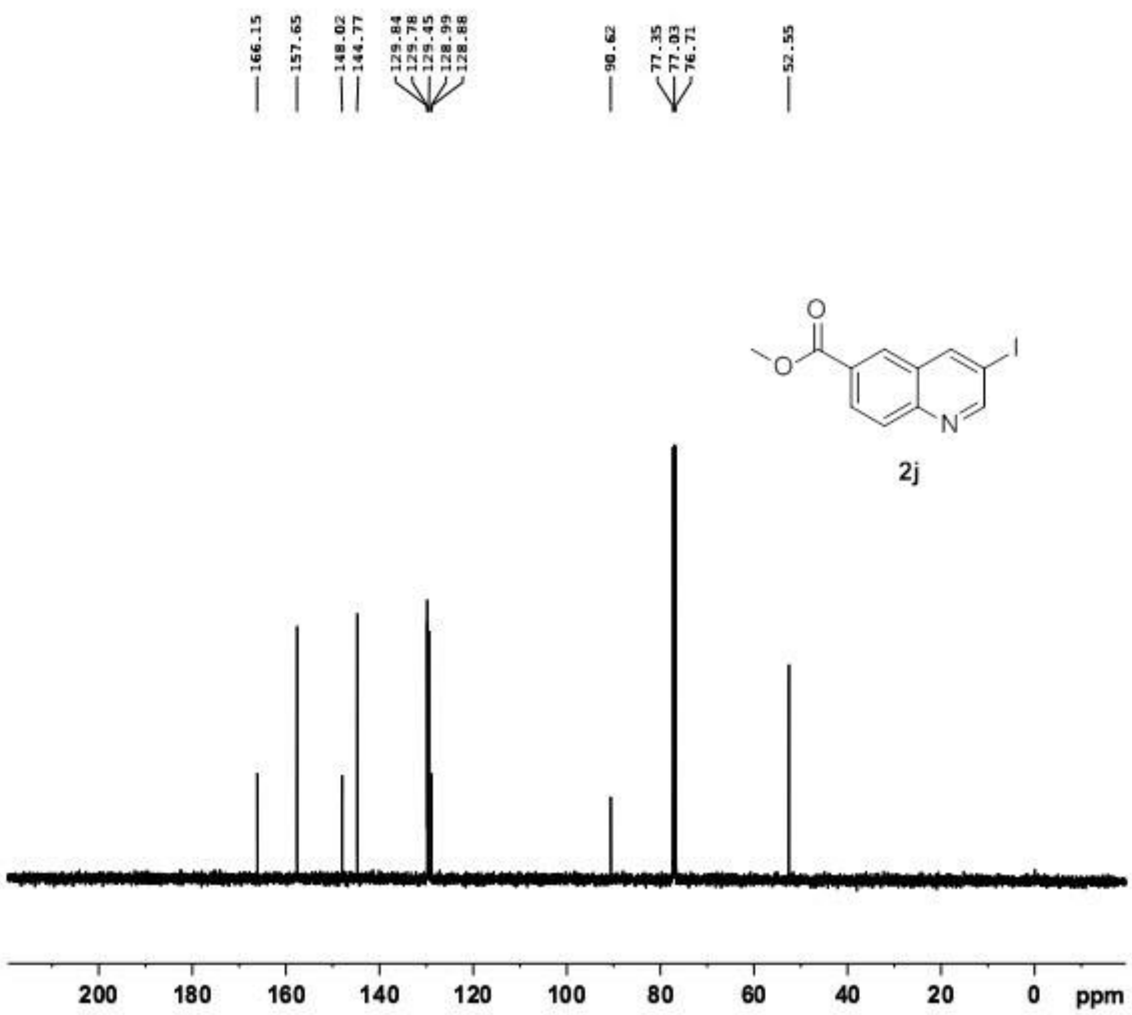
9.213
9.209
8.742
8.695
8.690
8.508
8.502
8.485
8.479
8.227
8.204
7.274
0.005
O2N
I
N
2i
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.06
1.01
1.00


159.12
148.23
145.95
145.21
131.56
128.60
123.40
123.38
92.08
77.33
77.02
76.70
O_2N
I
N
2i
200
180
160
140
120
100
80
60
40
20
0
ppm

