Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

For

Accessing indole-isoindole derivatives via palladium-catalyzed [3+2] cyclization of isocyanides with alkynyl imines

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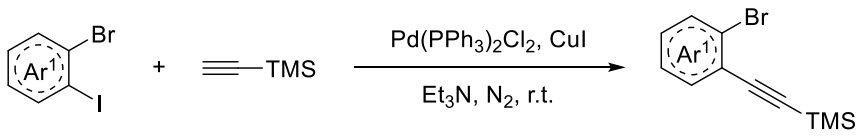
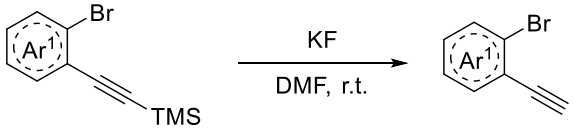
1. General information

All reactions were carried out in oven-dried glassware sealed with rubber septa under nitrogen condition. All solvents were distilled under nitrogen atmosphere prior to use. Purification of products was conducted by flash chromatography on silica gel (200-300 mesh). NMR spectra were measured on a Bruker magnetic resonance spectrometer (^{1}H at 500 MHz, ^{13}C at 126 MHz). Chemical shifts are reported in ppm using tetramethylsilane as internal standard (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet). HRMS data were obtained on a VG ZAB-HS mass spectrometer, Brucker Apex IV FTMS spectrometer. Absorption spectra were obtained on a HITACHI U-2910 spectrometer. Fluorescence spectra were collected on a Horiba Jobin Yvon-Edison Fluoromax-4 fluorescence spectrometer. X-Ray single-crystal diffraction data were collected on an Agilent Technologies Gemini single-crystal diffractometer. Compounds described in the literature were characterized by the comparison of ^{1}H and/or ^{13}C NMR spectra to the previously reported data.

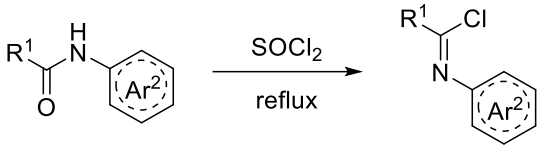
2. General procedure for substrates



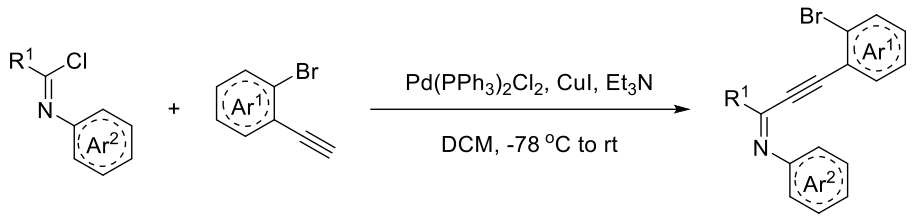
Under nitrogen condition, $Pd(PPh_3)_2Cl_2$ (5 mol %) and CuI (10 mol %) was successively added to a 50 mL vial equipped with a stir bar. A solution of *o*-bromoiodobenzene (10 mmol) and trimethylsilylacetylene (12 mmol) in Et_3N (20 mL) was added using a syringe. Then, the reaction was stirred 12 hours at room temperature. Solvent was removed in vacuo to leave a crude mixture, which was purified by silica gel column chromatography to afford the pure product.



KF (20 mmol) was added to a solution of above substrate (10 mmol) in DMF (10 mL) at room temperature. The resulting mixture was stirred for 30 minutes at room temperature. The reaction was monitored by TLC, and then quenched by adding 20 mL water and extracted with ether (3 × 20 mL). The combined organics were dried over anhydrous Na_2SO_4. Solvent was removed in vacuo to leave a crude mixture, which was purified by silica gel column chromatography to afford the pure product.

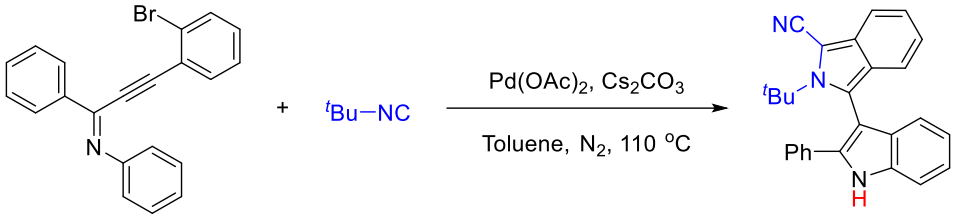


Under nitrogen condition, the amide (10.0 mmol) was added to $SOCl_2$ (6 mL, 82.5 mmol) at room temperature. Then, the resulting solution was heated to reflux for 2 hours. Corresponding imidoyl chloride was obtained by the removal of excessive $SOCl_2$, and the crude product could be directly used in the next step.



Under nitrogen condition, $Pd(PPh_3)_2Cl_2$ (5 mol %) and CuI (10 mol %) were successively added to a 50 mL vial equipped with a stir bar at -78 ^oC. A solution of the imidoyl chloride (10 mmol) in DCM (10 mL) was added using a syringe. Then, the corresponding alkyne (12 mmol) in DCM (10 mL) was added to the mixture. Et_3N (20 mmol) was added at last. The reaction was stirred for 30 minutes at -78 °C, and stirred for another 4 hours at room temperature. Solvent was removed in vacuo to leave a crude mixture, which was purified by silica gel column chromatography to afford the pure product.

3. Optimization of reaction conditions

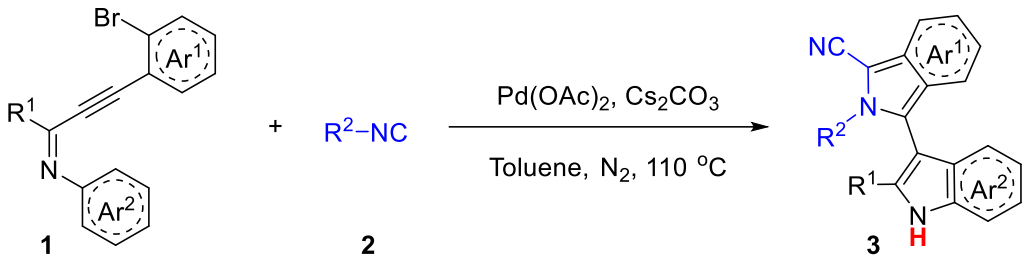


1a **2a** **3a**

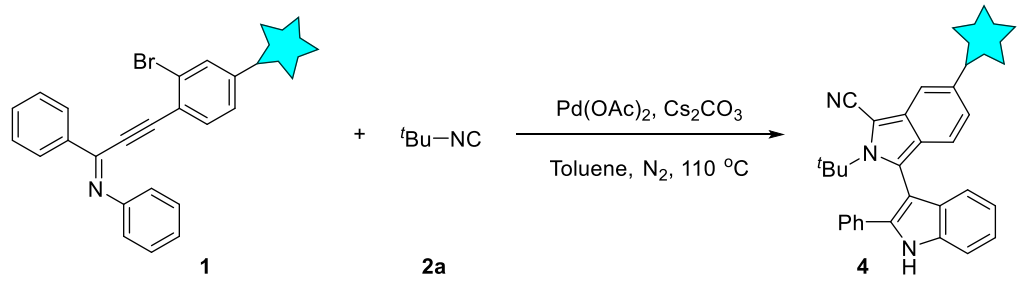
Entry	Deviation from standard conditions[a]	Yield of **3a** (%)[b]
1	None	83
2	Without $Pd(OAc)_2$	0
3	Without Cs_2CO_3	Trace
4	$PdCl_2$ instead of $Pd(OAc)_2$	66
5	$Pd(PPh_3)_4$ instead of $Pd(OAc)_2$	59
6	Na_2CO_3 instead of Cs_2CO_3	68
7	Et_3N or DBU instead of Cs_2CO_3	Trace
8	Xantphos was added	72
9	IPr was added	68
10	1,10-Phen was added	57
11	Acetonitrile instead of Toluene	34
12	DMF instead of Toluene	Complex
13	**5 mol% of $Pd(OAc)_2$**	**82**
14	2 mol% of $Pd(OAc)_2$	55
15	90 °C instead of 110 °C	41

[a] Conditions: **1a** (0.2 mmol), **2a** (0.5 mmol), $Pd(OAc)_2$ (10 mol%), Cs_2CO_3 (2.0 equiv) in 2 mL of toluene were stirred at 110 °C under a nitrogen atmosphere for 12 h; [b] Isolated yield based on **1a**.

4. General procedure for the reaction



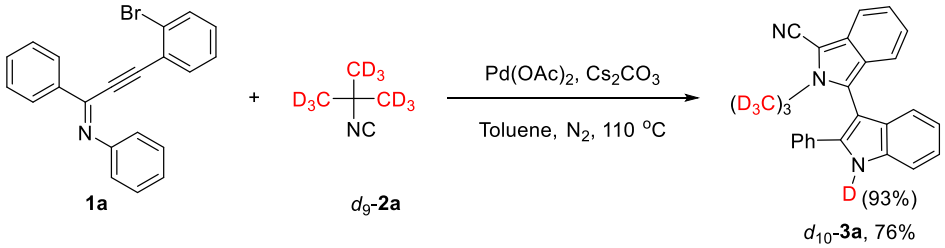
A solution of alkynyl imide **1** (0.2 mmol), isocyanide **2** (0.5 mmol), $Pd(OAc)_2$ (5 mol %) and Cs_2CO_3 (2 equiv) in toluene (2.0 mL) was stirred at 110 °C for 12 hours. After completion of the reaction as indicated by TLC, removal of the volatiles and purification by flash column chromatography provided the product **3**.



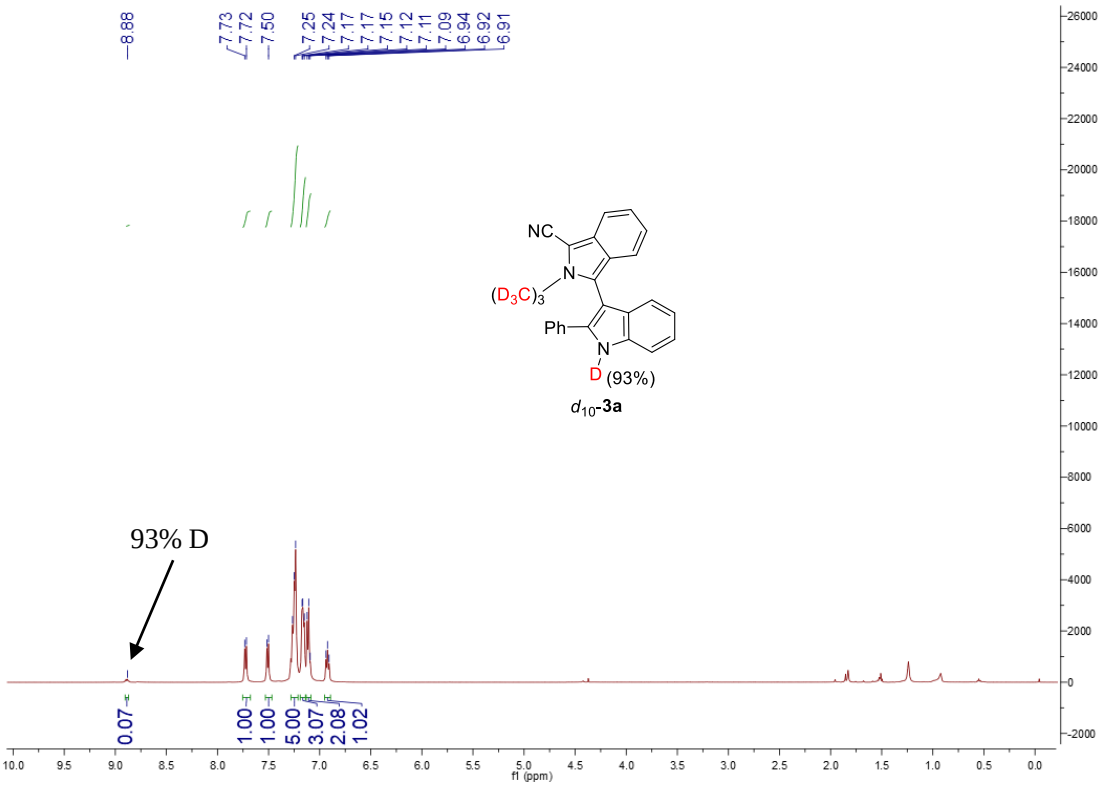
A solution of substrate **1** (0.2 mmol), *tert*-butylisocyanide **2a** (0.5 mmol), $Pd(OAc)_2$ (5 mol %) and Cs_2CO_3 (2 equiv) in toluene (2.0 mL) was stirred at 110 °C for 12 hours. After completion of the reaction as indicated by TLC, removal of the volatiles and purification by flash column chromatography provided the product **4**.

5. Mechanistic Studies

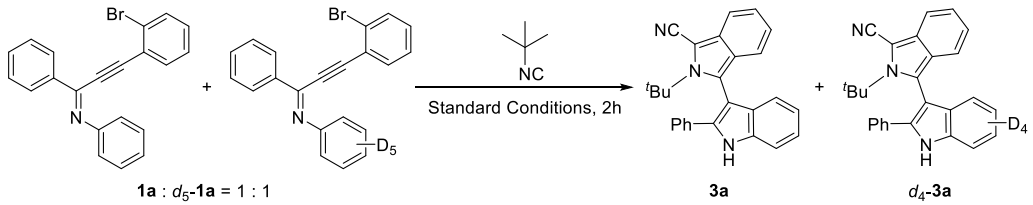
(a) The deuterium labeling study



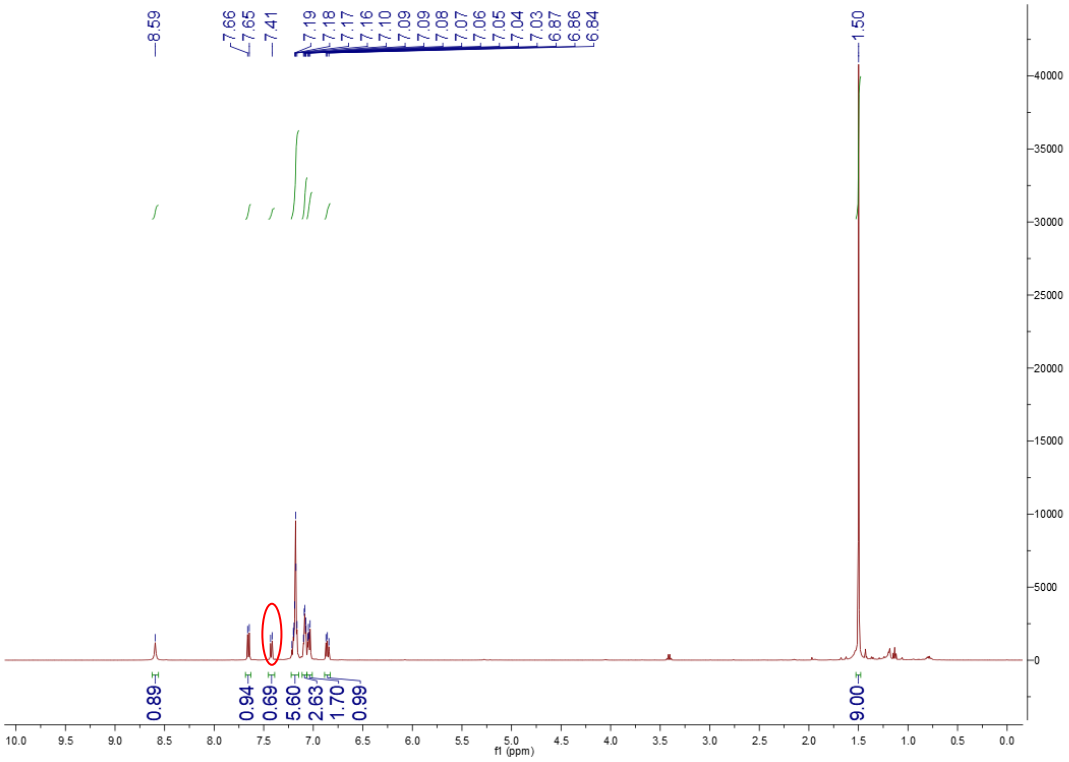
A solution of alkynyl imide **1a** (0.2 mmol), isocyanide d_9-**2a** (0.5 mmol), $Pd(OAc)_2$ (5 mol %) and Cs_2CO_3 (2 equiv) in dry Toluene (2.0 mL) was stirred at 110 °C for 12 hours. After completion of the reaction as indicated by TLC, removal of the volatiles and purification by flash column chromatography provided the corresponding product d_{10}-**3a** in 76% yield.



