Supporting Information

Hydrogen Bond Promoted Regio- and Stereoselective Synthesis of Isoindoline Derivatives through the Pd-Catalyzed Isocyanide Insertion Reaction Involving Aziridines

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Contents

1. General Information

Unless otherwise noted, all solvents and reagents were purchased from commercial suppliers without further purification. Oil bath was used for all required reactions with magnetic stirring. Column chromatography purifications were performed under "flash" conditions using 200-300 mesh silica gel. Analytical TLC was carried out on silica gel 60 F254 plates which were visualized by exposure to ultraviolet light. Melting points were determined with an X-4 model apparatus. Crystal was tested on a Bruker D8 Quest diffractometer. HRMS was measured on an Waters Xevo G2-XS Tof spectrometer. NMR spectra were recorded on a Bruker 400 spectrometer calibrated to $CDCl_3$ using tetramethylsilane (TMS) as internal standards. ^1H NMR spectral data are reported in terms of chemical shift (δ, ppm), multiplicity (s = single, d = doublet, t = triplet, q = quartet, m =multiplet), coupling constant (Hz), and integration. ^{13}C NMR spectral data are reported in terms of chemical shift.

All calculations in this work were performed using Gaussian 16 program package[1]. Full geometry optimizations were performed to locate all the stationary points, using the M06-2x method[2] with the def2tzvp[3-4], namely M06-2x/def2tzvp, as well as the frequency calculation all in M06-2x/def2tzvp level. Dispersion corrections were computed with Grimme's D3(BJ) method in optimization[5]. Harmonic vibrational frequency was performed at the same level to guarantee that there is no imaginary frequency in the molecules, i.e. they locate on the minima of potential energy surface. Convergence parameters of the default threshold were retained (maximum force within 4.5×10^{-4} Hartrees/Bohr and root mean square (RMS) force within 3.0×10^{-4} Hartrees/Radian) to obtain the optimized structure. The optimal structure was identified given that all calculations for structural optimization were successfully converged within the convergence threshold of no imaginary frequency, during the process of vibration analysis.

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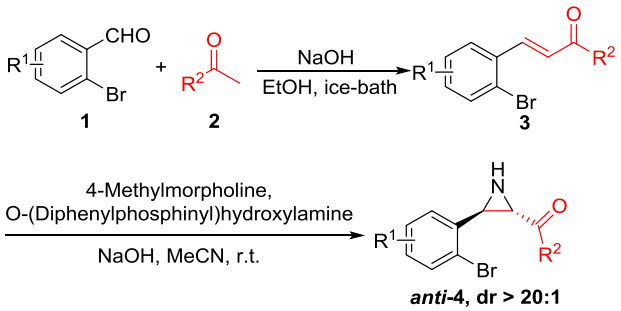
2. General Procedure for the Preparation of 3 and 4.

A mixture of benzaldehydes **1** (4 mmol) and ketones **2** (4 mmol) were subjected to a solution of 10% NaOH (1 mL) in an ice-bath of ethanol (12 mL) for 4 hours (Scheme S1). The reactions yielded chalcones **3**.[6] NMM (223 mg, 2.2 mmol) was added dropwise over 1 min to a solution of $DppONH_2$ (513 mg, 2.2 mmol) in MeCN (20 mL) at rt under N_2. The white mixture was allowed to stir for 30 min, then NaOH (160 mg, 4.0 mmol) and chalcones **3** (2.0 mmol) were added sequentially. The mixture was allowed to stir at rt for 10 h, then quenched by the addition of saturated NH_4Cl solution (30 mL). After completion, the solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel with ethylacetate/petroleum ether (1: 22-25) as the eluent to give products **4** in a yield of 70−85%.[7]

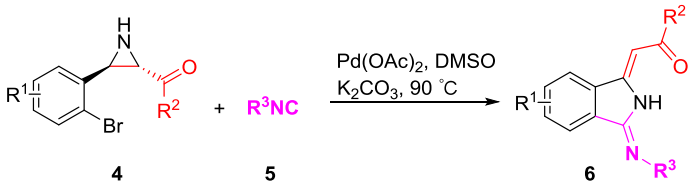


Comp.	R^1	R^2	yield[a] (%)	Comp.	R^1	R^2	yield (%)
4a	H	4-ClC_6H_4	80	**4g**	5-F	4-ClC_6H_4	77
4b	H	2,4-$Cl_2C_6H_3$	77	**4h**	5-Cl	C_6H_5	75
4c	H	4-FC_6H_4	74	**4i**	5-Cl	4-ClC_6H_4	85
4d	H	C_6H_5	78	**4j**	4-F	C_6H_5	79
4e	H	4-$CH_3C_6H_4$	70	**4k**	4-Cl	C_6H_5	80
4f	5-F	C_6H_5	76	**4l**	4-Cl	4-ClC_6H_4	82

[a] Yield of isolated product based on substrates **3**.

Scheme S1 Preparation of substrates **4**.

General Procedure for the Preparation of 6.



Scheme S2 Preparation of products **6**.

In an oven-dried 10 mL pressure tube, a mixture of substrates **4** (0.5 mmol), isocyanides **5** (0.6 mmol, 1.2 equiv.), K_2CO_3 (103.5 mg, 0.75 mmol, 1.5 equiv.) and $Pd(OAc)_2$ (5.6 mg, 0.025 mmol, 0.05 equiv.) were dissolved in DMSO (4 mL) at 90 ℃ by oil bath for 8 h (Scheme S2). The reactions were monitored by TLC. After completion, the solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel with ethylacetate/petroleum ether (1: 25-30) as the eluent to give products **6** in a yield of 62–81%.

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3. X-ray Crystallography Data of 6a

Crystal sample preparation of 6a: A solution of compound **6a** (20 mg) in AcOEt (0.8 mL) was placed in a vial (10 mL). Then petroleum ether (5 mL) was added to the solution with a dropper. The single crystal **6a** was obtained by slowly evaporating mixed solvent at room temperature under the air conditions. A suitable crystal was selected and tested on a Bruker D8 Quest diffractometer. The crystal was kept at 296.0 K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

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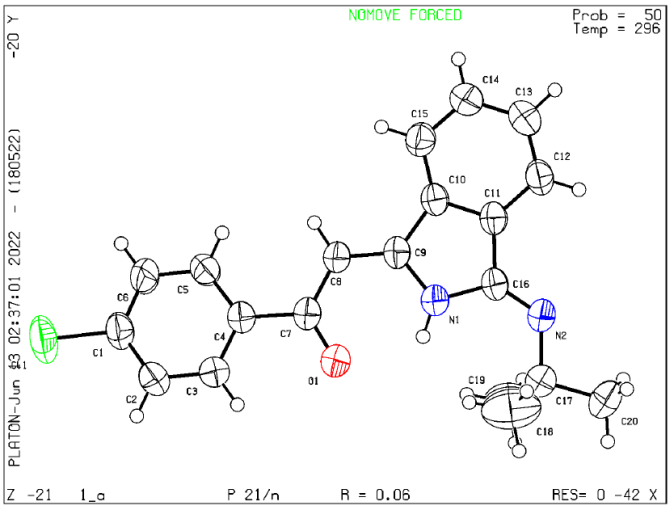


Figure S1. X-ray crystal structure of **6a** is drawn at the 50% probability.

Table S1 Crystal data and structure refinement for **6a.**

Identification code	**6a**	
Empirical formula	C20 H19 Cl N2 O	
Formula weight	338.82	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.876(5) Å	α= 90 °.
	b = 17.391(9) Å	β= 101.377(10) °.
	c = 10.776(5) Å	γ = 90 °.
Volume	1814.4(14) $Å^3$	
Z	4	
Density (calculated)	1.240 Mg/m^3	
Absorption coefficient	0.219 mm^{-1}	
F(000)	712	
Crystal size	0.200 x 0.200 x 0.200 mm^3	
Theta range for data collection	2.408 to 25.160 °.	

Index ranges	-11<=h<=10, -20<=k<=20, -12<=l<=12
Reflections collected	27362
Independent reflections	3220 [R(int) = 0.0748]
Completeness to theta = 25.160 °	98.8 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3220 / 0 / 220
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0595, wR2 = 0.1333
R indices (all data)	R1 = 0.1145, wR2 = 0.1648
Extinction coefficient	n/a
Largest diff. peak and hole	0.297 and -0.303 e.$Å^{-3}$

Table S2 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)
C(1)	-1845(3)	6315(2)	3084(3)	60(1)
C(2)	-1399(3)	5918(2)	4176(3)	62(1)
C(3)	-48(3)	5996(2)	4804(3)	58(1)
C(4)	874(3)	6462(2)	4333(3)	48(1)
C(5)	381(4)	6853(2)	3225(3)	78(1)
C(6)	-975(4)	6789(3)	2607(3)	89(1)
C(7)	2351(3)	6473(2)	5001(3)	50(1)
C(8)	3324(3)	6990(2)	4604(3)	50(1)
C(9)	4692(3)	6976(2)	5130(3)	46(1)
C(10)	5814(3)	7480(2)	4903(3)	47(1)
C(11)	7013(3)	7265(2)	5744(3)	47(1)
C(12)	8244(3)	7655(2)	5766(3)	58(1)
C(13)	8233(3)	8252(2)	4926(3)	69(1)
C(14)	7049(4)	8453(2)	4066(3)	67(1)
C(15)	5819(3)	8075(2)	4046(3)	58(1)
C(16)	6708(3)	6592(2)	6482(3)	46(1)
C(17)	7247(3)	5537(2)	7961(3)	63(1)
C(18)	6200(6)	5709(3)	8786(4)	121(2)

C(19)	6669(5)	4903(2)	7031(4)	99(1)
C(20)	8601(5)	5256(3)	8731(6)	173(3)
Cl(1)	-3557(1)	6226(1)	2303(1)	93(1)
N(1)	5288(2)	6466(1)	6051(2)	52(1)
N(2)	7584(2)	6236(1)	7297(2)	53(1)
O(1)	2714(2)	6013(1)	5893(2)	67(1)

Table S3 Bond lengths [Å] and angles [°] for **6a**.

	Bond lengths [Å]		angles [°]
C(1)-C(2)	1.360(4)	C(2)-C(1)-C(6)	120.8(3)
C(1)-C(6)	1.362(5)	C(2)-C(1)-Cl(1)	119.4(3)
C(1)-Cl(1)	1.740(3)	C(6)-C(1)-Cl(1)	119.8(3)
C(2)-C(3)	1.378(4)	C(1)-C(2)-C(3)	119.5(3)
C(2)-H(2)	0.9300	C(1)-C(2)-H(2)	120.2
C(3)-C(4)	1.388(4)	C(3)-C(2)-H(2)	120.2
C(3)-H(3)	0.9300	C(2)-C(3)-C(4)	121.3(3)
C(4)-C(5)	1.377(4)	C(2)-C(3)-H(3)	119.4
C(4)-C(7)	1.494(4)	C(4)-C(3)-H(3)	119.4
C(5)-C(6)	1.377(5)	C(5)-C(4)-C(3)	117.4(3)
C(5)-H(5)	0.9300	C(5)-C(4)-C(7)	123.8(3)
C(6)-H(6)	0.9300	C(3)-C(4)-C(7)	118.7(3)
C(7)-O(1)	1.247(4)	C(6)-C(5)-C(4)	121.5(3)
C(7)-C(8)	1.441(4)	C(6)-C(5)-H(5)	119.2
C(8)-C(9)	1.358(4)	C(4)-C(5)-H(5)	119.2
C(8)-H(8)	0.9300	C(1)-C(6)-C(5)	119.5(3)
C(9)-N(1)	1.374(4)	C(1)-C(6)-H(6)	120.3
C(9)-C(10)	1.471(4)	C(5)-C(6)-H(6)	120.3
C(10)-C(15)	1.387(4)	O(1)-C(7)-C(8)	121.5(3)
C(10)-C(11)	1.393(4)	O(1)-C(7)-C(4)	117.9(3)
C(11)-C(12)	1.389(4)	C(8)-C(7)-C(4)	120.6(3)
C(11)-C(16)	1.479(4)	C(9)-C(8)-C(7)	122.1(3)
C(12)-C(13)	1.376(5)	C(9)-C(8)-H(8)	118.9
C(12)-H(12)	0.9300	C(7)-C(8)-H(8)	118.9
C(13)-C(14)	1.386(5)	C(8)-C(9)-N(1)	124.2(3)
C(13)-H(13)	0.9300	C(8)-C(9)-C(10)	129.8(3)
C(14)-C(15)	1.377(5)	N(1)-C(9)-C(10)	106.0(2)

C(14)-H(14)	0.9300	C(15)-C(10)-C(11)	121.2(3)
C(15)-H(15)	0.9300	C(15)-C(10)-C(9)	131.1(3)
C(16)-N(2)	1.267(3)	C(11)-C(10)-C(9)	107.7(3)
C(16)-N(1)	1.404(4)	C(12)-C(11)-C(10)	120.6(3)
C(17)-N(2)	1.482(4)	C(12)-C(11)-C(16)	130.4(3)
C(17)-C(20)	1.510(5)	C(10)-C(11)-C(16)	109.0(2)
C(17)-C(18)	1.521(6)	C(13)-C(12)-C(11)	117.6(3)
C(17)-C(19)	1.523(5)	C(13)-C(12)-H(12)	121.2
C(18)-H(18A)	0.9600	C(11)-C(12)-H(12)	121.2
C(18)-H(18B)	0.9600	C(12)-C(13)-C(14)	121.7(3)
C(18)-H(18C)	0.9600	C(12)-C(13)-H(13)	119.1
C(19)-H(19A)	0.9600	C(14)-C(13)-H(13)	119.1
C(19)-H(19B)	0.9600	C(15)-C(14)-C(13)	121.0(3)
C(19)-H(19C)	0.9600	C(15)-C(14)-H(14)	119.5
C(20)-H(20A)	0.9600	C(13)-C(14)-H(14)	119.5
C(20)-H(20B)	0.9600	C(14)-C(15)-C(10)	117.7(3)
C(20)-H(20C)	0.9600	C(14)-C(15)-H(15)	121.2
N(1)-H(1)	0.8600	C(10)-C(15)-H(15)	121.2
		N(2)-C(16)-N(1)	130.9(3)
		N(2)-C(16)-C(11)	125.1(3)
		N(1)-C(16)-C(11)	104.0(2)
		N(2)-C(17)-C(20)	105.8(3)
		N(2)-C(17)-C(18)	111.4(3)
		C(20)-C(17)-C(18)	111.9(4)
		N(2)-C(17)-C(19)	111.5(3)
		C(20)-C(17)-C(19)	107.7(4)
		C(18)-C(17)-C(19)	108.5(3)
		C(17)-C(18)-H(18A)	109.5
		C(17)-C(18)-H(18B)	109.5
		H(18A)-C(18)-H(18B)	109.5
		C(17)-C(18)-H(18C)	109.5
		H(18A)-C(18)-H(18C)	109.5
		H(18B)-C(18)-H(18C)	109.5
		C(17)-C(19)-H(19A)	109.5
		C(17)-C(19)-H(19B)	109.5
		H(19A)-C(19)-H(19B)	109.5
		C(17)-C(19)-H(19C)	109.5

		H(19A)-C(19)-H(19C)	109.5
		H(19B)-C(19)-H(19C)	109.5
		C(17)-C(20)-H(20A)	109.5
		C(17)-C(20)-H(20B)	109.5
		H(20A)-C(20)-H(20B)	109.5
		C(17)-C(20)-H(20C)	109.5
		H(20A)-C(20)-H(20C)	109.5
		H(20B)-C(20)-H(20C)	109.5
		C(9)-N(1)-C(16)	113.3(2)
		C(9)-N(1)-H(1)	123.3
		C(16)-N(1)-H(1)	123.3
		C(16)-N(2)-C(17)	123.2(3)

Symmetry transformations used to generate equivalent atoms:

Table S4 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}
C(1)	42(2)	80(2)	55(2)	-5(2)	2(2)	-5(2)
C(2)	45(2)	66(2)	76(2)	5(2)	13(2)	-7(2)
C(3)	48(2)	62(2)	62(2)	12(2)	8(2)	-2(2)
C(4)	41(2)	52(2)	48(2)	-2(1)	6(1)	-1(1)
C(5)	51(2)	113(3)	66(2)	35(2)	-2(2)	-24(2)
C(6)	55(2)	134(4)	67(2)	42(2)	-12(2)	-19(2)
C(7)	42(2)	56(2)	49(2)	0(2)	2(1)	1(2)
C(8)	42(2)	54(2)	49(2)	3(1)	-1(1)	-3(1)
C(9)	40(2)	51(2)	46(2)	-4(1)	2(1)	0(1)
C(10)	42(2)	51(2)	46(2)	-6(1)	4(1)	-2(1)
C(11)	41(2)	51(2)	46(2)	-7(1)	3(1)	-1(1)
C(12)	41(2)	67(2)	63(2)	-1(2)	3(2)	-4(2)
C(13)	52(2)	76(2)	77(2)	5(2)	10(2)	-13(2)
C(14)	62(2)	67(2)	70(2)	11(2)	7(2)	-11(2)
C(15)	53(2)	59(2)	57(2)	1(2)	1(2)	-1(2)
C(16)	38(2)	52(2)	45(2)	-8(1)	5(1)	-2(1)
C(17)	56(2)	62(2)	68(2)	12(2)	1(2)	-3(2)
C(18)	183(5)	109(4)	87(3)	10(3)	69(3)	4(3)

C(19)	127(4)	62(2)	109(3)	4(2)	29(3)	-5(2)
C(20)	85(3)	153(5)	242(7)	133(5)	-61(4)	-28(3)
Cl(1)	45(1)	139(1)	86(1)	-7(1)	-6(1)	-14(1)
N(1)	43(2)	55(2)	55(2)	6(1)	1(1)	-4(1)
N(2)	44(1)	58(2)	54(2)	4(1)	0(1)	1(1)
O(1)	51(1)	77(2)	68(1)	20(1)	-2(1)	-6(1)

Table S5 Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for **6a**.

	x	y	z	U(eq)
H(2)	-2000	5597	4496	75
H(3)	251	5731	5558	69
H(5)	978	7166	2885	94
H(6)	-1294	7068	1871	107
H(8)	3004	7345	3968	60
H(12)	9048	7518	6329	70
H(13)	9041	8529	4935	82
H(14)	7086	8848	3493	81
H(15)	5021	8214	3478	69
H(18A)	5320	5821	8257	181
H(18B)	6503	6145	9315	181
H(18C)	6114	5271	9306	181
H(19A)	6613	4433	7485	148
H(19B)	7265	4832	6437	148
H(19C)	5764	5046	6586	148
H(20A)	8966	5634	9357	259
H(20B)	9245	5173	8183	259
H(20C)	8454	4782	9142	259
H(1)	4837	6105	6334	62

Table S6 Torsion angles [º] for **6a**.

C(6)-C(1)-C(2)-C(3)	-0.2(5)
Cl(1)-C(1)-C(2)-C(3)	-179.2(3)
C(1)-C(2)-C(3)-C(4)	-1.1(5)

C(2)-C(3)-C(4)-C(5)	0.9(5)
C(2)-C(3)-C(4)-C(7)	-175.1(3)
C(3)-C(4)-C(5)-C(6)	0.4(6)
C(7)-C(4)-C(5)-C(6)	176.3(4)
C(2)-C(1)-C(6)-C(5)	1.5(6)
Cl(1)-C(1)-C(6)-C(5)	-179.5(3)
C(4)-C(5)-C(6)-C(1)	-1.6(7)
C(5)-C(4)-C(7)-O(1)	-170.0(3)
C(3)-C(4)-C(7)-O(1)	5.9(4)
C(5)-C(4)-C(7)-C(8)	8.9(5)
C(3)-C(4)-C(7)-C(8)	-175.3(3)
O(1)-C(7)-C(8)-C(9)	3.6(5)
C(4)-C(7)-C(8)-C(9)	-175.1(3)
C(7)-C(8)-C(9)-N(1)	1.8(5)
C(7)-C(8)-C(9)-C(10)	-176.2(3)
C(8)-C(9)-C(10)-C(15)	-4.5(5)
N(1)-C(9)-C(10)-C(15)	177.2(3)
C(8)-C(9)-C(10)-C(11)	175.7(3)
N(1)-C(9)-C(10)-C(11)	-2.7(3)
C(15)-C(10)-C(11)-C(12)	1.6(4)
C(9)-C(10)-C(11)-C(12)	-178.5(3)
C(15)-C(10)-C(11)-C(16)	-176.9(3)
C(9)-C(10)-C(11)-C(16)	3.0(3)
C(10)-C(11)-C(12)-C(13)	-0.5(5)
C(16)-C(11)-C(12)-C(13)	177.6(3)
C(11)-C(12)-C(13)-C(14)	-1.3(5)
C(12)-C(13)-C(14)-C(15)	2.1(6)
C(13)-C(14)-C(15)-C(10)	-1.0(5)
C(11)-C(10)-C(15)-C(14)	-0.8(4)
C(9)-C(10)-C(15)-C(14)	179.4(3)
C(12)-C(11)-C(16)-N(2)	-1.0(5)
C(10)-C(11)-C(16)-N(2)	177.3(3)
C(12)-C(11)-C(16)-N(1)	179.6(3)
C(10)-C(11)-C(16)-N(1)	-2.2(3)

C(8)-C(9)-N(1)-C(16)	-177.1(3)
C(10)-C(9)-N(1)-C(16)	1.3(3)
N(2)-C(16)-N(1)-C(9)	-179.0(3)
C(11)-C(16)-N(1)-C(9)	0.5(3)
N(1)-C(16)-N(2)-C(17)	3.0(5)
C(11)-C(16)-N(2)-C(17)	-176.3(3)
C(20)-C(17)-N(2)-C(16)	174.1(4)
C(18)-C(17)-N(2)-C(16)	-64.0(4)
C(19)-C(17)-N(2)-C(16)	57.3(4)

Table S7 Hydrogen bonds for **6a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(1)	0.86	2.06	2.635(3)	123.3

Symmetry transformations used to generate equivalent atoms:

4. Characterization Datas

***Anti* (3-(2-bromophenyl)aziridin-2-yl)(4-chlorophenyl)methanone (4a):**

White solid, yield: 0.534g (80%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 25, mp 104–106 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.03-7.17 (m, 8H), 3.41-3.32 (m, 2H), 2.61 (s, *J* = 8.4 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 194.7, 140.4, 137.4, 134.0, 132.2, 129.9, 129.3, 129.1, 128.1, 127.6, 124.0, 44.2, 42.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{12}BrClNO$ 335.9785; Found 335.9800.

***Anti* (3-(2-bromophenyl)aziridin-2-yl)(2,4-dichlorophenyl)methanone (4b):**

White solid, yield: 0.568g (77%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 22, mp 90–92 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 7.69-7.14 (m, 7H), 3.57-3.22 (m, 2H), 2.63 (t, *J* = 8.4 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 196.9, 138.7, 137.0, 135.2, 133.4, 132.4, 131.2, 130.8, 129.3, 127.7, 127.5, 127.4, 124.1, 46.4, 45.0; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{11}BrCl_2NO$ 369.9396; Found 369.9408.

***Anti* (3-(2-bromophenyl)aziridin-2-yl)(4-fluorophenyl)methanone (4c):**

White solid, yield: 0.472g (74%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 22, mp 62–63 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.13-7.15 (m, 8H), 3.41-3.32 (m, 2H), 2.61 (t, J = 8.4 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 194.3, 166.2 (d, $J_{C\text{-}F}$ = 254.0 Hz), 137.5, 132.2, 131.3, 131.2, 129.2, 128.1, 127.6, 124.0, 116.0 (d, $J_{C\text{-}F}$ = 21.0 Hz), 44.0, 42.6; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{12}BrFNO$ 320.0081; Found 320.0085.

***Anti* (3-(2-bromophenyl)aziridin-2-yl)(phenyl)methanone (4d):**

White solid, yield: 0.470g (78%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 22, mp 89–90 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.08-7.16 (m, 9H), 3.42-3.38 (m, 2H), 2.62 (t, J = 8.0 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 195.8, 137.6, 135.7, 133.8, 132.2, 129.2, 128.7, 128.5, 128.0, 127.6, 124.1, 44.0, 42.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{13}BrNO$ 302.0175; Found 302.0180.

***Anti* (3-(2-bromophenyl)aziridin-2-yl)(p-tolyl)methanone (4e):**

White solid, yield: 0.472g (70%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 25, mp 102–103 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 7.99-7.16 (m, 8H), 3.39-3.36 (m, 2H), 2.60 (t, J = 8.0 Hz, 1H), 2.43 (s, 3H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 195.3, 144.9, 137.7, 133.2, 132.2, 129.4, 129.1, 128.7, 128.0, 127.6, 124.1, 43.8, 42.6, 21.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{14}BrNO$ 338.1186; Found 338.1194.

***Anti* (3-(2-bromo-5-fluorophenyl)aziridin-2-yl)(phenyl)methanone (4f):**

White solid, yield: 0.485g (76%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 22, mp 91–93 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.07-7.26 (m, 6H), 6.93-6.89 (m, 2H), 3.38-3.36 (m, 2H), 2.63 (t, J = 8.0 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 195.5, 162.3 (d, $J_{C\text{-}F}$ = 246.0 Hz), 140.0 (d, $J_{C\text{-}F}$ = 8.0 Hz), 135.7, 134.0, 133.4 (d, $J_{C\text{-}F}$ = 8.0 Hz), 128.8, 128.5, 117.9, 116.4 (d, $J_{C\text{-}F}$ = 23.0 Hz), 115.3 (d, $J_{C\text{-}F}$ = 24.0 Hz), 43.4, 42.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{12}BrFNO$ 320.0081; Found 320.0087.