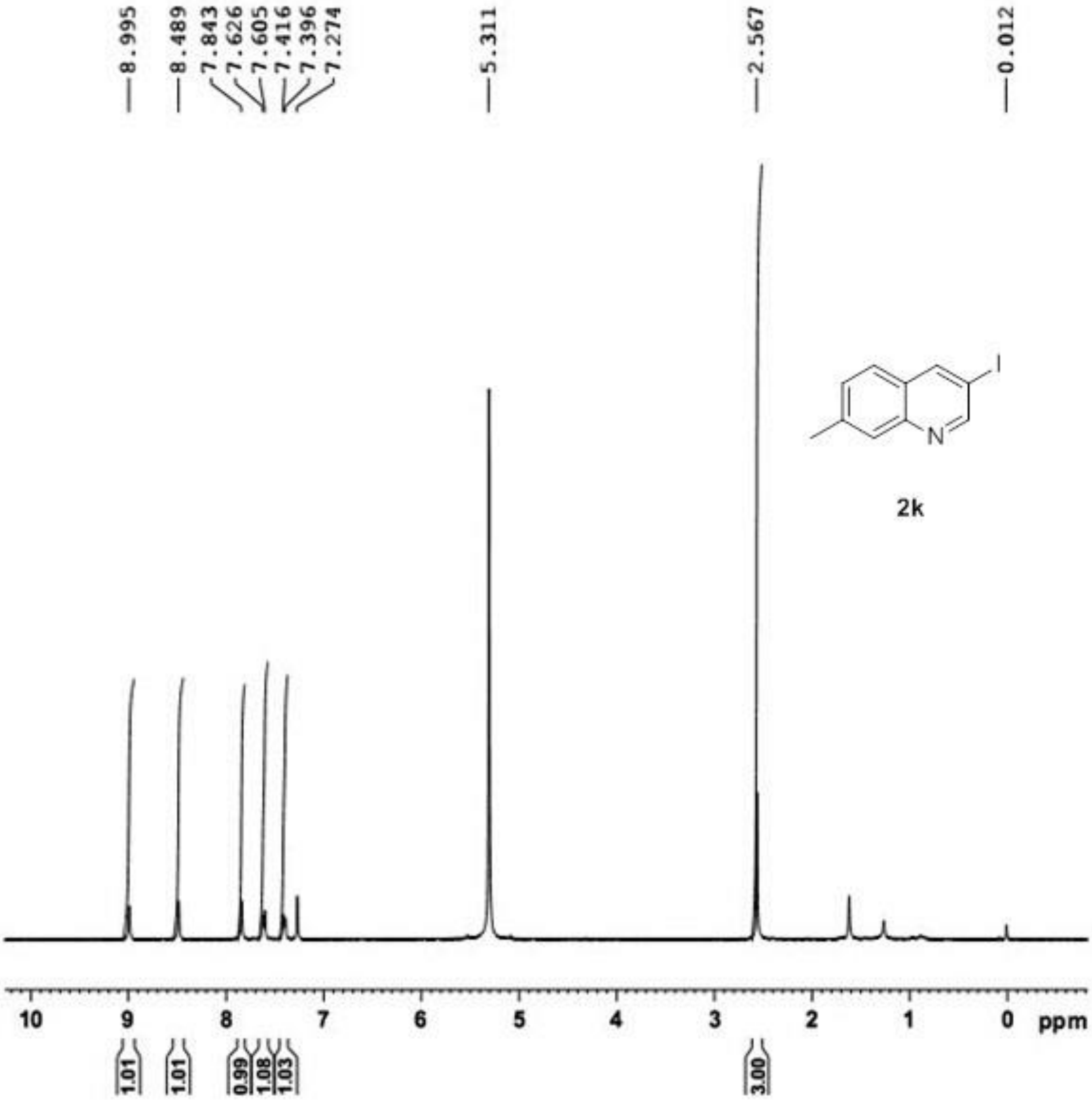
Compound 2j



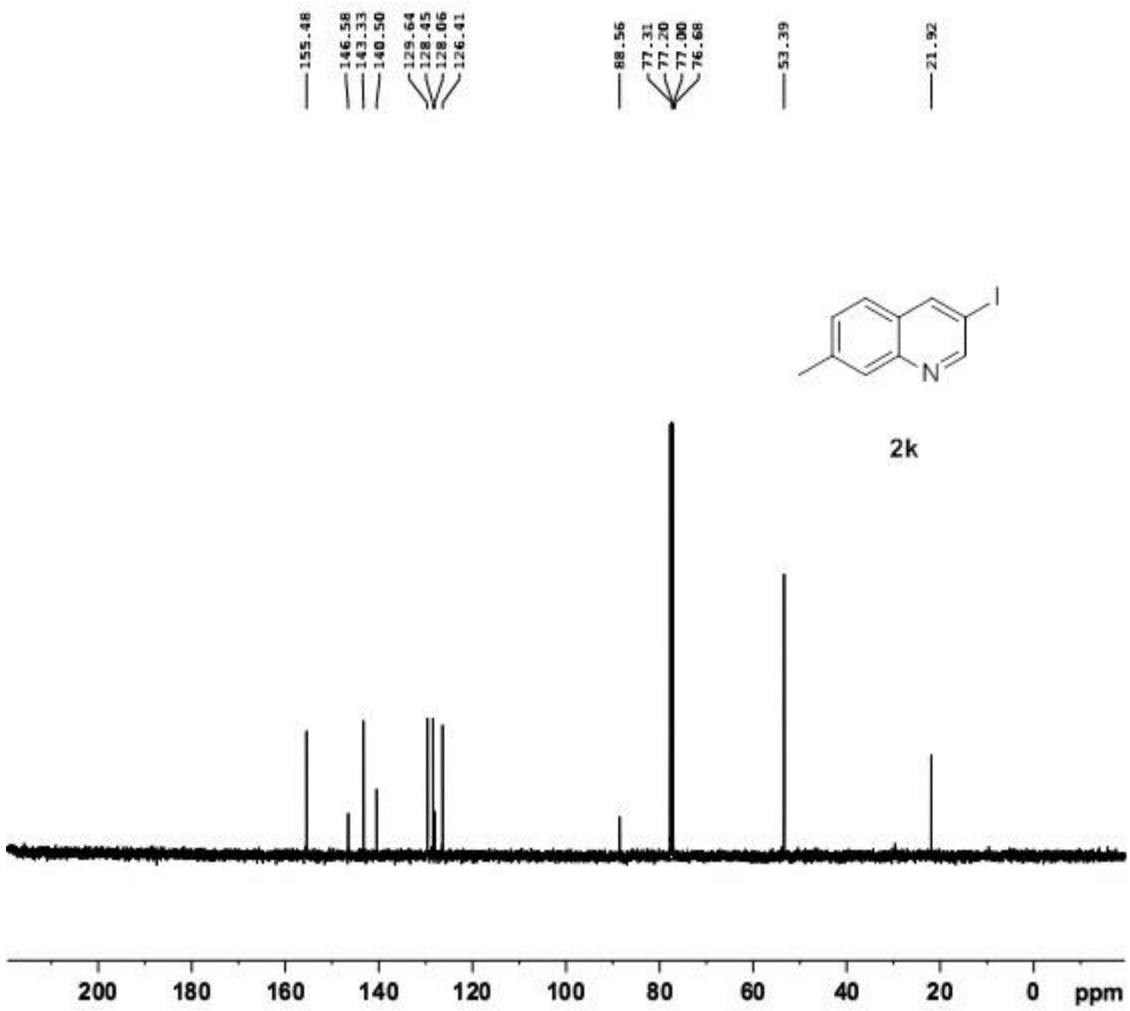
9.100
9.096
8.603
8.441
8.304
8.300
8.282
8.278
8.095
8.073
7.274
3.995
O
O
I
N
2j
10
9
8
7
6
5
4
3
2
1
0 ppm
0.90
1.02
1.01
1.00
0.99
3.00


166.15
157.65
148.02
144.77
129.84
129.78
129.45
128.99
128.88
90.62
77.35
77.03
76.71
52.55
2j
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 2k



8.995
8.489
7.843