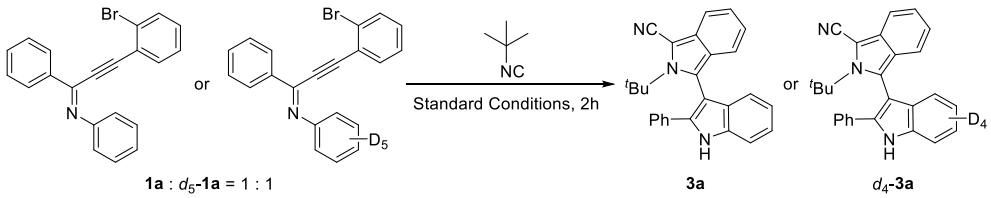
(b) The competition KIE experiment



A solution of substrate **1** (36mg of **1a** and 36mg of d_5-**1a**), *tert*-butylisocyanide **2a** (0.6 mmol), $Pd(OAc)_2$ (5 mol %) and Cs_2CO_3 (2 equiv) in toluene (2.0 mL) was stirred at 110 °C for 2 hours. After evaporation, chromatography on silica gel (eluent: hexane/EtOAc = 5:1) of the crude mixture afforded 12 mg of the product mixture as light yellow solid. The KIE value (K_H/K_D= 2.23) was determined from the ^{1}H NMR.



(c) The parallel KIE experiment



A solution of substrate **1a** (0.2 mmol), *tert*-butylisocyanide **2a** (0.6 mmol), $Pd(OAc)_2$ (5 mol %) and Cs_2CO_3 (2 equiv) in toluene (2.0 mL) was stirred at 110 °C for 2 hours. After evaporation, chromatography on silica gel (eluent: hexane/EtOAc =

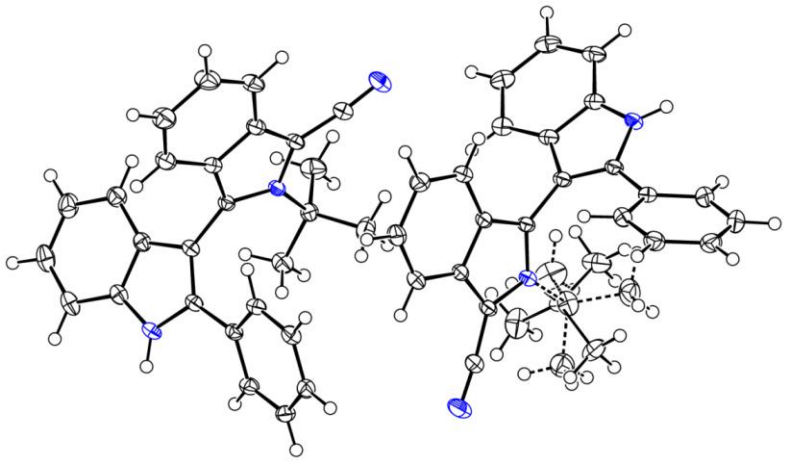
5:1) of the crude mixture afforded the desired product **3a** in 27.63% yield (21.5mg).

A solution of substrate d_5-**1a** (0.2 mmol), *tert*-butylisocyanide **2a** (0.6 mmol), $Pd(OAc)_2$ (5 mol %) and Cs_2CO_3 (2 equiv) in toluene (2.0 mL) was stirred at 110 °C for 2 hours. After evaporation, chromatography on silica gel (eluent: hexane/EtOAc = 5:1) of the crude mixture afforded the desired product d_4-**3a** in 11.23% yield (8.8 mg).

Consequently, the parallel kinetic isotopic effect value equals 2.46. (KIE = 27.63%/11.23%)

6. The single crystal data of 3a

The crystal of **3a** was obtained by crystallization from a solution in methanol after purification by column chromatography. The crystallographic data was deposited with the Cambridge Crystallographic Data Centreas supplementary publication with a CCDC number: **2264478**.



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Temperature:   120 K
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Hall group	-P 1	-P 1
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Sum formula	C27 H23 N3	C27 H23 N3
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Dx,g cm-3	1.211	1.211
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F000'	824.27	
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Nref	9905	9892
Tmin,Tmax	0.983,0.989	0.598,0.746
Tmin'	0.972	

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S = 1.036                 Npar= 587
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7. The Photophysical Properties of 3bf

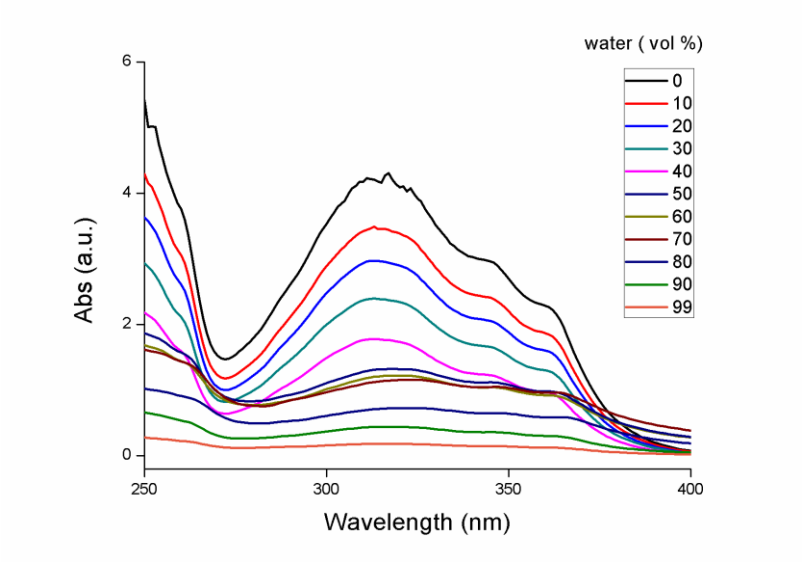


Figure S1 Absorption spectra of **3bf** in THF/water mixtures. Excited width = 5.0 nm, emission width = 5.0 nm.

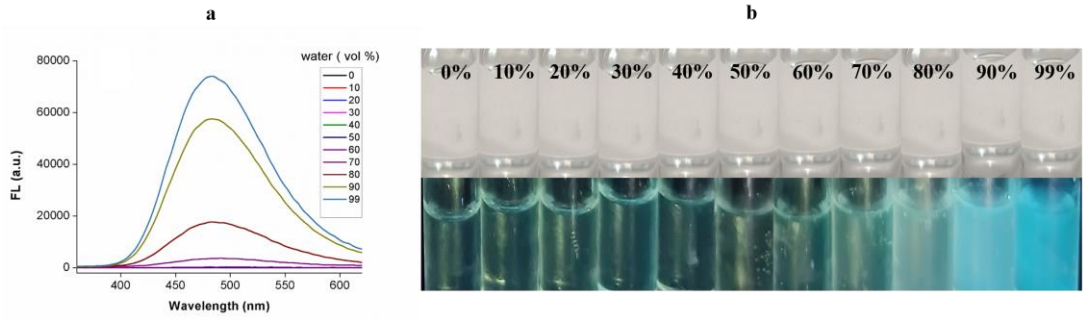


Figure S2 (a) Emission spectra of **3bf** in THF/water mixtures. (b) Solution color of **3bf** under UV light (365 nm). Excited width = 5.0 nm, emission width = 5.0 nm.

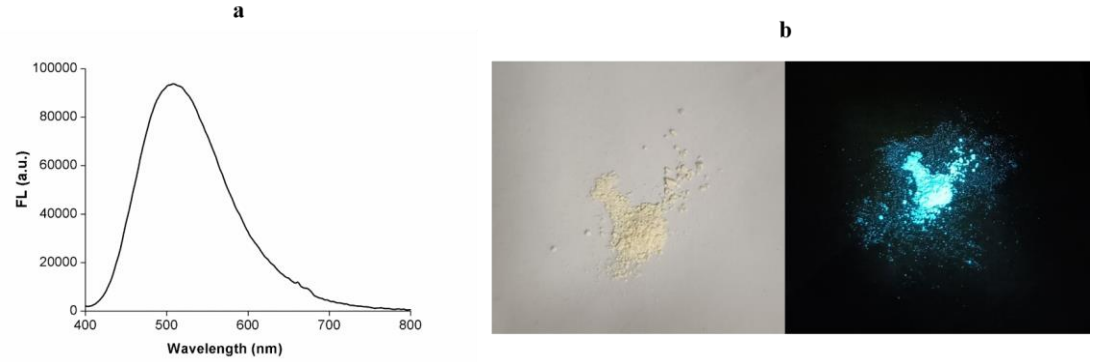


Figure S3 (a) Solid emission spectra of **3bf**. (b) Images of compound **3bf** under white light (left) and under UV light (365 nm) (right)

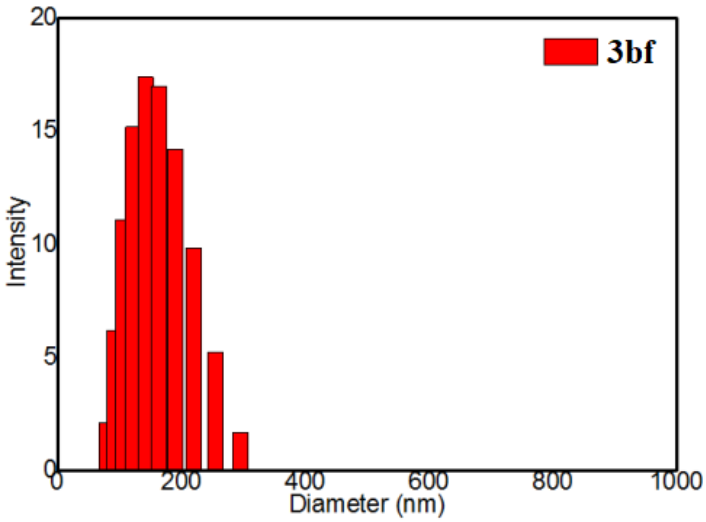
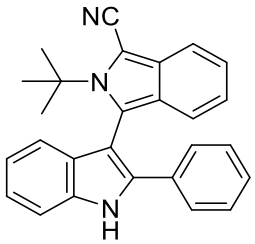


Figure S4 The size distribution of nano-particles of **3bf** in H_2O-THF (90:10, v/v)

8. Characterization data



3a

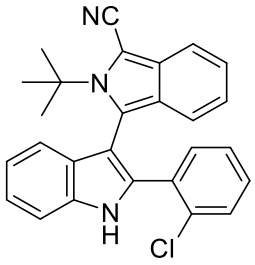
2-(*tert*-butyl)-3-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3a)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3a** 81 mg (83% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.88 (br, 1H), 7.73 (d, *J* = 9.0 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.28 (s, 1H), 7.24 (d, *J* = 7.0 Hz, 4H), 7.18–7.14 (m, 3H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.92 (t, *J* = 8.0 Hz, 1H), 1.57 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.7, 135.5, 133.4, 131.7, 131.0, 129.2, 128.3, 126.2, 125.9, 124.9, 123.3, 122.4, 121.3, 121.1, 119.6, 117.5, 117.5, 111.2, 106.0, 92.8, 62.8, 31.4;

HRMS (EI-TOF) calcd for $C_{27}H_{23}N_3$ 389.1892, found 389.1890.



3b

2-(*tert*-butyl)-3-(2-(2-chlorophenyl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3b)

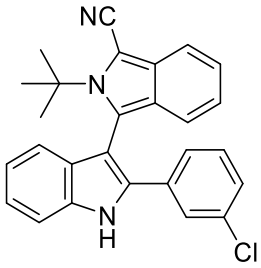
Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3b** 66 mg (62% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.95 (br, 1H), 7.72 (d, *J* = 9.0 Hz, 1H), 7.55 (d, *J*

= 8.0 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.36–7.33 (m, 1H), 7.29 (d, *J* = 2.0 Hz, 1H), 7.27 (d, *J* = 7.0 Hz, 1H), 7.24–7.21 (m, 1H), 7.19–7.16 (m, 2H), 7.01–6.97 (m, 2H), 6.86 (dd, *J* = 8.0, 2.0 Hz, 1H), 1.59 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 140.8, 139.9, 136.3, 135.6, 133.4, 131.1, 130.4, 128.9, 127.7, 126.8, 126.5, 126.0, 124.9, 123.3, 122.5, 121.3, 121.2, 119.6, 117.5, 111.2, 106.1, 92. 9, 62.9, 31.4;

HRMS (EI-TOF) calcd for $C_{27}H_{22}ClN_3$ 423.1502, found 423.1505.



3c

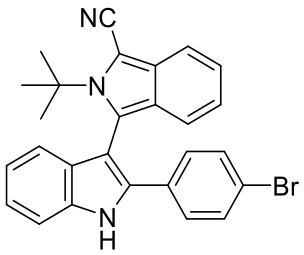
2-(*tert*-butyl)-3-(2-(3-chlorophenyl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3c)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3c** 70 mg (69% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.94 (br, 1H), 7.77 (d, *J* = 9.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.36 (t, *J* = 2.0 Hz, 1H), 7.35–7.31 (m, 1H), 7.31–7.27 (m, 1H), 7.24 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.16 (m, 2H), 7.10 (d, *J* = 8.5 Hz, 1H), 6.98–6.92 (m, 2H), 1.65 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 135.7, 135.1, 135.0, 133.4, 130.9, 130.5, 128.2, 126.2, 126.0, 124.4, 124.3, 123.8 122.7, 121.4, 121.0, 119.8, 117.6, 117.4, 111.4, 106.9, 93.0, 62.9, 31.4;

HRMS (EI-TOF) calcd for $C_{27}H_{22}ClN_3$ 423.1502, found 423.1505.



3d

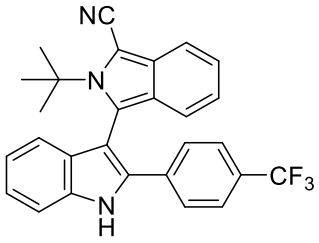
3-(2-(4-bromophenyl)-1*H*-indol-3-yl)-2-(*tert*-butyl)-2*H*-isoindole-1-carbonitrile (3d)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3d** 50 mg (85% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (br, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.44–7.40 (m, 2H), 7.31 (m, 2H), 7.19–7.14 (m, 2H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 9.0 Hz, 2H), 6.96 (dd, *J* = 9.0, 6.0 Hz, 1H), 1.62 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 135.6, 135.4, 133.3, 132.4, 131.0, 130.6, 127.6, 126.2, 126.0, 124.7, 123.6, 122.6, 122.4, 121.4, 121.0, 119.8, 117.6, 117.2, 111.2, 106.6, 93.1, 62.9, 31.4;

HRMS (EI-TOF) calcd for $C_{27}H_{22}BrN_3$ 467.0997, found 467.0999.



3e

2-(*tert*-butyl)-3-(2-(4-(trifluoromethyl)phenyl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3e)

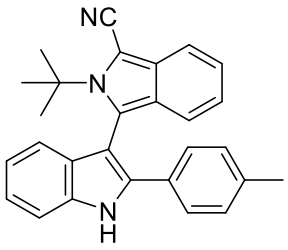
Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3e** 80 mg (70% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.86 (br, 1H), 7.76 (d, *J* = 9.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 3H), 7.37–7.29 (m, 4H), 7.18 (m, 2H), 7.10 (d, *J* = 9.0 Hz, 1H), 6.97 (dd, *J*

= 9.0, 7.0 Hz, 1H), 1.62 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 135.7, 135.0, 134.7, 132.1 (d, $J_{C\text{-}F}$ = 301.1 Hz), 128.8 (q, $J_{C\text{-}F}$ = 32.8 Hz), 126.3, 126.2, 126.1 (q, $J_{C\text{-}F}$ = 3.8 Hz), 126.0, 125.9, 124.1, 123.8, 122.8, 121.6, 120.8, 120.0, 117.6, 117.1, 111.4, 107.7, 93.3, 62.9, 31.4.

HRMS (EI-TOF) calcd for $C_{28}H_{22}F_3N_3$ 457.1766, found 457.1765.



3f

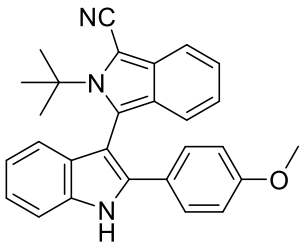
2-(*tert*-butyl)-3-(2-(p-tolyl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3f)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3f** 80 mg (78% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (br, 1H), 7.76 (d, *J* = 9.0 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.31–7.27 (m, 2H), 7.20–7.13 (m, 3H), 7.10 (s, 4H), 6.98–6.93 (m, 1H), 2.32 (s, 3H), 1.63 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.3, 136.9, 135.4, 133.4, 131.1, 129.9, 128.8, 126.2, 126.1, 125.9, 125.2, 123.1, 122.4, 121.3, 121.1, 119.5, 117.6, 117.5, 111.1, 105.4, 92.7, 62.8, 31.4, 21.2;

HRMS (EI-TOF) calcd for $C_{28}H_{25}N_3$ 403.2048, found 403.2050.