***Anti* (3-(2-bromo-5-fluorophenyl)aziridin-2-yl)(4-chlorophenyl)methanone (4g):**

White solid, yield: 0.544g (77%), dr > 20:1, determined by ^{1}H NMR spectrum,

ethylacetate/petroleum ether = 1: 22, mp 108–109 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.01-6.92 (m, 7H), 3.37-3.31 (m, 2H), 2.63 (t, J = 8.0 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 194.3, 162.3 (d, J_{C-F} = 246.0 Hz), 140.6, 139.8 (d, J_{C-F} = 8.0 Hz), 133.9, 133.5 (d, J_{C-F} = 8.0 Hz), 129.9, 129.2, 117.8 (d, J_{C-F} = 3.0 Hz), 116.5 (d, J_{C-F} = 22.0 Hz), 115.4 (d, J_{C-F} = 24.0 Hz), 43.7, 42.6; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $C_{15}H_{11}BrClFNO$ 353.9691; Found 353.9693.

***Anti* (3-(2-bromo-5-chlorophenyl)aziridin-2-yl)(phenyl)methanone (4h):**

White solid, yield: 0.503g (75%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 22, mp 106–108 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.07-7.15 (m, 8H), 3.39-3.34 (m, 2H), 2.63 (t, J = 8.4 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 195.4, 139.4, 135.6, 134.0, 133.3, 129.9, 129.3, 128.8, 128.5, 128.2, 121.7, 43.3, 42.7; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $C_{15}H_{12}BrClNO$ 335.9785; Found 335.9794.

***Anti* (3-(2-bromo-5-chlorophenyl)aziridin-2-yl)(4-chlorophenyl)methanone (4i):**

White solid, yield: 0.627g (85%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 25, mp 146–147 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.01-7.15 (m, 7H), 3.36-3.32 (m, 2H), 2.62 (t, J = 8.0 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 194.3, 140.6, 139.2, 134.0, 133.9, 133.3, 129.9, 129.4, 129.2, 128.3, 121.6, 43.6, 42.6; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $C_{15}H_{11}BrCl_2NO$ 369.9396; Found 369.9403.

***Anti* (3-(2-bromo-4-fluorophenyl)aziridin-2-yl)(phenyl)methanone (4j):**

White solid, yield: 0.504g (79%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 22, mp 95–96 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.08-7.03 (m, 8H), 3.37-3.34 (m, 2H), 2.62 (t, J = 8.4 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 195.6, 161.9 (d, J_{C-F} = 250.0 Hz), 135.7, 133.9, 133.6 (d, J_{C-F} = 3.0 Hz), 129.2 (d, J_{C-F} = 8.0 Hz), 128.8, 128.5, 123.9 (d, J_{C-F} = 10.0 Hz), 119.5 (d, J_{C-F} = 24.0 Hz), 114.7(d, J_{C-F} = 20.0 Hz), 43.3, 42.7; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $C_{15}H_{12}BrFNO$ 320.0081; Found 320.0086.

***Anti* (3-(2-bromo-4-chlorophenyl)aziridin-2-yl)(phenyl)methanone (4k):**

White solid, yield: 0.536g (80%), dr > 20:1, determined by ^{1}H NMR spectrum,

ethylacetate/petroleum ether = 1: 22, mp 106–107 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.07-7.48 (m, 8H), 3.36-3.34 (m, 2H), 2.62 (t, *J* = 7.6 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 195.5, 136.4, 135.7, 134.2, 134.0, 131.9, 128.9, 128.8, 128.5, 127.9, 124.2, 43.3, 42.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{12}BrClNO$ 335.9785; Found 335.9792.

***Anti* (3-(2-bromo-4-chlorophenyl)aziridin-2-yl)(4-chlorophenyl)methanone (4l):**

White solid, yield: 0.605g (82%), dr > 20:1, determined by ^{1}H NMR spectrum, ethylacetate/petroleum ether = 1: 25, mp 120–122 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 8.01-7.31 (m, 7H), 3.35-3.28 (m, 2H), 2.62 (t, *J* = 8.0 Hz, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 194.4, 140.6, 136.2, 134.3, 133.9, 131.9, 129.9, 129.2, 129.0, 127.9, 124.1, 43.5, 42.6; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{11}BrC_{l2}NO$ 369.9396; Found 369.9399.

2-((1Z,3Z)-3-(Tert-butylimino)isoindolin-1-ylidene)-1-(4-chlorophenyl)ethan-1-one (6a):

Light yellow solid, yield: 0.125g (74%), ethylacetate/petroleum ether = 1: 25, mp 123–125 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.47 (s, 1H), 7.98-7.26 (m, 8H), 6.59 (s, 1H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 189.8, 153.7, 148.2, 138.4, 137.5, 135.0, 134.6, 131.7, 130.5, 129.0, 128.8, 122.9, 120.8, 89.0, 54.8, 30.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{20}ClN_2O$ 339.1259; Found 339.1268.

2-((1Z,3Z)-3-(Tert-butylimino)isoindolin-1-ylidene)-1-(3,5-dichlorophenyl)ethan-1-one (6b):

Light yellow solid, yield: 0.145g (78%), ethylacetate/petroleum ether = 1: 30, mp 169–171 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.27 (s, 1H), 7.94-7.33 (m, 7H), 6.38 (s, 1H), 1.54 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 191.2, 153.3, 148.1, 136.6, 135.0, 134.4, 132.0, 131.8, 130.6, 130.6, 130.2, 127.3, 122.9, 121.0, 93.3, 55.0, 30.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{19}Cl_2N_2O$ 373.0869; Found 373.0876.

2-((1Z,3Z)-3-(Tert-butylimino)isoindolin-1-ylidene)-1-(4-fluorophenyl)ethan-1-one (6c):

Light yellow solid, yield: 0.116g (72%), ethylacetate/petroleum ether = 1: 25, mp

142–143 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.45 (s, 1H), 8.08-7.14 (m, 8H), 6.60 (s, 1H), 1.54 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 189.7, 165.2 (d, J_{C-F} = 252.0 Hz), 153.5, 148.2, 135.5 (d, J_{C-F} = 3.0 Hz), 134.7, 131.6, 130.4, 130.1 (d, J_{C-F} = 9.0 Hz), 122.8, 120.8, 115.6 (d, J_{C-F} = 21.0 Hz), 89.0, 54.8, 30.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{20}FN_2O$ 323.1554; Found 323.1559.

2-((1Z,3Z)-3-(Tert-butylimino)isoindolin-1-ylidene)-1-phenylethan-1-one (6d):

Light yellow solid, yield: 0.106g (70%), ethylacetate/petroleum ether = 1: 28, mp 120–122 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.48 (s, 1H), 8.05-7.50 (m, 9H), 6.67 (s, 1H), 1.55 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 191.4, 153.3, 148.4, 139.2, 135.1, 134.8, 132.2, 131.5, 130.4, 128.6, 127.6, 122.8, 89.4, 54.7, 30.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{21}N_2O$ 305.1648; Found 305.1658.

2-((1Z,3Z)-3-(Tert-butylimino)isoindolin-1-ylidene)-1-(p-tolyl)ethan-1-one (6e):

Light yellow solid, yield: 0.108g (68%), ethylacetate/petroleum ether = 1: 30, mp 117–118 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.40 (s, 1H), 7.88-7.20 (m, 8H), 6.57 (s, 1H), 2.34 (s, 3H), 1.46 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 191.0, 152.9, 148.5, 142.9, 136.5, 135.1, 134.8, 131.4, 130.4, 129.2, 127.1, 120.7, 89.4, 54.6, 30.4, 21.6; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{23}N_2O$ 319.1805; Found 319.1809.

2-((1Z,3Z)-3-(Tert-butylimino)-6-fluoroisoindolin-1-ylidene)-1-phenylethan-1-one(6f):

Light yellow solid, yield: 0.111g (69%), ethylacetate/petroleum ether = 1: 28, mp 102–104 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.44 (s, 1H), 8.04-7.24 (m, 8H), 6.60 (s, 1H), 1.53 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 191.3, 164.4 (d, J_{C-F} = 248.0 Hz), 152.0 (d, J_{C-F} = 3.0 Hz), 147.3, 138.9, 136.8 (d, J_{C-F} = 10.0 Hz), 132.3, 128.6, 127.6, 124.7 (d, J_{C-F} = 9.0 Hz), 119.0 (d, J_{C-F} = 23.0 Hz), 107.7 (d, J_{C-F} = 25.0 Hz), 89.8, 54.8, 30.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{20}FN_2O$ 323.1554; Found 323.1558.

2-((1Z,3Z)-3-(Tert-butylimino)-6-fluoroisoindolin-1-ylidene)-1-(4-chlorophenyl)ethan-1-one (6g):

Light yellow solid, yield: 0.134g (75%), ethylacetate/petroleum ether = 1: 30, mp

145–147 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.42 (s, 1H), 7.98-7.25 (m, 7H), 6.54 (s, 1H), 1.53 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 189.9, 164.4 (d, J_{C-F} = 248.0 Hz), 152.5, 147.1, 138.7, 137.3, 136.6 (d, J_{C-F} = 10.0 Hz), 131.0, 129.0, 128.9, 124.8, 124.7, 119.2 (d, J_{C-F} = 24.0 Hz), 107.8 (d, J_{C-F} = 24.0 Hz), 89.4, 54.9, 30.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{19}ClFN_2O$ 357.1164; Found 357.1172.

2-((1Z,3Z)-3-(Tert-butylimino)-6-chloroisoindolin-1-ylidene)-1-phenylethan-1-one(6h):

Light yellow solid, yield: 0.122g (72%), ethylacetate/petroleum ether = 1: 25, mp 113–114 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.44 (s, 1H), 8.04-7.48 (m, 8H), 6.62 (m, 1H), 1.53 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 191.3, 147.3, 138.9, 136.6, 136.3, 133.5, 132.4, 131.6, 128.6,128.1, 127.7, 121.0, 89.8, 54.9, 30.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{20}ClN_2O$ 339.1259; Found 339.1268.

2-((1Z,3Z)-3-(Tert-butylimino)-6-chloroisoindolin-1-ylidene)-1-(4-chlorophenyl)ethan-1-one (6i):

Light yellow solid, yield: 0.145g (78%), ethylacetate/petroleum ether = 1: 25, mp 181–183 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.35 (s, 1H), 7.90-7.19 (m, 7H), 6.48 (s, 1H), 1.45 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 189.9, 152.3, 147.2, 138.7, 137.2, 136.8, 136.2, 133.4, 131.8, 129.1, 128.9, 124.2, 121.1, 89.5, 55.0, 30.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{19}Cl_2N_2O$ 373.0869; Found 373.0875.

2-((1Z,3Z)-3-(Tert-butylimino)-5-fluoroisoindolin-1-ylidene)-1-phenylethan-1-one(6j):

Light yellow solid, yield: 0.121g (75%), ethylacetate/petroleum ether = 1: 30, mp 132–133 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.49 (s, 1H), 8.04-7.22 (m, 8H), 6.62 (s, 1H), 1.53 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 191.3, 165.1 (d, J_{C-F} = 250.0 Hz), 152.4, 147.3, 139.1, 137.9 (d, J_{C-F} = 10.0 Hz), 132.3, 130.6, 130.6, 128.6, 127.6, 122.7, 122.6, 118.1 (d, J_{C-F} = 25.0 Hz), 110.0 (d, J_{C-F} = 24.0 Hz), 89.5, 54.9, 30.3; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{20}FN_2O$ 323.1554; Found 323.1562.

2-((1Z,3Z)-3-(Tert-butylimino)-5-chloroisoindolin-1-ylidene)-1-phenylethan-1-one(6k):

Light yellow solid, yield: 0.130g (77%), ethylacetate/petroleum ether = 1: 28, mp 129–131 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.39 (s, 1H), 7.95-7.18 (m, 8H), 6.55 (s, 1H), 1.45 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 191.3, 152.2, 147.1, 139.0, 137.8, 136.8, 133.0, 132.3, 130.6, 128.6, 127.6, 123.1, 121.9, 89.7, 54.9, 30.3; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{20}ClN_2O$ 339.1259; Found 339.1265.

2-((1Z,3Z)-3-(Tert-butylimino)-5-chloroisoindolin-1-ylidene)-1-(4-chlorophenyl)ethan-1-one (6l):

Light yellow solid, yield: 0.151g (81%), ethylacetate/petroleum ether = 1: 25, mp 168–170 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.45 (s, 1H), 7.97-7.45 (m, 7H), 6.55 (s, 1H), 1.52 (s, 9H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 189.8, 152.7, 146.9, 138.6, 138.0, 137.3, 136.8, 132.8, 130.7, 129.0, 128.9, 123.2, 121.9, 89.3, 55.0, 30.3; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{19}Cl_2N_2O$ 373.0869; Found 373.0874.

2-((1Z,3Z)-3-(((3s,5s,7s)-Adamantan-1-yl)imino)isoindolin-1-ylidene)-1-(4-chlorophenyl)ethan-1-one (6m):

Light yellow solid, yield: 0.150g (72%), ethylacetate/petroleum ether = 1: 30, mp 157–158 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.53 (s, 1H), 7.97-7.46 (m, 8H), 6.58 (s, 1H), 2.22-1.80 (m, 15H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 189.9, 153.7, 147.5, 138.4, 137.6, 135.2, 134.5, 131.7, 130.5, 129.1, 128.8, 123.0, 120.8, 88.9, 56.0, 43.0, 36.5, 29.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{26}H_{26}ClN_2O$ 417.1728; Found 417.1734.

2-((1Z,3Z)-3-(((3s,5s,7s)-Adamantan-1-yl)imino)-6-chloroisoindolin-1-ylidene)-1-(4-chlorophenyl)ethan-1-one (6n):

Light yellow solid, yield: 0.171g (76%), ethylacetate/petroleum ether = 1: 28, mp 182–183 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.40 (s, 1H), 7.90-7.38 (m, 7H), 6.46 (s, 1H), 2.14-1.69 (m, 15H); ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 189.8, 152.2, 146.4, 138.6, 137.3, 136.6, 136.1, 133.6, 131.7, 129.1, 128.8, 124.1, 121.0,

89.2, 56.1, 43.0, 36.5, 29.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{26}H_{25}Cl_2N_2O$ 451.1338; Found 451.1348.

2-((1Z,3Z)-3-(((3s,5s,7s)-Adamantan-1-yl)imino)-5-chloroisoindolin-1-ylidene)-1-(4-chlorophenyl)ethan-1-one (6o):

Light yellow solid, yield: 0.160g (71%), ethylacetate/petroleum ether = 1: 28, mp 216–218 ℃. ^1H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.50 (s, 1H), 7.97-7.44 (m, 7H), 6.52 (s, 1H), 2.22-1.76 (m, 15H); ^{13}C {^1H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 189.8, 152.7, 146.0, 138.5, 137.9, 137.4, 137.0, 132.7, 130.6, 129.0, 128.8, 123.2, 121.9, 89.1, 56.2, 43.0, 36.5, 29.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{26}H_{25}Cl_2N_2O$ 451.1338; Found 451.1345.

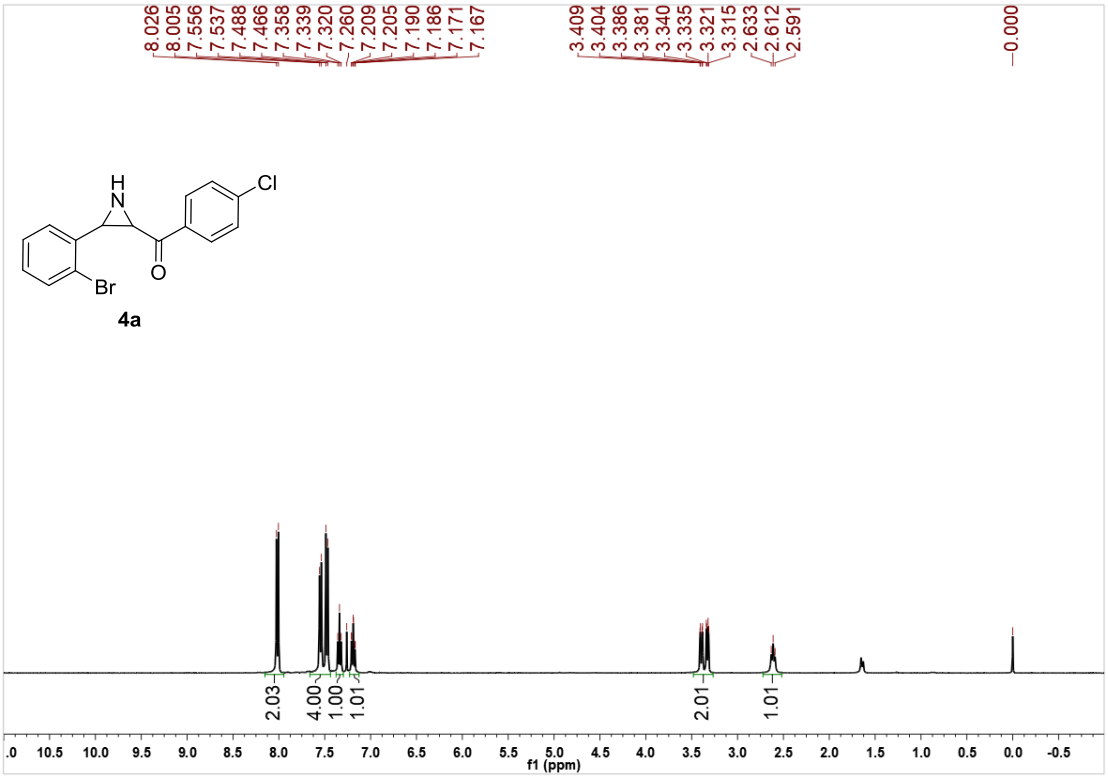
2-((1Z,3Z)-6-Chloro-3-((2,4,4-trimethylpentan-2-yl)imino)isoindolin-1-ylidene)-1-phenylethan-1-one (6p):

Light yellow solid, yield: 0.122g (62%), ethylacetate/petroleum ether = 1: 25, mp 110–111 ℃. ^1H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.45 (s, 1H), 8.04-7.45 (m, 8H), 6.61 (s, 1H), 1.81 (s, 2H), 1.58 (s, 6H), 1.04 (s, 9H); ^{13}C {^1H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 191.2, 152.1, 145.8, 139.0, 136.5, 136.3, 133.7, 132.3, 131.7, 128.6, 127.6, 124.1, 120.9, 89.5, 59.0, 56.5, 32.2, 31.8, 30.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{28}ClN_2O$ 395.1885; Found 395.1892.

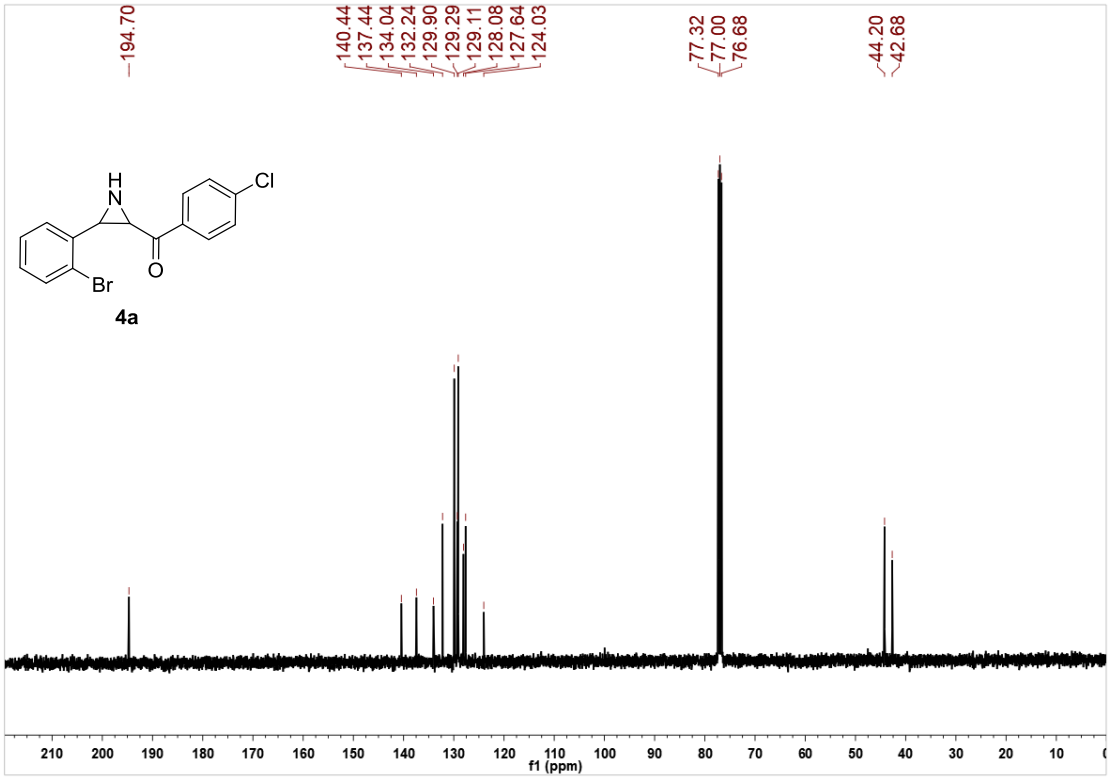
2-((1Z,3Z)-6-Chloro-3-((2,4,4-trimethylpentan-2-yl)imino)isoindolin-1-ylidene)-1-(4-chlorophenyl)ethan-1-one (6q):

Light yellow solid, yield: 0.139g (65%), ethylacetate/petroleum ether = 1: 25, mp 130–132 ℃. ^1H NMR ($CDCl_3$, 400 MHz) δ (ppm) 11.43 (s, 1H), 7.98-7.45 (m, 7H), 6.54 (s, 1H), 1.80 (s, 2H), 1.57 (s, 6H), 1.03 (s, 9H); ^{13}C {^1H} NMR ($CDCl_3$, 100 MHz) δ (ppm) 189.7, 152.5, 145.5, 138.6, 137.3, 136.5, 136.1, 133.7, 131.8, 129.0, 128.9, 124.1, 121.0, 89.0, 59.1, 56.6, 32.2, 31.8, 30.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{27}Cl_2N_2O$ 429.1495; Found 429.1499.