7.626
7.605
7.416
7.396
7.274
5.311
2.567
0.012
I
N
2k
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.01
0.99
1.08
1.03
3.00


155.48
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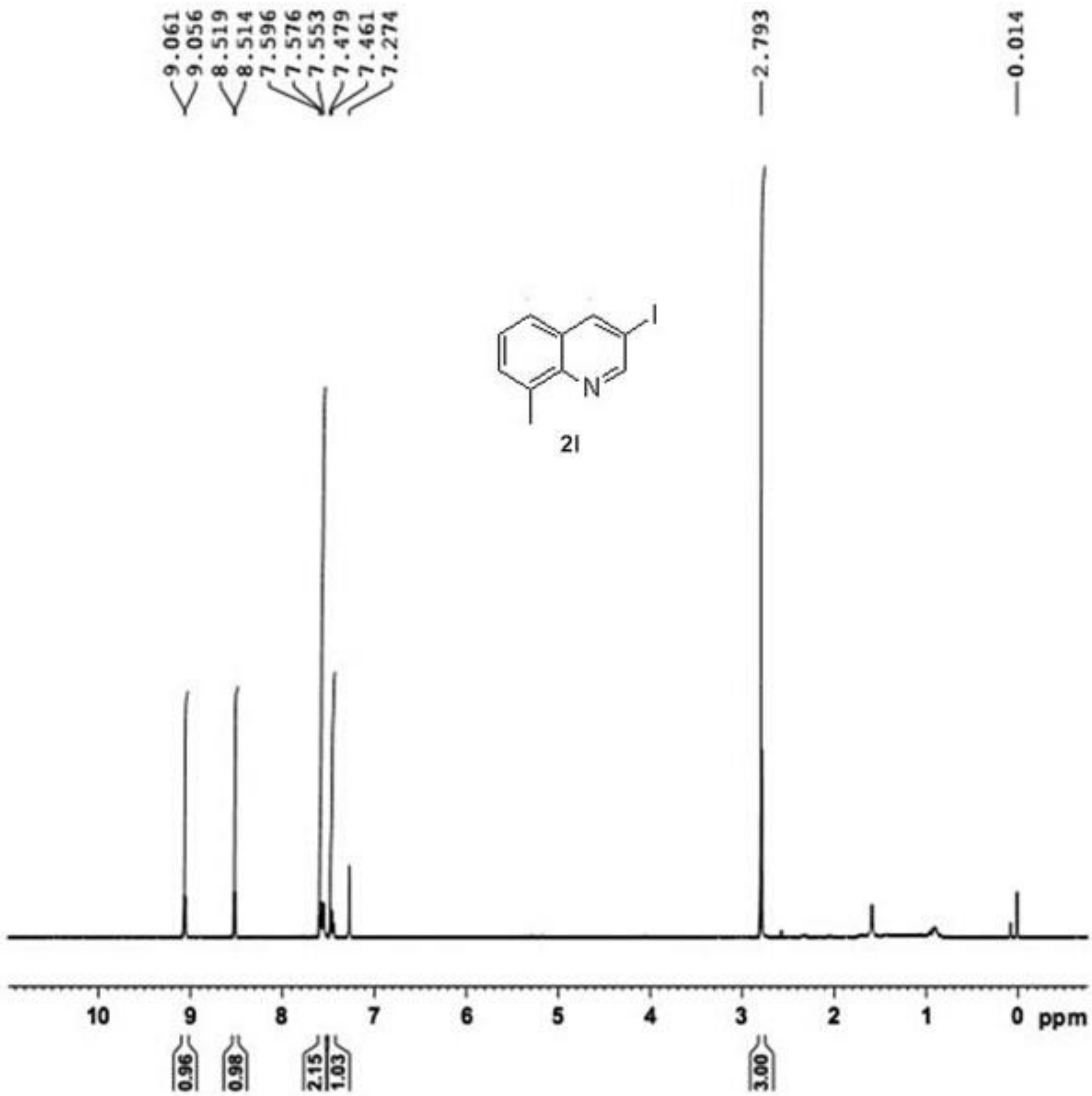
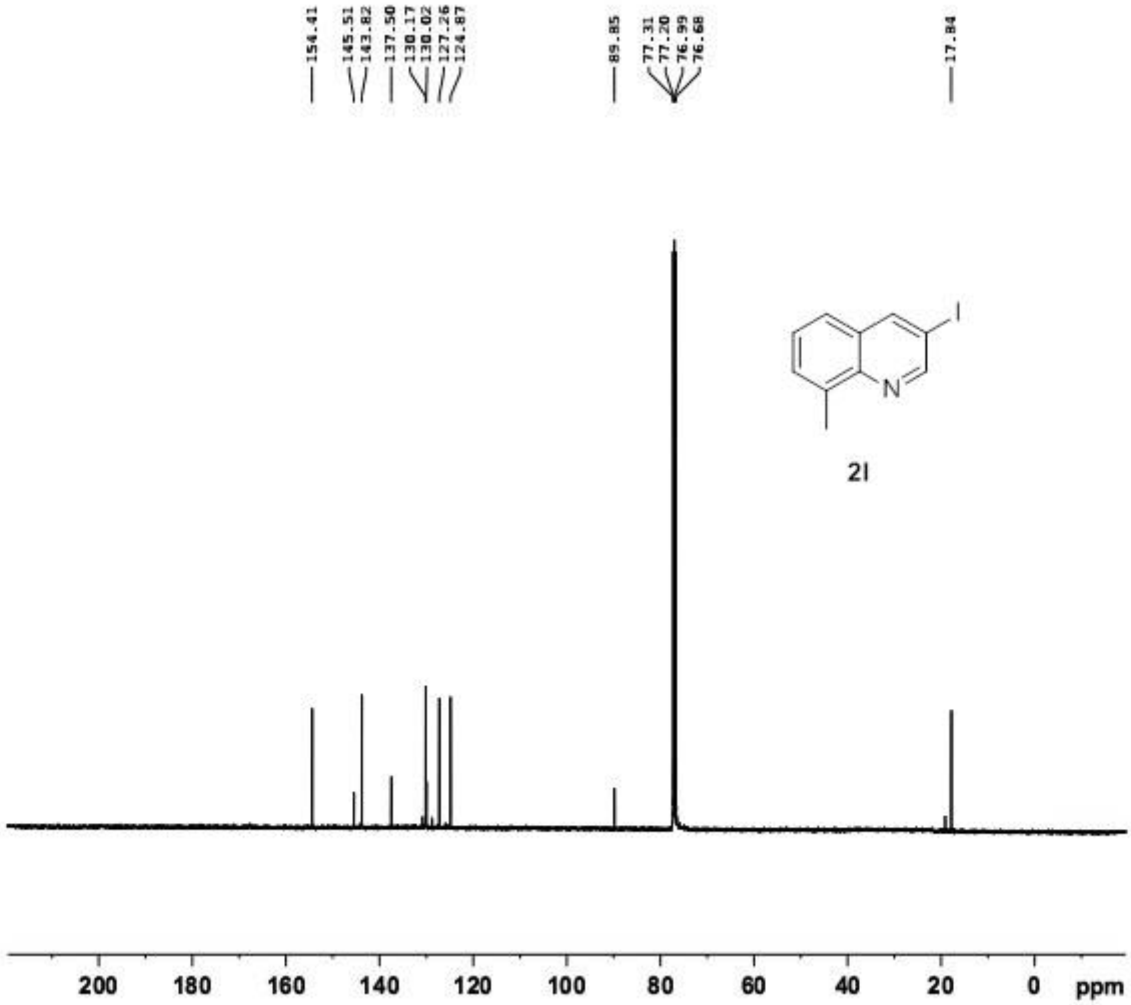
143.33
140.50
129.64
128.45
128.06
126.41
88.56
77.31
77.20
77.00
76.68
53.39
21.92
I
N
2k
200
180
160
140
120
100
80
60
40
20
0
ppm