3g

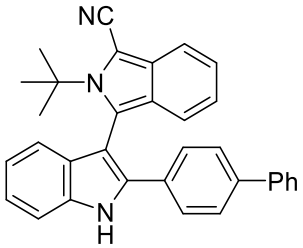
2-(*tert*-butyl)-3-(2-(4-methoxyphenyl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3g)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 4/1) to give **3g** 85 mg (81% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61 (br, 1H), 7.75 (d, *J* =9.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.29 (t, *J* = 5.0 Hz, 2H), 7.18–7.10 (m, 5H), 6.96 (t, *J* = 8.0 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 2H), 3.78 (s, 3H), 1.61 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.6, 136.8, 135.3, 133.4, 131.1, 127.5, 126.3, 125.9, 125.1, 124.2, 122.9, 122.4, 121.3, 121.1, 119.4, 117.5, 117.5, 114.7, 111.0, 104.9, 92.7, 62.8, 55.3, 31.4;

HRMS (EI-TOF) calcd for $C_{28}H_{25}N_3O$ 419.1998, found 419.1994.



3h

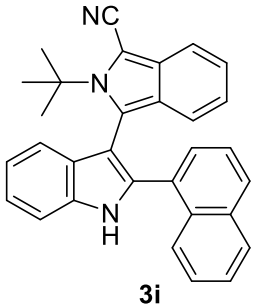
3-(2-([1,1'-biphenyl]-4-yl)-1*H*-indol-3-yl)-2-(*tert*-butyl)-2*H*-isoindole-1-carbonitrile (3h)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3h** 84 mg (80% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.95 (br, 1H), 7.78 (d, *J* = 9.0 Hz, 1H), 7.58–7.52 (m, 5H), 7.44 (t, *J* = 8.0 Hz, 2H), 7.38–7.34 (m, 1H), 7.34–7.27 (m, 4H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.17–7.13 (m, 2H), 6.97 (dd, *J* = 9.0, 7.0 Hz, 1H), 1.64 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 140.87, 139.9, 136.3, 135.6, 133.4, 131.1, 130.4, 128.9, 127.7, 126.8, 126.5, 126.2, 126.0, 124.9, 123.3, 122.5, 121.3, 121.2, 119.6, 117.5, 117.4, 111.2, 106.1, 92.9, 62.9, 31.4;

HRMS (EI-TOF) calcd for $C_{33}H_{27}N_3$ 465.2205, found 465.2201.



3i

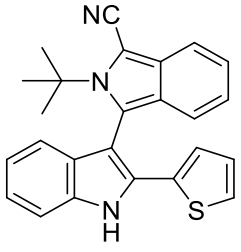
2-(*tert*-butyl)-3-(2-(naphthalen-1-yl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3i)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3i** 69 mg (70% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64 (br, 1H), 8.05 (d, *J* = 9.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 9.0 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.0 Hz, 1H), 7.43–7.39 (m, 1H), 7.35–7.32 (m, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.25–7.21 (m, 3H), 7.20–7.16 (m, 2H), 6.96 (dd, *J* = 8.0, 7.0 Hz, 1H), 1.48 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 137.2, 136.2, 133.8, 132.8, 131.5, 130.1, 130.0, 129.4, 128.9, 128.2, 127.1, 126.7, 126.4, 126.1, 126.1, 125.7, 122.8, 122.6, 121.6, 120.9, 119.33, 117.2, 112.3, 106.5, 91.8, 62.8, 31.1;

HRMS (EI-TOF) calcd for $C_{31}H_{25}N_3$ 439.2048, found 439.2050.



3j

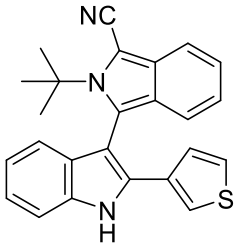
2-(*tert*-butyl)-3-(2-(thiophen-2-yl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3j)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3j** 70 mg (65% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (br, 1H), 7.76 (d, *J* = 9.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 7.0 Hz, 1H), 7.27 (d, *J* = 3.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 7.0 Hz, 1H), 7.11 (d, *J* = 9.0 Hz, 1H), 7.00 (dd, *J* = 3.0, 1.0 Hz, 1H), 6.95 (dd, *J* = 9.0, 7.0 Hz, 1H), 6.73 (dd, *J* = 5.0, 1.0 Hz, 1H), 1.65 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 136.3, 133.6, 133.3, 132.9, 130.7, 127.8, 127.8, 126.5, 126.1, 125.3, 125.0, 123.2, 122.9, 121.2, 121.0, 118.9, 117.2, 117.1, 112.0, 103.9, 92.8, 63.1, 31.1;

HRMS (EI-TOF) calcd for $C_{25}H_{21}N_3S$ 395.1456, found 395.1454.



3k

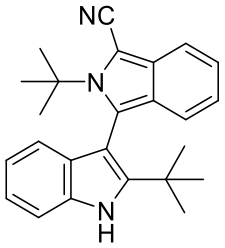
2-(*tert*-butyl)-3-(2-(thiophen-3-yl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3k)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3k** 81 mg (77% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.60 (br, 1H), 7.78–7.74 (m, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.32–7.29 (m, 1H), 7.28–7.25 (m, 1H), 7.21–7.17 (m, 2H), 7.14 (t, *J* = 7.0 Hz, 1H), 7.08–7.05 (m, 1H), 6.99 (d, *J* = 4.0 Hz, 2H), 6.94 (dd, *J* = 9.0, 7.0 Hz, 1H), 1.71 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 136.0, 133.8, 133.1, 132.9, 130.7, 128.0, 126.6, 126.2, 125.7, 125.6, 122.9, 122.8, 122.5, 121.4, 120.9, 119.0, 117.3, 117.2, 112.0, 103.5, 92.2, 63.1, 31.1;

HRMS (EI-TOF) calcd for $C_{25}H_{21}N_3S$ 395.1456, found 395.1454.



3l

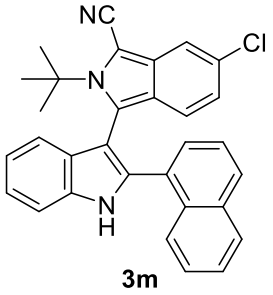
2-(*tert*-butyl)-3-(2-(*tert*-butyl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3j)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3l** 69 mg (66% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (br, 1H), 7.67 (d, *J* = 9.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.23–7.17 (m, 2H), 7.05–7.02 (m, 2H), 6.96 (d, *J* = 8.0 Hz, 1H), 6.91 (dd, *J* = 9.0, 7.0 Hz, 1H), 1.77 (s, 9H), 1.24 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.1, 134.2, 133.1, 131.3, 126.3, 125.8, 122.2, 122.0, 121.6, 120.5, 119.0, 117.6, 117.3, 110.5, 103.3, 92.4, 62.8, 33.3, 31.5, 30.4;

HRMS (EI-TOF) calcd for $C_{25}H_{27}N_3$ 369.2205, found 369.2202.



3m

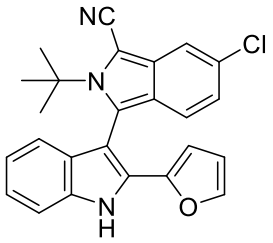
2-(*tert*-butyl)-6-chloro-3-(2-(naphthalen-1-yl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3m)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3m** 68 mg (60% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (br, 1H), 8.02 (d, *J* = 9.0 Hz, 1H), 7.90–7.86 (m, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 2.0 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.52–7.49 (m, 1H), 7.43 (m, 1H), 7.34 (m, 1H), 7.28 (d, *J* = 7.0 Hz, 2H), 7.20 (m, 1H), 7.17–7.11 (m, 2H), 6.88 (dd, *J* = 9.0, 2.0 Hz, 1H), 1.48 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.9, 135.4, 134.0, 133.3, 132.0, 131.2, 129.9, 129.5, 129.0, 128.9, 128.3, 126.9, 126.3, 125.4, 125.1, 125.0, 124.9, 123.8, 123.3, 122.8, 121.3, 119.7, 116.5, 111.22, 107.6, 92.6, 63.0, 31.4;

HRMS (EI-TOF) calcd for $C_{31}H_{24}ClN_3$ 473.1659, found 473.1655.



3n

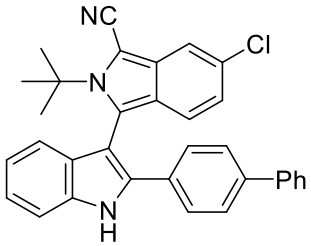
2-(*tert*-butyl)-6-chloro-3-(2-(furan-2-yl)-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3n)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3n** 66 mg (57% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, DMSO-d_6) δ 7.69–7.63 (m, 1H), 7.54–7.50 (m, 2H), 7.37 (dd, *J* = 3.0, 1.0 Hz, 1H), 7.20 (m, 1H), 7.05–7.00 (m, 2H), 6.94–6.88 (m, 2H), 6.68 (dd, *J* = 5.0, 1.0 Hz, 1H), 1.60 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 136.0, 134.0, 133.1, 132.7, 131.8, 130.6, 128.1, 127.0, 125.6, 124.0, 123.9, 123.7, 122.9, 122.7, 121.0, 118.9, 116.5, 116.1, 112.0, 102.8, 92.3, 63.6, 31.0;

HRMS (EI-TOF) calcd for $C_{25}H_{20}ClN_3O$ 413.1295, found 413.1299.



3o

3-(2-([1,1'-biphenyl]-4-yl)-1*H*-indol-3-yl)-2-(*tert*-butyl)-6-chloro-2*H*-isoindol

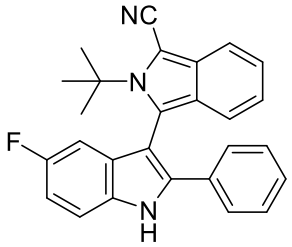
e-1-carbonitrile (3o)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3o** 84 mg (79% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (br, 1H), 7.74 (d, *J* = 2.0 Hz, 1H), 7.56–7.51 (m, 5H), 7.42 (t, *J* = 8.0 Hz, 2H), 7.37–7.33 (m, 1H), 7.30 (m, 1H), 7.24–7.20 (m, 2H), 7.17–7.13 (m, 2H), 7.06 (d, *J* = 9.0 Hz, 1H), 6.88 (dd, *J* = 9.0, 2.0 Hz, 1H), 1.61 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 141.0, 139.7, 136.4, 135.5, 133.5, 132.4, 130.9, 130.2, 128.9, 127.8, 126.9, 126.4, 125.4, 124.4, 124.0, 123.5, 122.8, 121.4, 119.4, 116.7, 116.5, 111.2, 105.5, 92.8, 63.2, 31.3;

HRMS (EI-TOF) calcd for $C_{35}H_{32}ClN_3$ 499.1815, found 499.1814.



3p

2-(*tert*-butyl)-3-(5-fluoro-2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitril e (3p)

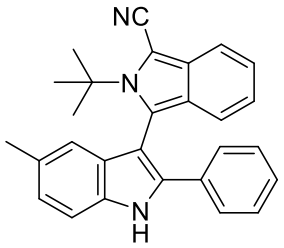
Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3p** 77 mg (75% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (br, 1H), 7.76 (d, *J* =9.0 Hz, 1H), 7.46 (dd, *J* = 9.0, 4.0 Hz, 1H), 7.31–7.28 (m, 4H), 7.18–7.15 (m, 2H), 7.14 (s, 1H), 7.04 (m, 1H), 6.99 (m, 1H), 6.84 (dd, *J* = 9.0, 3.0 Hz, 1H), 1.59 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.8 (d, *J* = 240.0 Hz), 138.6, 133.3, 131.9, 131.4, 131.3 (d, *J* = 10.0 Hz), 129.3, 128.6, 126.3, 126.2, 126.0, 124.0, 122.6, 121.0, 117.6, 117.3, 112.1 (d, *J* = 10.0 Hz), 111.8 (d, *J* = 30.0 Hz), 106.1 (d, *J* = 5.0 Hz),

104.5 (d, *J* = 24.0 Hz), 93.1, 62.8, 31.4;

HRMS (EI-TOF) calcd for $C_{27}H_{22}FN_3$ 407.1798, found 407.1799.



3q

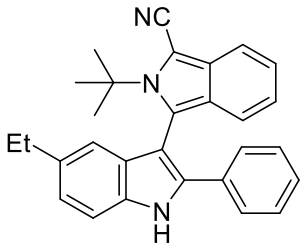
2-(*tert*-butyl)-3-(5-methyl-2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3q)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3q** 87 mg (80% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (br, 1H), 7.77 (m, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.31–7.26 (m, 4H), 7.18–7.15 (m, 3H), 7.13 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.99–6.95 (m, 2H), 2.40 (s, 3H), 1.60 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.7, 133.8, 133.4, 131.8, 131.3, 130.6, 129.2, 128.2, 126.2, 126.1, 125.9, 125.1, 125.0, 122.4, 121.3, 119.2, 117.5, 110.8, 105.6, 92.7, 62.8, 31.4, 21.5;

HRMS (EI-TOF) calcd for $C_{28}H_{25}N_3$ 403.2048, found 403.2044.



3r

2-(*tert*-butyl)-3-(5-ethyl-2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3q)

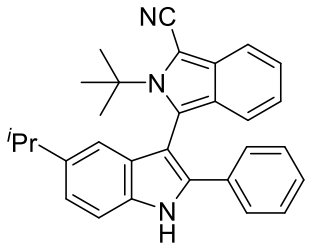
Following the General Procedure, and target product was purified by flash

chromatography (PE/EA = 5/1) to give **3r** 85 mg (76% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (br, 1H), 7.77 (dd, *J* = 9.0, 1.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.31–7.26 (m, 4H), 7.17 (dd, *J* = 8.0, 2.0 Hz, 4H), 7.00–6.95 (m, 2H), 2.69 (m, 2H), 1.62 (s, 9H), 1.24 (t, *J* = 8.0 Hz, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.4, 136.7, 134.0, 133.4, 131.8, 131.2, 129.2, 128.2, 126.2, 126.1, 125.9, 125.2, 123.9, 122.4, 121.4, 118.0, 117.5, 117.5, 110.9, 105.7, 92.8, 62.8, 31.4, 29.0, 16.4;

HRMS (EI-TOF) calcd for $C_{29}H_{27}N_3$ 417.2205, found 417.2204.



3s

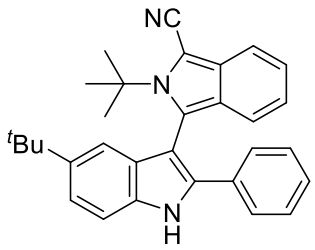
2-(*tert*-butyl)-3-(5-isopropyl-2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3s)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3s** 82 mg (71% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64 (br, 1H), 7.77 (dd, *J* = 9.0, 1.0 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.31–7.26 (m, 4H), 7.21 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.19–7.16 (m, 3H), 7.01 (d, *J* = 2.0 Hz, 1H), 6.98–6.94 (m, 1H), 2.96 (m, 1H), 1.63 (s, 9H), 1.26 (dd, *J* = 7.0, 3.0 Hz, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 142.1, 136.7, 134.1, 133.4, 131.8, 131.2, 129.2, 128.1, 126.2, 126.1, 125.9, 125.2, 122.4, 122.3, 121.4, 117.5, 117.4, 116.6, 110.9, 105.8, 92.8, 62.8, 34.2, 31.4, 24.8, 24.4;

HRMS (EI-TOF) calcd for $C_{30}H_{29}N_3$ 431.2361, found 431.2360.



3t

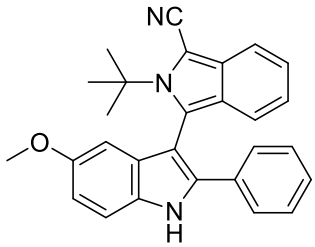
2-(*tert*-butyl)-3-(5-(*tert*-butyl)-2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3t)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3t** 83 mg (70% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.65 (br, 1H), 7.77 (m, 1H), 7.47 (d, *J* = 9.0 Hz, 1H), 7.40 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.30–7.25 (m, 4H), 7.19–7.15 (m, 4H), 6.96 (m, 1H), 1.65 (s, 9H), 1.33 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.4, 136.7, 133.7, 133.4, 131.8, 130.9, 129.2, 128.1, 126.1, 125.9, 125.3, 122.3, 121.6, 121.4, 117.5, 117.4, 115.5, 110.6, 106.1, 92.8, 62.8, 34.7, 31.9, 31.4;

HRMS (EI-TOF) calcd for $C_{31}H_{31}N_3$ 445.2518, found 445.2518.