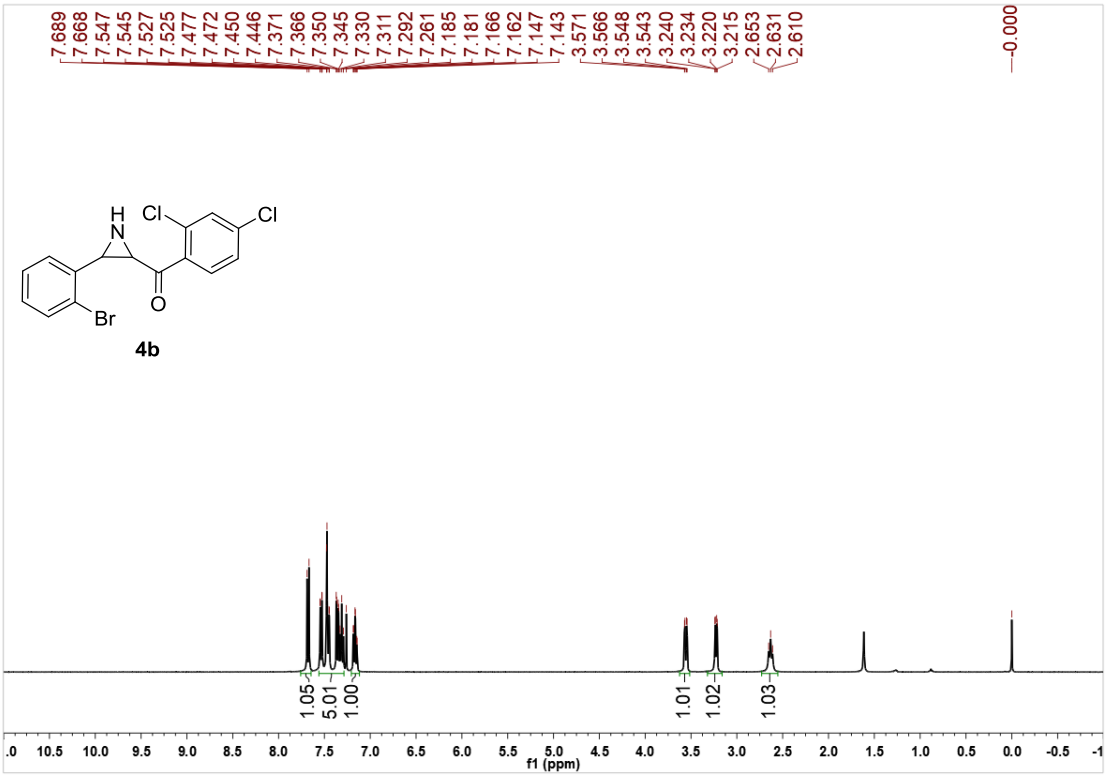
5. Copies of ^{1}H and ^{13}C NMR Spectrum