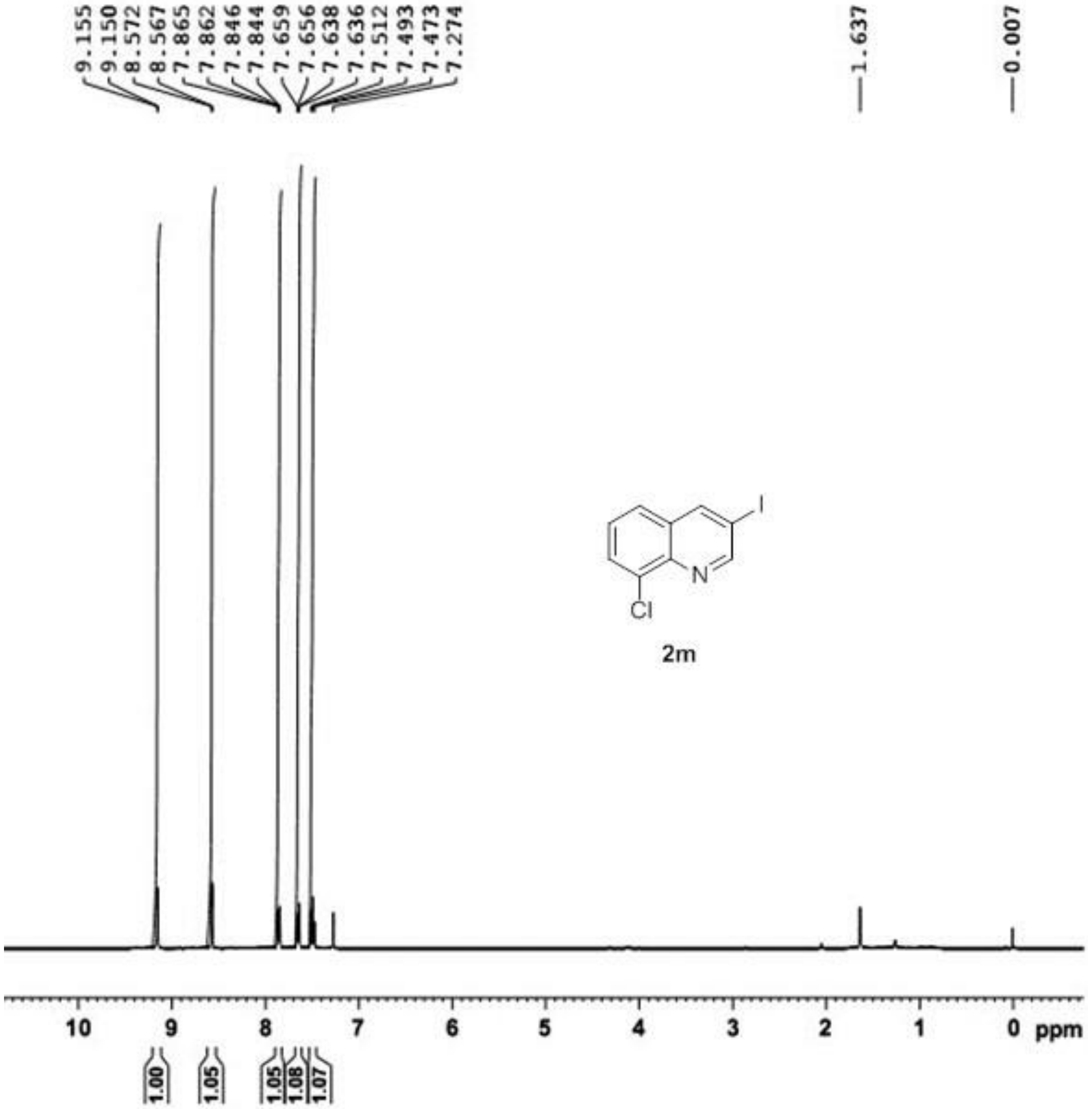
Compound 2l

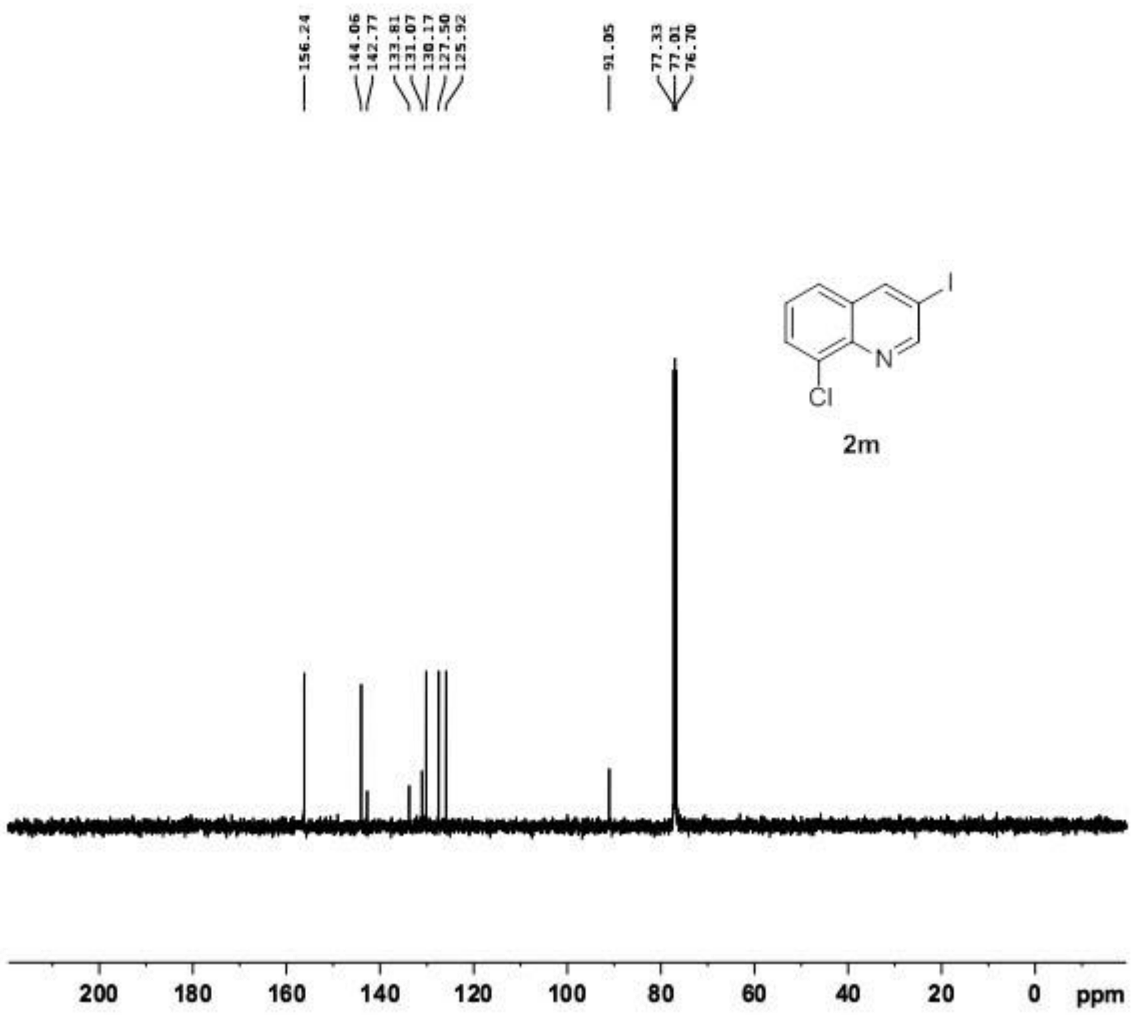

9.061
9.056
8.519
8.514
7.596
7.576
7.553
7.479
7.461
7.274
2.793
0.014
2l
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
0.98
2.15
1.03
3.00



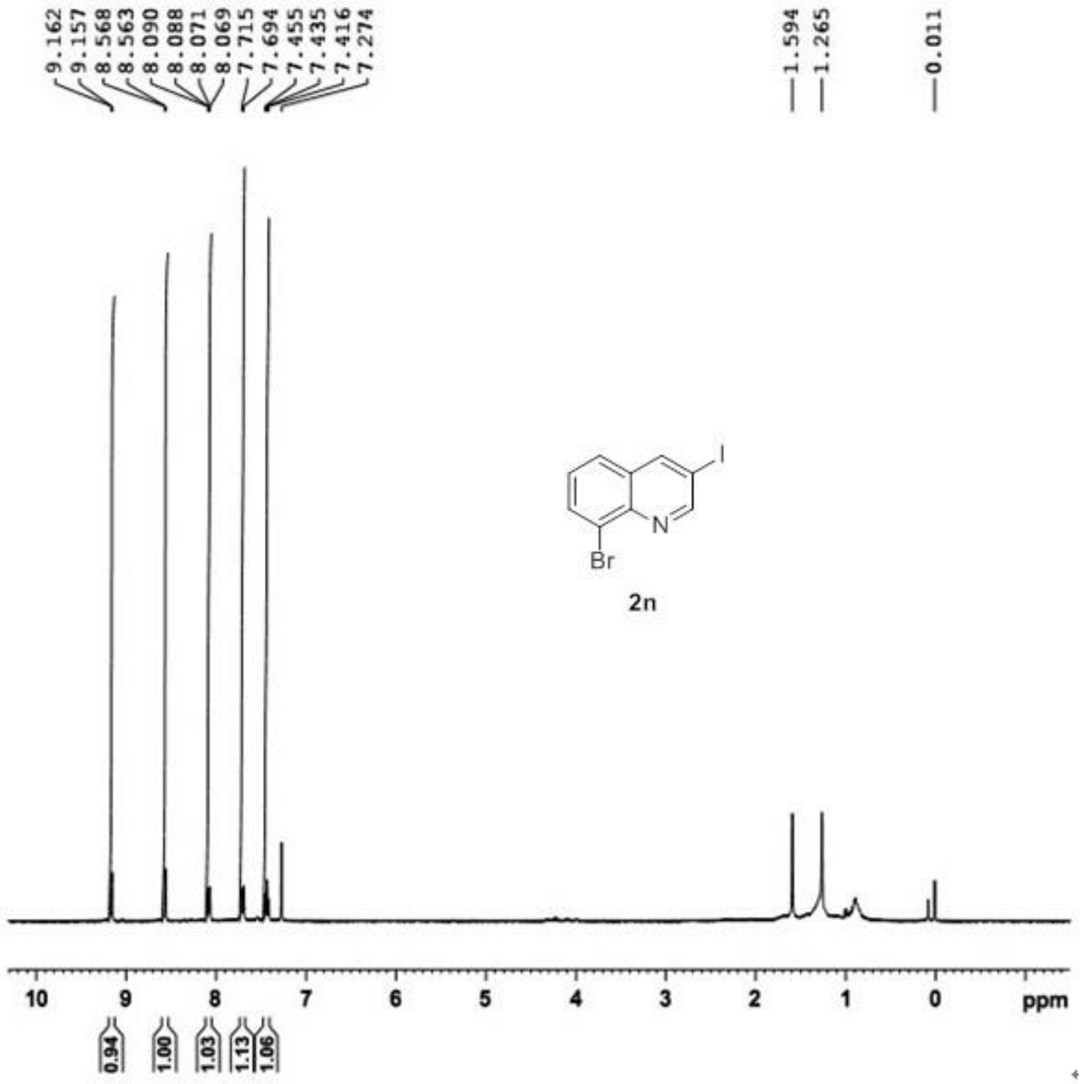
154.41
145.51
143.82
137.50
130.17
130.02
127.26
124.87
89.85
77.31
77.20
76.99
76.68
17.84
I
N
2l
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 2m


9.155
9.150
8.572
8.567
7.865
7.862
7.846
7.844
7.659
7.656
7.638
7.636
7.512
7.493
7.473
7.274
1.637
0.007
I
N
Cl
2m
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.05
1.05
1.08
1.07