3u

2-(*tert*-butyl)-3-(5-methoxy-2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3u)

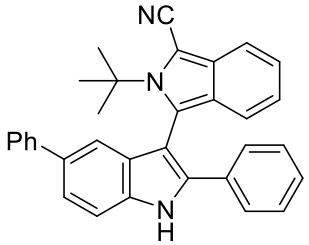
Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 4/1) to give **3u** 93 mg (83% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.70 (br, 1H), 7.77 (dd, *J* = 9.0, 1.0 Hz, 1H), 7.42

(d, *J* = 9.0 Hz, 1H), 7.32–7.26 (m, 3H), 7.25 (s, 1H), 7.19 (m, 1H), 7.17–7.14 (m, 2H), 7.00–6.94 (m, 2H), 6.60 (d, *J* = 2.0 Hz, 1H), 3.74 (s, 3H), 1.61 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 137.4, 133.4, 131.8, 131.4, 130.6, 129.2, 128.2, 126.2, 126.1, 126.0, 125.0, 122.5, 121.3, 117.5, 113.6, 112.1, 105.8, 100.8, 92.8, 62.8, 55.9, 31.4;

HRMS (EI-TOF) calcd for $C_{28}H_{25}N_3O$ 419.1998, found 419.1996.



3v

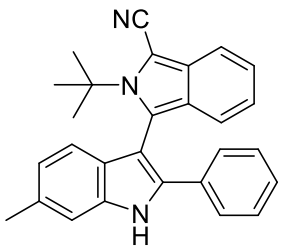
2-(*tert*-butyl)-3-(2,5-diphenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3v)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3v** 104 mg (84% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (br, 1H), 7.78 (dd, *J* = 9.0, 1.0 Hz, 1H), 7.60–7.56 (m, 4H), 7.43–7.39 (m, 3H), 7.30 (m, 5H), 7.20 (m, 3H), 7.00–6.96 (m, 1H), 1.63 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 141.8, 137.4, 135.0, 134.8, 133.4, 131.6, 131.5, 129.3, 128.7, 128.4, 127.3, 126.7, 126.3, 126.2, 126.0, 124.6, 123.1, 122.6, 121.2, 117.8, 117.5, 117.4, 111.5, 106.4, 93.0, 62.8, 31.4;

HRMS (EI-TOF) calcd for $C_{33}H_{27}N_3$ 465.2205, found 465.2204.



3w

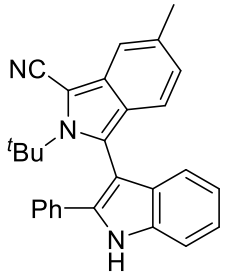
2-(*tert*-butyl)-3-(6-methyl-2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3w)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3w** 70 mg (69% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (br, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.32–7.27 (m, 4H), 7.22 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.15 (d, *J* = 9.0 Hz, 1H), 7.12 (d, *J* = 7.0 Hz, 1H), 7.09–7.03 (m, 2H), 6.98–6.94 (m, 1H), 2.66 (s, 3H), 1.60 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.5, 135.1, 133.3, 131.8, 130.6, 129.2, 128.2, 126.3, 126.3, 125.9, 125.0, 123.9, 122.4, 121.3, 121.3, 120.4, 117.5, 117.4, 106.6, 92.8, 62.8, 31.4, 16.7;

HRMS (EI-TOF) calcd for $C_{28}H_{25}N_3$ 403.2048, found 403.2044.



3x

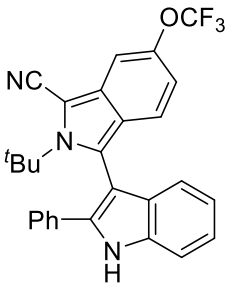
2-(*tert*-butyl)-6-methyl-3-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-1-carbonitrile (3x)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3x** 84 mg (78% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, DMSO-d_6) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.37 (s, 1H), 7.32 (t, *J* = 8.0 Hz, 2H), 7.25 (m, 3H), 7.21 (m, 1H), 7.02 (d, *J* = 4.0 Hz, 2H), 6.85 (d, *J* = 9.0 Hz, 1H), 6.76 (d, *J* = 9.0 Hz, 1H), 2.38 (s, 3H), 1.54 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 136.9, 136.3, 136.2, 133.7, 132.0, 130.8, 129.4, 128.4, 126.6, 126.2, 125.6, 124.3, 123.0, 121.2, 120.9, 119.0, 117.5, 115.7, 112.2, 104.5, 91.3, 62.7, 31.0, 22.1;

HRMS (EI-TOF) calcd for $C_{28}H_{25}N_3$ 403.2048, found 403.2044.



3y

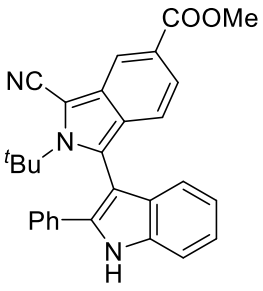
2-(*tert*-butyl)-3-(2-phenyl-1*H*-indol-3-yl)-6-(trifluoromethoxy)-2*H*-isoindole-1-carbonitrile (3y)

Following the General Procedure **1**, and target product was purified by flash chromatography (PE/EA = 4/1) to give **3y** 75 mg (60% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, DMSO-d_6) δ 7.58–7.50 (m, 2H), 7.37–7.32 (m, 2H), 7.29–7.19 (m, 4H), 7.06 (m, 3H), 6.88 (dd, *J* = 9.0, 3.0 Hz, 1H), 1.57 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 137.2, 136.3, 132.1, 131.8, 130.7, 129.5, 128.6, 127.2, 126.6, 124.5, 124.0, 123.1, 121.1, 119.0, 117.6, 116.5, 112.3, 108.3, 103.6, 93.2, 63.7, 30.9;

HRMS (EI-TOF) calcd for $C_{28}H_{22}F_3N_3O$ 473.1715, found 473.1717.



3z

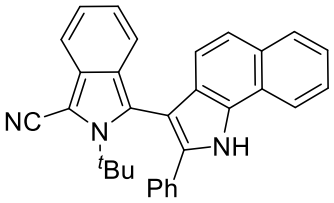
methyl 2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-5-carboxylate (3z)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 3/1) to give **3z** 72 mg (64% yield) as a yellow solid;

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.31 (t, *J* = 1.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.44 (dd, *J* = 9.0, 1.0 Hz, 1H), 7.32 (dd, *J* = 8.0, 7.0 Hz, 2H), 7.28–7.25 (m, 1H), 7.24–7.21 (m, 3H), 7.08–7.02 (m, 3H), 3.89 (s, 3H), 1.58 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.8, 137.3, 136.3, 131.8, 131.7, 130.7, 129.5, 128.6, 127.7, 127.0, 126.8, 126.7, 123.1, 122.0, 121.9, 121.1, 120.6, 119.0, 116.3, 112.3, 103.7, 94.4, 63.9, 52.7, 31.0;

HRMS (EI-TOF) calcd for $C_{29}H_{25}N_3O_2$ 447.1947, found 447.1946.



3ba

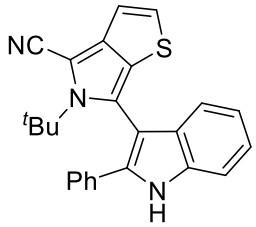
2-(*tert*-butyl)-3-(2-phenyl-1*H*-benzo[*g*]indol-3-yl)-2*H*-isoindole-1-carbonitrile (3ba)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3ba** 80 mg (68% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (br, 1H), 8.03 (d, *J* = 9.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 9.0 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 7.0 Hz, 1H), 7.41–7.37 (m, 1H), 7.33–7.30 (m, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.24–7.19 (m, 3H), 7.19–7.14 (m, 2H), 6.95 (dd, *J* = 8.0, 7.0 Hz, 1H), 1.46 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 137.2, 136.2, 133.8, 132.8, 131.5, 130.1, 123.0, 129.4, 128.9, 128.2, 127.1, 126.7, 126.4, 126.1, 126.1, 125.7, 122.8, 122.6, 121.6, 120.9, 119.3, 117.2, 112.3, 106.5, 91.8, 62.8, 31.1;

HRMS (EI-TOF) calcd for $C_{31}H_{25}N_3$ 439.2048, found 439.2044.



3bb

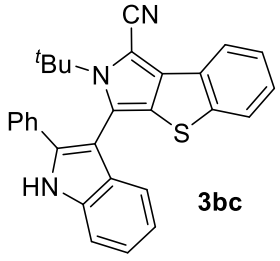
5-(*tert*-butyl)-6-(2-phenyl-1*H*-indol-3-yl)-5*H*-thieno[2,3-*c*]pyrrole-4-carbonitrile (3bb)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 4/1) to give **3bb** 71 mg (72% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.58 (br, 1H), 7.74–7.72 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.30–7.26 (m, 1H), 7.25–7.22 (m, 1H), 7.19–7.14 (m, 2H), 7.12 (t, *J* = 7.0 Hz, 1H), 7.06–7.03 (m, 1H), 6.96 (d, *J* = 4.0 Hz, 2H), 6.91 (dd, *J* = 9.0, 7.0 Hz, 1H), 1.69 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 141.3, 136.4, 136.2, 133.0, 132.0, 129.7, 129.5, 129.1, 128.6, 127.9, 126.7, 123.5, 123.0, 121.0, 119.0, 115.7, 112.3, 105.3, 91.4, 62.6, 31.0;

HRMS (EI-TOF) calcd for $C_{25}H_{21}N_3S$ 395.1456, found 395.1454.



3bc

2-(*tert*-butyl)-3-(2-phenyl-1*H*-indol-3-yl)-2*H*-benzo[4,5]thieno[2,3-*c*]pyrrole-1-carbonitrile (3bc)

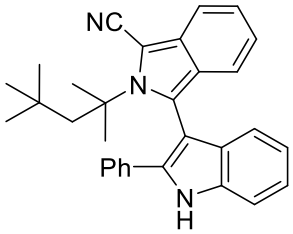
Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 3/1) to give **3bc** 68 mg (63% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.07 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.83 (d, *J* = 8.0

Hz, 1H), 7.54–7.50 (m, 2H), 7.45 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.43–7.39 (m, 3H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.32–7.28 (m, 1H), 7.22 (m, 2H), 7.08 (m, 1H), 1.52 (s, 9H);

^{13}C NMR (126 MHz, DMSO-d_6) δ 144.2, 136.7, 136.3, 135.6, 131.9, 129.7, 129.6, 129.5, 128.6, 127.4, 126.8, 125.9, 125.7, 124.8, 124.3, 123.1, 122.0, 121.0, 119.0, 116.6, 112.3, 104.9, 93.1, 62.9, 31.0;

HRMS (EI-TOF) calcd for $C_{29}H_{23}N_3S$ 445.1613, found 445.1610.



3bd

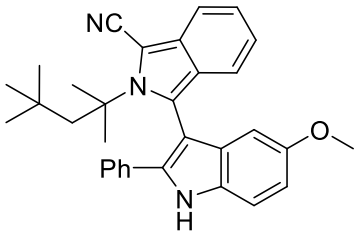
3-(2-phenyl-1*H*-indol-3-yl)-2-(2,4,4-trimethylpentan-2-yl)-2*H*-isoindole-1-carbonitrile (3bd)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 6/1) to give **3bd** 86 mg (77% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (br, 1H), 7.77 (d, *J* = 9.0 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.32–7.28 (m, 5H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.21 (d, *J* = 9.0 Hz, 1H), 7.14 (m, 3H), 7.01 (dd, *J* = 9.0, 7.0 Hz, 1H), 2.55 (d, *J* = 16.0 Hz, 1H), 1.80 (d, *J* = 16.0 Hz, 1H), 1.56 (s, 3H), 1.38 (s, 3H), 0.68 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.2, 135.5, 133.1, 132.0, 130.5, 129.3, 128.4, 126.9, 126.8, 125.8, 124.8, 123.2, 122.5, 121.3, 121.1, 120.0, 117.7, 117.6, 111.2, 106.3, 93.6, 66.6, 55.0, 31.7, 31.6, 31.0, 30.6;

HRMS (EI-TOF) calcd for $C_{31}H_{31}N_3$ 445.2518, found 445.2515.



3be

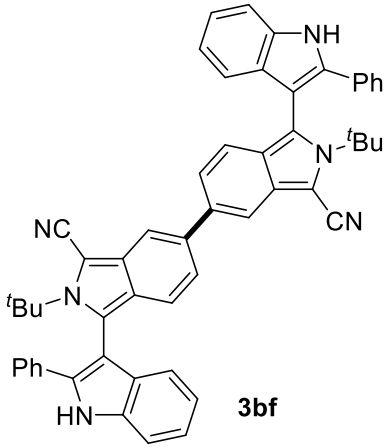
3-(5-methoxy-2-phenyl-1*H*-indol-3-yl)-2-(2,4,4-trimethylpentan-2-yl)-2*H*-isoindole-1-carbonitrile (3be)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 3/1) to give **3be** 96 mg (81% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (br, 1H), 7.78 (d, *J* = 9.0 Hz, 1H), 7.42 (d, *J* = 9.0 Hz, 1H), 7.32 (dd, *J* = 9.0, 7.0 Hz, 1H), 7.28–7.23 (m, 4H), 7.10 (dd, *J* = 7.0, 3.0 Hz, 2H), 7.02 (dd, *J* = 9.0, 7.0 Hz, 1H), 6.95 (dd, *J* = 9.0, 2.0 Hz, 1H), 6.65 (d, *J* = 2.0 Hz, 1H), 3.72 (s, 3H), 2.61 (d, *J* = 16.0 Hz, 1H), 1.77 (d, *J* = 16.0 Hz, 1H), 1.56 (s, 3H), 1.39 (s, 3H), 0.71 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.1, 137.8, 133.2, 132.1, 131.0, 130.5, 129.2, 128.3, 126.8, 126.6, 125.9, 125.1, 122.5, 121.3, 117.7, 113.8, 112.1, 106.0, 101.0, 93.6, 66.6, 55.7, 55.0, 31.8, 31.7, 30.8, 30.7;

HRMS (EI-TOF) calcd for $C_{32}H_{33}N_3O$ 475.2624, found 475.2625.



3bf

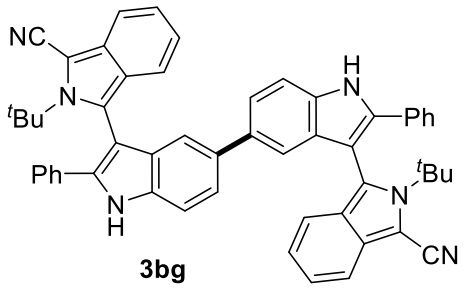
2,2'-di-*tert*-butyl-1,1'-bis(2-phenyl-1*H*-indol-3-yl)-2*H*,2'*H*-[5,5'-biisoindole]-3,3'-dicarbonitrile (3bf)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 1/1) to give **3bf** 56 mg (52% yield) as a yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.92 (br, 1H), 7.78–7.70 (m, 1H), 7.56–7.51 (m, 1H), 7.33–7.28 (m, 4H), 7.19–7.14 (m, 4H), 7.07 (d, *J* = 9.0 Hz, 1H), 6.89 (dd, *J* = 9.0, 2.0 Hz, 1H), 1.59 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.9, 135.5, 133.5, 132.3, 131.5, 130.8, 129.3, 128.4, 126.2, 125.5, 124.4, 123.9, 123.4, 122.9, 121.3, 119.4, 116.8, 116.5, 111.3, 105.3, 92.6, 65.9, 31.3;

HRMS (EI-TOF) calcd for $C_{54}H_{44}N_6$ 776.3627, found 776.3626.



3bg

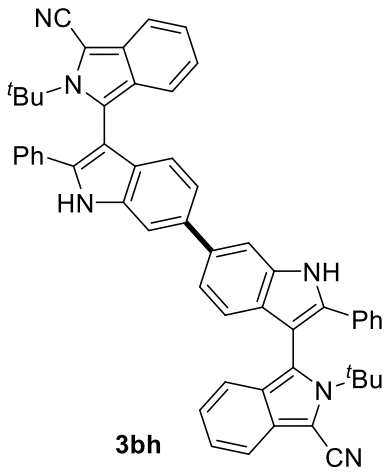
3,3'-(2,2'-diphenyl-1*H*,1'*H*-[5,5'-biindole]-3,3'-diyl)bis(2-(*tert*-butyl)-2*H*-isoindole-1-carbonitrile) (3bh)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 2/1) to give **4a** 56 mg (58% yield) as a yellow solid;

^{1}H NMR (500 MHz, DMSO) δ 7.63 (dd, *J* = 9.0, 1.0 Hz, 1H), 7.56 (d, *J* = 9.0 Hz, 1H), 7.34 (dd, *J* = 8.0, 7.0 Hz, 2H), 7.30–7.27 (m, 2H), 7.22 (m, 3H), 7.05 (d, *J* = 2.0 Hz, 1H), 6.99–6.94 (m, 2H), 1.54 (s, 9H);

^{13}C NMR (126 MHz, DMSO) δ 138.8, 134.7, 133.0, 131.8, 131.5, 129.5, 128.9, 126.7, 126.7, 125.8, 125.5, 125.1, 123.1, 121.2, 118.0, 117.4, 117.1, 113.9, 104.1, 92.5, 63.1, 31.1;

HRMS (EI-TOF) calcd for $C_{54}H_{44}N_6$ 776.3627, found 776.3625.