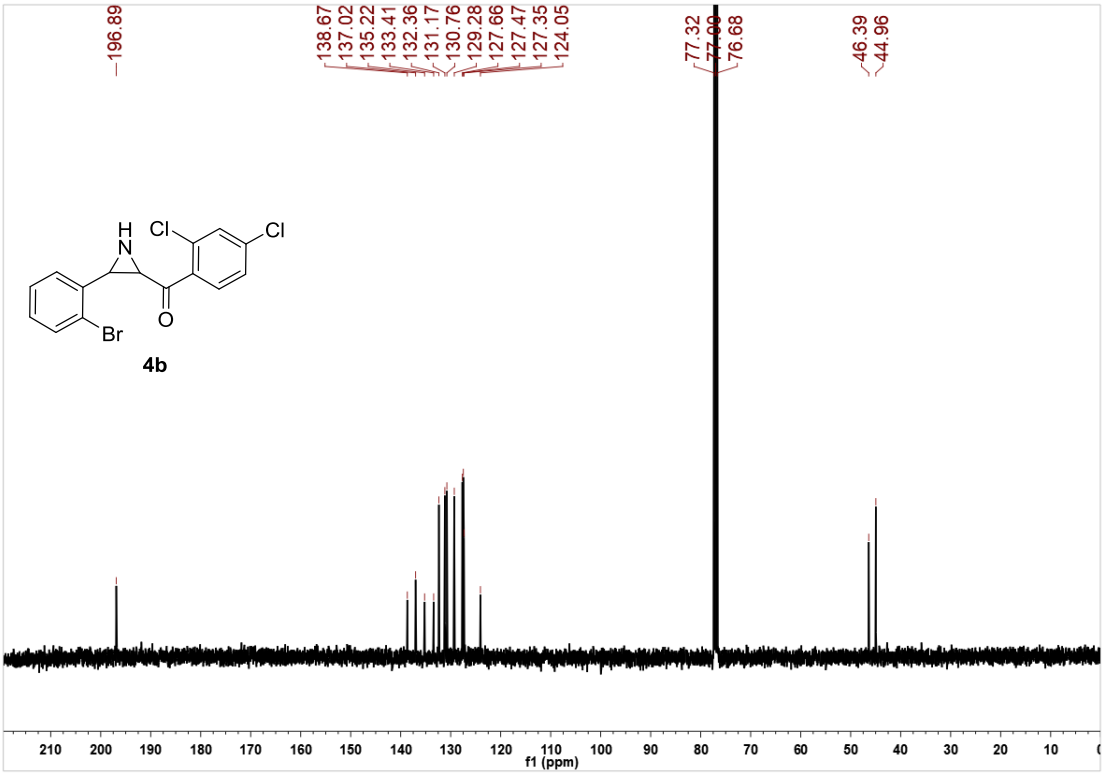
^{1}H NMR (400 MHz), $CDCl_3$



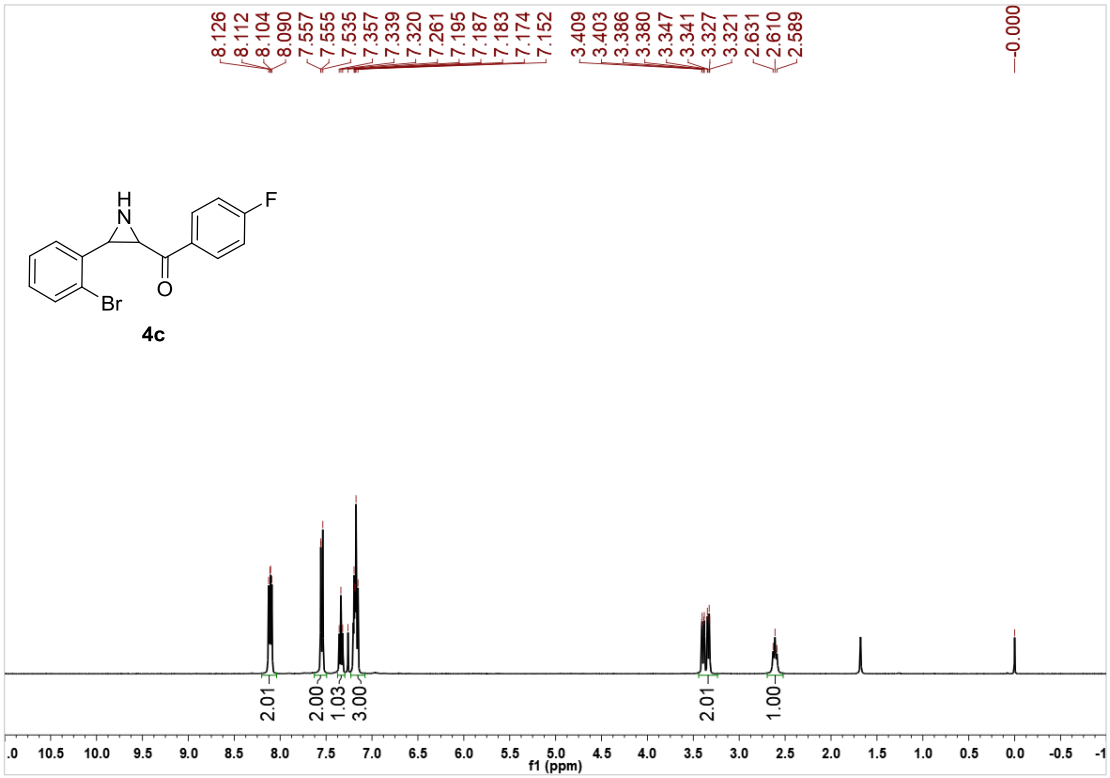
^{13}C NMR (100 MHz), $CDCl_3$



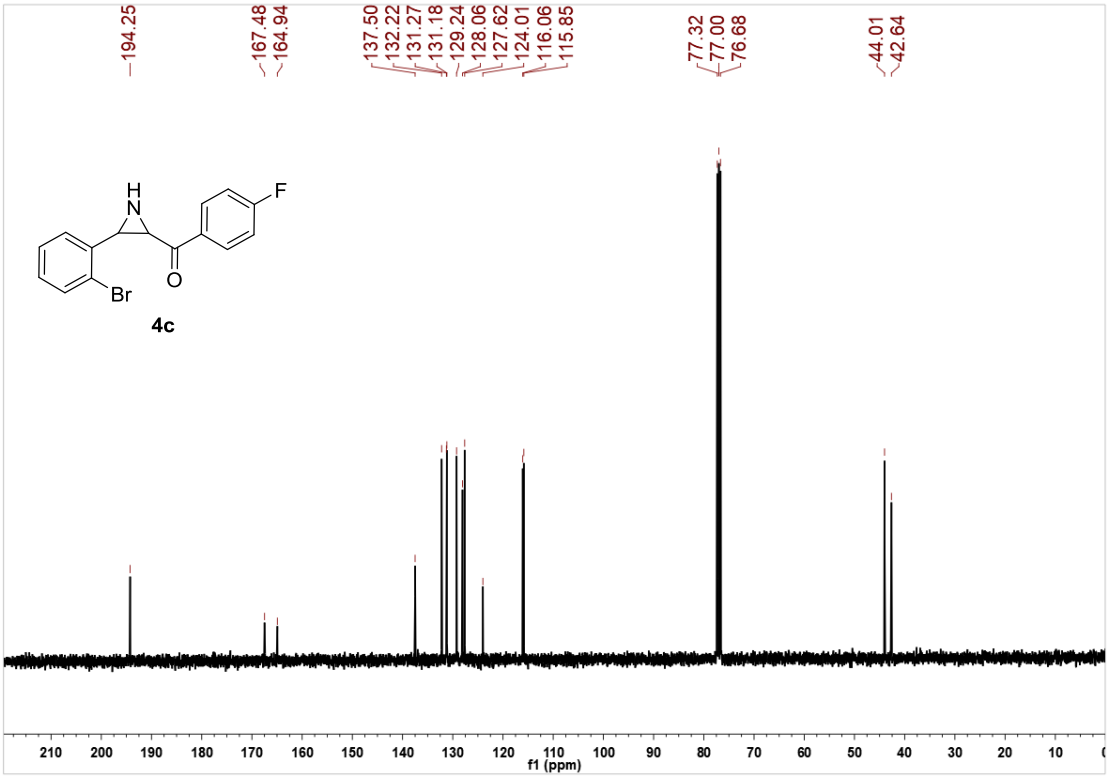
^{1}H NMR (400 MHz), $CDCl_3$



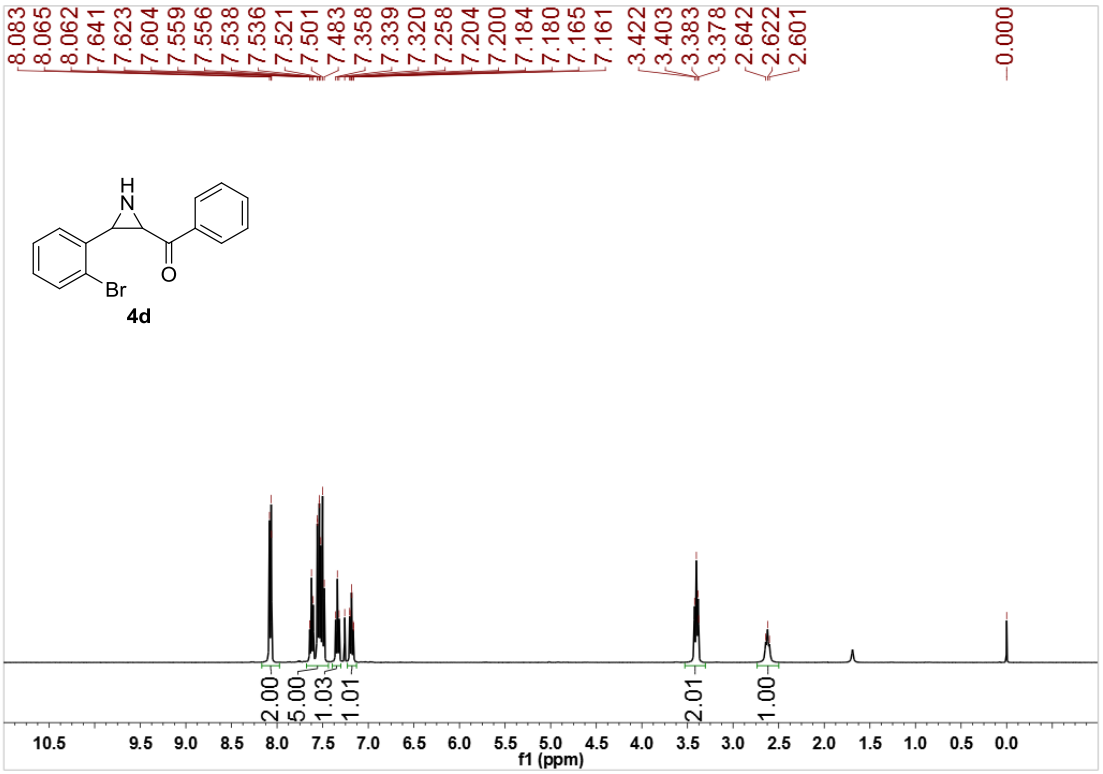
^{13}C NMR (100 MHz), $CDCl_3$



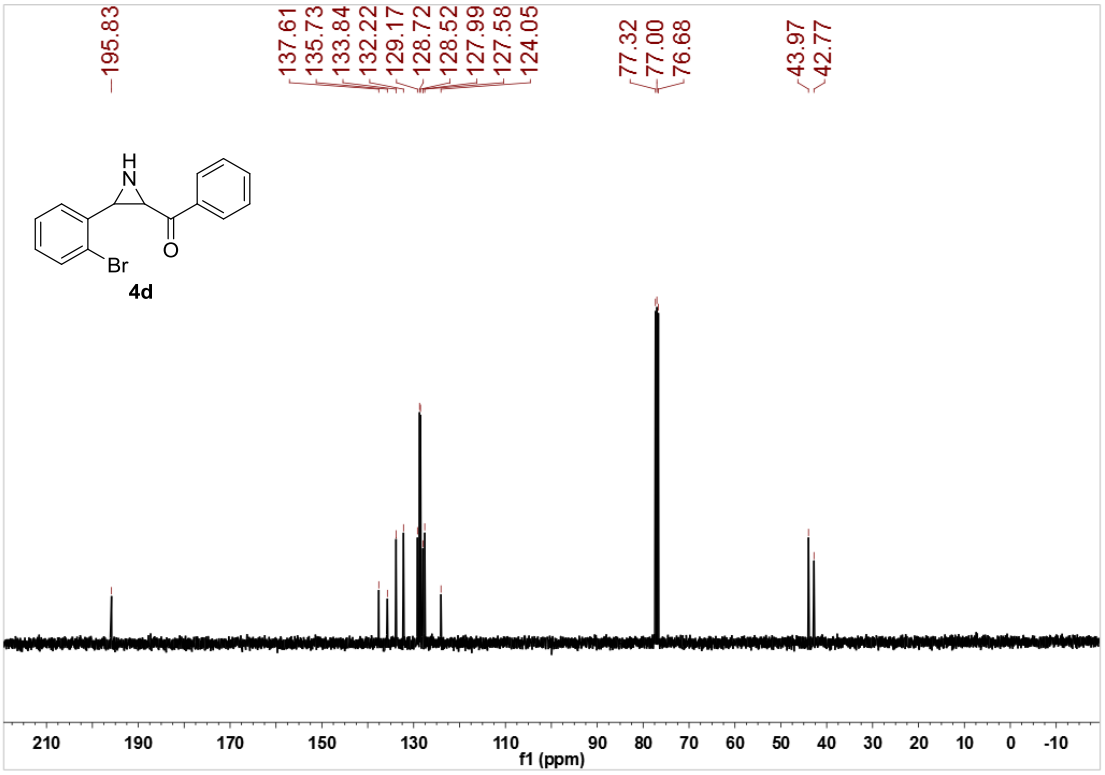
^{1}H NMR (400 MHz), $CDCl_3$



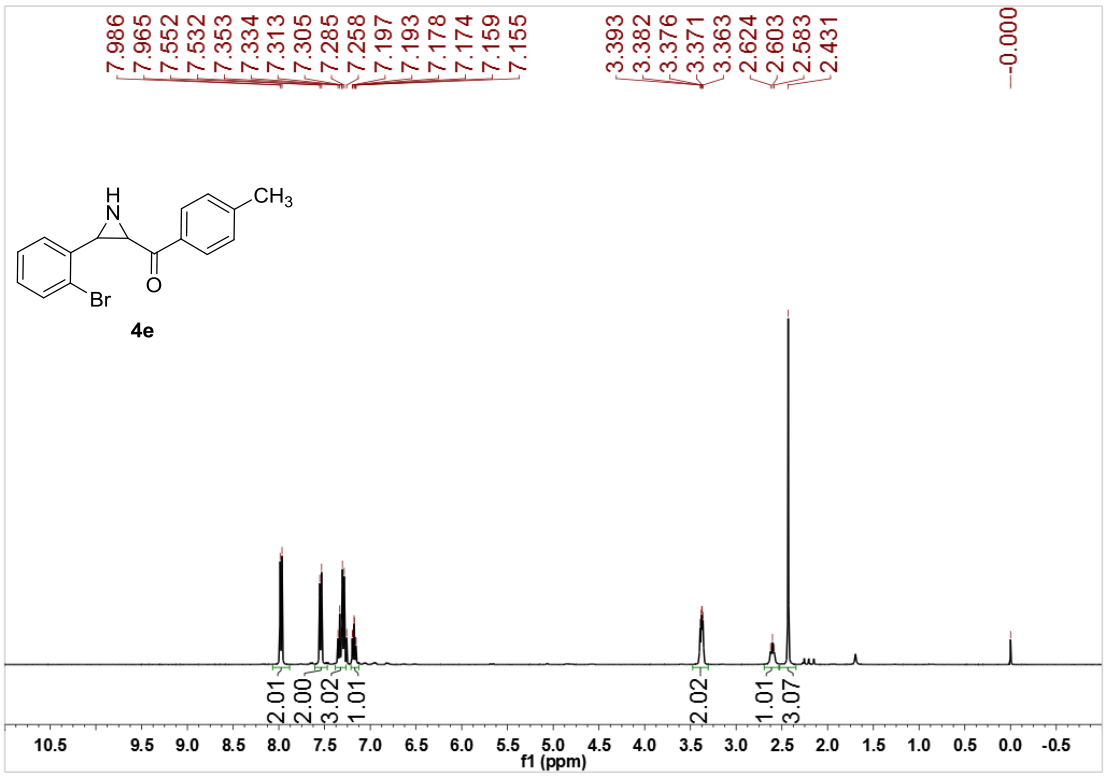
^{13}C NMR (100 MHz), $CDCl_3$



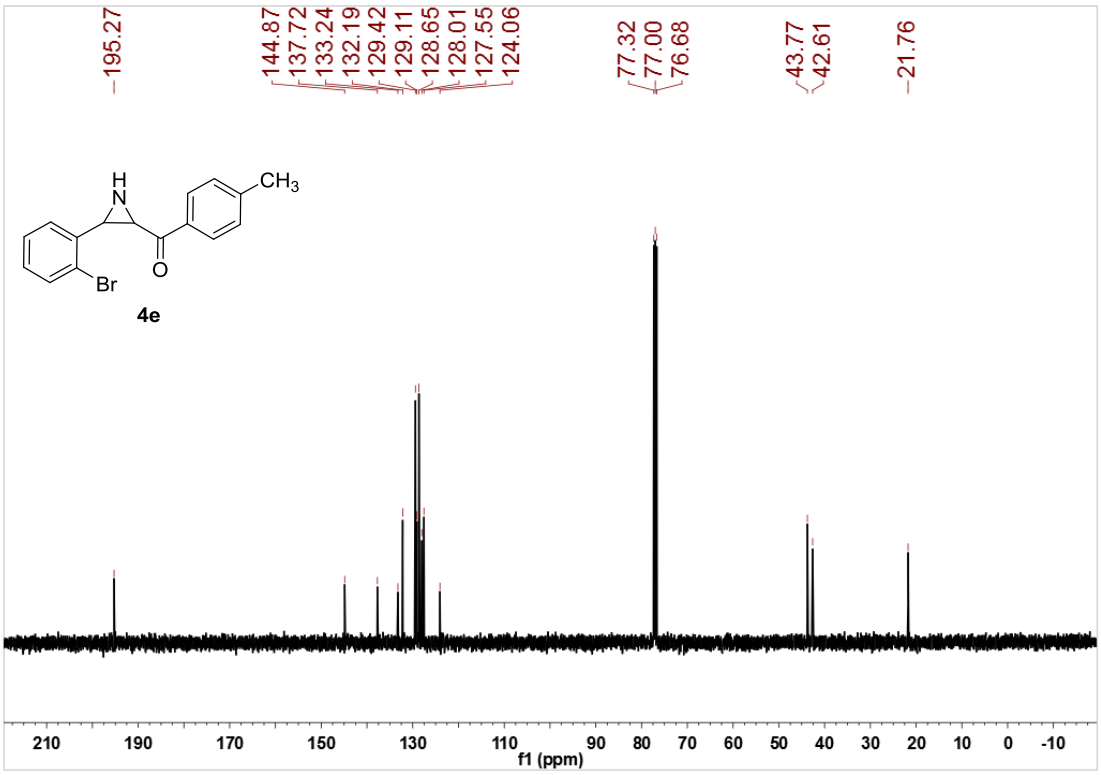
^{1}H NMR (400 MHz), $CDCl_3$



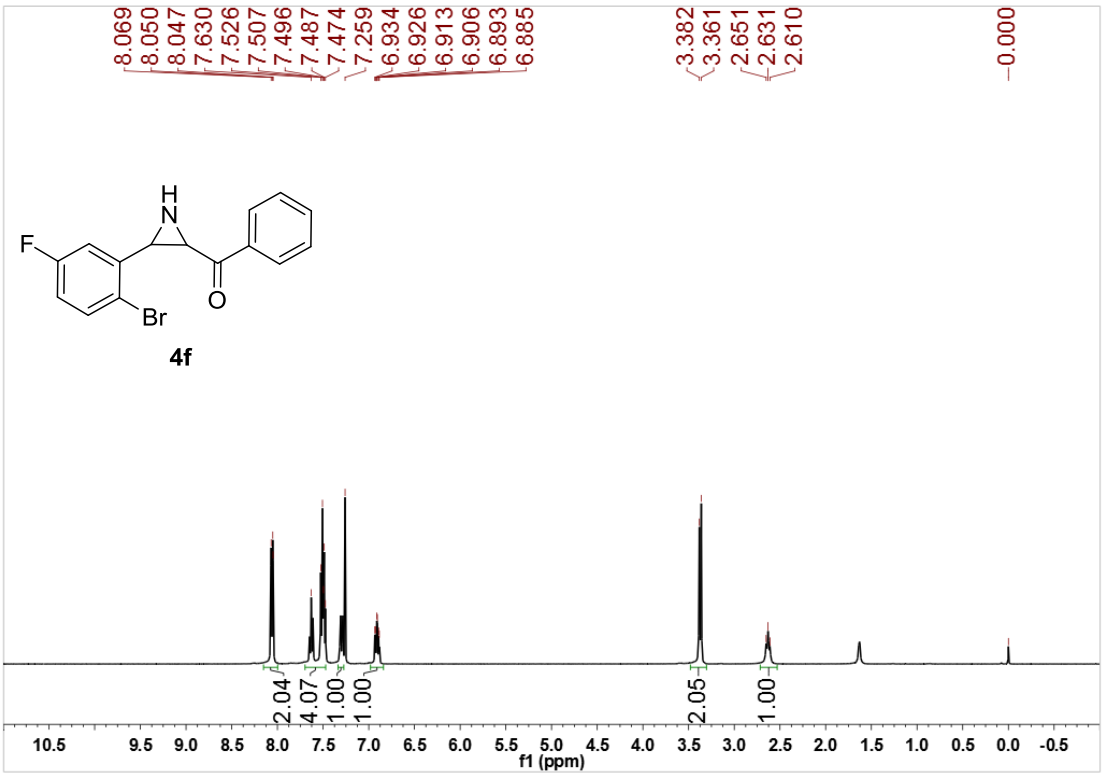
^{13}C NMR (100 MHz), $CDCl_3$



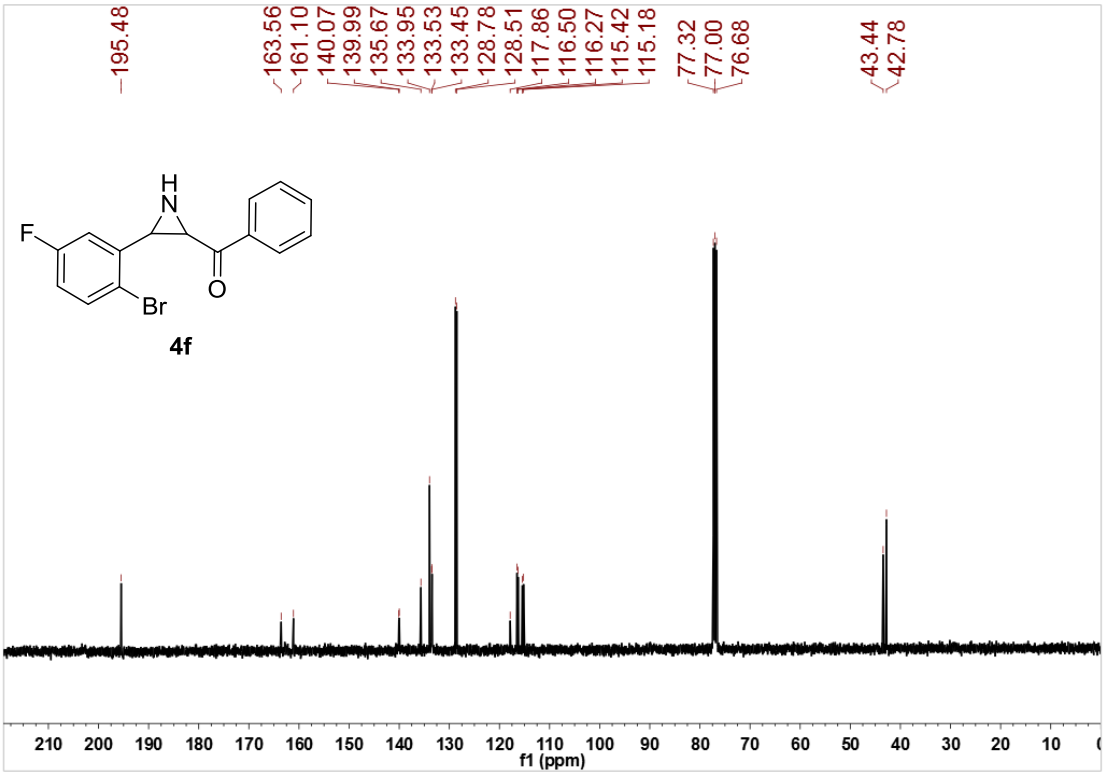
^{1}H NMR (400 MHz), $CDCl_3$



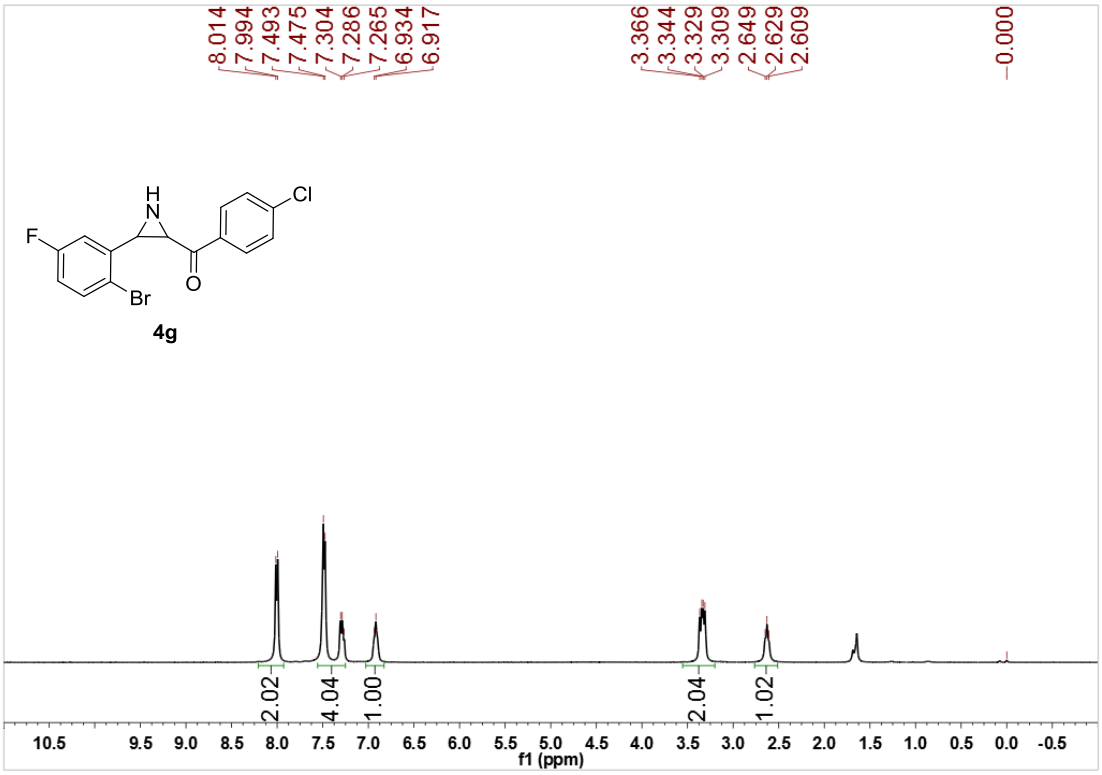
^{13}C NMR (100 MHz), $CDCl_3$



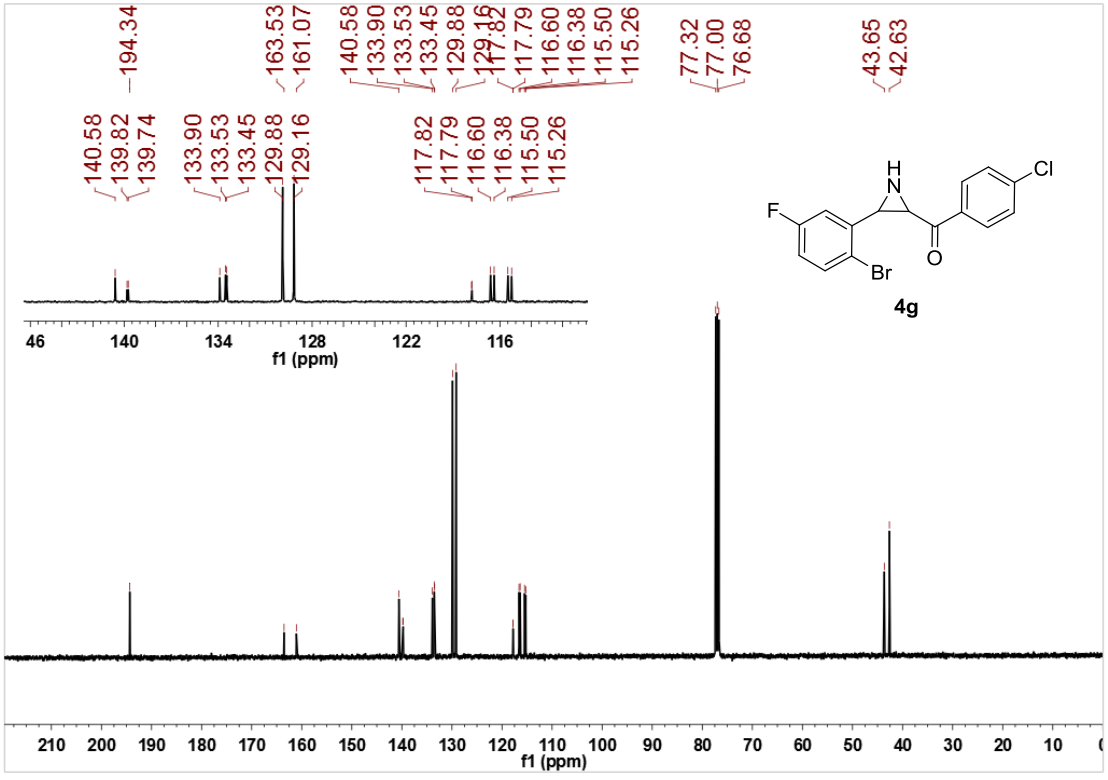
^{1}H NMR (400 MHz), $CDCl_3$



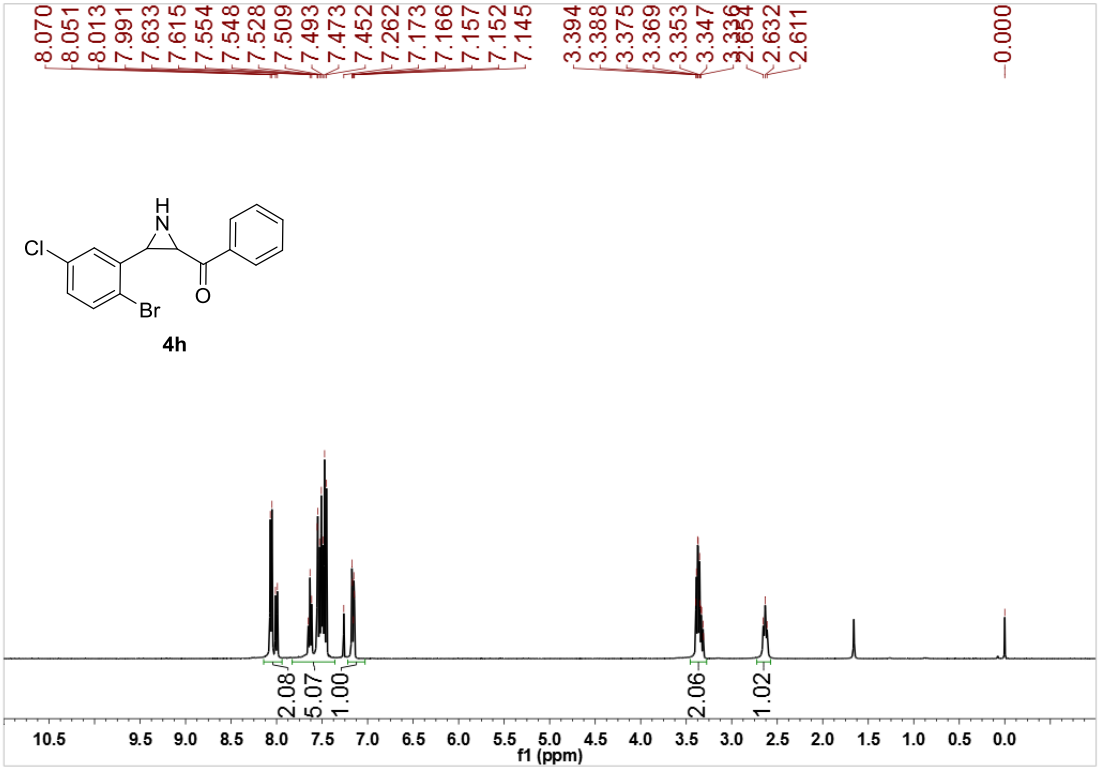