156.24
144.06
142.77
133.81
131.07
130.17
127.50
125.92
91.05
77.33
77.01
76.70
I
N
Cl
2m
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 2n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9.157
8.568
8.563
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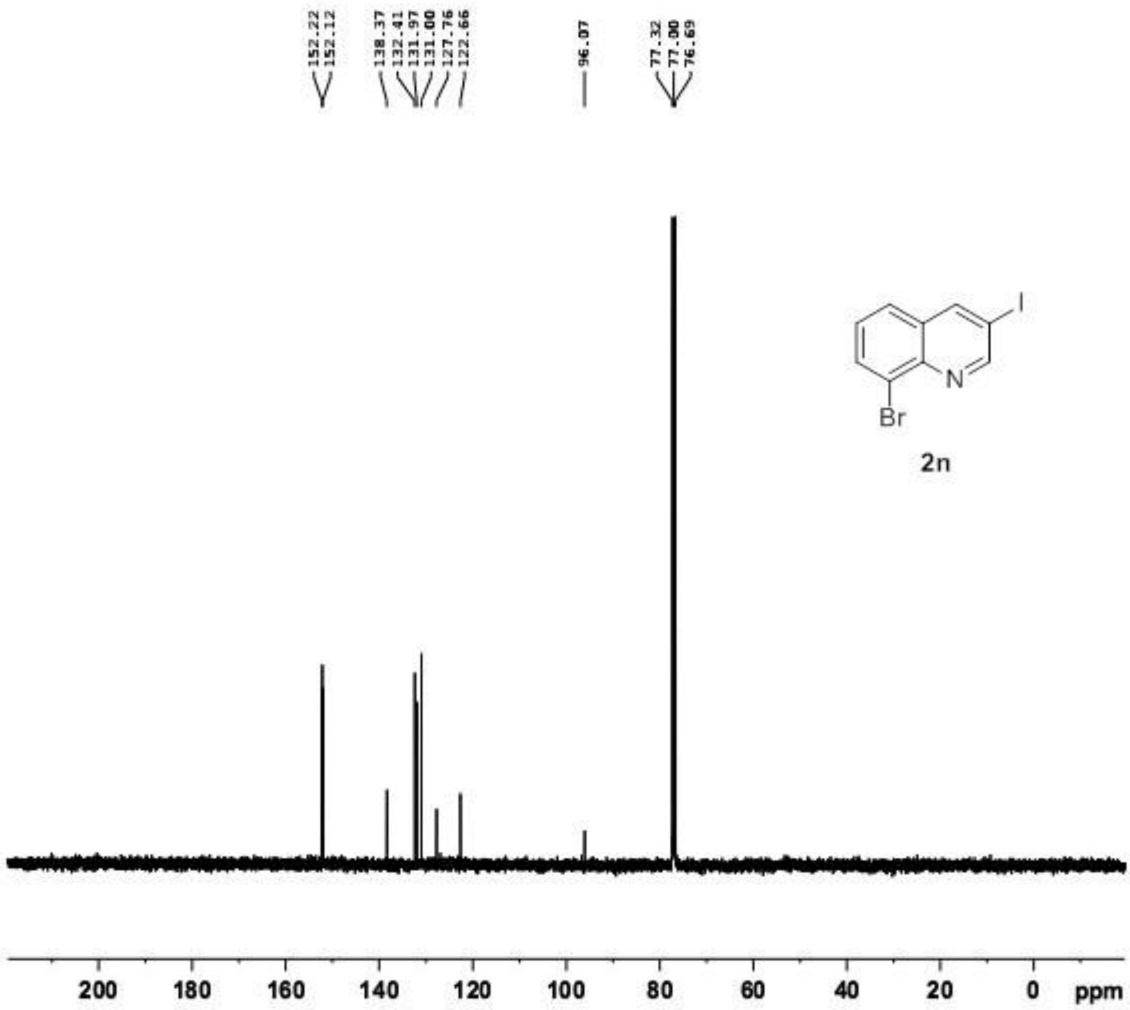
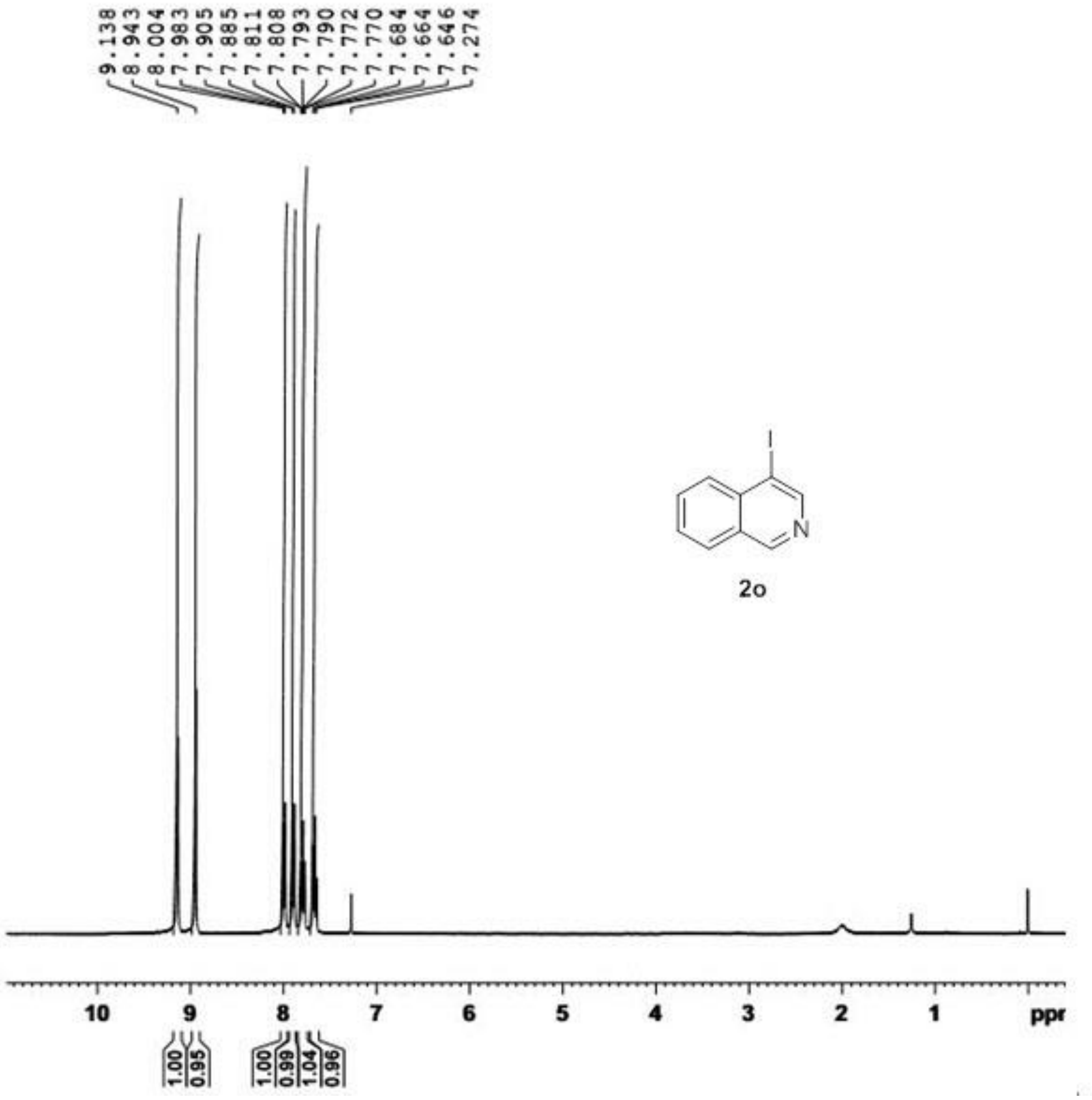
8.088
8.071
8.069
7.715
7.694
7.455
7.435
7.416
7.274
1.594
1.265
0.011
I
N
Br
2n
10
9
8
7
6
5
4
3
2
1
0
ppm
0.94
1.00
1.03
1.13
1.06



152.22
152.12
138.37
132.41
131.97
131.00
127.76
122.66
96.07
77.32
77.00
76.69
I
N
Br
2n
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 2o