3bh

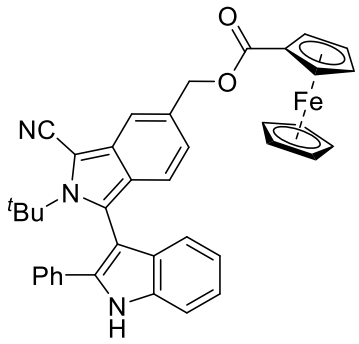
3,3'-(2,2'-diphenyl-1*H*,1'*H*-[6,6'-biindole]-3,3'-diyl)bis(2-(*tert*-butyl)-2*H*-isoindole-1-carbonitrile) (3bh)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 1/1) to give **3bh** 58 mg (60% yield) as a yellow solid;

^{1}H NMR (500 MHz, DMSO) δ 7.60 (d, *J* = 9.0 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.34–7.26 (m, 4H), 7.25–7.19 (m, 3H), 7.06 (d, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 6.96 (dd, *J* = 9.0, 6.0 Hz, 1H), 1.55 (s, 9H);

^{13}C NMR (126 MHz, DMSO) δ 157.6, 138.3, 137.7, 132.7, 131.4, 129.4, 128.9, 127.0, 126.7, 126.7, 126.6, 126.0, 124.3, 123.8, 122.9, 121.5, 121.2, 117.1, 111.6, 103.3, 91.7, 62.9, 31.0;

HRMS (EI-TOF) calcd for $C_{54}H_{44}N_6$ 776.3627, found 776.3622.



4a

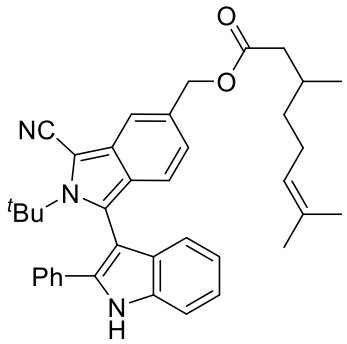
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl) ferronece formate (4a)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 3/1) to give **4a** 42 mg (53% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (br, 1H), 7.84 (s, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.29–7.27 (m, 1H), 7.20–7.15 (m, 4H), 7.14 (dd, *J* = 5.0, 3.0 Hz, 3H), 7.10 (t, *J* = 7.0 Hz, 1H), 7.02 (d, *J* = 9.0 Hz, 1H), 5.39–5.32 (m, 2H), 4.85 (m, 2H), 4.41–4.38 (m, 2H), 4.11–4.08 (m, 5H), 1.56 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 171.7, 136.8, 135.5, 134.4, 133.1, 131.6, 130.9, 129.2, 128.3, 126.2, 125.9, 125.0, 123.3, 123.0, 121.7, 121.2, 119.6, 117.2, 117.0, 111.2, 105.8, 93.2, 71.4, 71.0, 70.3, 69.8, 66.2, 62.9, 31.3.

HRMS (EI-TOF) calcd for $C_{39}H_{33}FeN_3O_2$ 631.1922, found 631.1919.



4b

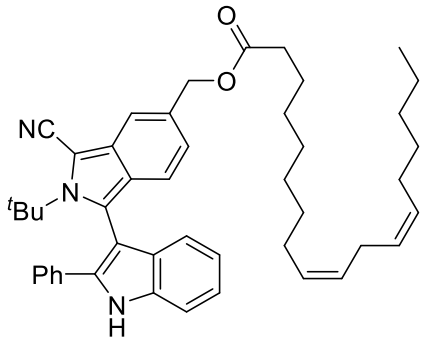
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 3,7-dimethyloct-6-enoate (4b)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 2/1) to give **4b** 45 mg (62% yield) as a pale yellow oil;

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.00 (br, *J* = 7.0 Hz, 1H), 7.75 (s, 1H), 7.54 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.33–7.28 (m, 4H), 7.21 (m, 2H), 7.16 (dd, *J* = 7.0, 5.0 Hz, 3H), 6.92 (dd, *J* = 9.0, 2.0 Hz, 1H), 5.23 (s, 2H), 5.10 (m, 1H), 2.47–2.41 (m, 1H), 2.27–2.21 (m, 1H), 2.05–2.00 (m, 2H), 1.74 (d, *J* = 30.0 Hz, 1H), 1.70–1.66 (m, 3H), 1.60 (d, *J* = 2.0 Hz, 12H), 1.43–1.37 (m, 1H), 1.28 (m, 1H), 0.99 (dd, *J* = 7.0, 2.0 Hz, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.3, 136.8, 135.6, 133.8, 133.1, 131.7, 131.6, 130.9, 130.9, 129.2, 128.3, 126.3, 125.9, 125.1, 124.3, 123.3, 122.7, 121.8, 121.2, 119.5, 117.2, 116.8, 111.3, 105.7, 93.2, 66.6, 63.0, 41.9, 36.8, 31.3, 25.7, 25.4, 19.7, 17.7;

HRMS (EI-TOF) calcd for $C_{33}H_{41}N_3O_2$ 571.3199, found 571.3202.



4c

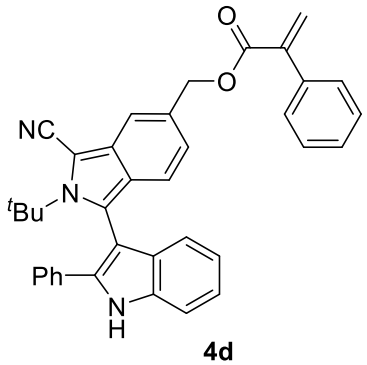
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl (9*Z*,12*Z*)-octadeca-9,12-dienoate (3bh)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 3/1) to give **4c** 55 mg (46% yield) as a pale yellow oil;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.82 (br, *J* = 10.0 Hz, 1H), 7.74 (s, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.32–7.27 (m, 4H), 7.20–7.17 (m, 2H), 7.17–7.12 (m, 3H), 6.92 (dd, *J* = 9.0, 2.0 Hz, 1H), 5.42–5.33 (m, 4H), 5.22 (s, 2H), 2.79 (t, *J* = 7.0 Hz, 2H), 2.41 (t, *J* = 8.0 Hz, 2H), 2.09–2.04 (m, 4H), 1.59 (s, 9H), 1.38–1.29 (m, 16H), 0.91 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.9, 136.8, 135.5, 133.8, 131.6, 130.9, 130.2, 130.1, 129.2, 128.3, 128.1, 128.0, 126.3, 125.9, 125.0, 123.3, 122.7, 121.8, 121.2, 119.5, 117.2, 116.8, 111.3, 105.7, 93.2, 66.6, 63.0, 34.4, 31.5, 31.3, 29.6, 29.4, 29.2, 29.2, 29.1, 27.2, 25.7, 25.0, 22.6, 14.1;

HRMS (EI-TOF) calcd for $C_{46}H_{55}N_3O_2$ 681.4294, found 681.4260.



4d

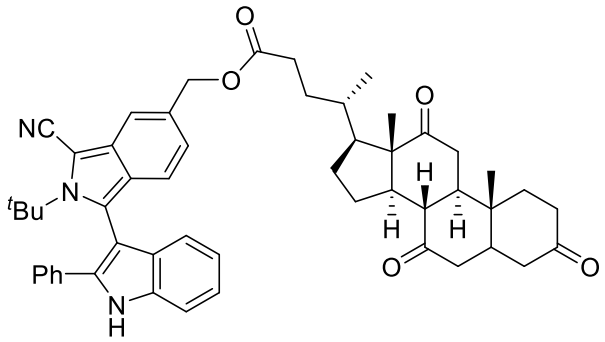
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 2-phenylacrylate (4d)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 3/1) to give **4d** 41 mg (58% yield) as a white solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.70 (br, 1H), 7.66 (t, *J* = 1.0 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.38–7.34 (m, 2H), 7.30–7.28 (m, 1H), 7.27–7.24 (m, 2H), 7.21–7.17 (m, 4H), 7.07 (m, 3H), 7.05–7.02 (m, 2H), 6.84 (dd, *J* = 9.0, 1.0 Hz, 1H), 6.35 (d, *J* = 1.0 Hz, 1H), 5.85 (d, *J* = 1.0 Hz, 1H), 5.27 (s, 2H), 1.49 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.7, 141.2, 136.7, 136.6, 135.5, 133.6, 133.1, 131.6, 130.9, 129.3, 128.8, 128.4, 128.2, 128.2, 127.3, 126.2, 125.9, 125.0, 123.3, 122.7, 121.8, 121.2, 119.6, 117.1, 116.8, 111.2, 105.8, 93.3, 67.3, 63.0, 31.3;

HRMS (EI-TOF) calcd for $C_{37}H_{31}N_3O_2$ 549.2419, found 549.2417.



4e

(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl (4*S*)-4-((8*S*,9*R*,10*R*,13*S*,14*R*,17*S*)-10,13-dimethyl-3,7,12-trioxohexadecahydro-1*H*

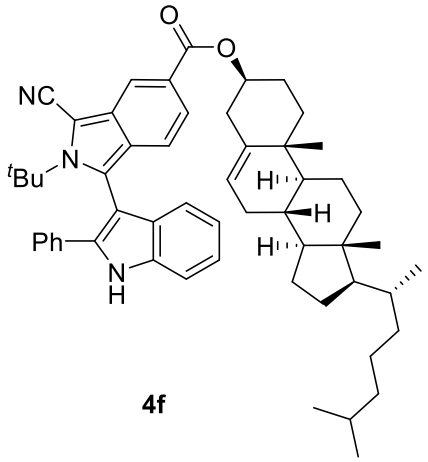
-cyclopenta[*a*]phenanthren-17-yl)pentanoate (4e)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 1/1) to give **4e** 74 mg (31% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (br, *J* = 4.0 Hz, 1H), 7.70 (s, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.29–7.26 (m, 2H), 7.26–7.24 (m, 2H), 7.16–7.14 (m, 2H), 7.13–7.09 (m, 3H), 6.89 (m, 1H), 5.18 (d, *J* = 3.0 Hz, 2H), 2.93–2.86 (m, 2H), 2.85–2.80 (m, 1H), 2.47 (m, 1H), 2.38–2.28 (m, 4H), 2.28–2.21 (m, 3H), 2.19 (d, *J* = 5.0 Hz, 1H), 2.12 (dd, *J* = 13.0, 5.0 Hz, 2H), 2.05–2.00 (m, 3H), 1.94 (m, 2H), 1.89–1.79 (m, 2H), 1.61–1.57 (m, 1H), 1.56 (s, 9H), 1.39 (d, *J* = 1.0 Hz, 3H), 1.31 (m, 2H), 1.06 (d, *J* = 2.0 Hz, 3H), 0.85 (d, *J* = 7.0 Hz, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 212.0, 209.2, 208.8, 174.0, 136.7, 135.5, 133.8, 133.0, 131.6, 130.9, 129.3, 128.4, 126.2, 125.8, 124.9, 123.3, 122.8, 121.7, 121.2, 119.5, 117.1, 116.9, 111.2, 105.8, 93.3, 66.7, 62.9, 56.9, 51.7, 49.0, 46.9, 45.7, 45.5, 45.0, 42.8, 38.6, 36.5, 36.0, 35.5, 35.3, 31.7, 31.3, 30.5, 27.6, 25.1, 21.9, 18.7, 11.9;

HRMS (EI-TOF) calcd for $C_{52}H_{57}N_3O_5$ 803.4298, found 803.4300.



4f

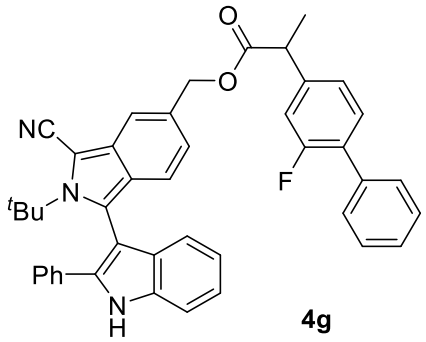
(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindole-5-carboxylate (4f)

Following the General Procedure **1**, and target product was purified by flash chromatography (PE/EA = 3/1) to give **4f** 80 mg (40% yield) as a white solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.89 (d, *J* = 11.7 Hz, 1H), 8.56 (br, 1H), 7.58–7.52 (m, 2H), 7.32–7.26 (m, 4H), 7.16 (m, 5H), 5.45 (d, *J* = 5.0 Hz, 1H), 4.93 (m, 1H), 2.52 (t, *J* = 10.0 Hz, 2H), 2.08–2.00 (m, 3H), 1.96 (m, 1H), 1.89–1.78 (m, 2H), 1.67 (d, *J* = 4.0 Hz, 2H), 1.61 (s, 9H), 1.59–1.47 (m, 6H), 1.34 (s, 6H), 1.25–1.18 (m, 3H), 1.12 (s, 3H), 1.08–0.99 (m, 4H), 0.95 (d, *J* = 6.0 Hz, 3H), 0.89 (dd, *J* = 7.0, 2.0 Hz, 6H), 0.72 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.5, 139.8, 137.0, 135.5, 132.1, 131.6, 130.8, 129.2, 128.4, 128.3, 127.6, 126.3, 125.1, 123.4, 122.7, 122.2, 121.3, 121.3, 121.2, 119.4, 116.6, 111.3, 105.4, 95.0, 63.5, 56.7, 56.2, 50.3, 50.1, 42.4, 39.8, 39.5, 38.3, 37.1, 36.7, 36.2, 35.8, 32.0, 31.9, 31.3, 29.6, 28.3, 28.0, 28.0, 23.9, 22. 6, 21.1, 19.4, 18.7, 11.9;

HRMS (EI-TOF) calcd for $C_{55}H_{67}N_3O_2$ 801.5233, found 801.5234.



4g

(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (4g)

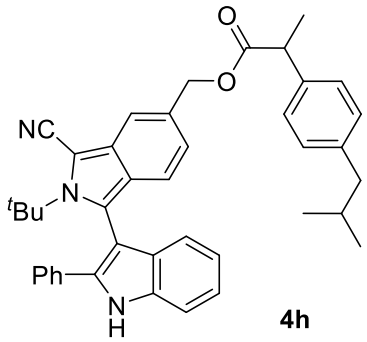
Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 3/1) to give **4g** 73 mg (45% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (br, 1H), 7.72 (d, *J* = 1.0 Hz, 1H), 7.55 (t, *J* = 2.0 Hz, 1H), 7.46–7.36 (m, 5H), 7.32–7.30 (m, 1H), 7.28–7.25 (m, 3H), 7.21–7.15 (m, 6H), 7.14–7.10 (m, 2H), 6.86–6.83 (m, 1H), 5.29 (dd, *J* = 13.0, 3.4 Hz, 1H), 5.21 (dd,

J = 13.0, 2.0 Hz, 1H), 3.88 (q, *J* = 7.0 Hz, 1H), 1.60 (d, *J* = 7.0 Hz, 3H), 1.59 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 174.0, 159.7 (d, *J* = 250 Hz), 141.7 (d, *J* = 8 Hz), 136.7, 135.5, 135.5, 133.5, 133.0, 131.6, 130.9, 130.8, 129.2, 129.0 (d, *J* = 2 Hz), 128.4, 128.3, 127.8 (d, *J* = 14 Hz), 127.6, 126.2, 125.8, 125.0, 123.7, 123.6, 123.3, 122.5, 121.8, 121.2, 119.5, 116.7 (d, *J* = 38 Hz), 115.3 (d, *J* = 24 Hz), 111.2, 105.7, 93.3, 67.2, 63.0, 45.1, 31.3, 18.5;

HRMS (EI-TOF) calcd for $C_{43}H_{36}FN_3O_2$ 645.2792, found 645.2793.



4h

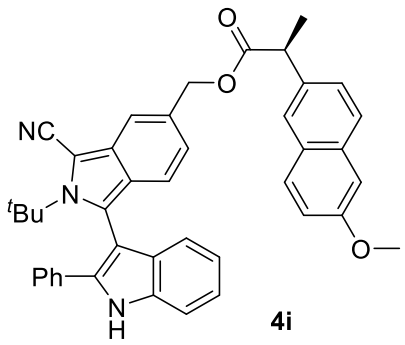
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 2-(4-isobutylphenyl)propanoate (4h)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 3/1) to give **4h** 87 mg (59% yield) as a white solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.70 (br, 1H), 7.57 (d, *J* = 2.0 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.22–7.17 (m, 4H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.07 (m, 2H), 7.06–7.02 (m, 2H), 7.00 (dd, *J* = 8.0, 2.0 Hz, 2H), 6.98–6.96 (m, 1H), 6.68 (m, 1H), 5.14 (dd, *J* = 13.0, 5.0 Hz, 1H), 5.06 (dd, *J* = 13.0, 4.0 Hz, 1H), 3.73–3.68 (m, 1H), 2.34 (d, *J* = 7.0 Hz, 2H), 1.73 (m, 1H), 1.48 (d, *J* = 1.0 Hz, 9H), 1.45 (d, *J* = 7.0 Hz, 3H), 0.78 (d, *J* = 7.0 Hz, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 174.7, 140.6, 137.6, 136.7, 135.5, 133.8, 133.0, 131.6, 130.9, 129.4, 129.3, 128.3, 127.2, 126.2, 125.8, 124.9, 123.3, 122.4, 121.6, 121.2, 119.6, 117.1, 116.5, 111.2, 105.8, 93.3, 66.9, 62.9, 45.2, 45.0, 31.3, 30.2, 22.4, 18.5;

HRMS (EI-TOF) calcd for $C_{41}H_{41}N_3O_2$ 607.3199, found 607.3121.