^{13}C NMR (100 MHz), $CDCl_3$



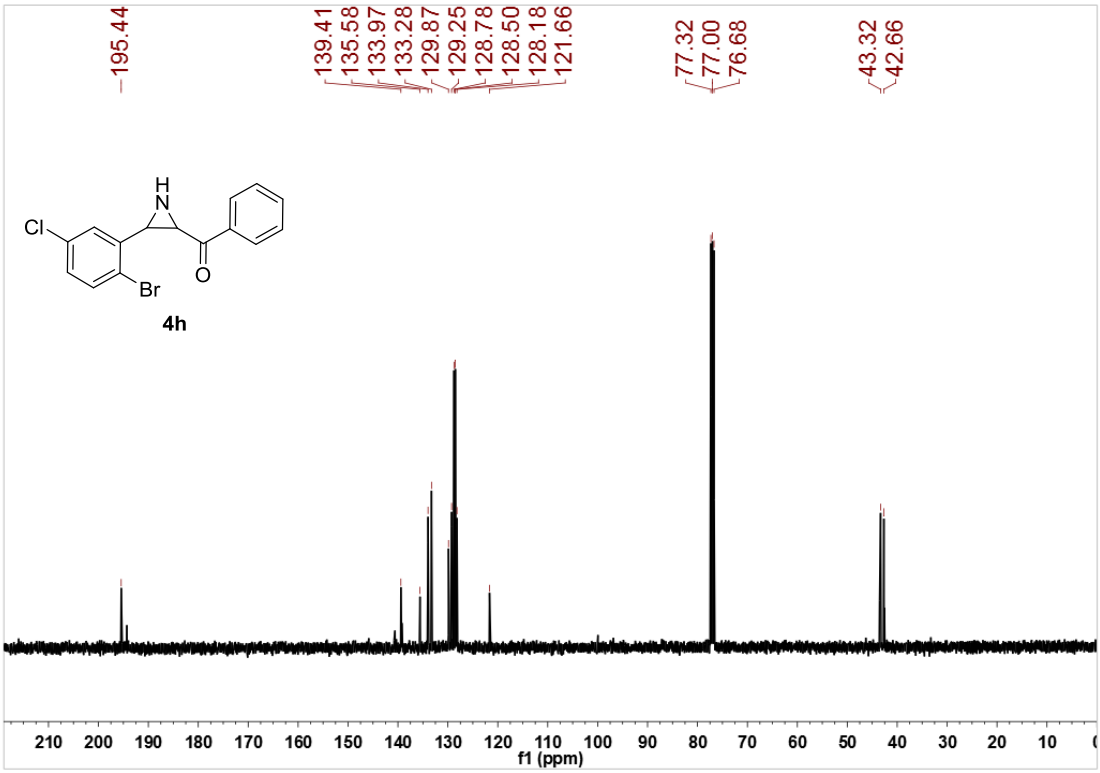
^{1}H NMR (400 MHz), $CDCl_3$



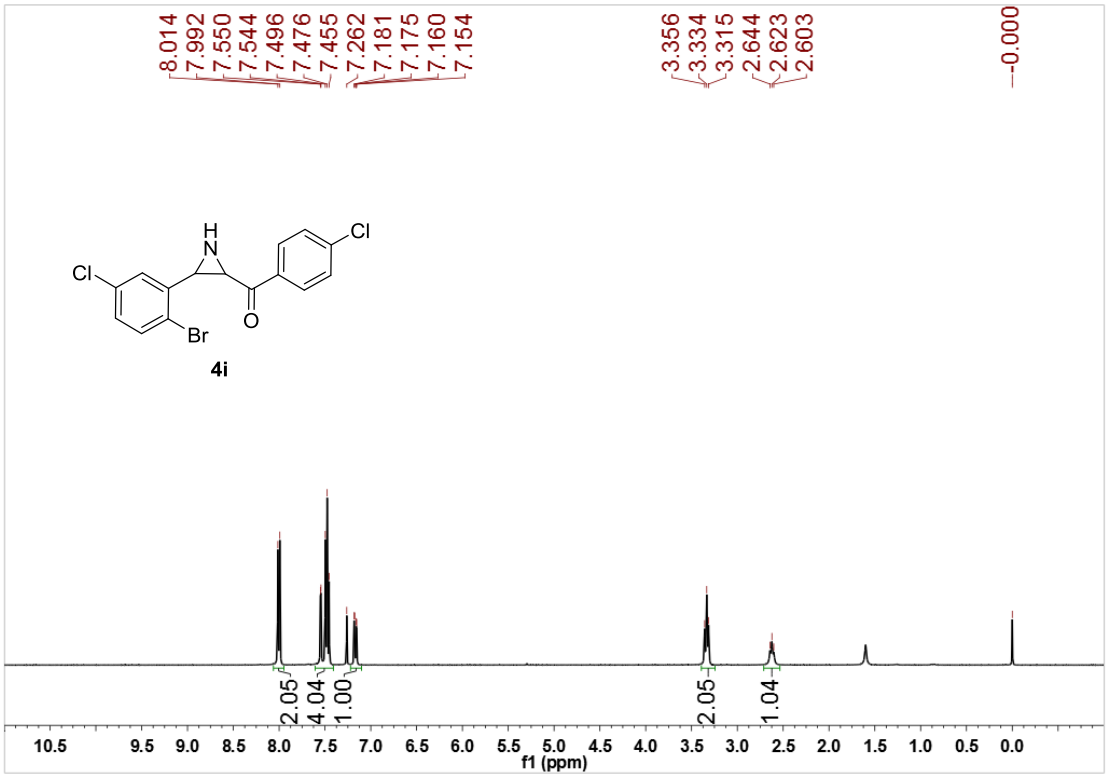
^{13}C NMR (100 MHz), $CDCl_3$



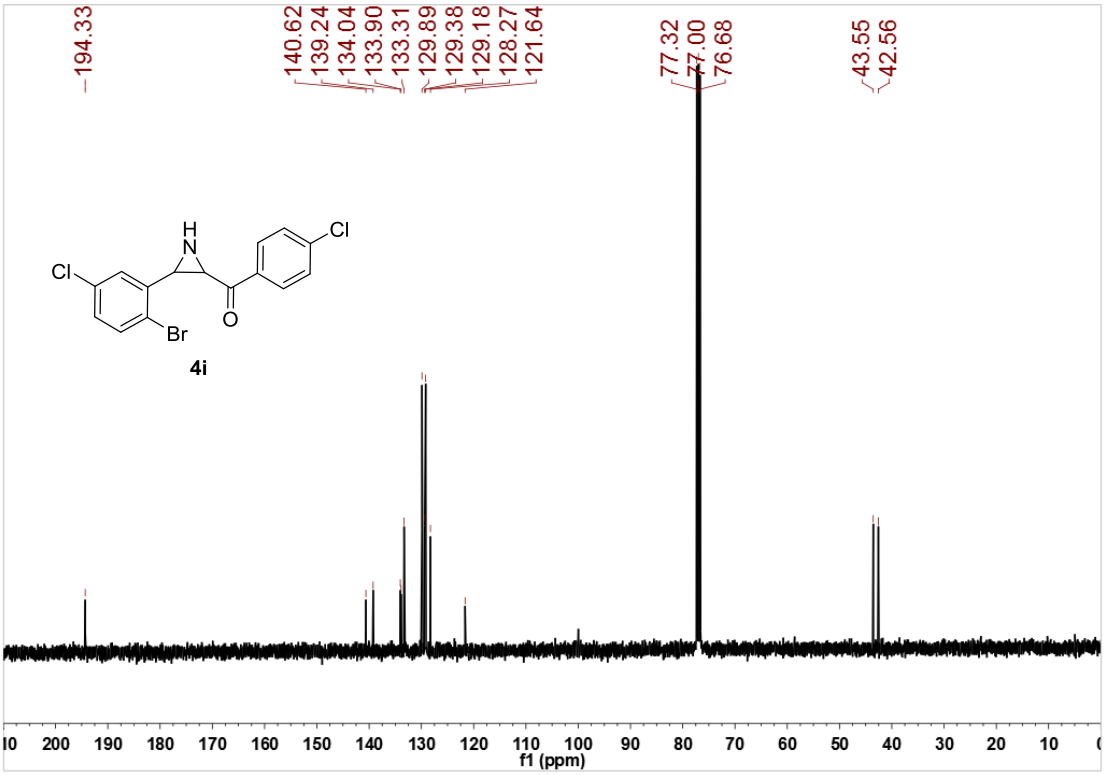
^{1}H NMR (400 MHz), $CDCl_3$



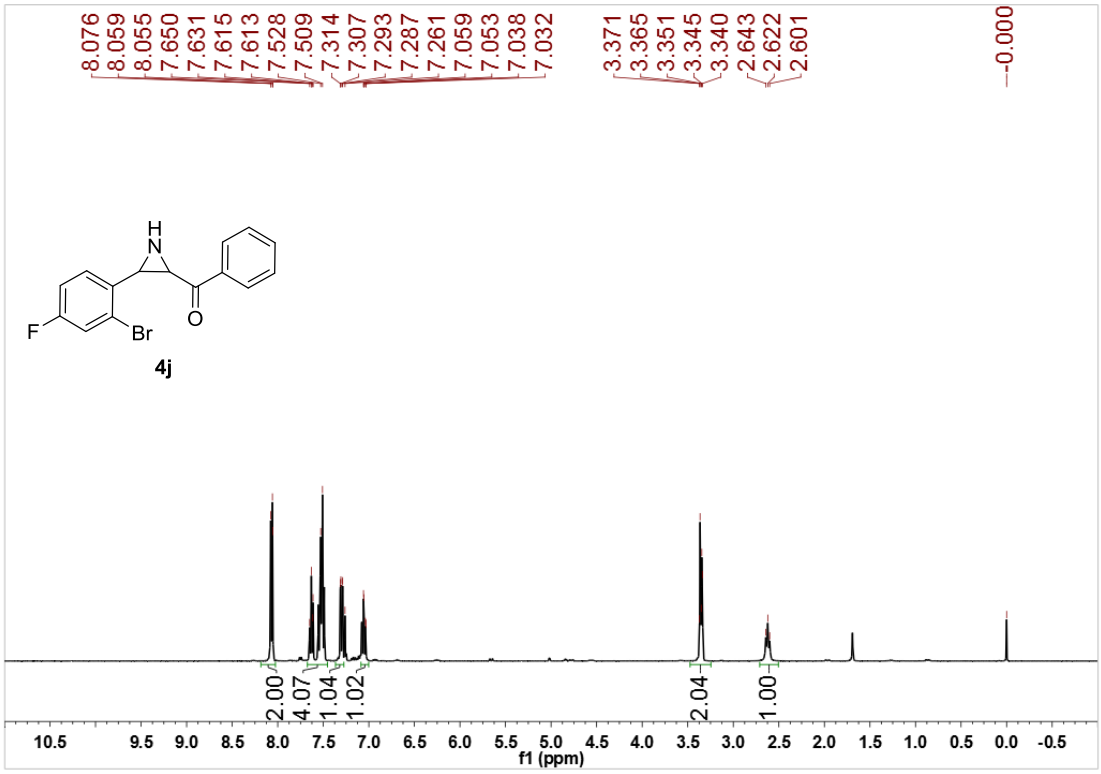
^{13}C NMR (100 MHz), $CDCl_3$



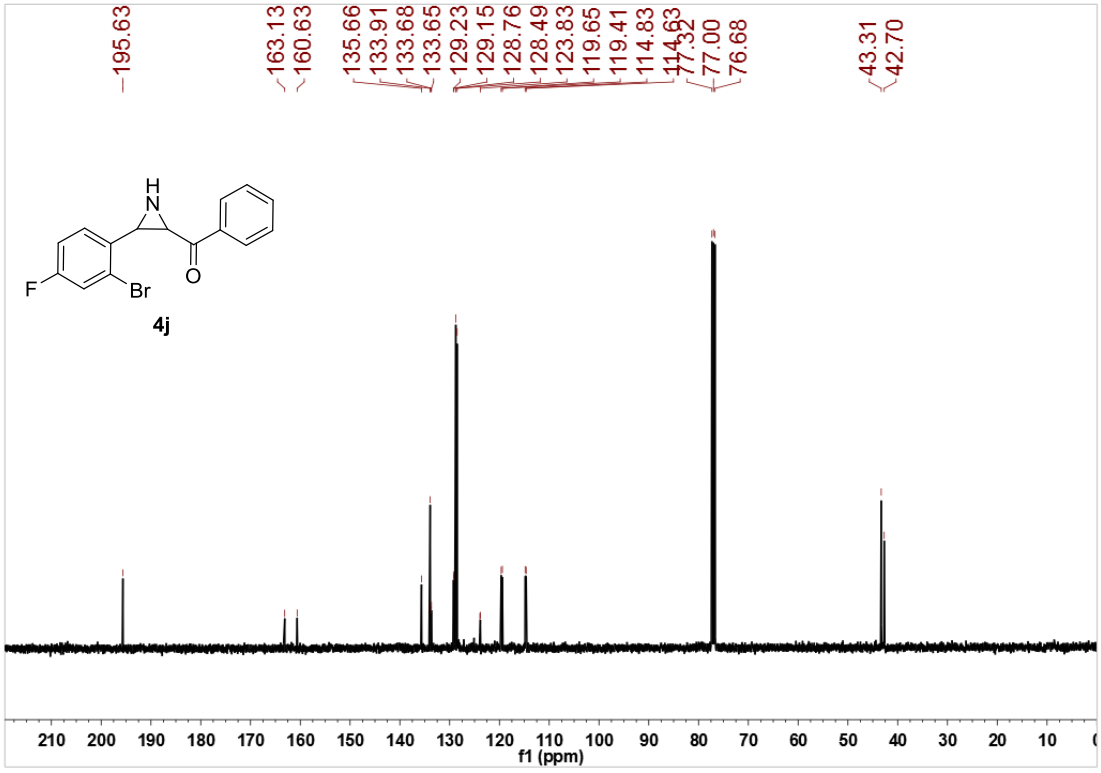
^{1}H NMR (400 MHz), $CDCl_3$



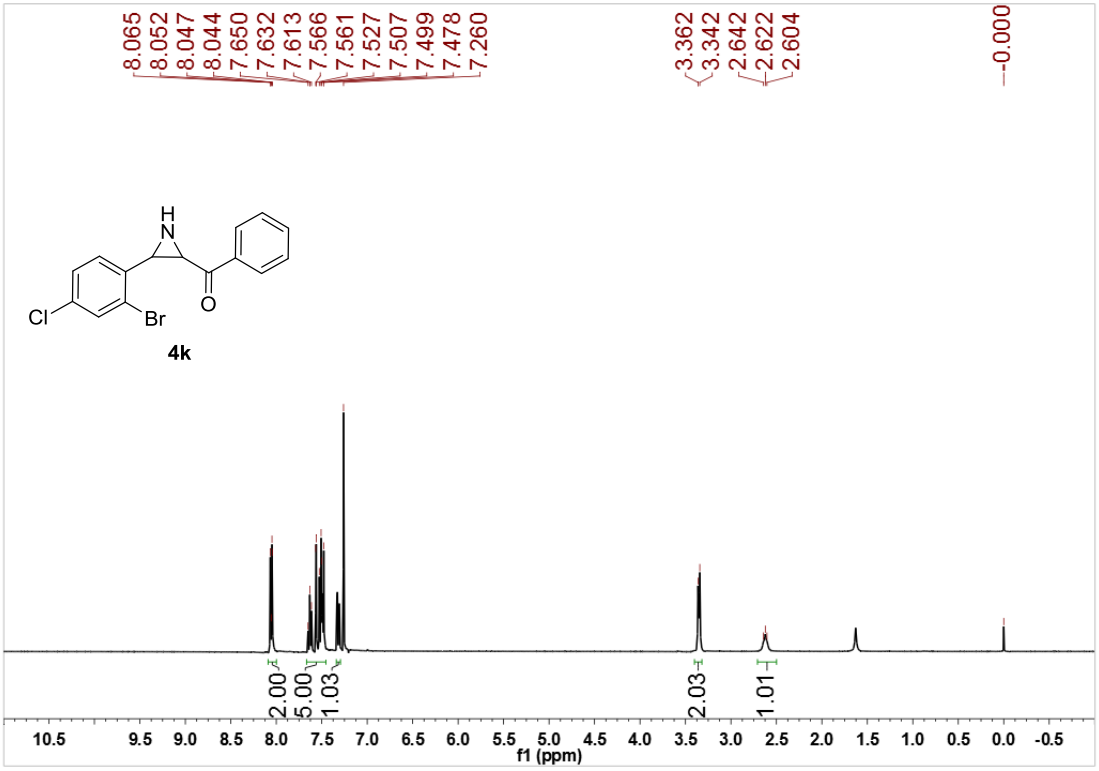
^{13}C NMR (100 MHz), $CDCl_3$



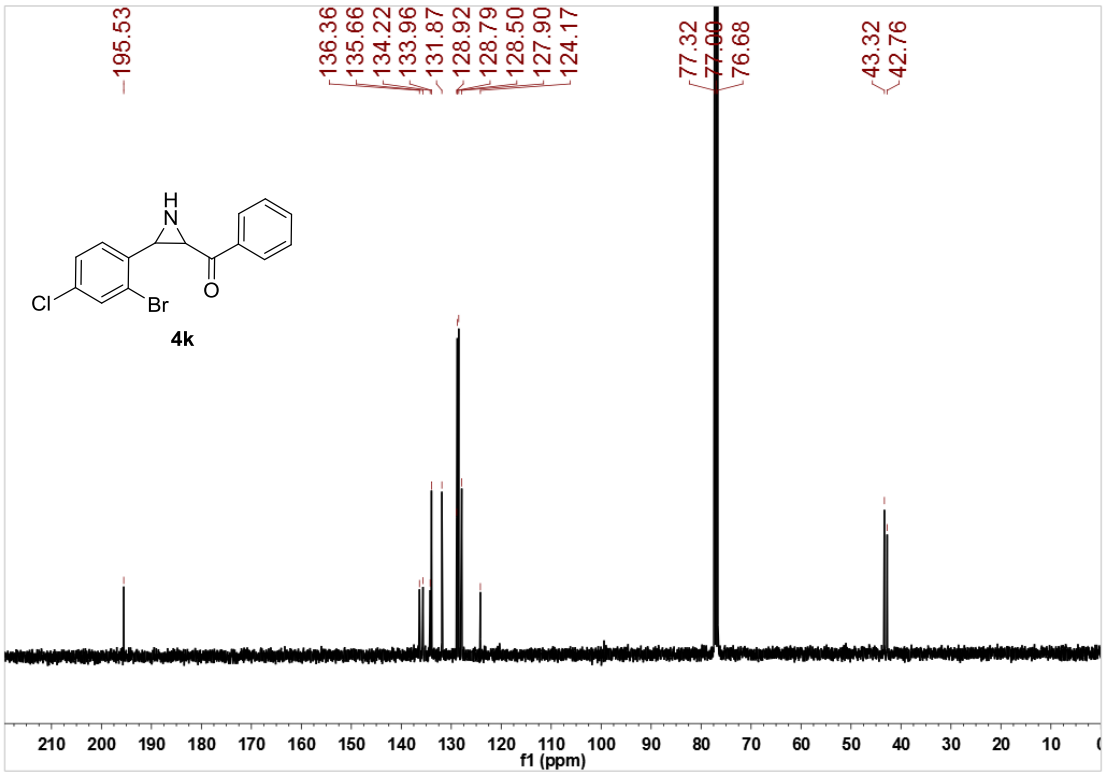
^{1}H NMR (400 MHz), $CDCl_3$



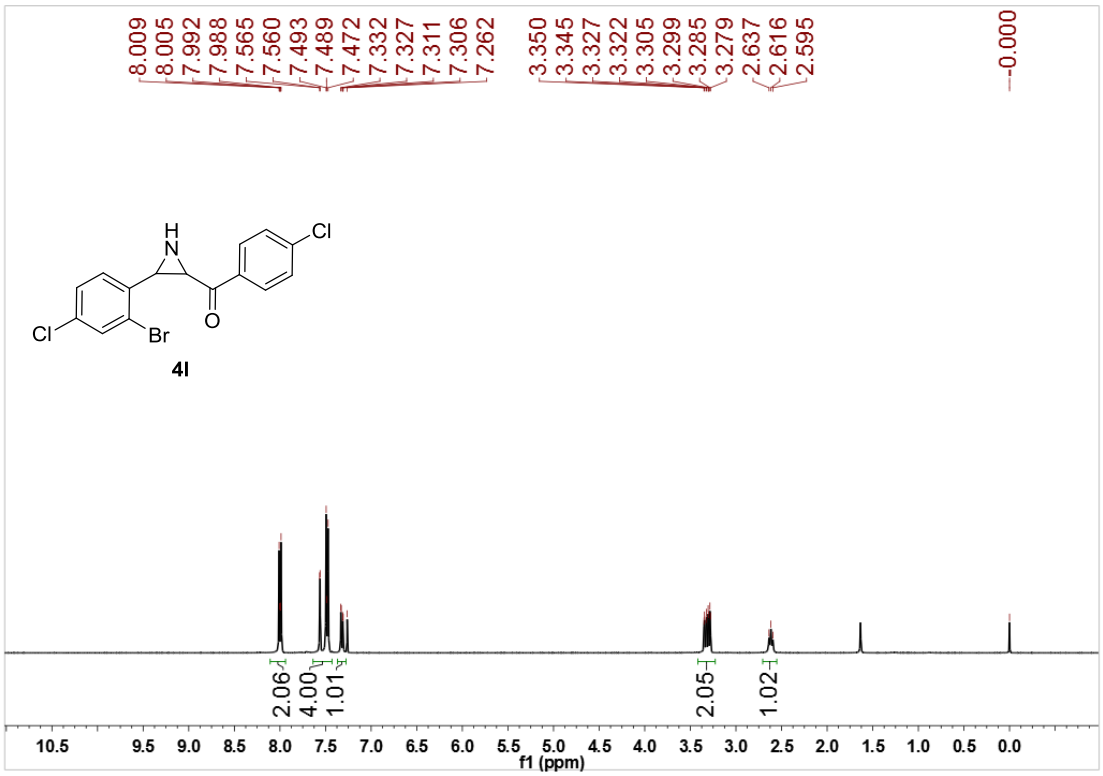
^{13}C NMR (100 MHz), $CDCl_3$



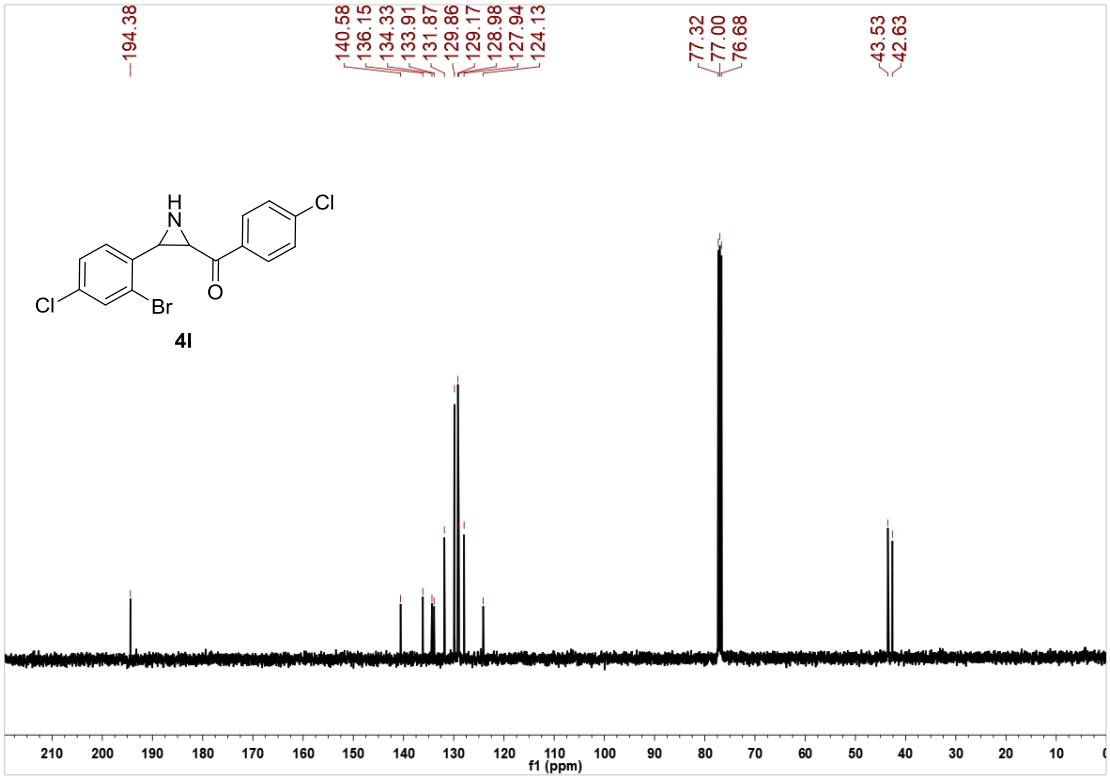
^{1}H NMR (400 MHz), $CDCl_3$



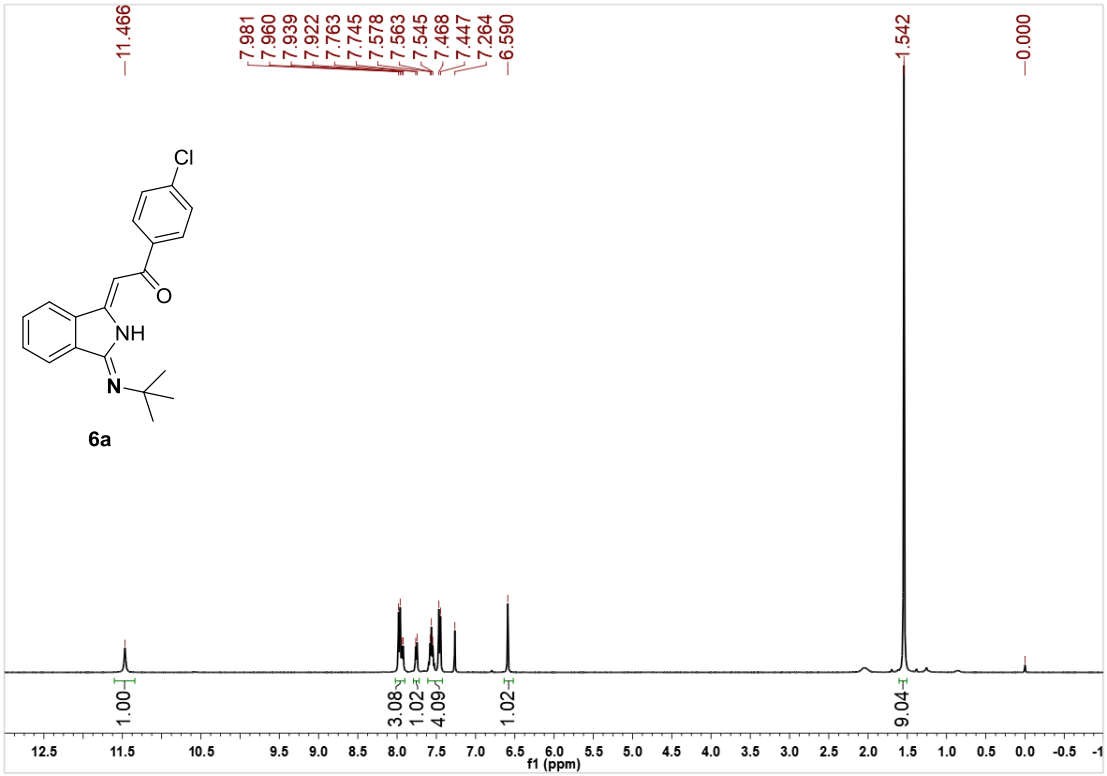
^{13}C NMR (100 MHz), $CDCl_3$



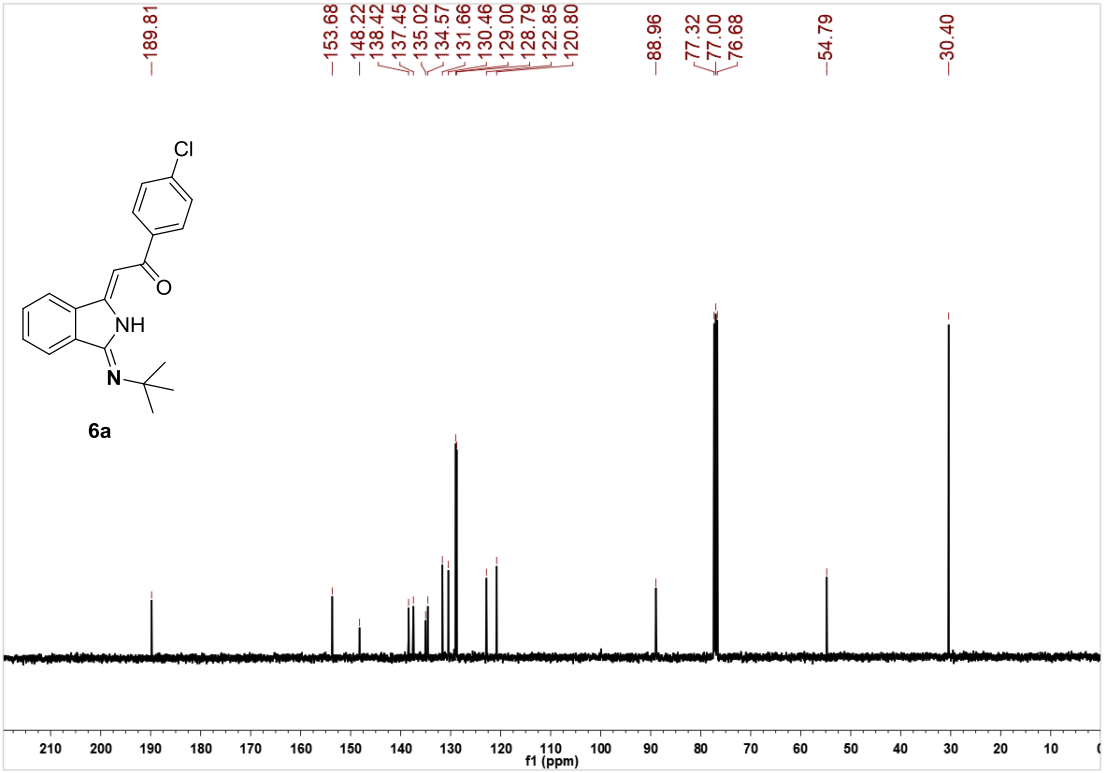
^{1}H NMR (400 MHz), $CDCl_3$



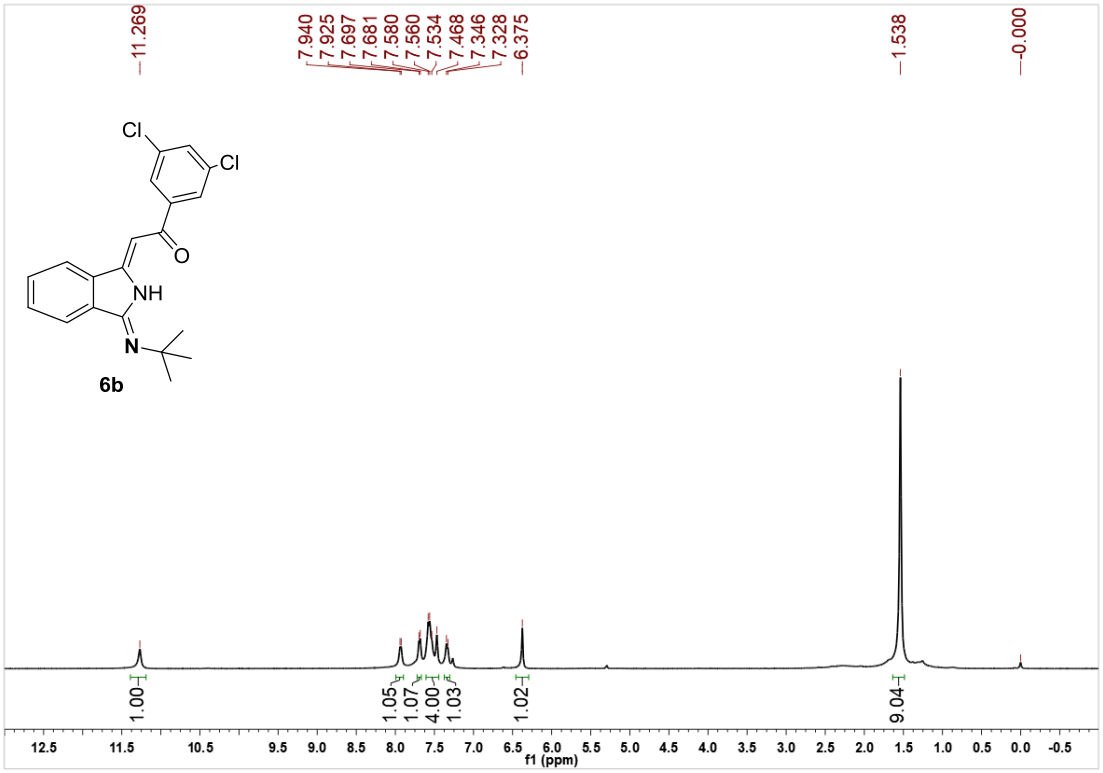