9.138
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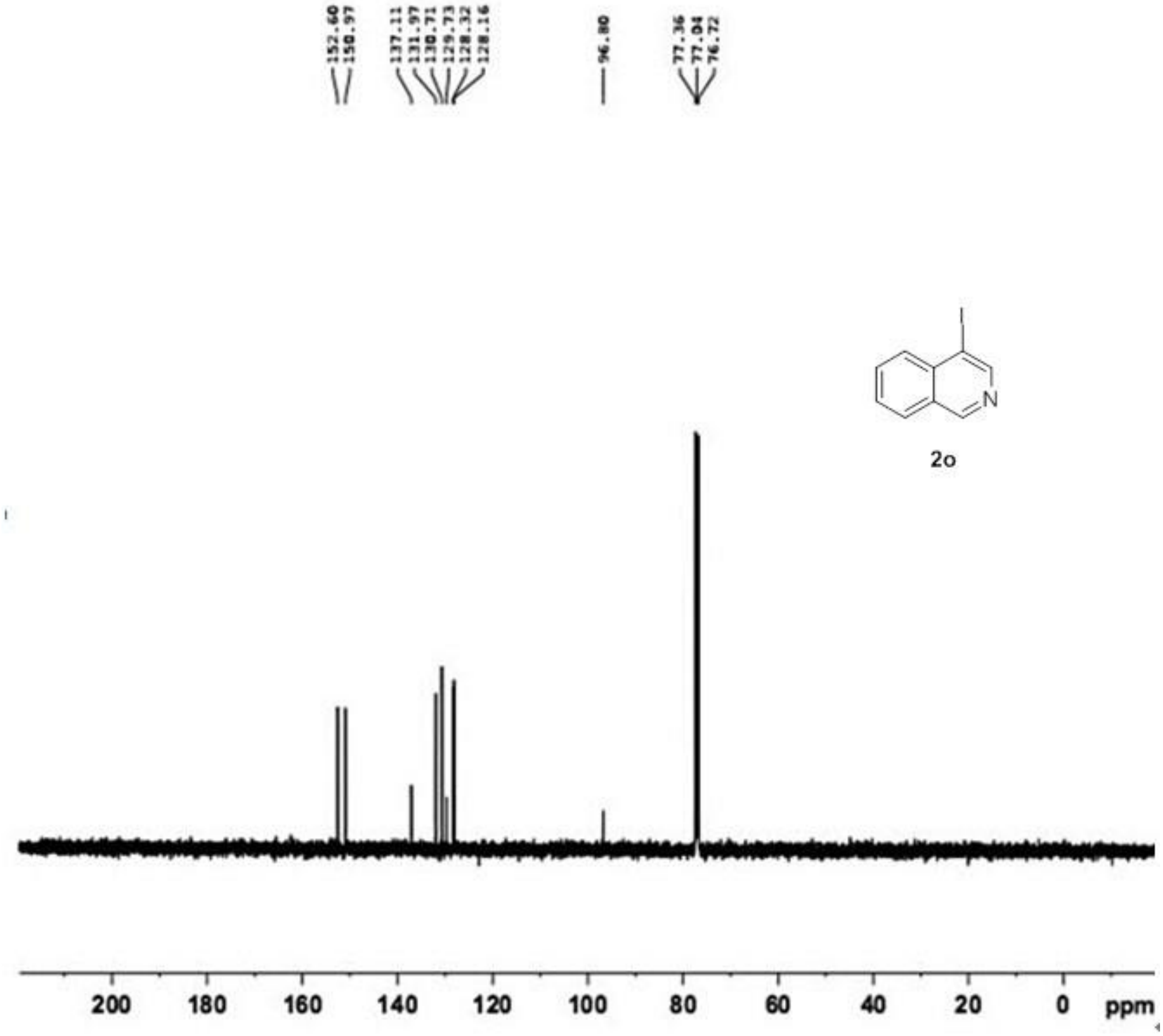
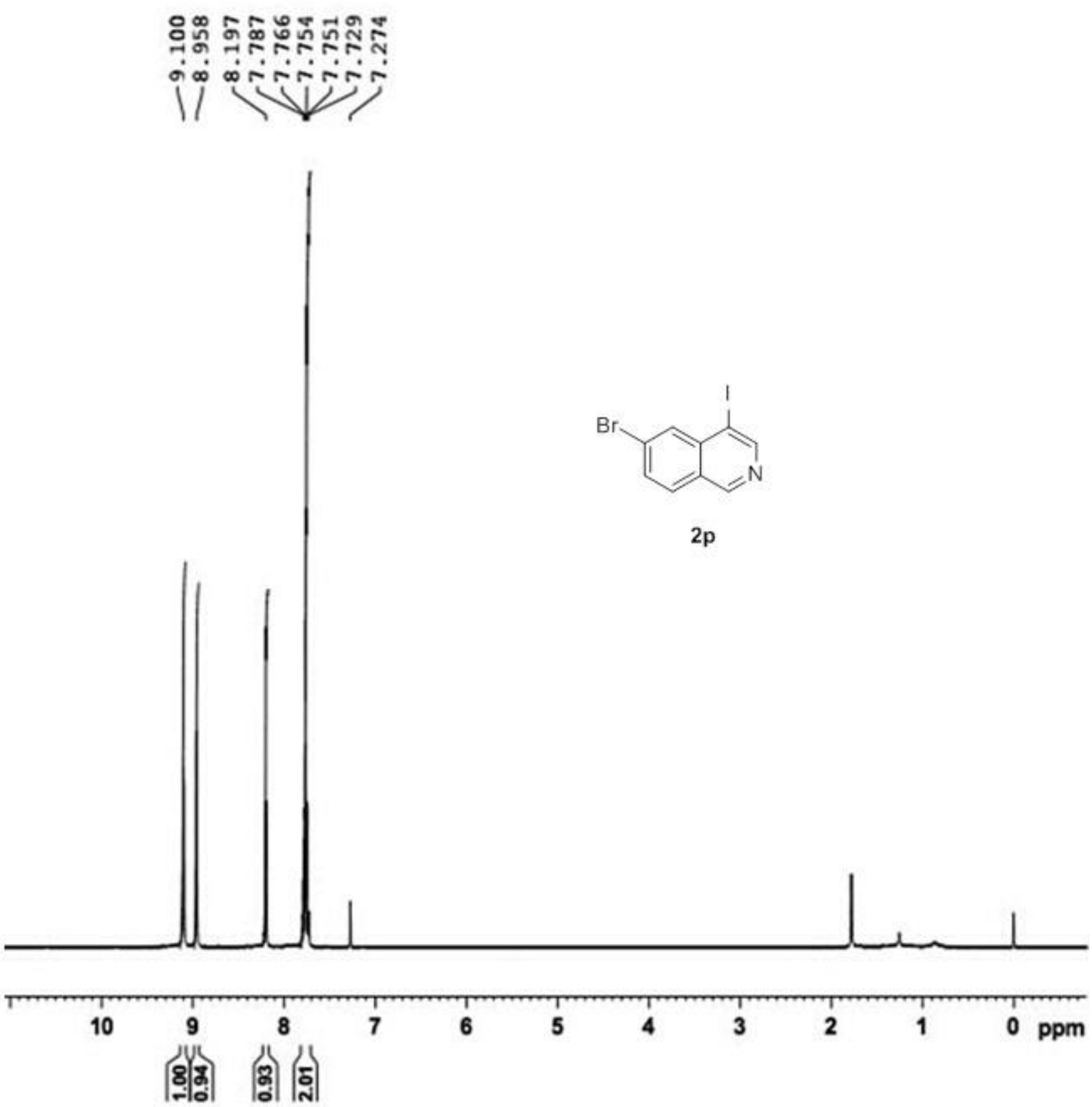
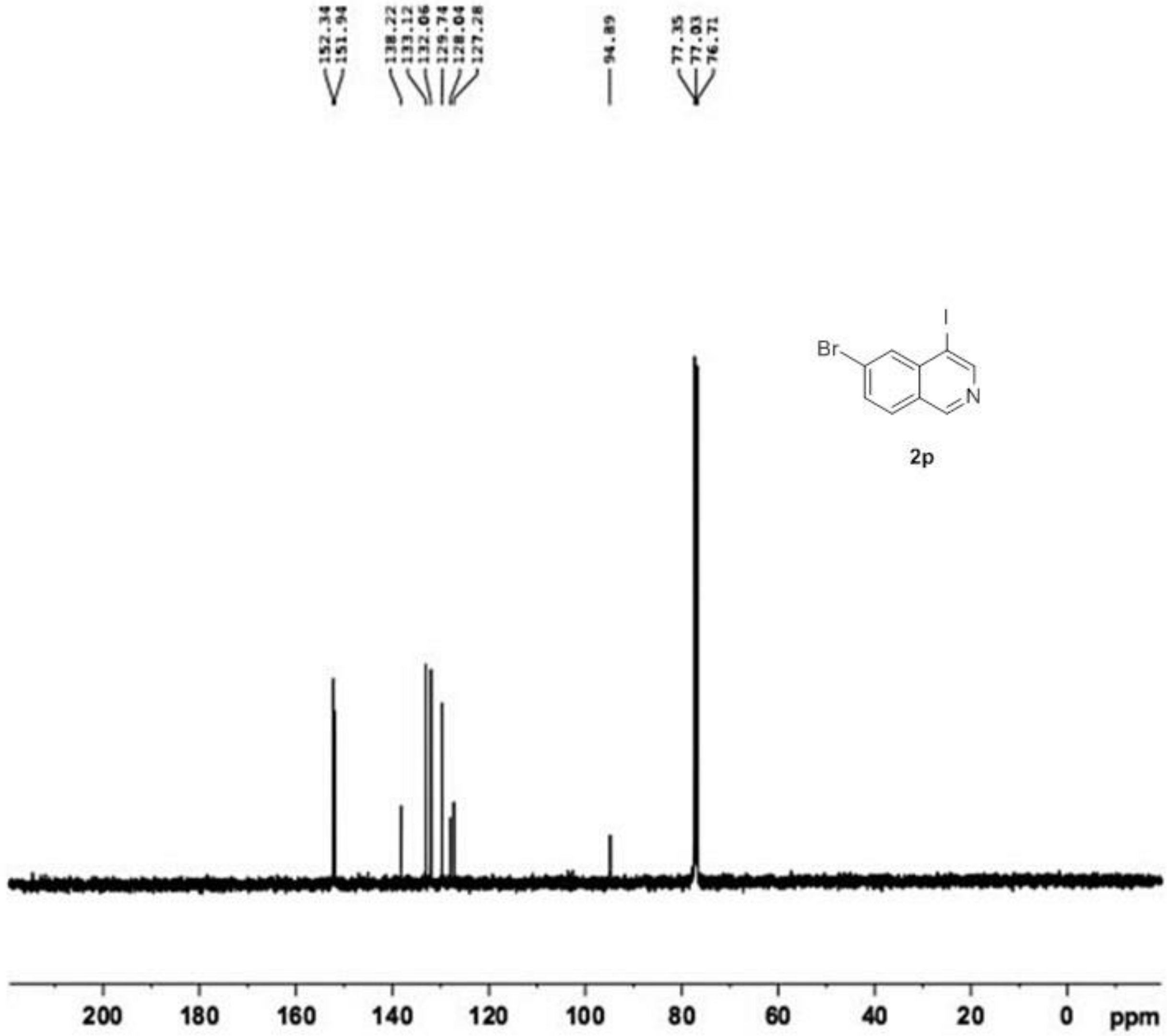
8.004
7.983
7.905
7.885
7.811
7.808
7.793
7.790
7.772
7.770
7.684
7.664
7.646
7.274
I
N
2o
10
9
8
7
6
5
4
3
2
1
ppr
1.00
0.95
1.00
0.99
1.04
0.96