4i

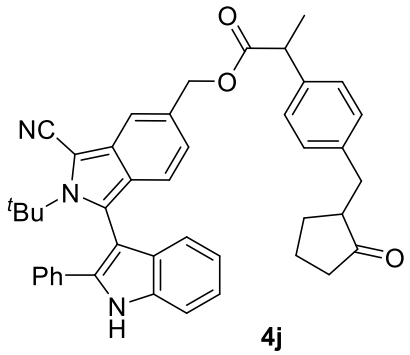
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl (*S*)-2-(6-methoxynaphthalen-2-yl)propanoate (4i)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 2/1) to give **4i** 93 mg (59% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.87 (br, 1H), 7.74–7.66 (m, 4H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.48–7.44 (m, 1H), 7.29 (dd, *J* = 12.0, 5.0 Hz, 4H), 7.16 (m, 4H), 7.12–7.08 (m, 2H), 7.06 (d, *J* = 9.0 Hz, 1H), 6.80 (dd, *J* = 9.0, 4.0 Hz, 1H), 5.29–5.15 (m, 2H), 3.98 (q, *J* = 7.0 Hz, 1H), 3.91 (t, *J* = 1.0 Hz, 3H), 1.64 (d, *J* = 7.0 Hz, 3H), 1.59 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 174.7, 157.6, 136.7, 135.6, 135.5, 133.7, 133.0, 131.6, 130.90, 129.3, 129.2, 128.9, 128.3, 127.3, 126.3, 126.2, 126.0, 125.8, 124.9, 123.3, 122.5, 121.7, 121.2, 119.5, 118.9, 117.1, 116.6, 111.2, 105.8, 105.7, 93.3, 67.0, 62.9, 55.3, 45.5, 31.3, 14.2;

HRMS (EI-TOF) calcd for $C_{42}H_{37}N_3O_3$ 631.2835, found 631.2833.



4j

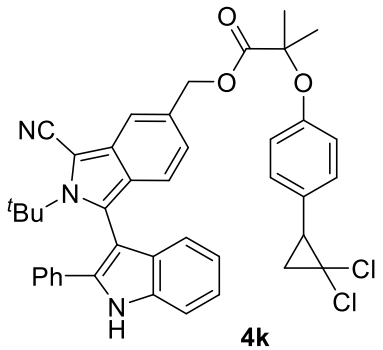
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 2-(4-((2-oxocyclopentyl)methyl)phenyl)propanoate (4j)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 1/1) to give **4j** 76 mg (47% yield) as a pale yellow oil;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.99–8.94 (br, 1H), 7.67 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.31–7.29 (m, 2H), 7.28–7.23 (m, 4H), 7.20–7.16 (m, 2H), 7.16–7.08 (m, 4H), 7.07–7.03 (m, 1H), 6.78–6.71 (m, 1H), 5.20 (m, 2H), 3.81 (m, 1H), 3.11 (m, 1H), 2.47 (m, 1H), 2.36–2.27 (m, 2H), 2.12 (m, 1H), 2.05 (m, 1H), 1.91 (m, 1H), 1.67 (m, 1H), 1.59 (d, *J* = 1.9 Hz, 9H), 1.54 (d, *J* = 1.1 Hz, 4H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 174.6, 138.9, 138.2, 136.7, 135.6, 133.7, 133.0, 131.7, 130.9, 129.2, 128.3, 127.6, 126.3, 125.8, 125.1, 123.3, 122.3, 121.7, 121.1, 119.5, 117.2, 116.4, 111.3, 105.6, 93.8, 66.9, 62.9, 51.0, 45.2, 38.2, 35.2, 31.3, 20.5, 18.5, 14.2;

HRMS (EI-TOF) calcd for $C_{43}H_{41}N_3O_3$ 647.3148, found 647.3143.



4k

(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 2-(4-(2,2-dichlorocyclopropyl)phenoxy)-2-methylpropanoate (4k)

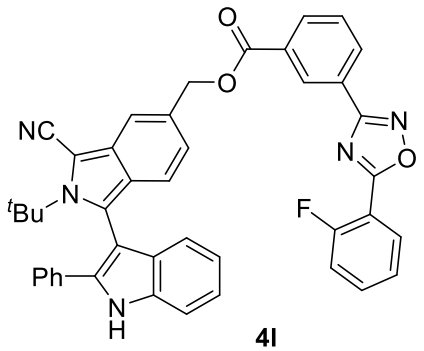
Following the General Procedure **1**, and target product was purified by flash chromatography (PE/EA = 2/1) to give **4k** 65 mg (38% yield) as a pale yellow oil;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (br, 1H), 7.65 (q, *J* = 2.0, 2.0 Hz, 1H), 7.50 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.30–7.26 (m, 2H), 7.25 (d, *J* = 2.0 Hz, 1H), 7.17–7.12 (m, 4H), 7.04 (m, 3H), 6.81–6.76 (m, 2H), 6.76–6.73 (m, 1H), 5.26 (d, *J* = 2.0 Hz, 2H),

2.76 (m, 1H), 1.84 (m Hz, 1H), 1.69 (q, *J* = 8.0 Hz, 1H), 1.63 (d, *J* = 2.0 Hz, 6H), 1.57 (d, *J* = 1.0 Hz, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 174.12 154.9, 154.9, 136.7, 135.5, 133.0, 132.9, 131.6, 130.9, 129.7, 129.3, 128.4, 128.5, 126.2, 125.8, 124.9, 123.4, 122.7, 121.7, 121.3, 119.5, 118.7, 117.2, 117.0, 111.2, 105.8, 93.4, 67.7, 63.0, 60.9, 34.8, 31.3, 25.8, 25.5, 25.4.

HRMS (EI-TOF) calcd for $C_{41}H_{37}Cl_2N_3O_3$ 689.2212, found 689.2211.



4l

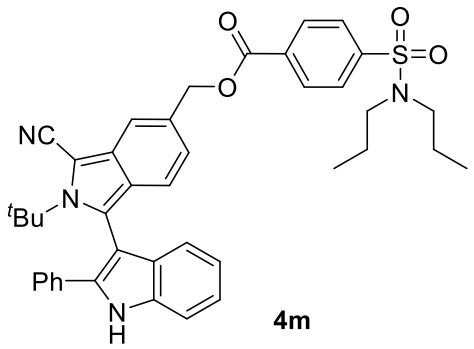
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 3-(5-(2-fluorophenyl)-1,2,4-oxadiazol-3-yl)benzoate (4l)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 1/1) to give **4l** 70 mg (41% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (br, 1H), 8.28 (m, 1H), 8.19–8.12 (m, 2H), 7.75 (t, *J* = 1.0 Hz, 1H), 7.50 (m, 2H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.25 (m, 1H), 7.21–7.18 (m, 2H), 7.17–7.12 (m, 4H), 7.11–7.05 (m, 4H), 7.02 (m, 1H), 6.95 (dd, *J* = 9.0, 1.0 Hz, 1H), 5.41 (s, 2H), 1.48 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.1, 168.1, 165.9, 161.1 (d, *J* = 260 Hz), 136.8, 135.5, 134.7 (d, *J* = 8 Hz), 133.6, 133.1, 132.4, 131.9, 131.6, 131.1, 131.0, 130.9, 129.2, 129.1, 128.9, 128.3, 127.3, 126.3, 126.0, 125.1, 124.8 (d, *J* = 4 Hz), 123.2 (d, *J* = 40 Hz), 121.9, 121.2, 119.5, 117.4, 117.3, 117.1 (d, *J* = 5 Hz), 112.8 (d, *J* = 12 Hz), 111.2, 105.7, 93.4, 67.6, 63.0, 31.3;

HRMS (EI-TOF) calcd for $C_{43}H_{32}FN_5O_3$ 685.2489, found 685.2488.



4m

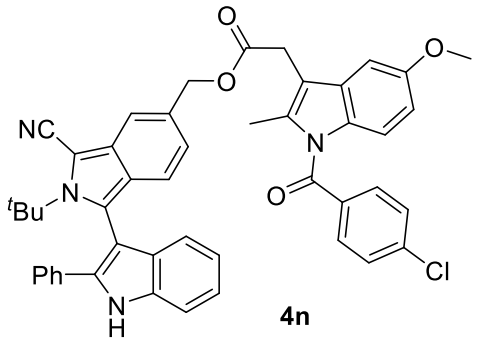
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 4-(*N*,*N*-dipropylsulfamoyl)benzoate (4m)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 1/1) to give **4m** 70 mg (46% yield) as a white solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.91 (br, 1H), 8.22 (d, *J* = 8.0 Hz, 2H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.82 (s, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.28 (t, *J* = 7.0 Hz, 4H), 7.21–7.12 (m, 5H), 7.01 (d, *J* = 9.0 Hz, 1H), 5.48 (s, 2H), 3.14–3.08 (m, 4H), 1.59 (s, 9H), 1.55 (dd, *J* = 15.0, 8.0 Hz, 4H), 0.89 (t, *J* = 7.0 Hz, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.2, 144.3, 136.8, 135.5, 133.5, 133.2, 133.0, 131.6, 130.9, 130.4, 129.2, 128.3, 127.0, 126.2, 125.9, 125.2, 123.3, 122.8, 122.0, 121.2, 119.5, 117.3, 117.1, 111.3, 105.6, 93.4, 67.9, 50.0, 31.3, 22.0, 11.2;

HRMS (EI-TOF) calcd for $C_{41}H_{42}N_4O_4S$ 686.2927, found 686.2925.



4n

(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)acetate (4n)

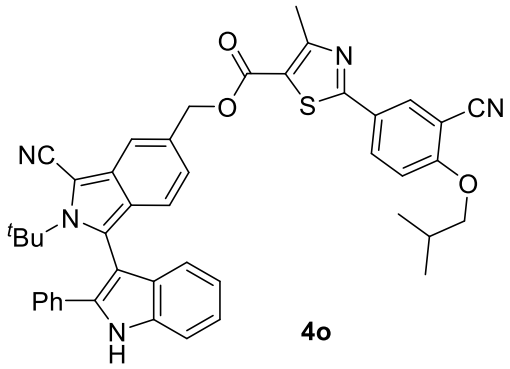
Following the General Procedure, and target product was purified by flash

chromatography (PE/EA = 3/1) to give **4n** 71 mg (31% yield) as a white solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.86 (br, 1H), 7.73 (s, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.32–7.27 (m, 4H), 7.16 (m, 4H), 7.11 (d, *J* = 9.0 Hz, 1H), 6.98 (d, *J* = 3.0 Hz, 1H), 6.91–6.85 (m, 2H), 6.67 (dd, *J* = 9.0, 3.0 Hz, 1H), 5.25 (s, 2H), 3.77 (s, 2H), 3.74 (s, 3H), 2.40 (s, 3H), 1.59 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.8, 168.3, 156.1, 139.2, 136.7, 136.0, 135.5, 133.9, 133.4, 133.0, 131.6, 131.2, 130.9, 130.8, 130.6, 129.2, 129.1, 128.4, 126.2, 125.8, 125.0, 123.4, 122.6, 121.8, 121.2, 119.5, 117.0, 116.9, 115.0, 112.5, 112.0, 111.2, 105.7, 101.1, 93.3, 67.3, 63.0, 55.6, 31.3, 30.4, 13.4;

HRMS (EI-TOF) calcd for $C_{47}H_{39}ClN_4O_4$ 758.2660, found 758.2665.



4o

(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 2-(3-cyano-4-isobutoxyphenyl)-4-methylthiazole-5-carboxylate (4o)

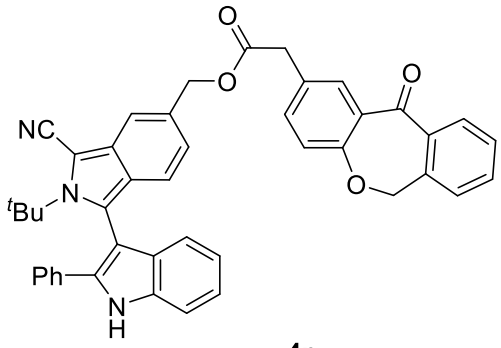
Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 1/1) to give **4o** 61 mg (35% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.90 (br, 1H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.99 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.69 (s, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.17 (d, *J* = 7.0 Hz, 4H), 7.11–7.08 (m, 2H), 7.07–7.01 (m, 3H), 6.94–6.88 (m, 2H), 5.32 (s, 2H), 3.81 (d, *J* = 6.0 Hz, 2H), 2.70 (s, 3H), 2.11 (m, 1H), 1.49 (s, 9H), 1.00 (d, *J* = 7.0 Hz, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 167.5, 162.5, 161.9, 161.7, 136.8, 135.5, 133.3, 133.0, 132.7, 132.1, 131.6, 130.9, 129.2, 128.3, 126.2, 126.0, 125.9, 125.1, 123.3, 122.7, 122.0, 121.5, 121.2, 119.5, 117.1, 117.1, 115.4, 112.6, 111.7, 105.6, 103.0, 93.4,

67.5, 63.0, 31.3, 28.2, 19.1, 17.6;

HRMS (EI-TOF) calcd for $C_{44}H_{39}N_5O_3S$ 717.2774, found 717.2775.



4p

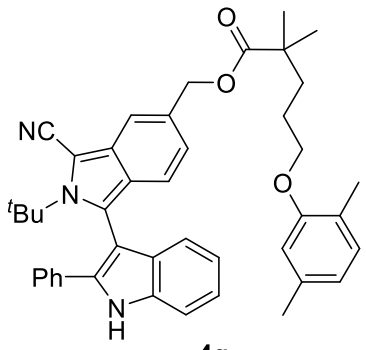
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 2-(11-oxo-6,11-dihydrodibenzo[*b*,*e*]oxepin-2-yl)acetate (4p)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 1/1) to give **4p** 84 mg (50% yield) as a pale yellow oil;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.78 (br, 1H), 8.06 (d, *J* = 2.0 Hz, 1H), 7.79 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.61 (t, *J* = 1.0 Hz, 1H), 7.48–7.45 (m, 1H), 7.42–7.40 (m, 1H), 7.38–7.35 (m, 2H), 7.27 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.20–7.18 (m, 1H), 7.18–7.15 (m, 3H), 7.09–7.05 (m, 3H), 7.04–7.01 (m, 2H), 6.95 (d, *J* = 9.0 Hz, 1H), 6.80 (dd, *J* = 9.0, 1.0 Hz, 1H), 5.14 (s, 2H), 5.08 (s, 2H), 3.64 (s, 2H), 1.48 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 190.9, 171.4, 140.5, 136.8, 136.5, 135.6, 135.5, 133.4, 133.0, 132.8, 132.6, 131.6, 131.0, 129.5, 129.2, 128.3, 127.8, 127.7, 126.2, 125.9, 125.2, 125.0, 123.3, 122.7, 121.8, 121.2, 121.1, 119.5, 117.1, 117.0, 111.2, 105.7, 93.3, 73.6, 67.3, 63.0, 40.2, 31.3;

HRMS (EI-TOF) calcd for $C_{44}H_{35}N_3O_4$ 669.2628, found 669.2629.



4q

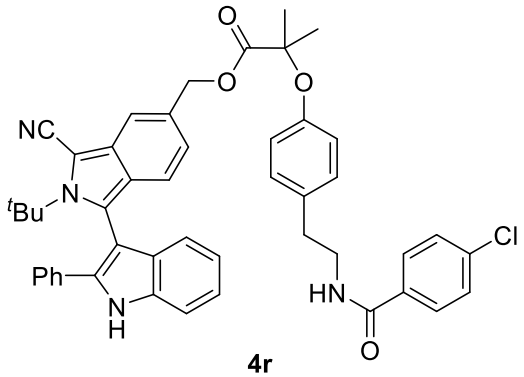
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (4q)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 2/1) to give **4q** 83 mg (51% yield) as a pale yellow oil;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (br, 1H), 7.55 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.17–7.12 (m, 4H), 7.02 (d, *J* = 8.0 Hz, 3H), 6.97 (dd, *J* = 13.0, 8.0 Hz, 2H), 6.81 (s, 1H), 6.74 (d, *J* = 9.0 Hz, 1H), 6.49 (d, *J* = 8.0 Hz, 1H), 6.45 (s, 1H), 5.09–5.01 (m, 2H), 3.79–3.72 (m, 2H), 2.14 (s, 3H), 1.98 (s, 3H), 1.46 (s, 4H), 1.43 (s, 9H), 1.13 (s, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 177.7, 157.0, 136.7, 136.4, 135.4, 134.1, 133.0, 131.6, 130.9, 130.2, 129.3, 128.4, 126.2, 125.8, 124.8, 123.6, 123.4, 122.4, 121.6, 121.2, 120.6, 119.6, 117.0, 116.4, 112.0, 111.1, 105.9, 93.3, 67.9, 66.6, 62.9, 42.3, 37.2, 31.3, 25.2, 25.1, 21.4, 15.8;

HRMS (EI-TOF) calcd for $C_{43}H_{45}N_3O_3$ 651.3461, found 651.3460.