^{13}C NMR (100 MHz), $CDCl_3$



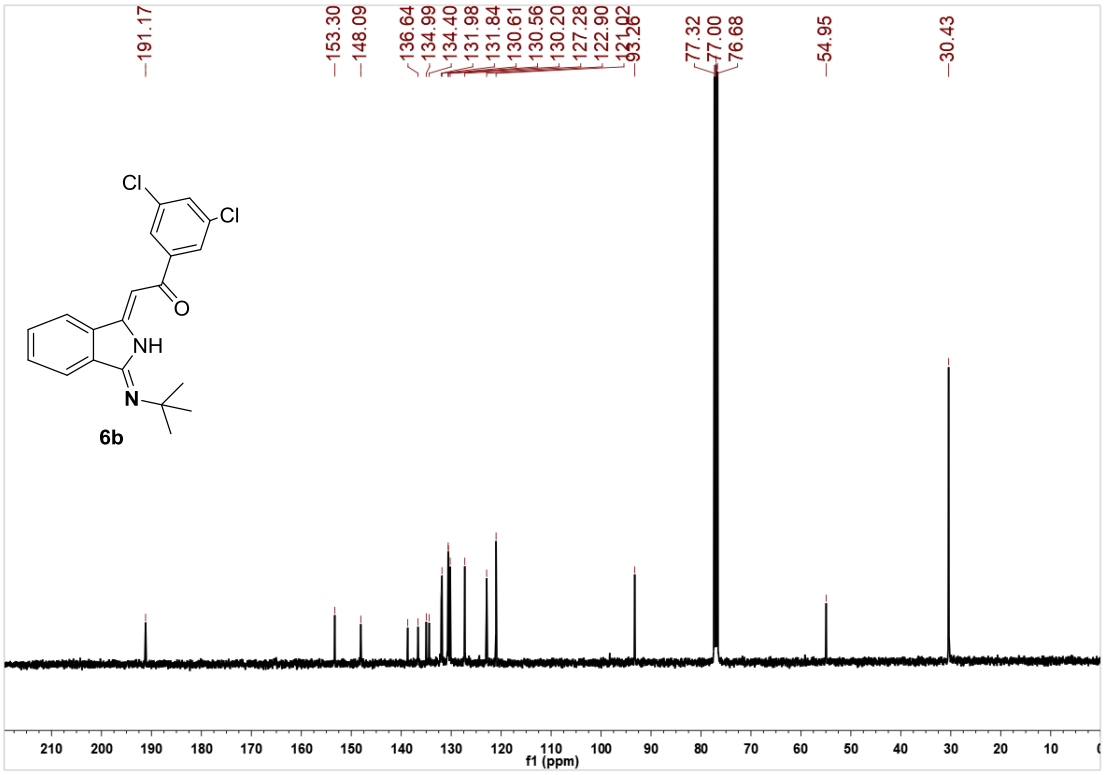
^{1}H NMR (400 MHz), $CDCl_3$



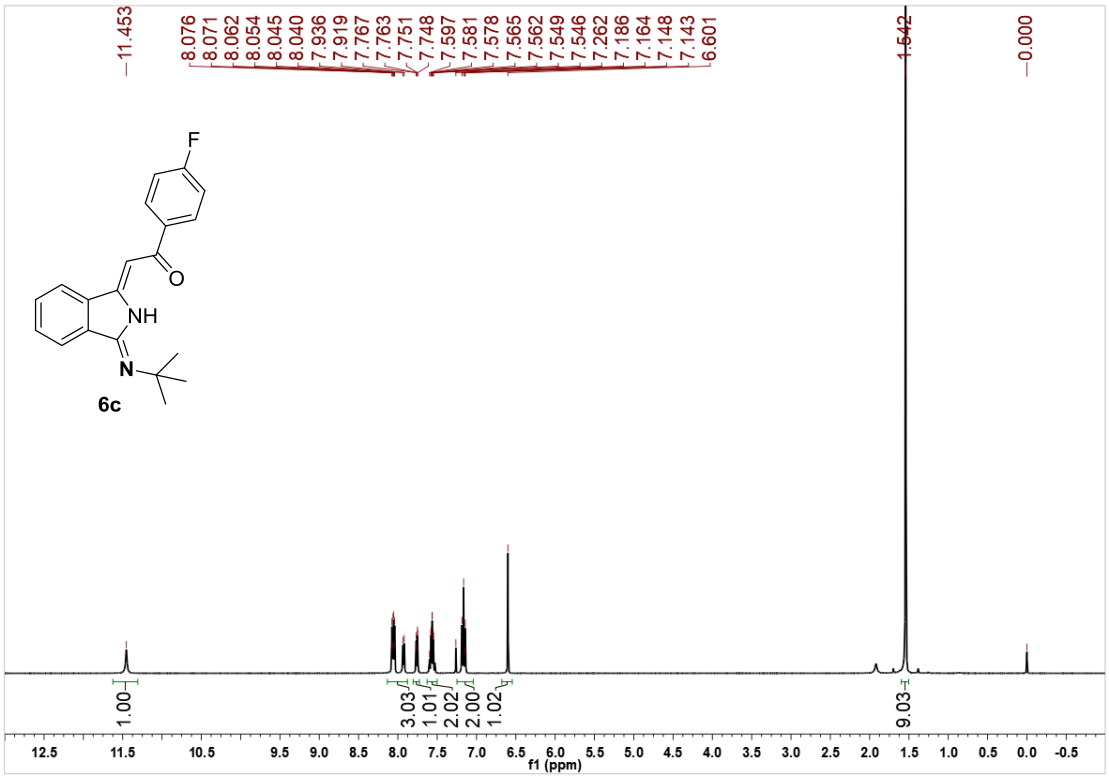
^{13}C NMR (100 MHz), $CDCl_3$



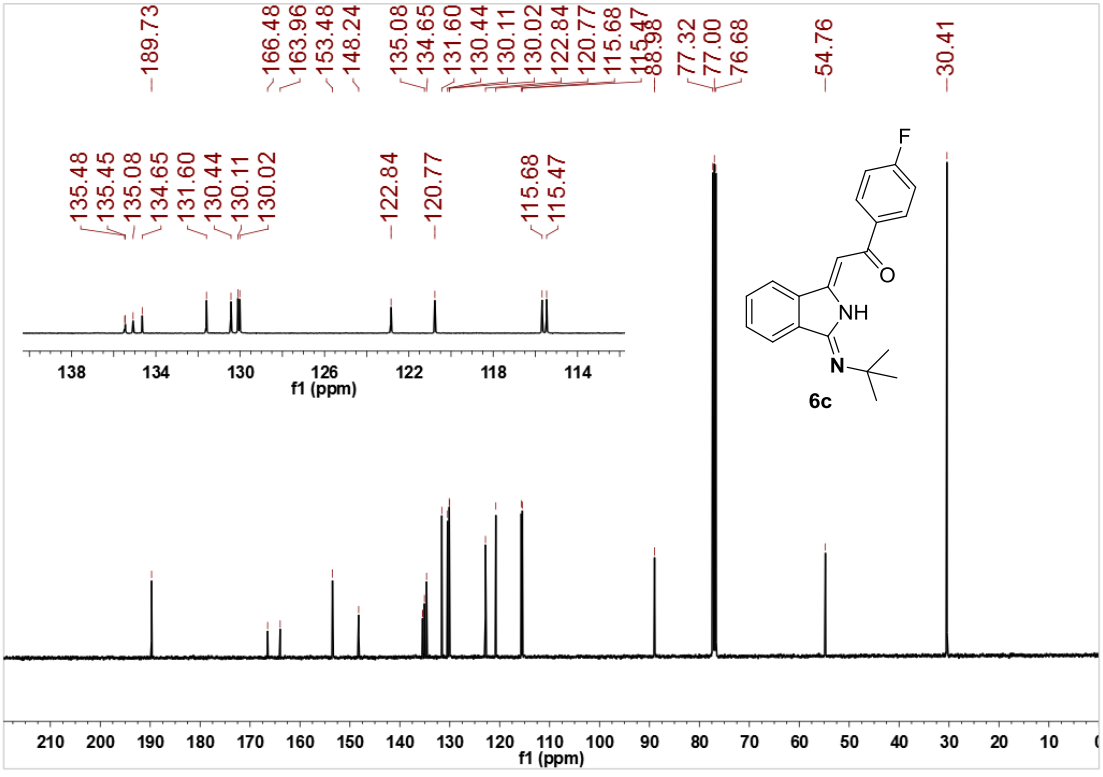
^{1}H NMR (400 MHz), $CDCl_3$



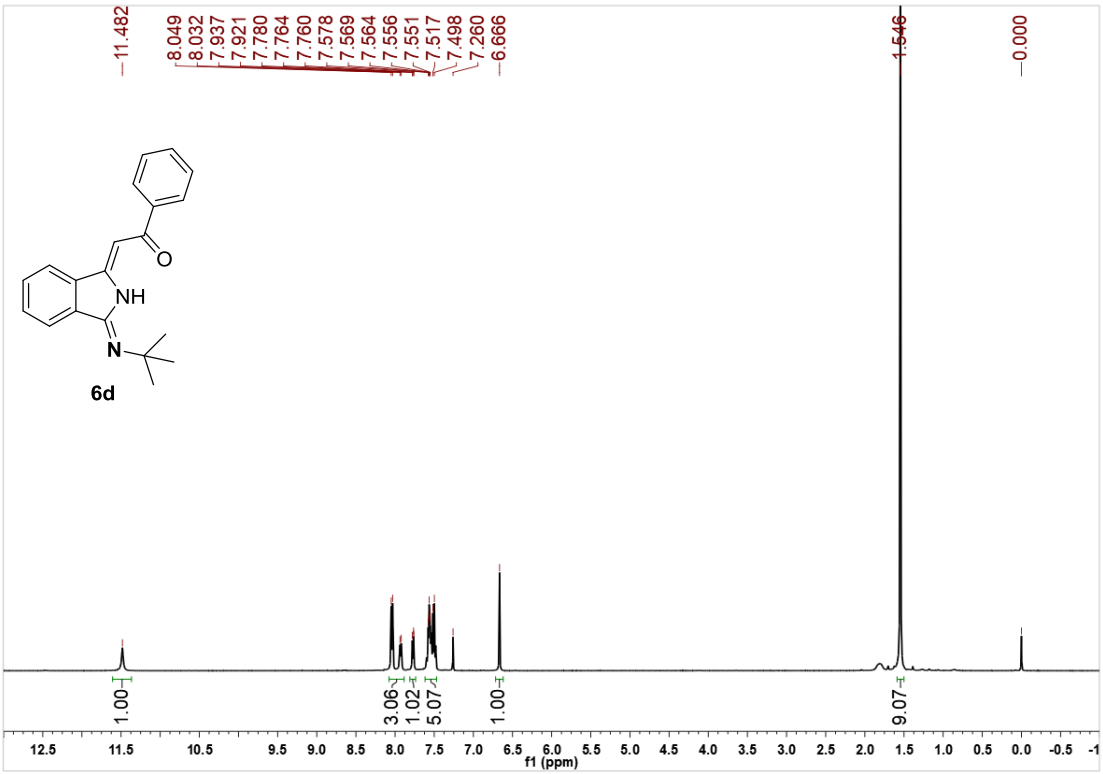
^{13}C NMR (100 MHz), $CDCl_3$



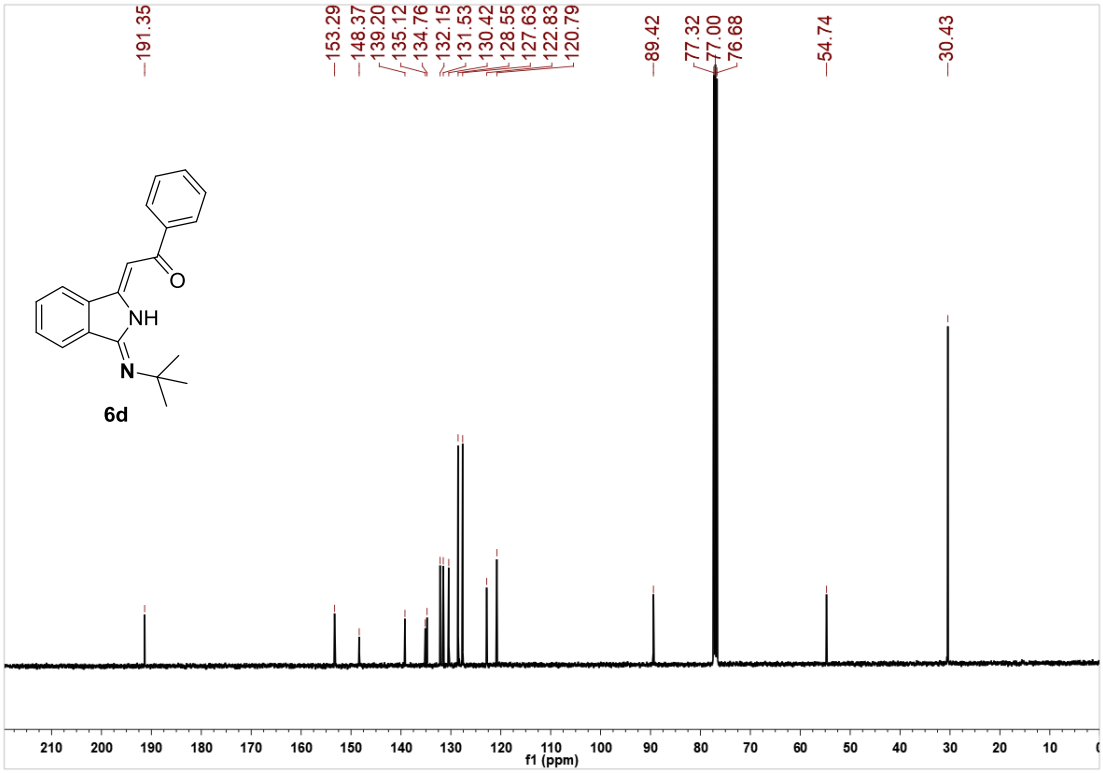
^{1}H NMR (400 MHz), $CDCl_3$



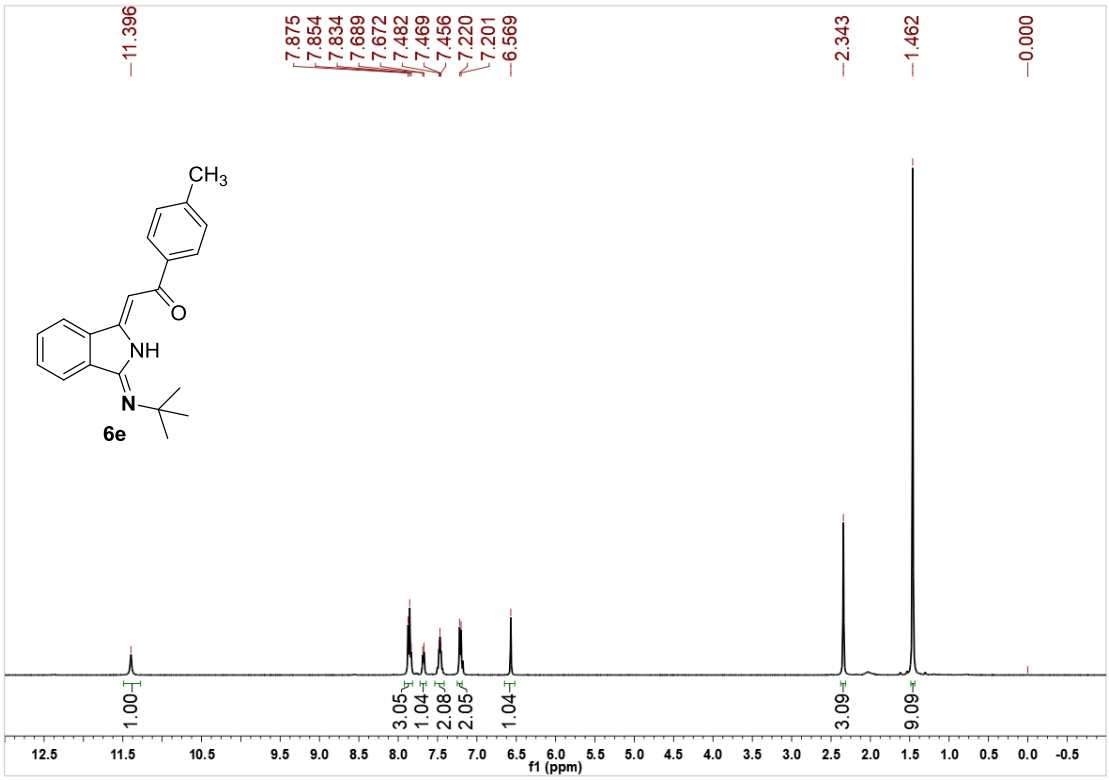
^{13}C NMR (100 MHz), $CDCl_3$



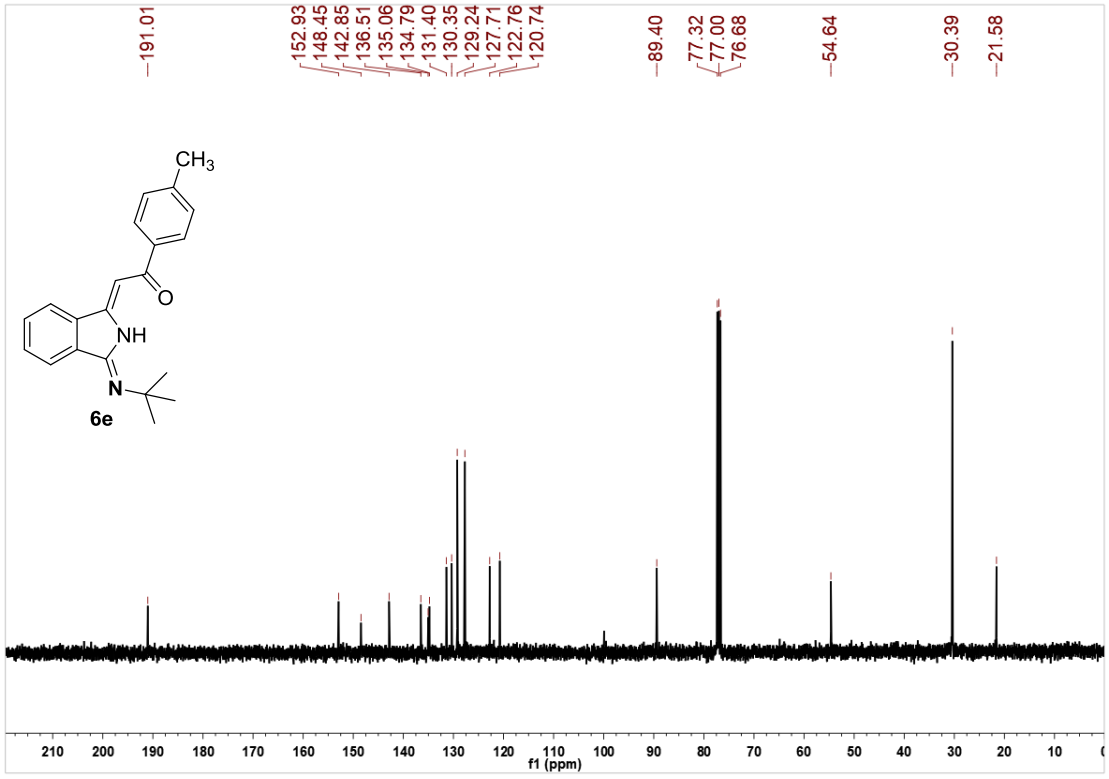
^{1}H NMR (400 MHz), $CDCl_3$



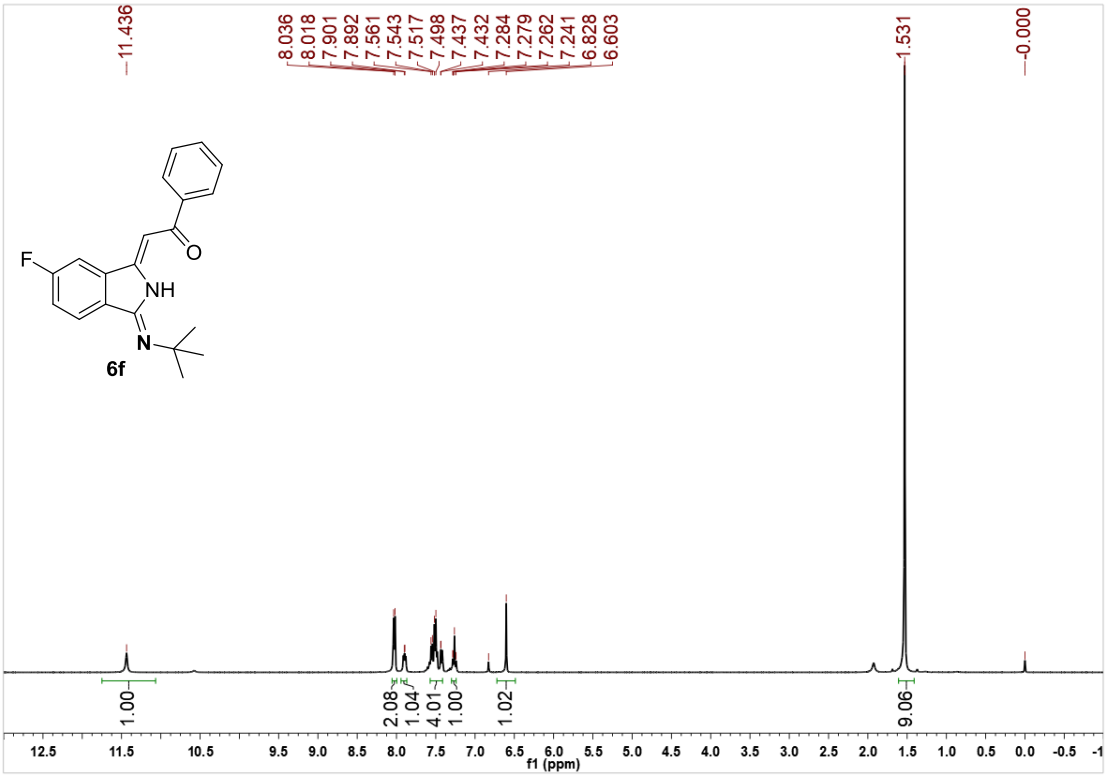
^{13}C NMR (100 MHz), $CDCl_3$



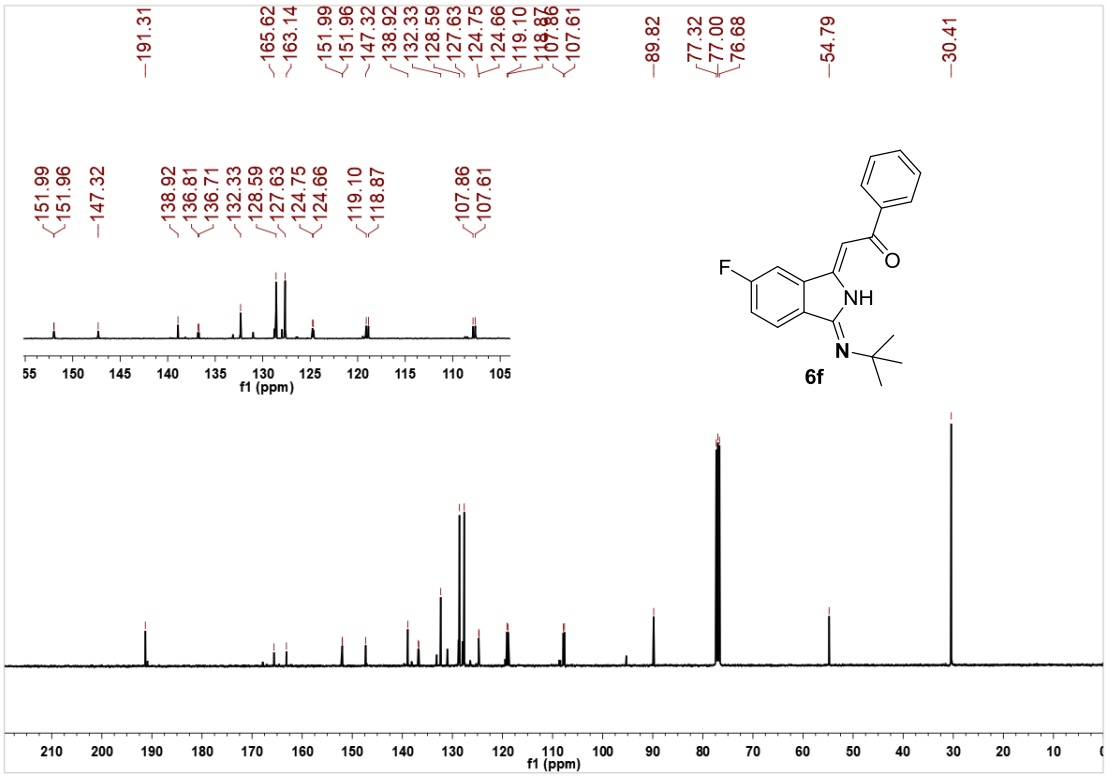
^{1}H NMR (400 MHz), $CDCl_3$



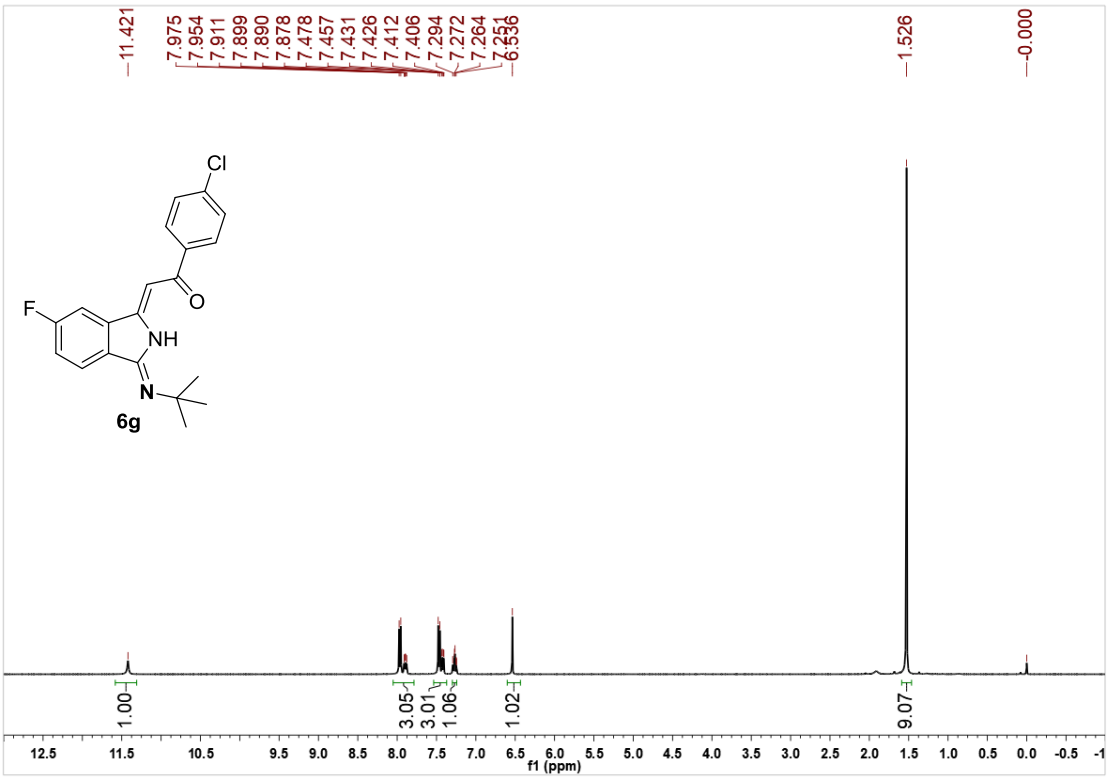
^{13}C NMR (100 MHz), $CDCl_3$



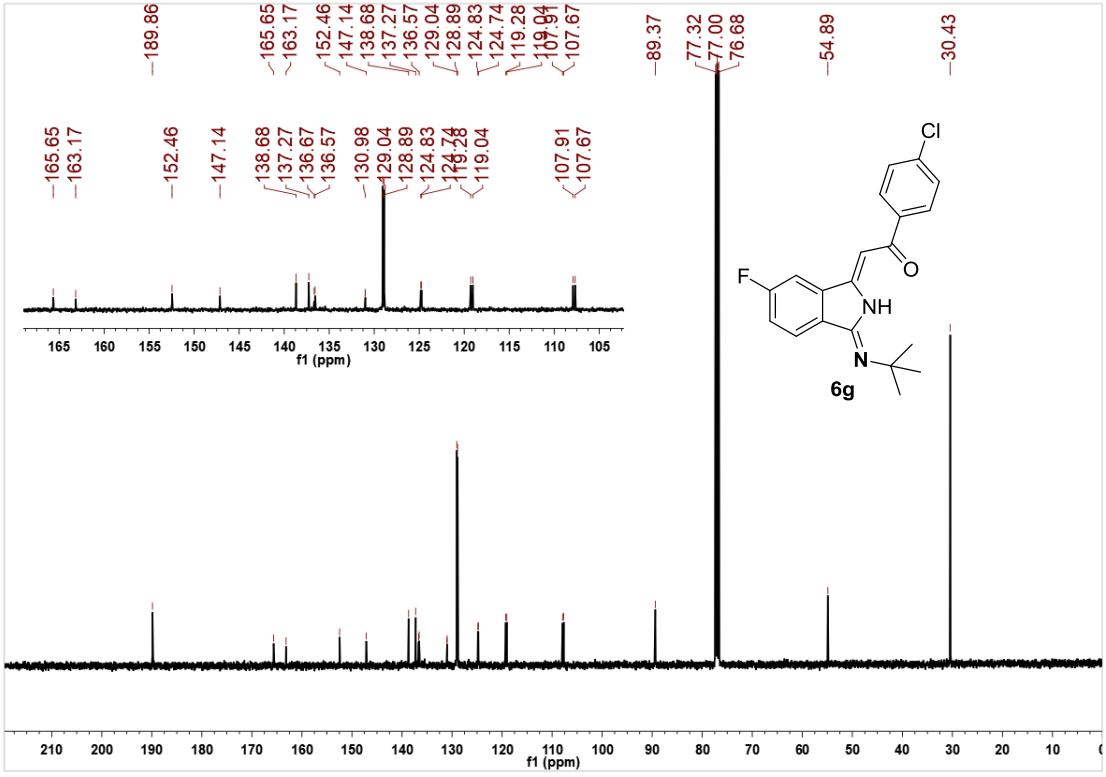
^{1}H NMR (400 MHz), $CDCl_3$



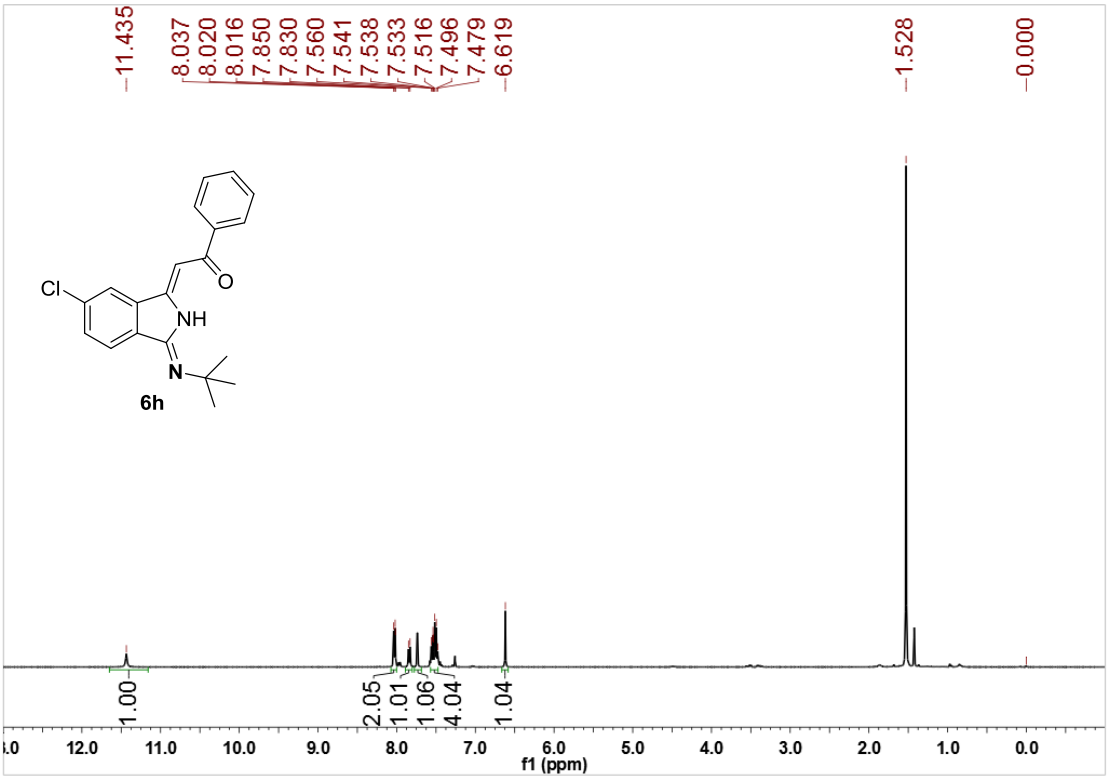