152.60
150.97
137.11
131.97
130.71
129.73
128.32
128.16
96.80
77.36
77.04
76.72
200
180
160
140
120
100
80
60
40
20
0
ppm
I
N

2o

Compound 2p

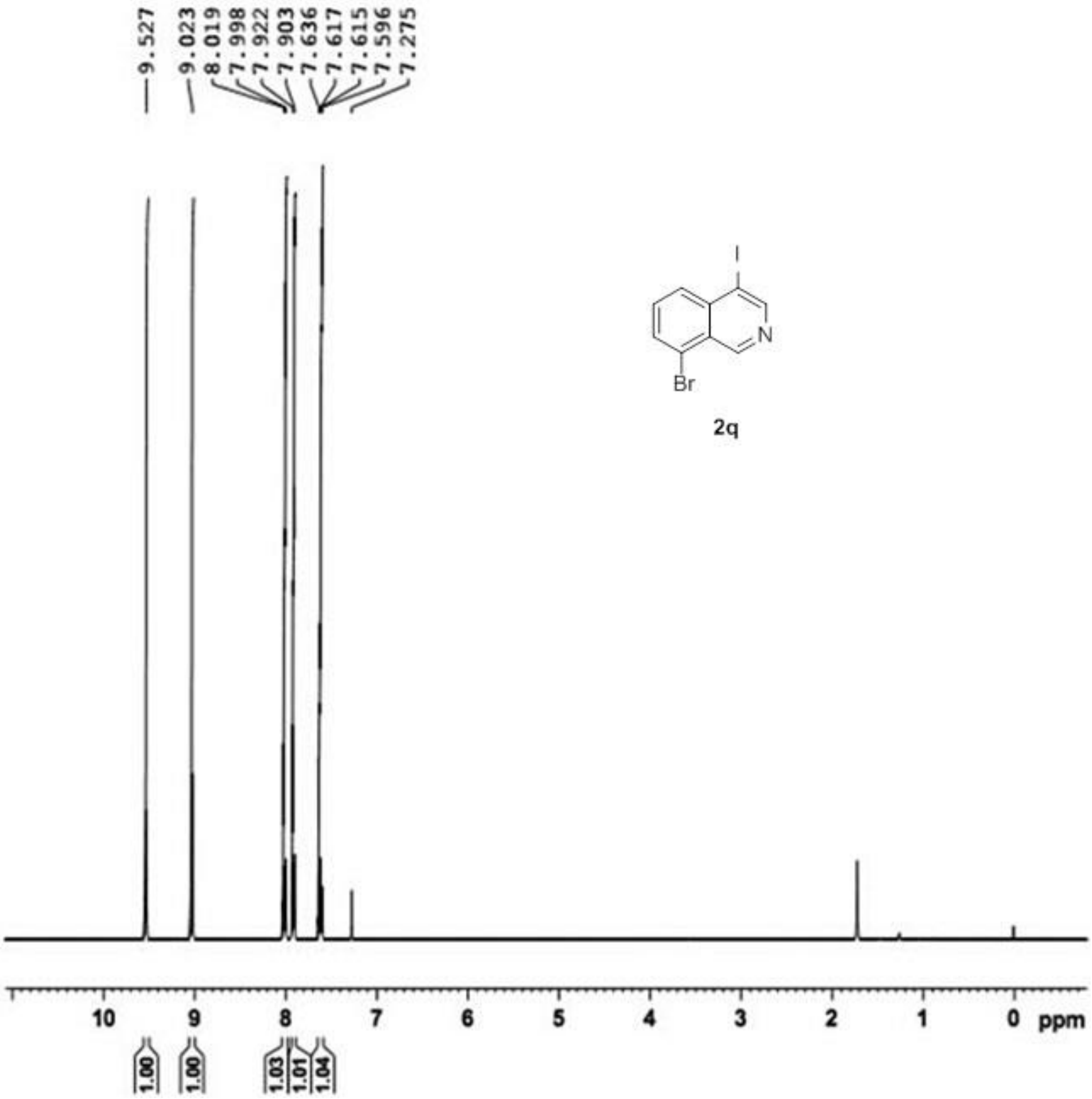

9.100
8.958
8.197
7.787
7.766
7.754
7.751
7.729
7.274
Br
I
N
2p
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.94
0.93
2.01

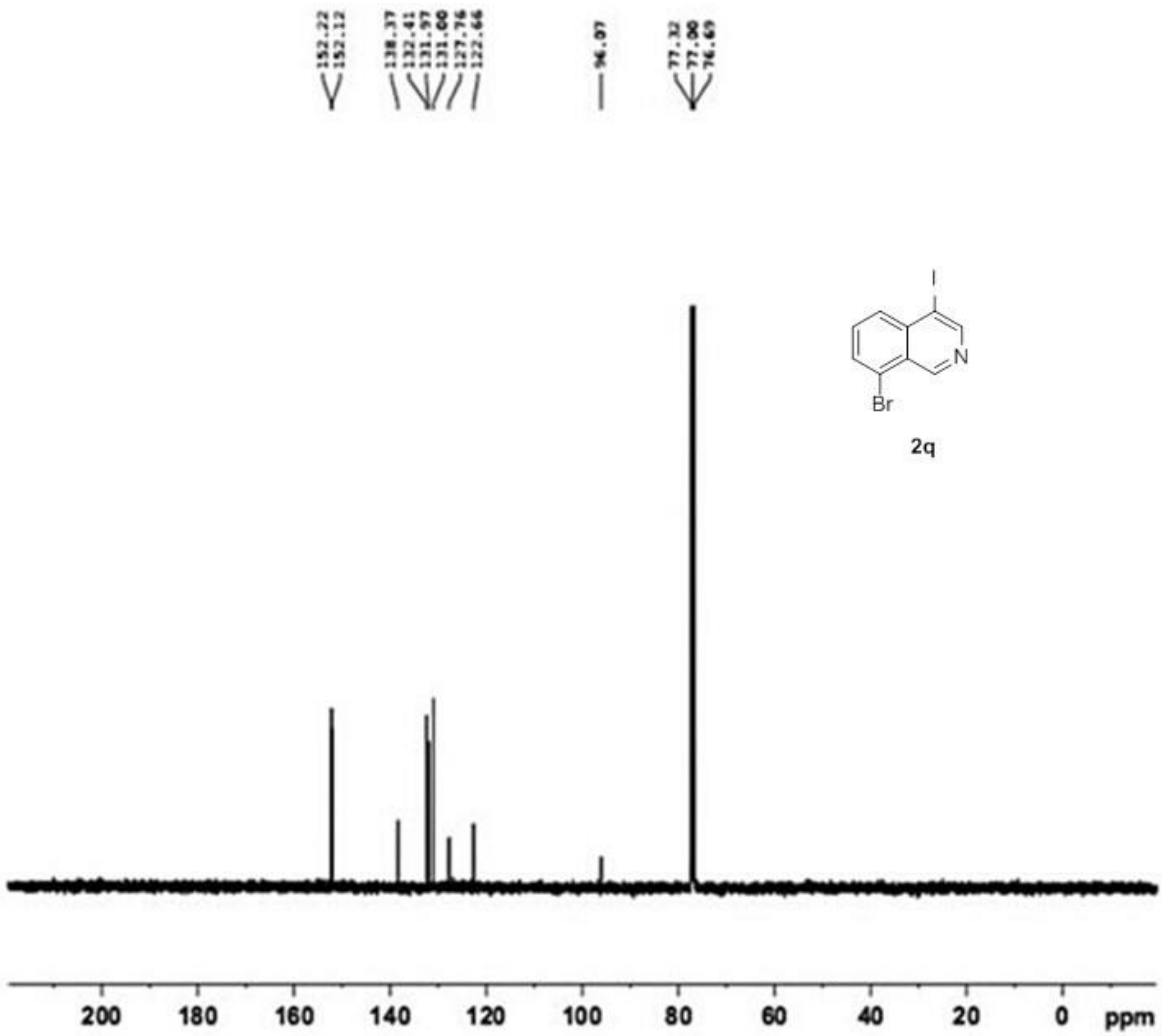


152.34
151.94
138.22
133.12
132.06
129.74
128.04
127.28
94.89
77.35
77.03
76.71
Br
I
N
200
180
160
140
120
100
80
60
40
20
0
ppm