4r

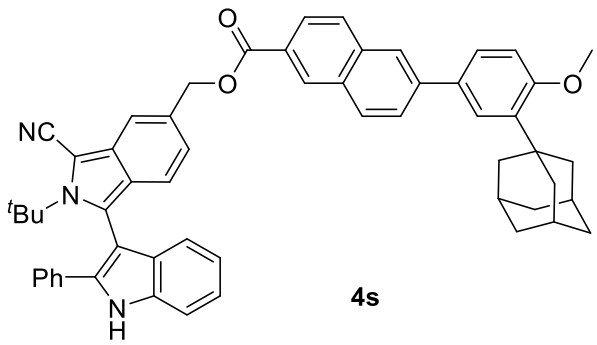
(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 2-(4-(2-(4-chlorobenzamido)ethyl)phenoxy)-2-methylpropanoate (4r)

Following the General Procedure, and target product was purified by flash chromatography (PE/EA = 1/1) to give **4r** 88 mg (46% yield) as a white solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (br, 1H), 7.55 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.17–7.12 (m, 4H), 7.02 (d, *J* = 8.0 Hz, 3H), 6.97 (dd, *J* = 13.0, 8.0 Hz, 2H), 6.81 (s, 1H), 6.74 (d, *J* = 9.0 Hz, 1H), 6.49 (d, *J* = 8.0 Hz, 1H), 6.45 (br, 1H), 5.09–5.01 (m, 2H), 3.79–3.72 (m, 2H), 2.14 (s, 3H), 1.98 (s, 3H), 1.46 (s, 4H), 1.43 (s, 9H), 1.13 (s, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 174.3, 166.5, 154.1, 137.6, 136.8, 135.6, 133.2, 133.0, 132.9, 132.4, 131.6, 130.8, 129.6, 129.2, 128.8, 128.3, 126.2, 125.9, 125.2, 123.3, 122.6, 121.7, 121.2, 119.4, 119.3, 117.1, 116.9, 111.3, 105.6, 93.2, 67.6, 63.0, 41.1, 34.5, 31.3, 25.5, 25.4;

HRMS (EI-TOF) calcd for $C_{47}H_{43}ClN_4O_4$ 762.2973, found 762.2977.



4s

(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 6-(3-((3*r*,5*r*,7*r*)-adamantan-1-yl)-4-methoxyphenyl)-2-naphthoate (4s)

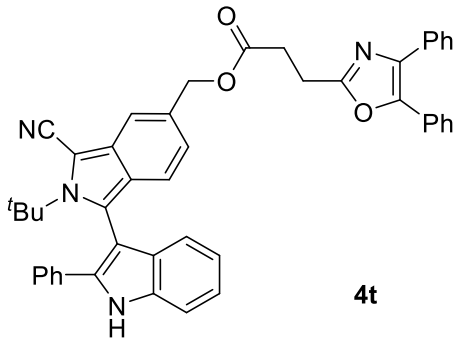
Following the General Procedure **1**, and target product was purified by flash chromatography (PE/EA = 2/1) to give **4s** 52 mg (51% yield) as a pale yellow solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (br, 1H), 8.69 (s, 1H), 8.14 (dd, *J* = 9.0, 2.0 Hz, 1H), 8.05 – 8.03 (m, 1H), 8.01 (d, *J* = 9.0 Hz, 1H), 7.94 (d, *J* = 9.0 Hz, 1H), 7.90 (t, *J* = 1.0 Hz, 1H), 7.81 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.63 (d, *J* = 2.0 Hz, 1H), 7.57 (dd, *J*

= 8.0, 2.0 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.33 – 7.28 (m, 4H), 7.22–7.18 (m, 4H), 7.15 (m, 1H), 7.10 (dd, *J* = 9.0, 1.0 Hz, 1H), 7.02 (d, *J* = 9.0 Hz, 1H), 5.54 (s, 2H), 3.93 (s, 3H), 2.22 (d, *J* = 3.0 Hz, 6H), 2.13 (s, 3H), 1.84 (d, *J* = 3.0 Hz, 6H), 1.61 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.8, 158.9, 141.4, 139.0, 136.7, 136.1, 135.5, 133.9, 133.1, 132.6, 131.6, 131.3, 131.1, 130.9, 129.8, 129.3, 128.4, 128.3, 126.9, 126.5, 126.2, 126.0, 125.9, 125.8, 125.7, 124.9, 124.7, 123.4, 123.0, 121.8, 121.3, 119.6, 117.2, 117.1, 112.1, 111.2, 105.8, 93.4, 67.4, 63.0, 55.2, 40.6, 37.2, 37.2, 31.3, 29.1;

HRMS (EI-TOF) calcd for $C_{56}H_{51}N_3O_3$ 813.3930, found 813.3933.



4t

(2-(*tert*-butyl)-3-cyano-1-(2-phenyl-1*H*-indol-3-yl)-2*H*-isoindol-5-yl)methyl 3-(4,5-diphenyloxazol-2-yl)propanoate (4t)

Following the General Procedure **1**, and target product was purified by flash chromatography (PE/EA = 1/1) to give **4t** 76 mg (44% yield) as a pale yellow oil;

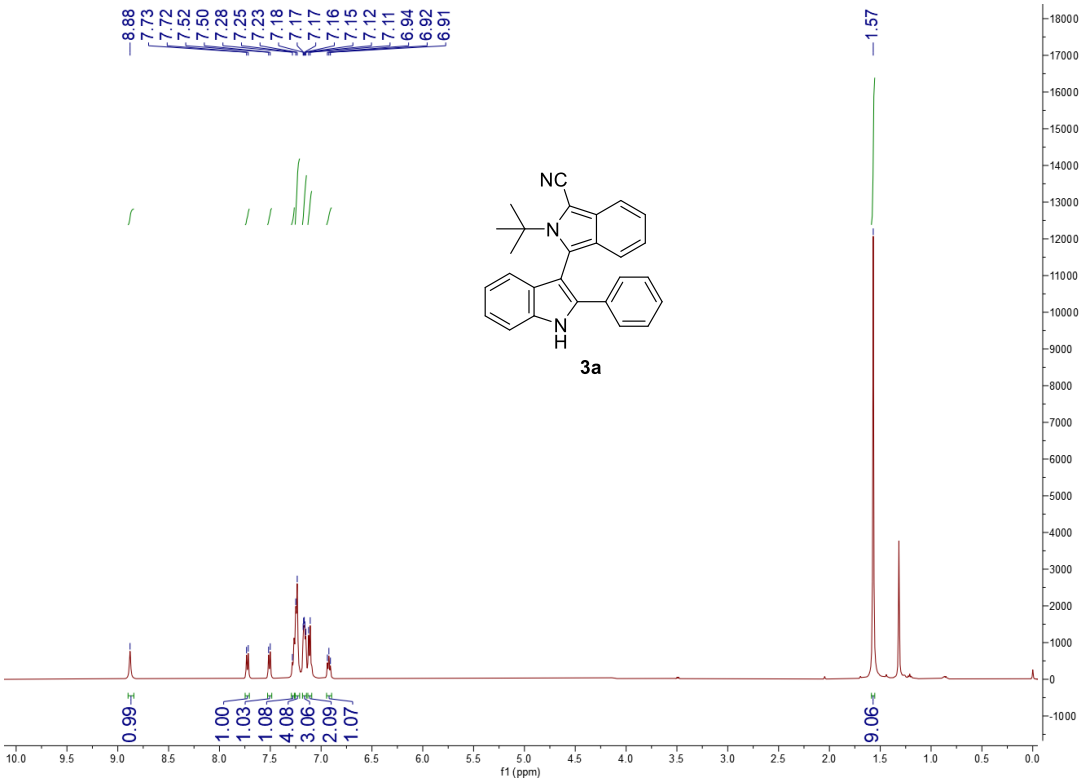
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.89 (br, 1H), 7.71 (t, *J* = 1.0 Hz, 1H), 7.62–7.59 (m, 2H), 7.56–7.52 (m, 2H), 7.50 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.33–7.26 (m, 7H), 7.25–7.22 (m, 3H), 7.16–7.13 (m, 2H), 7.11–7.08 (m, 2H), 7.03 (dd, *J* = 9.0, 1.0 Hz, 1H), 6.87 (dd, *J* = 9.0, 1.0 Hz, 1H), 5.24 (s, 2H), 3.21 (t, *J* = 8.0 Hz, 2H), 2.98 (t, *J* = 8.0 Hz, 2H), 1.56 (s, 9H);

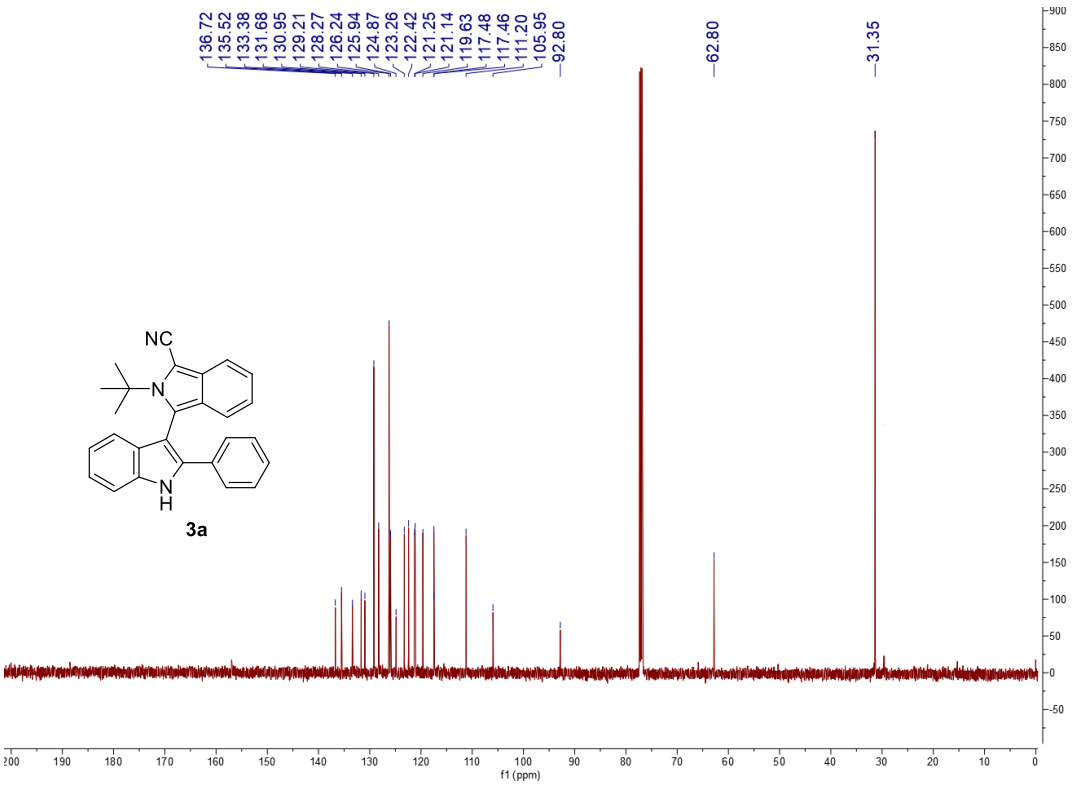
^{13}C NMR (126 MHz, $CDCl_3$) δ 172.0, 161.7, 145.5, 136.8, 135.5, 135.1, 133.5, 133.0, 132.4, 131.6, 130.9, 129.2, 129.0, 128.6, 128.5, 128.4, 128.3, 128.0, 127.9,

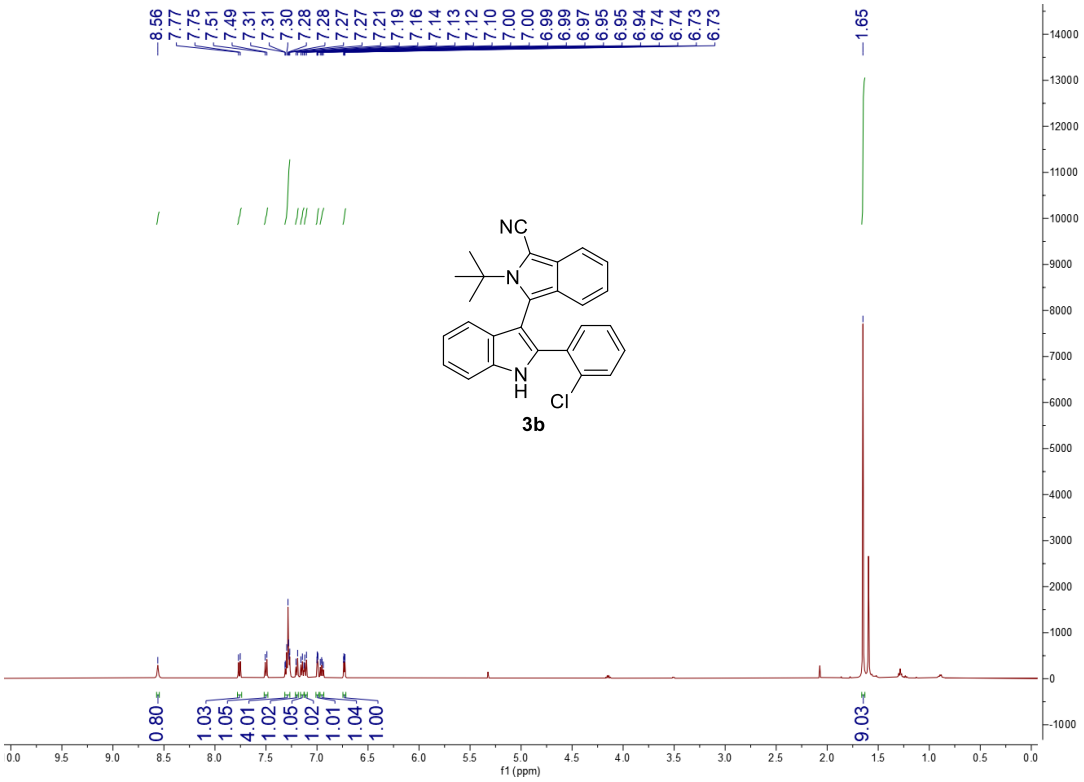
126.5, 126.3, 125.9, 125.0, 123.3, 122.7, 121.8, 121.2, 119.6, 117.1, 117.0, 111.2, 105.7, 93.3, 67.2, 63.0, 31.3, 31.2, 23.6;

HRMS (EI-TOF) calcd for $C_{46}H_{38}N_4O_3$ 694.2944, found 694.2940.