^{13}C NMR (100 MHz), $CDCl_3$



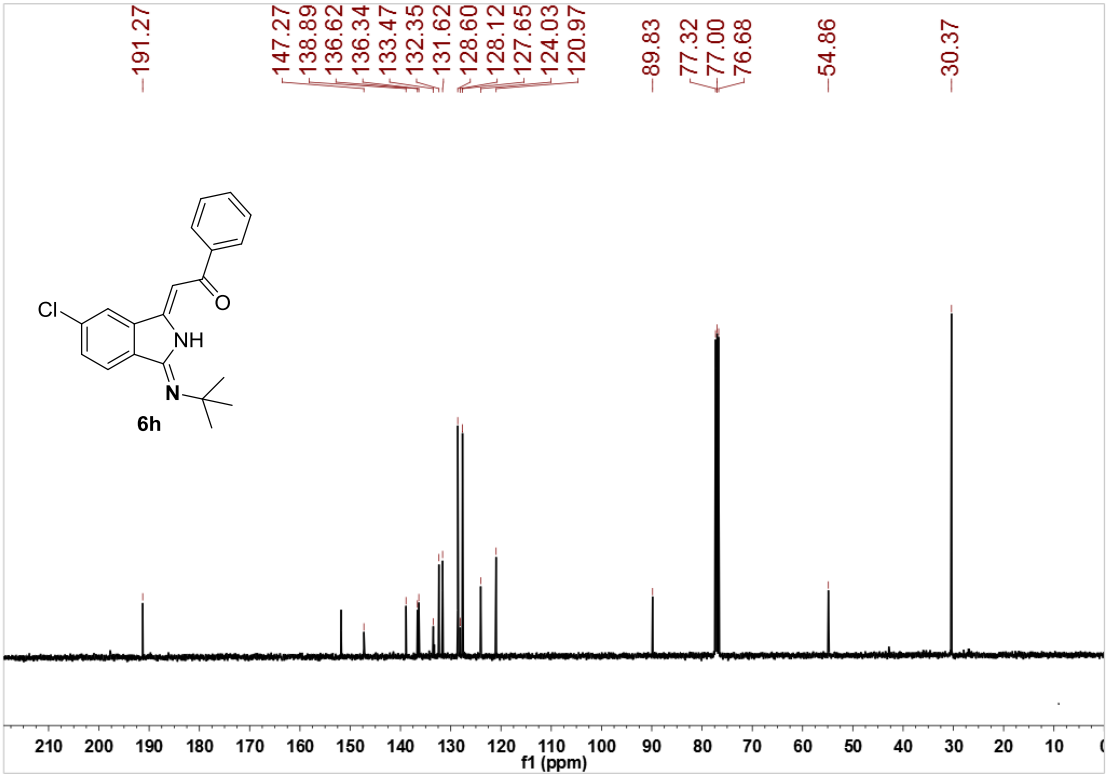
^{1}H NMR (400 MHz), $CDCl_3$



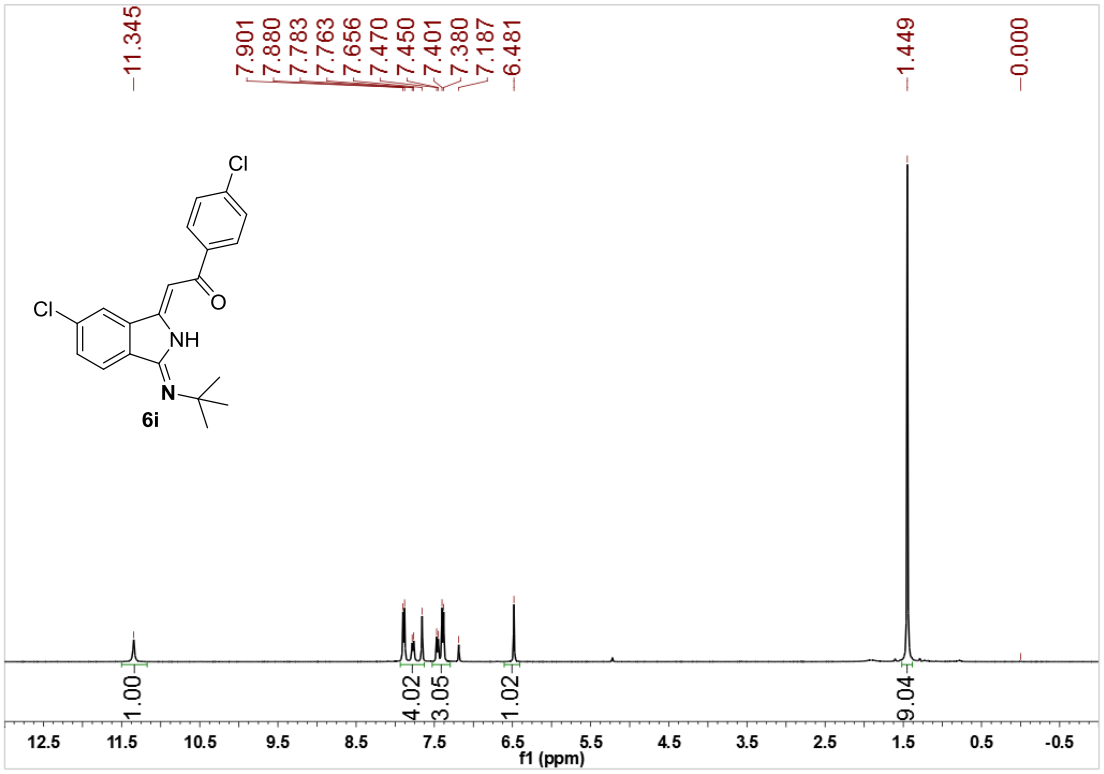
^{13}C NMR (100 MHz), $CDCl_3$



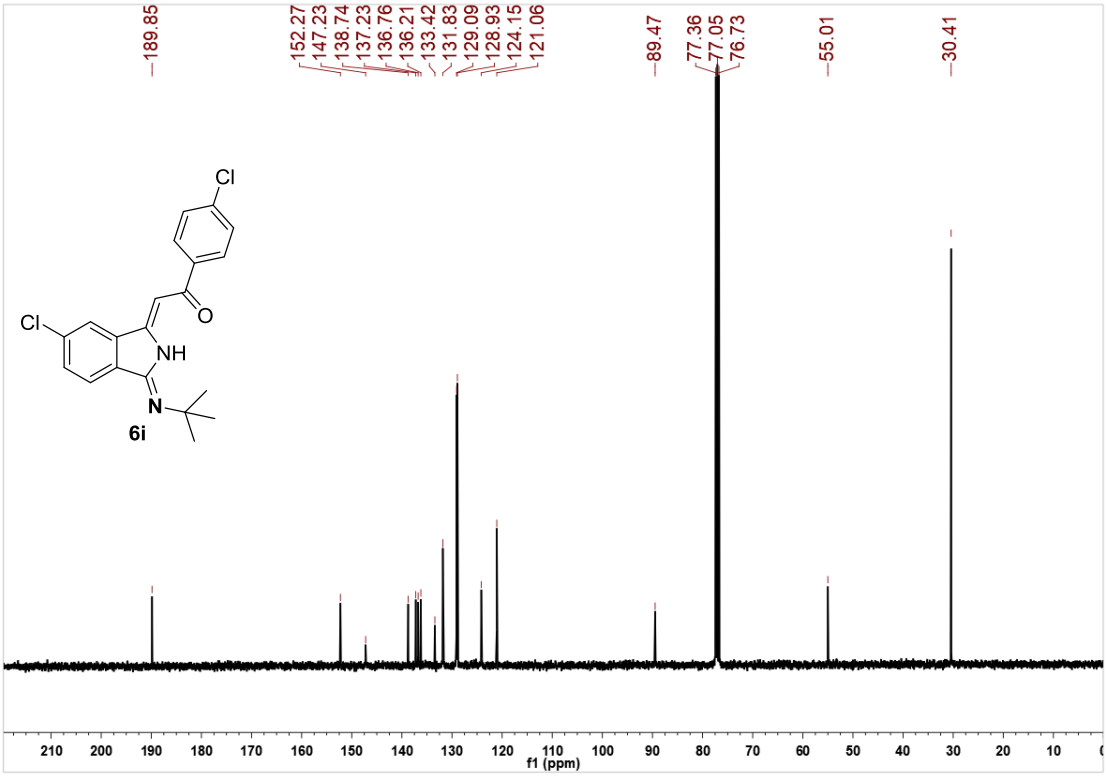
^{1}H NMR (400 MHz), $CDCl_3$



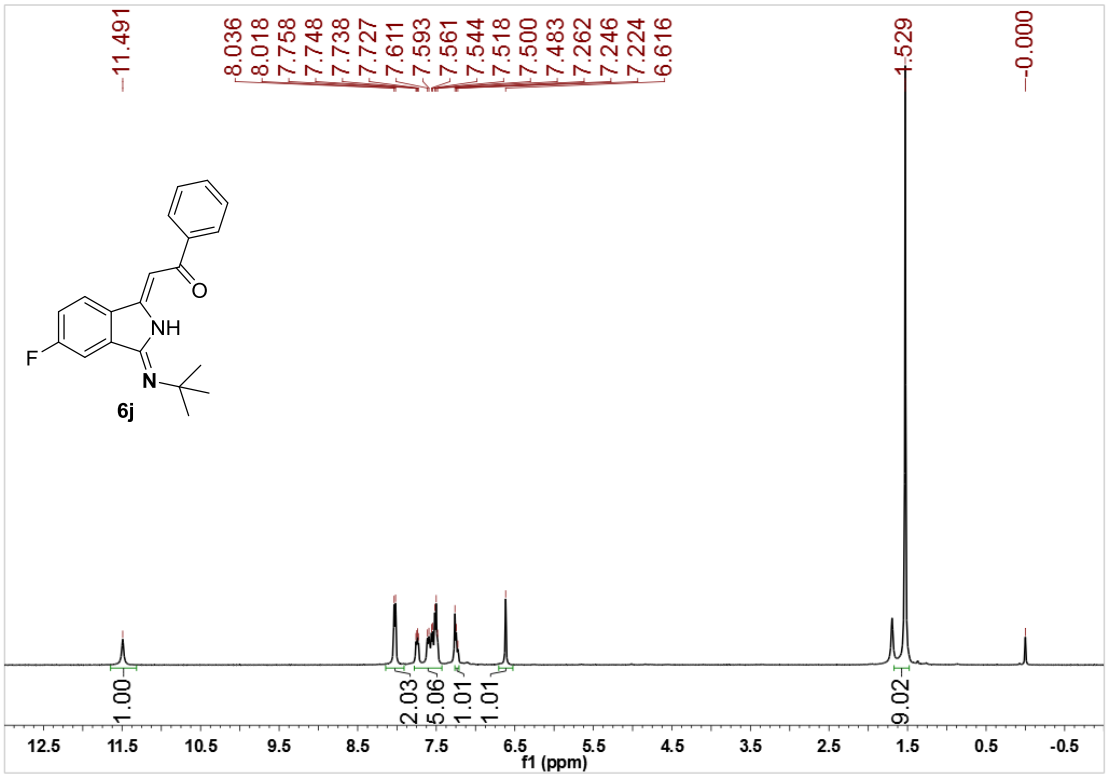
^{13}C NMR (100 MHz), $CDCl_3$



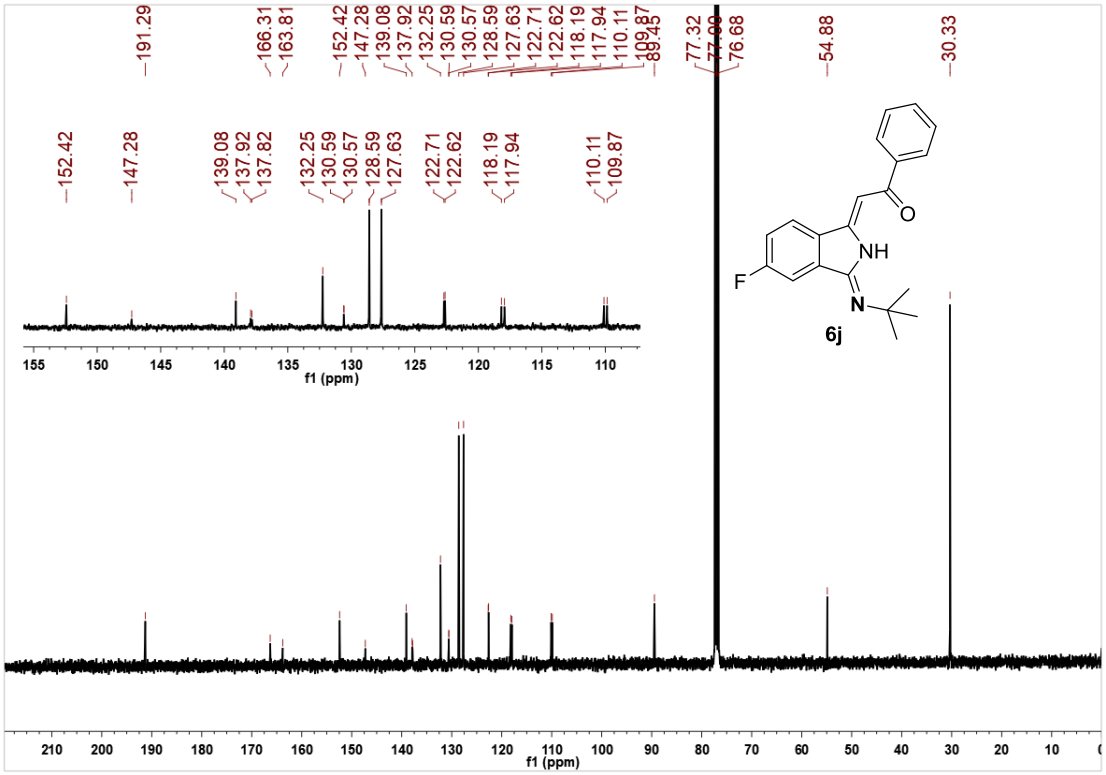
^{1}H NMR (400 MHz), $CDCl_3$



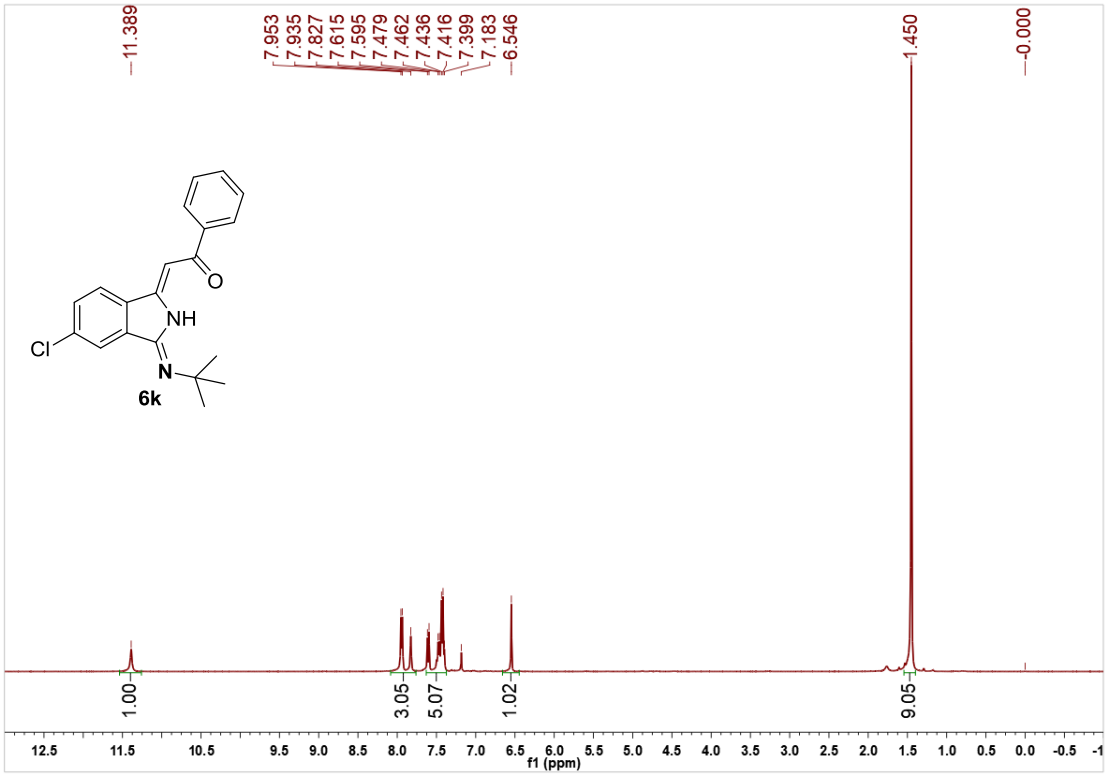
^{13}C NMR (100 MHz), $CDCl_3$



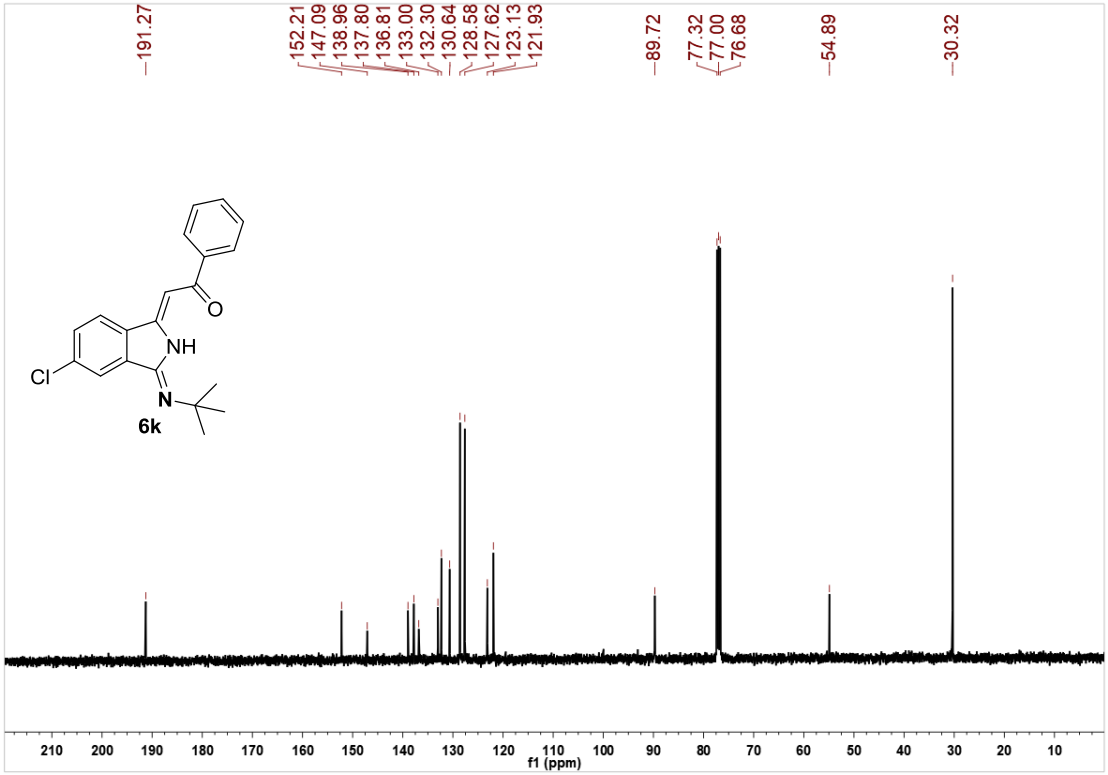
^{1}H NMR (400 MHz), $CDCl_3$



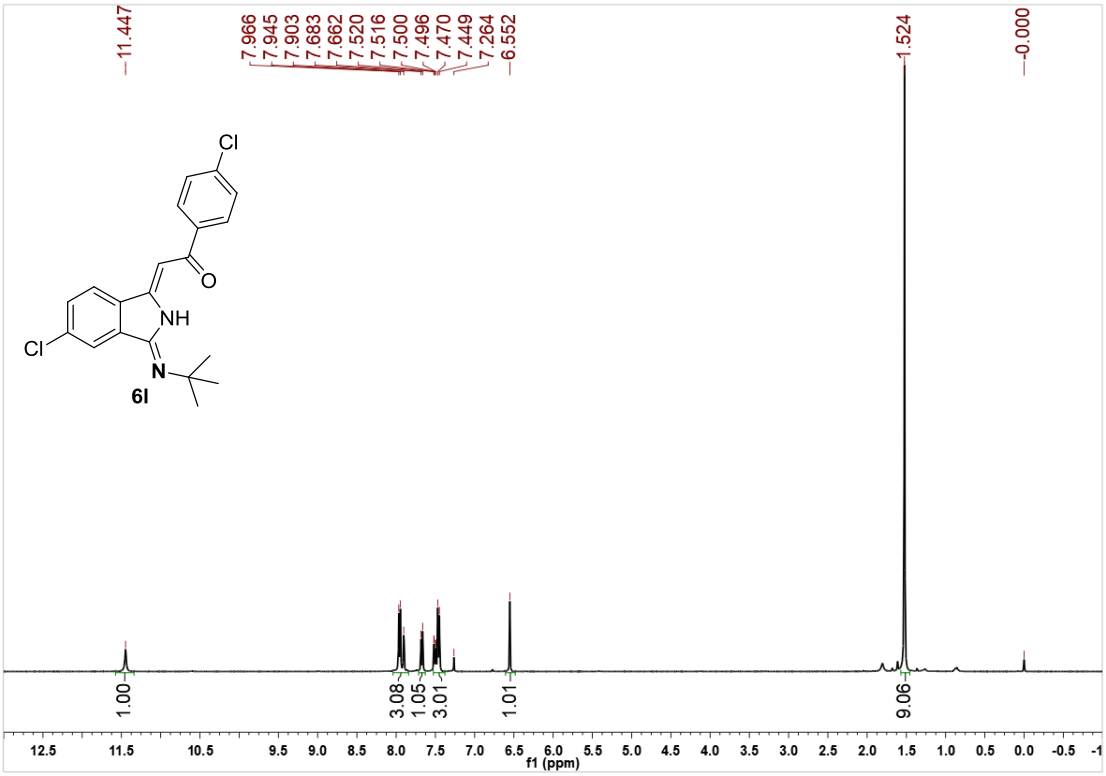
^{13}C NMR (100 MHz), $CDCl_3$



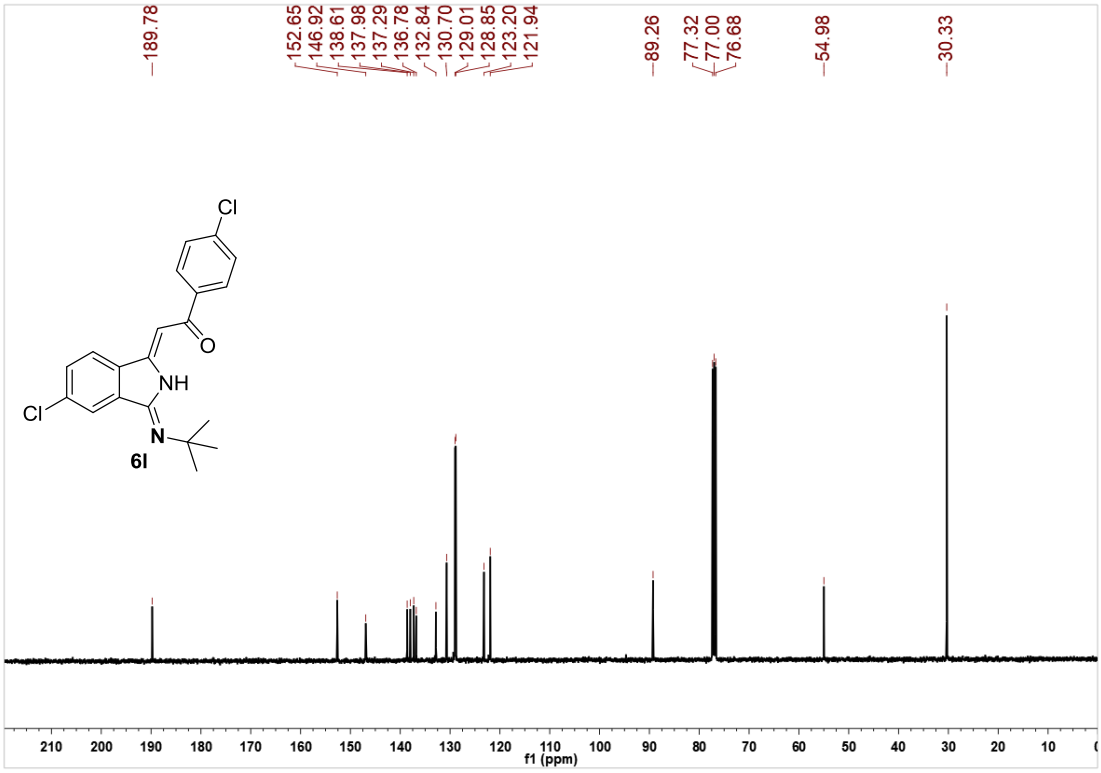
^{1}H NMR (400 MHz), $CDCl_3$



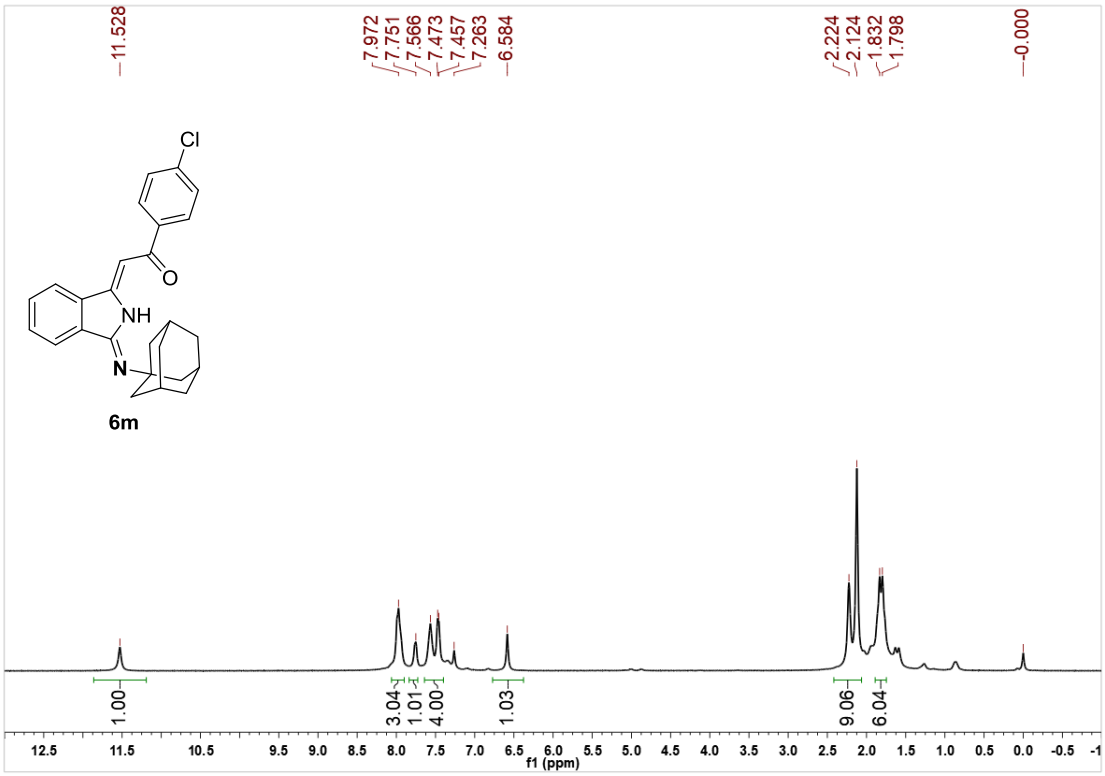
^{13}C NMR (100 MHz), $CDCl_3$



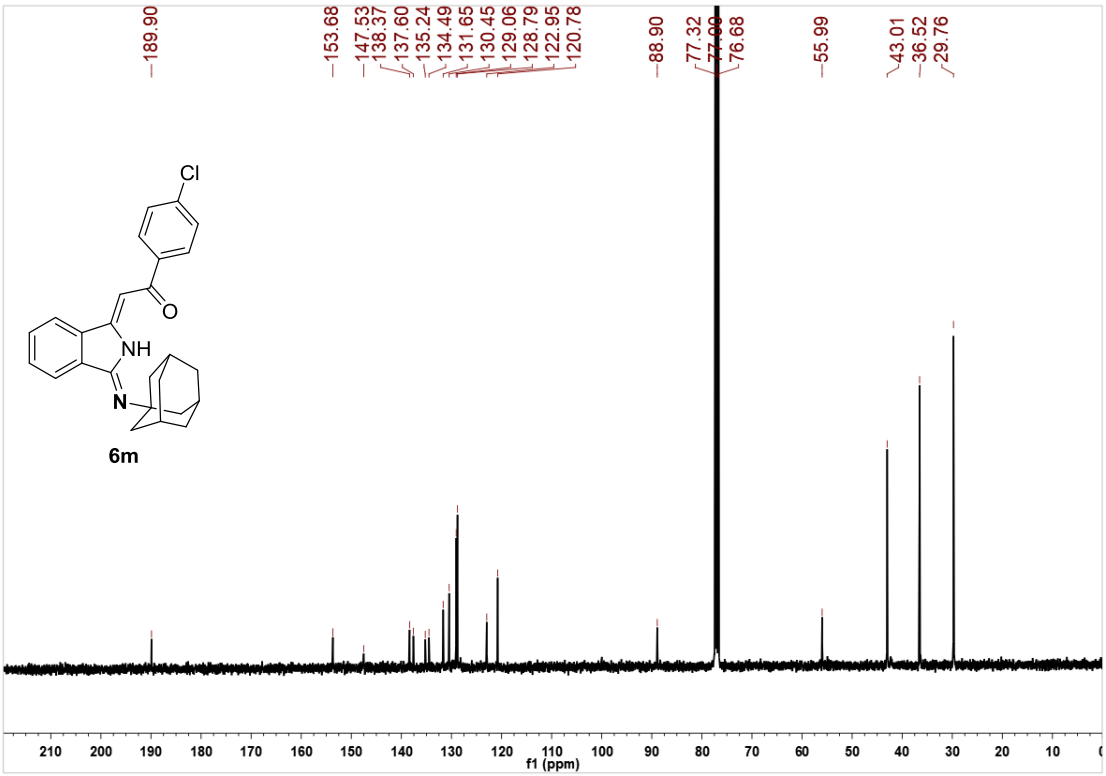
^{1}H NMR (400 MHz), $CDCl_3$