2p

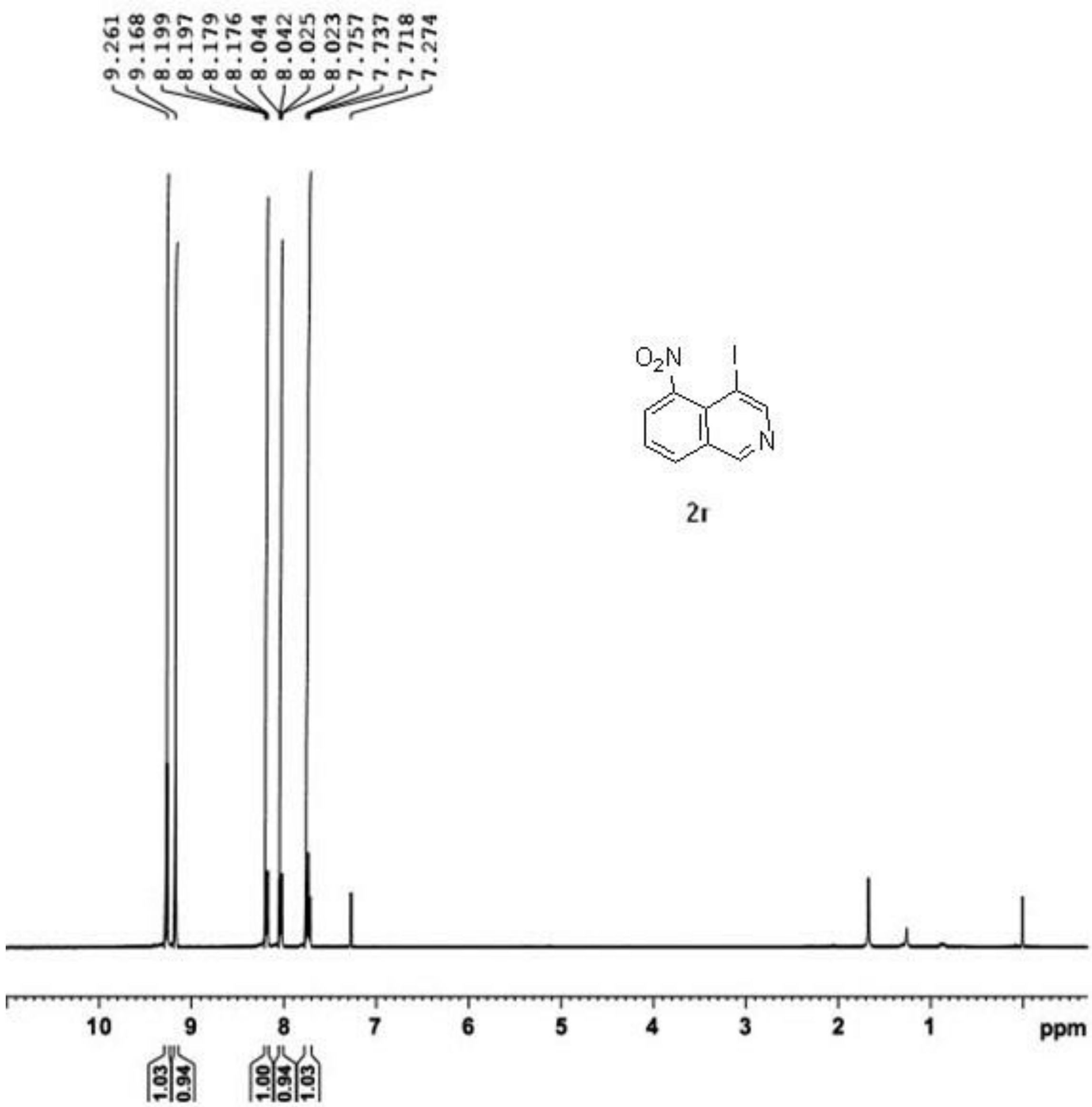
Compound 2q


9.527
9.023
8.019
7.998
7.922
7.903
7.636
7.617
7.615
7.596
7.275
I
N
Br
2q
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.03
1.01
1.04

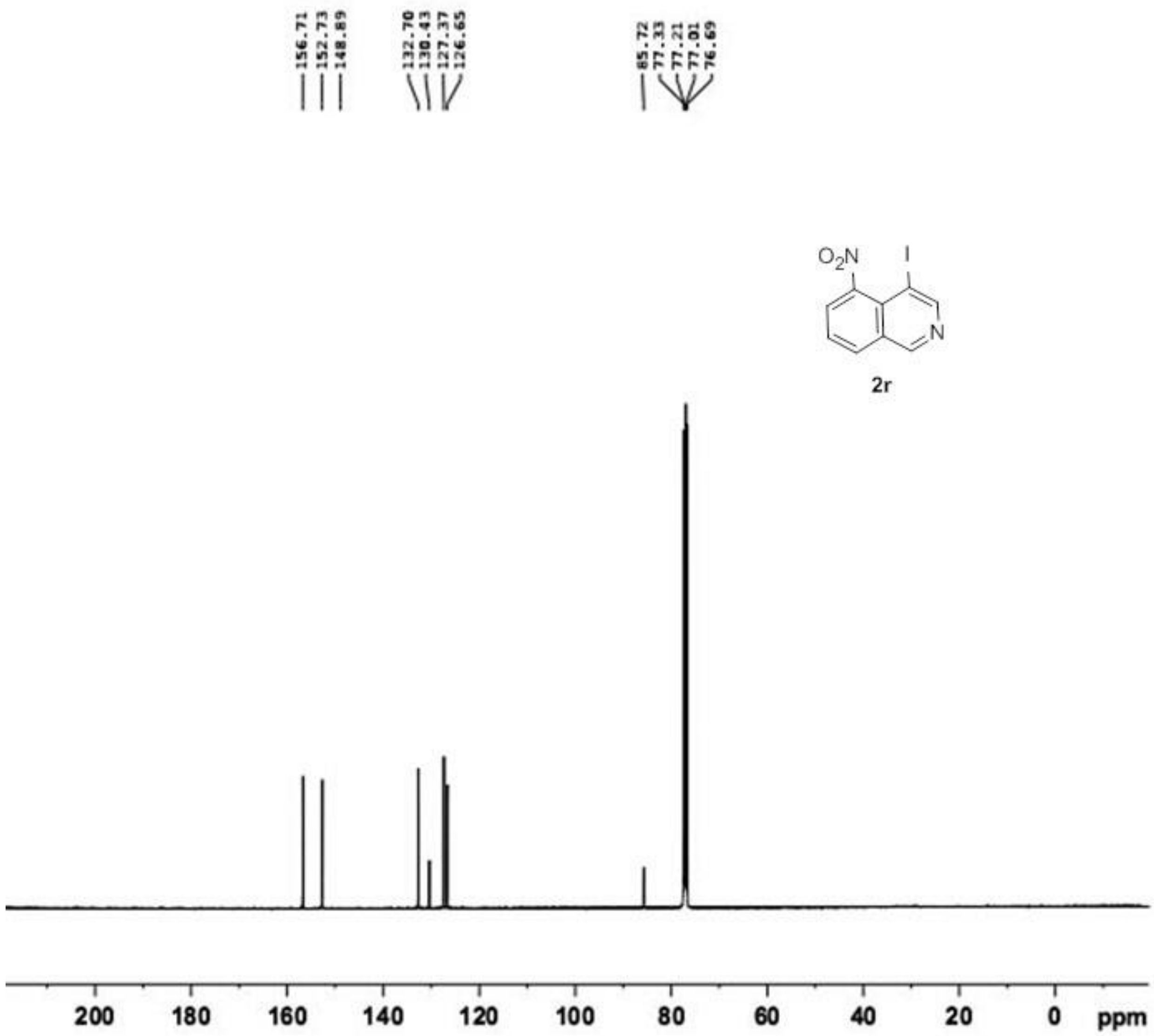


152.22
152.12
138.37
132.41
131.97
131.00
127.76
122.66
96.07
77.32
77.00
76.69
I
N
Br
2q
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 2r



9.261
9.168
8.199
8.197
8.179
8.176
8.044
8.042
8.025
8.023
7.757
7.737
7.718
7.274
O2N
I
N
2r
10
9
8
7
6
5
4
3
2
1
ppm
1.03
0.94
1.00
0.94
1.03


156.71
152.73
148.89
132.70
130.43
127.37
126.65
85.72
77.33
77.21
77.01
76.69
O_2N
I
N
2r
200
180
160
140
120
100
80
60
40
20
0
ppm