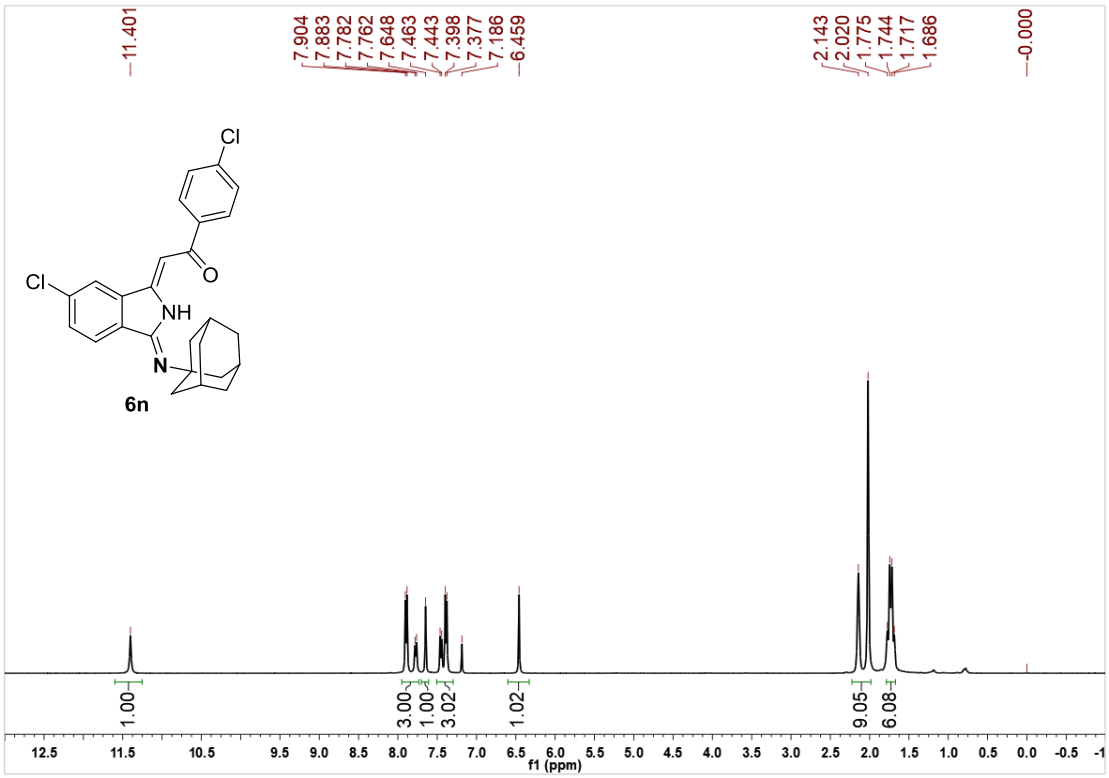
^{13}C NMR (100 MHz), $CDCl_3$



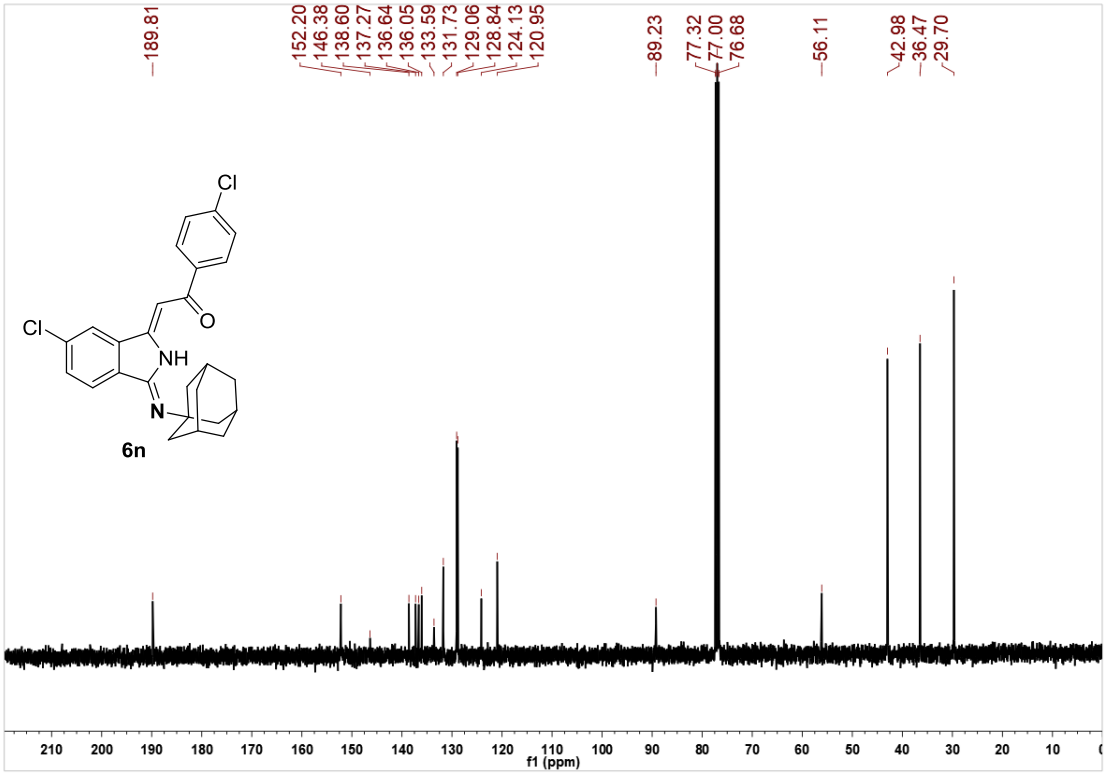
^{1}H NMR (400 MHz), $CDCl_3$



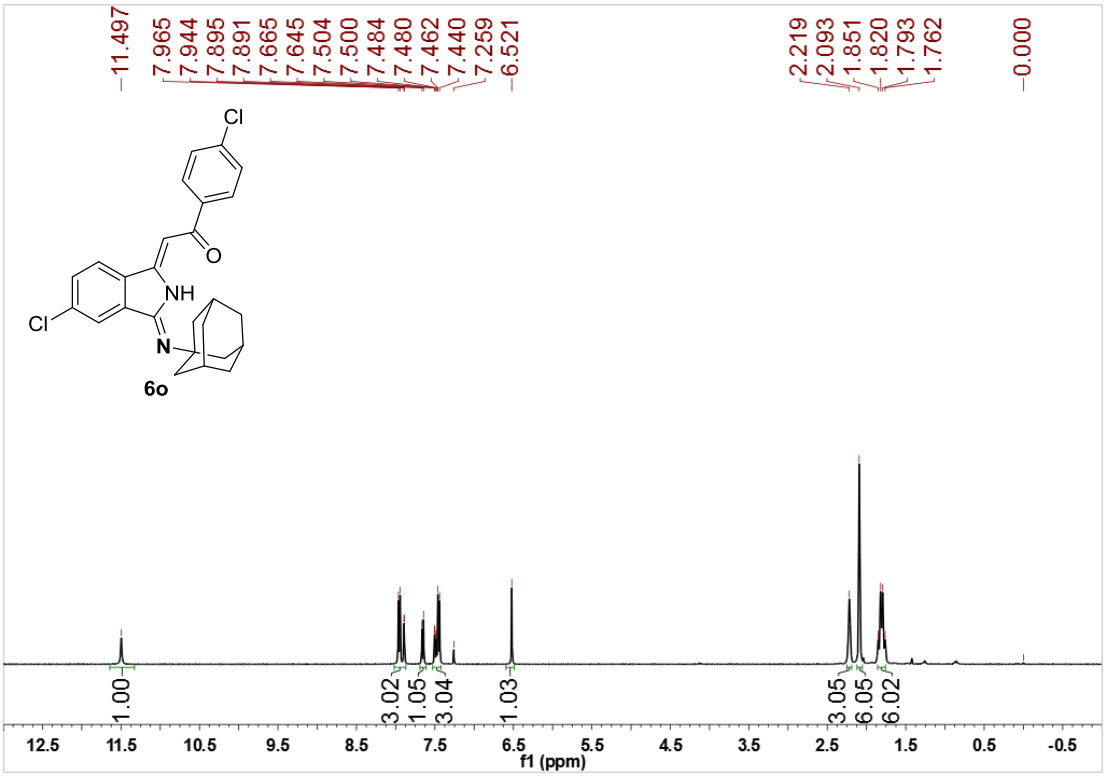
^{13}C NMR (100 MHz), $CDCl_3$



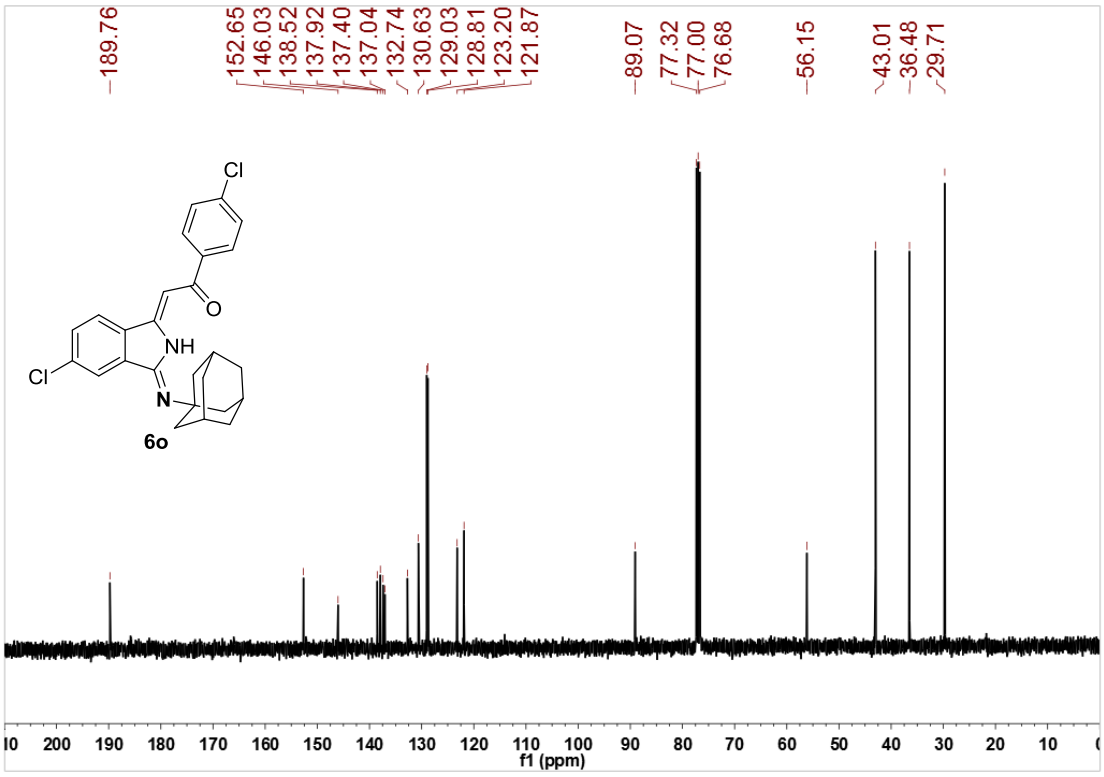
^{1}H NMR (400 MHz), $CDCl_3$



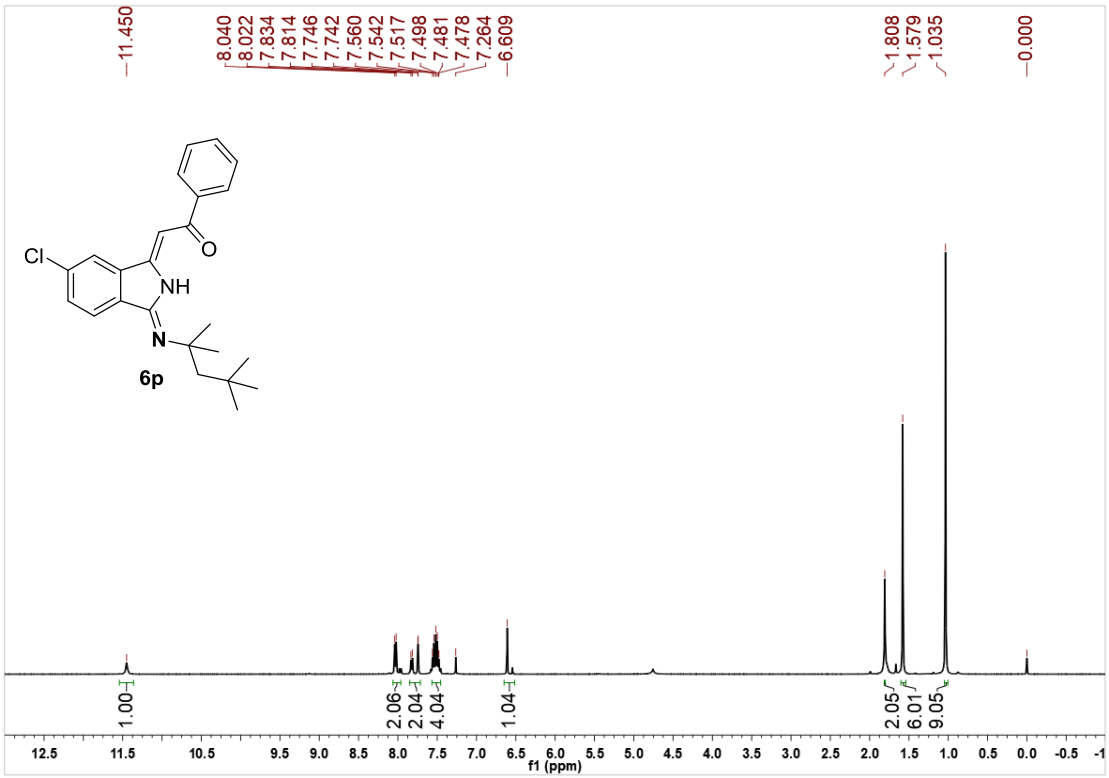
^{13}C NMR (100 MHz), $CDCl_3$



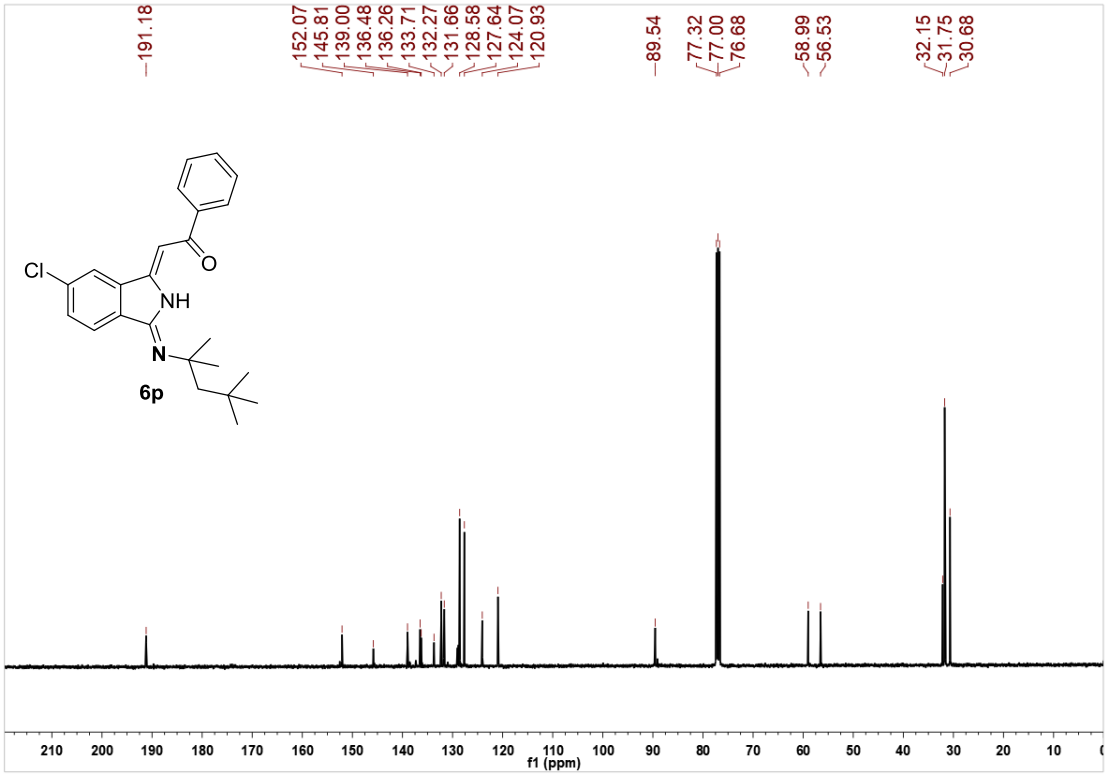
^{1}H NMR (400 MHz), $CDCl_3$



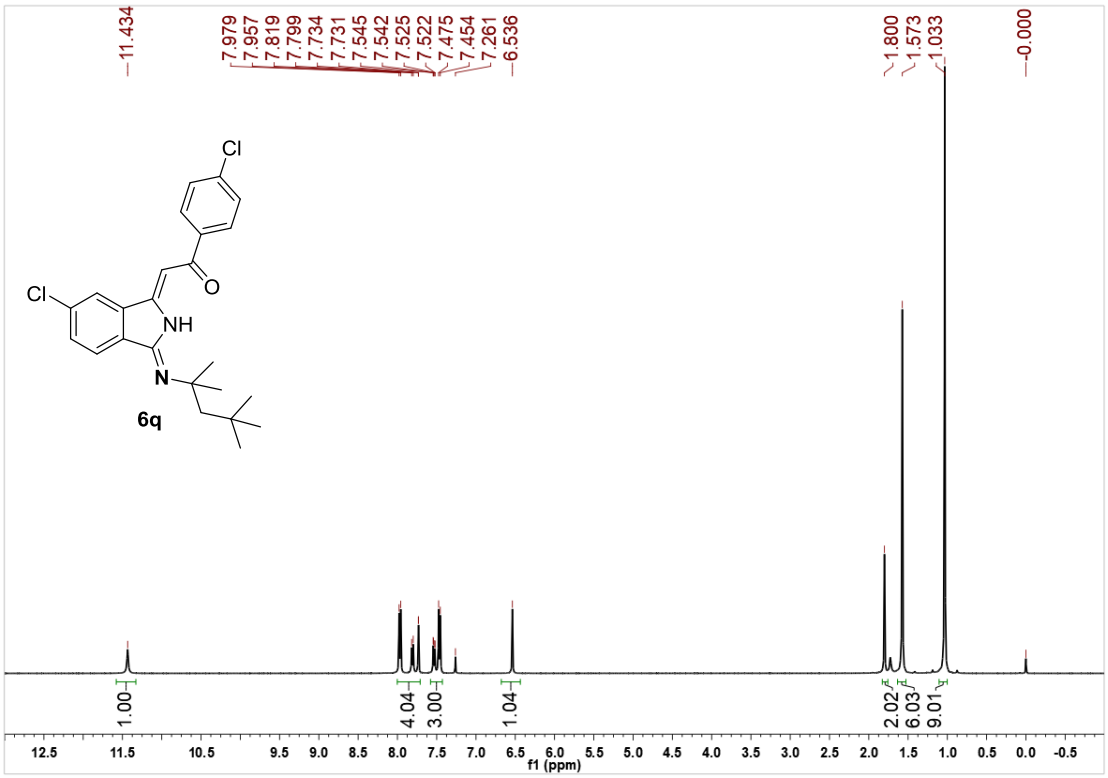
^{13}C NMR (100 MHz), $CDCl_3$



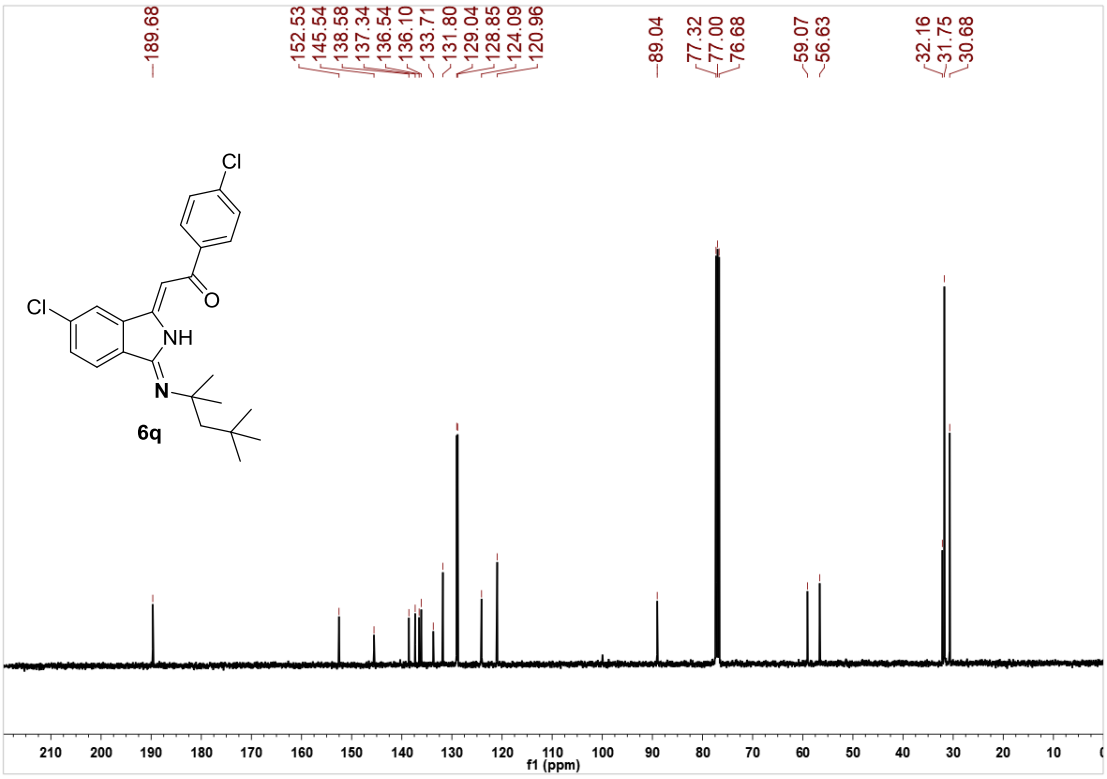
^{1}H NMR (400 MHz), $CDCl_3$



^{13}C NMR (100 MHz), $CDCl_3$

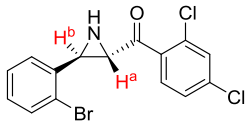


^{1}H NMR (400 MHz), $CDCl_3$



^{13}C NMR (100 MHz), $CDCl_3$

6. Copies of 2D ^{1}H NMR Spectrum of 4b



4b

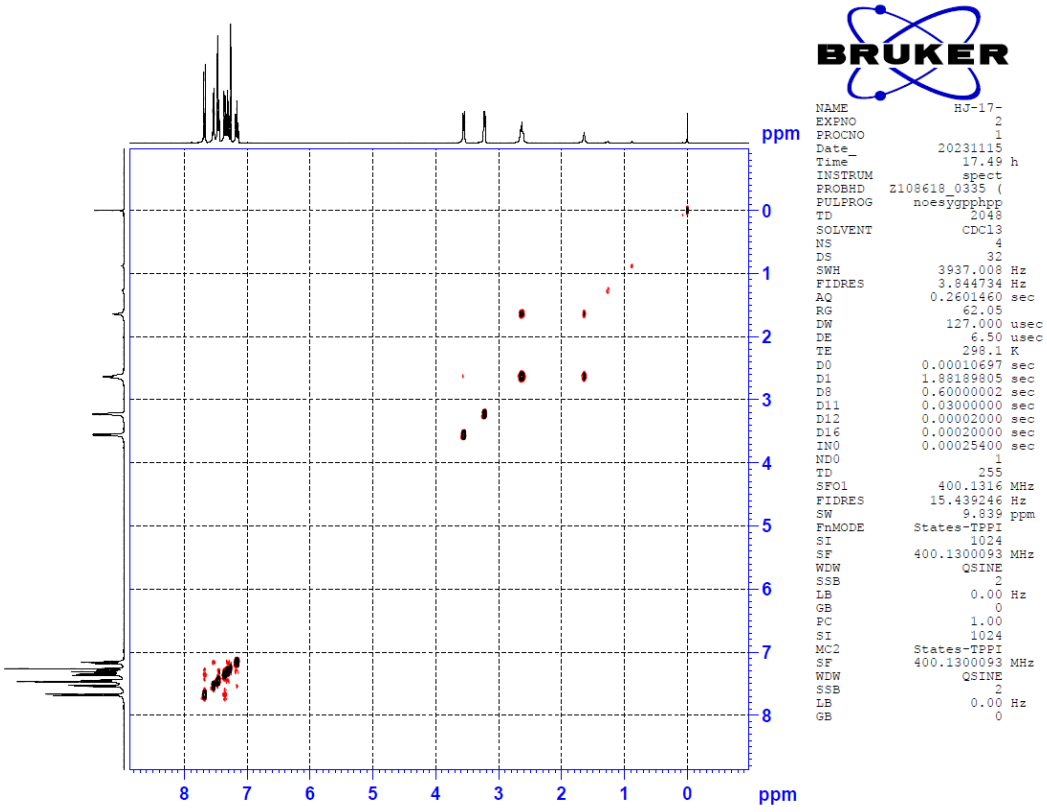


Figure S2. Copies of 2D ^{1}H NMR Spectrum of **4b**.