9. The ^{1}H and ^{13}C NMR spectra of compounds



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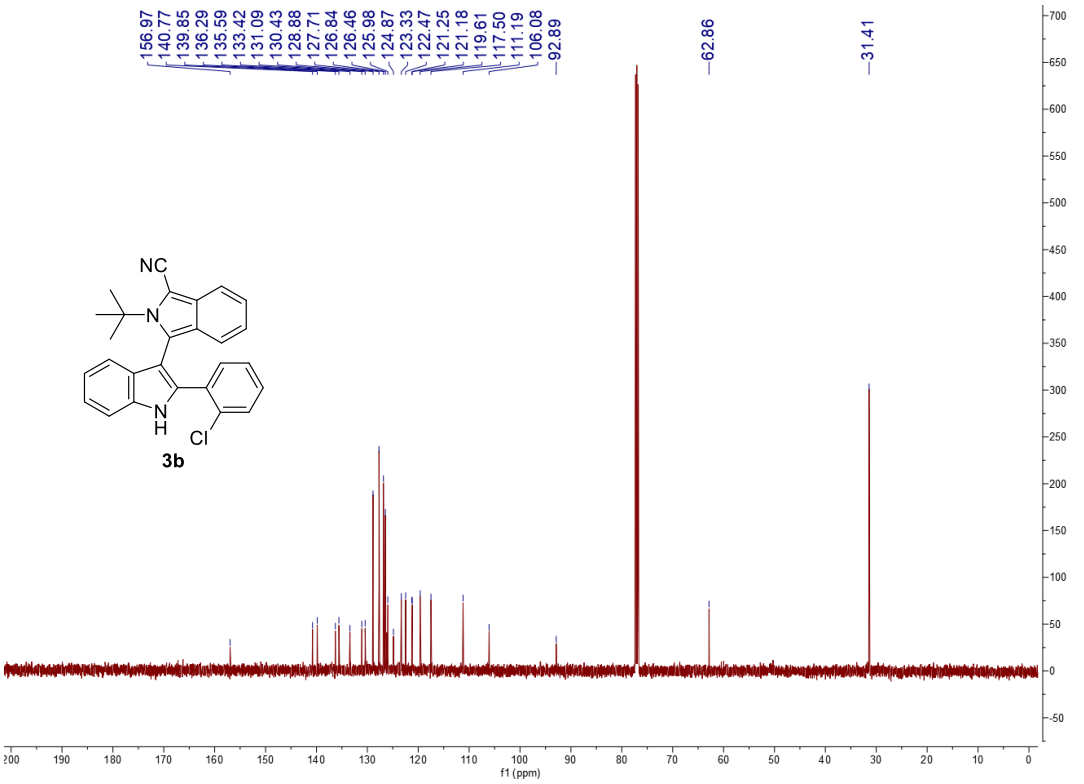
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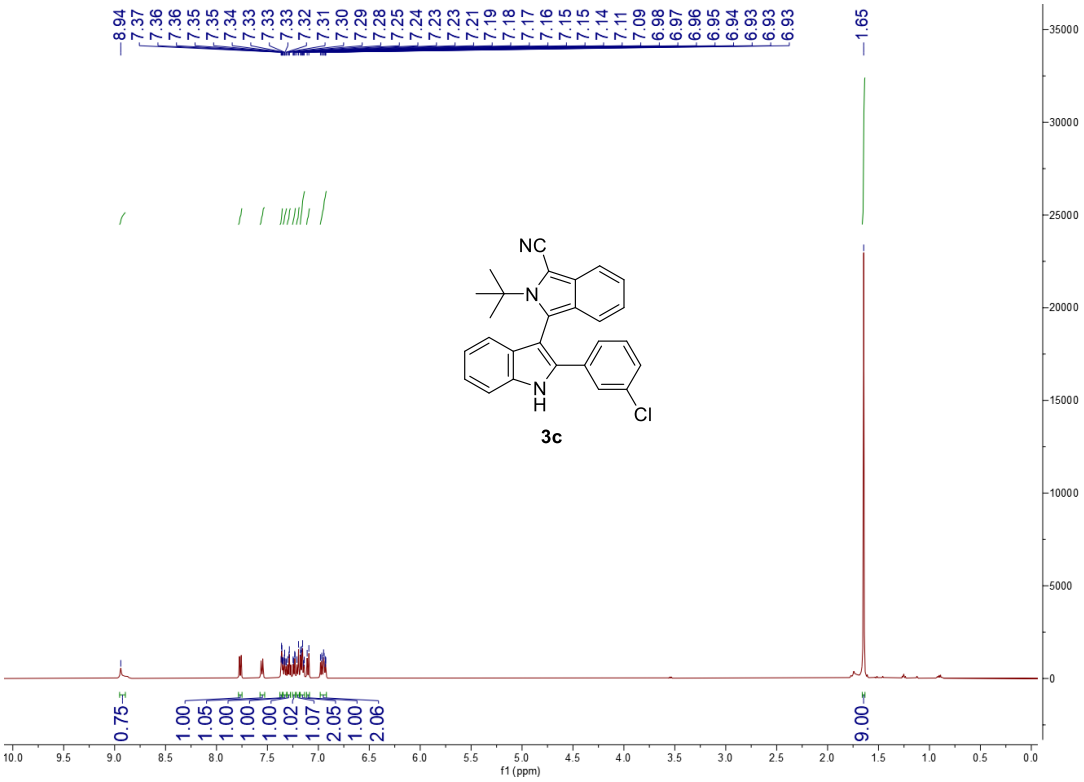
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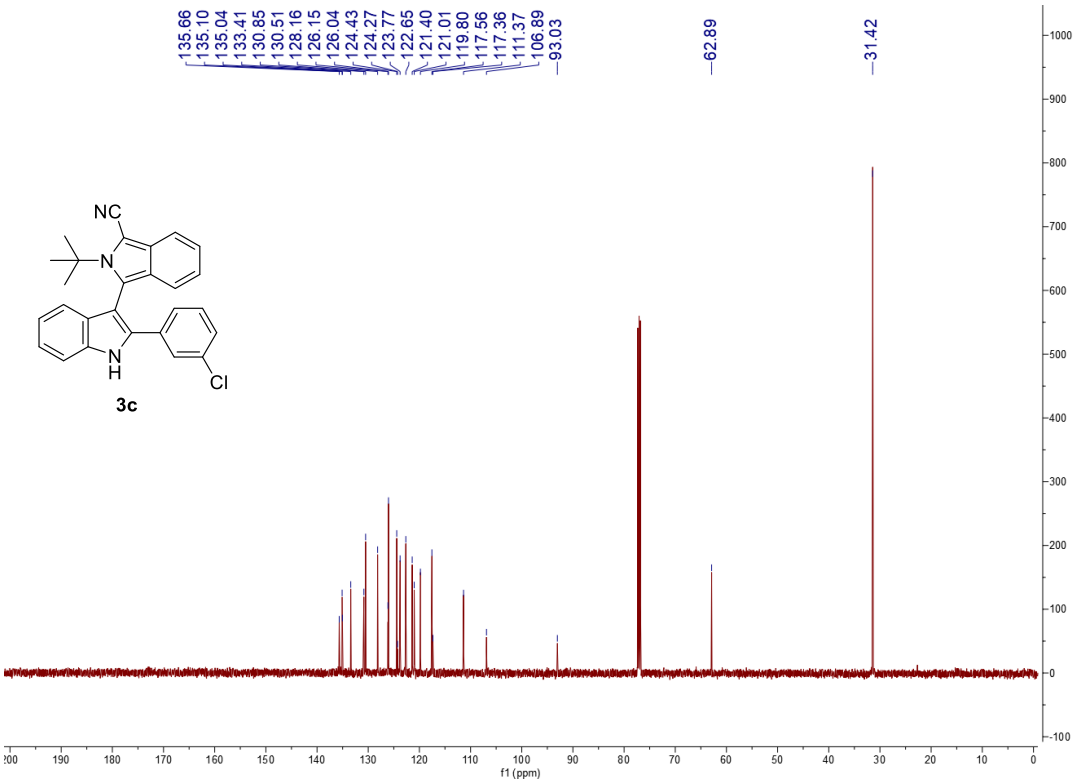
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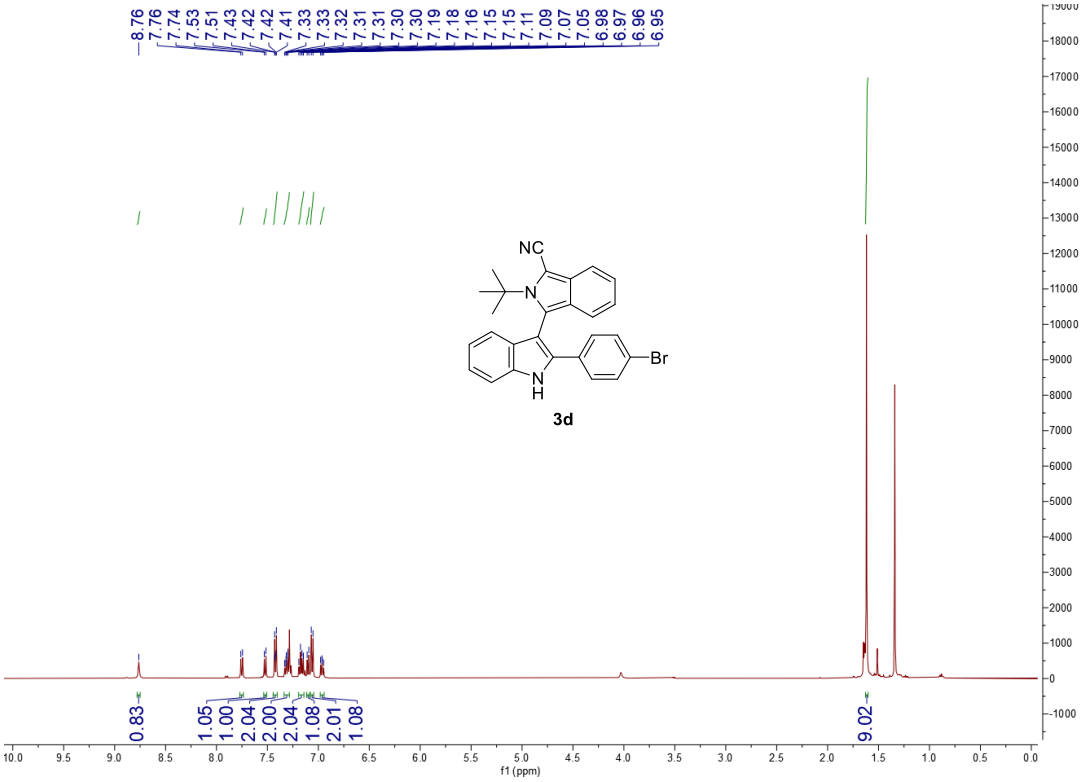
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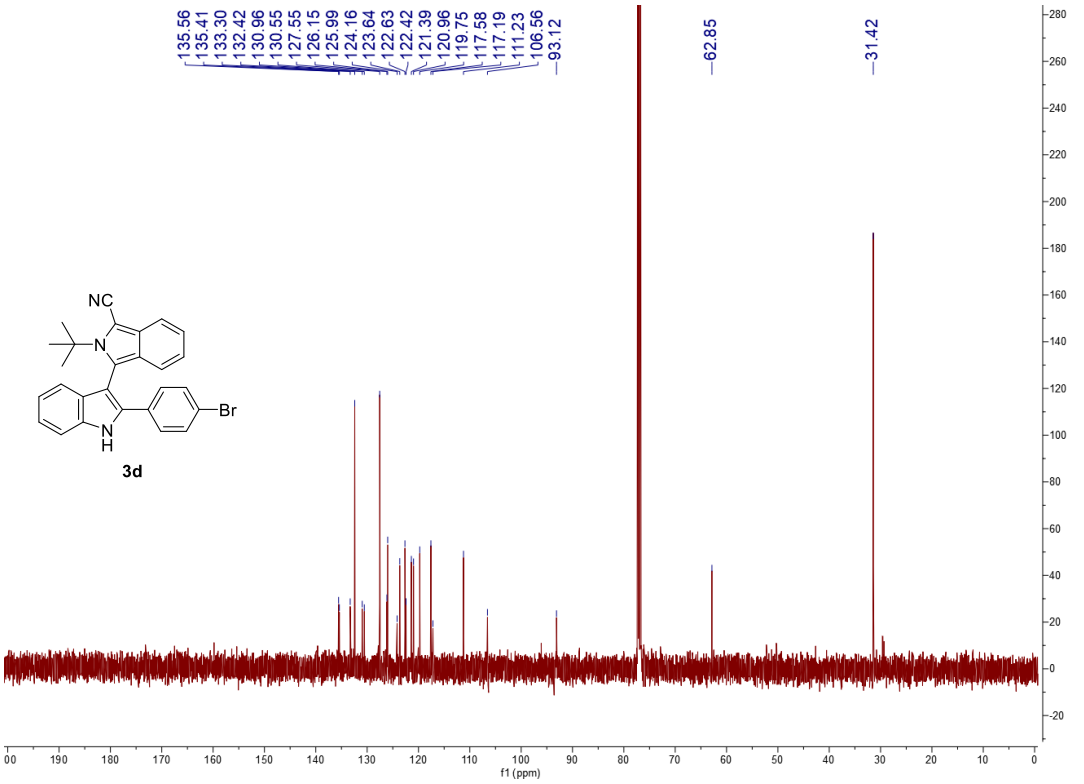
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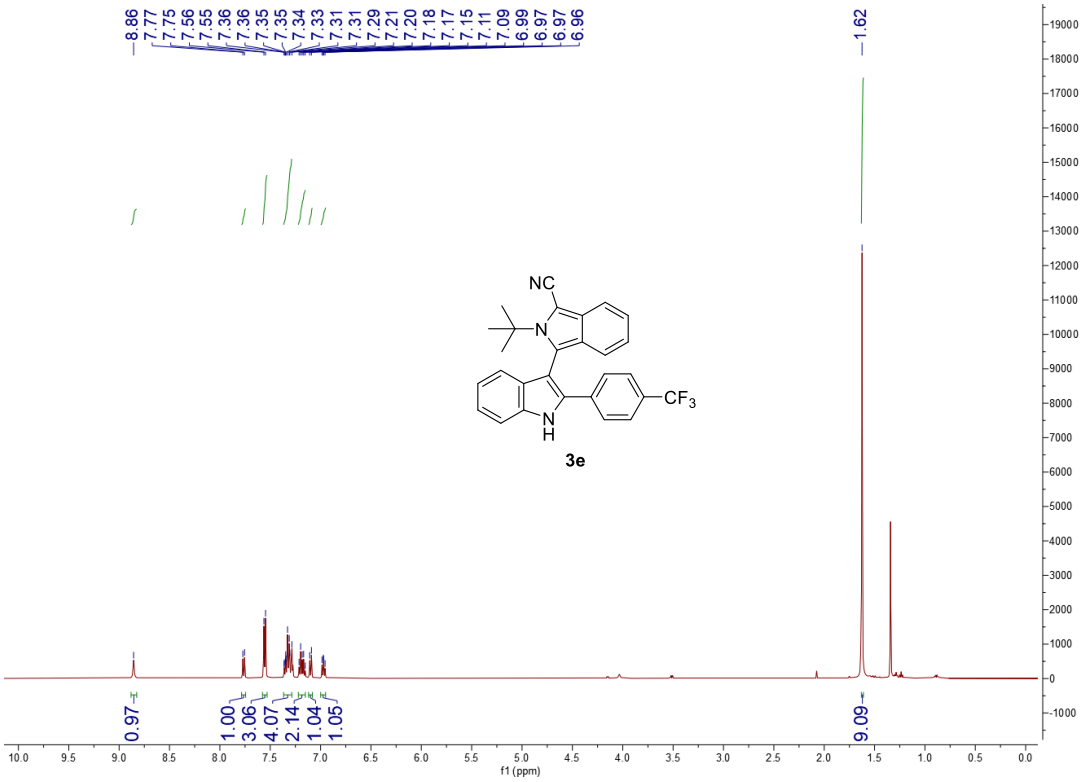
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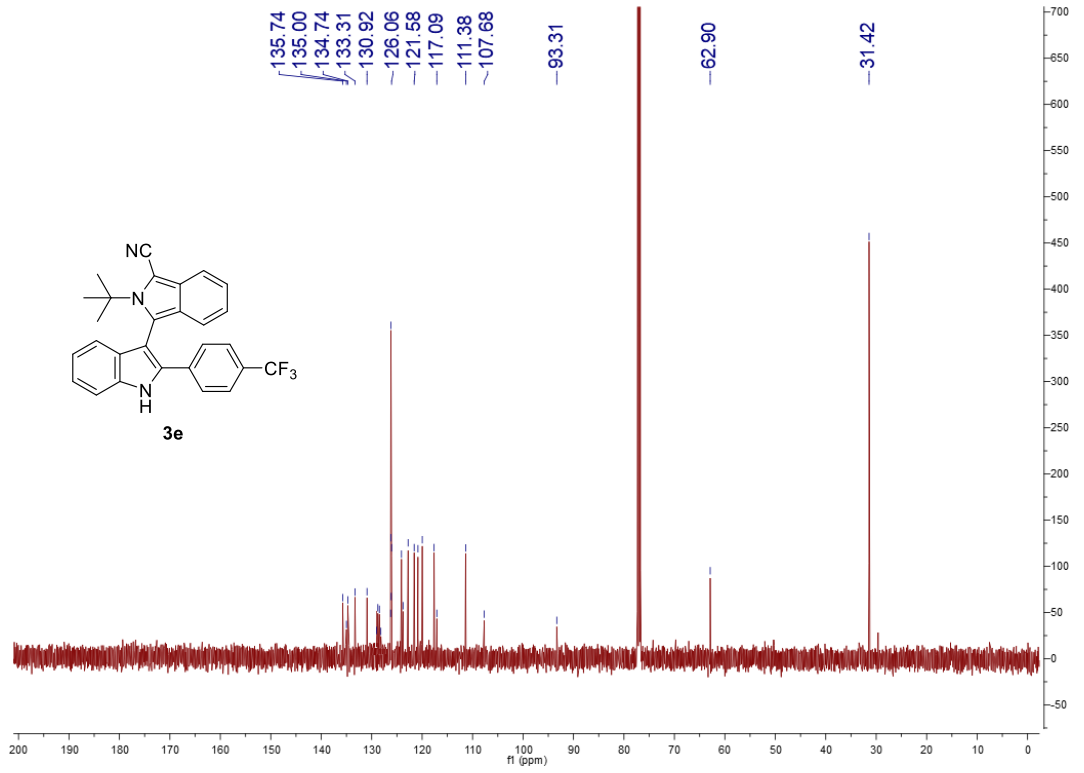
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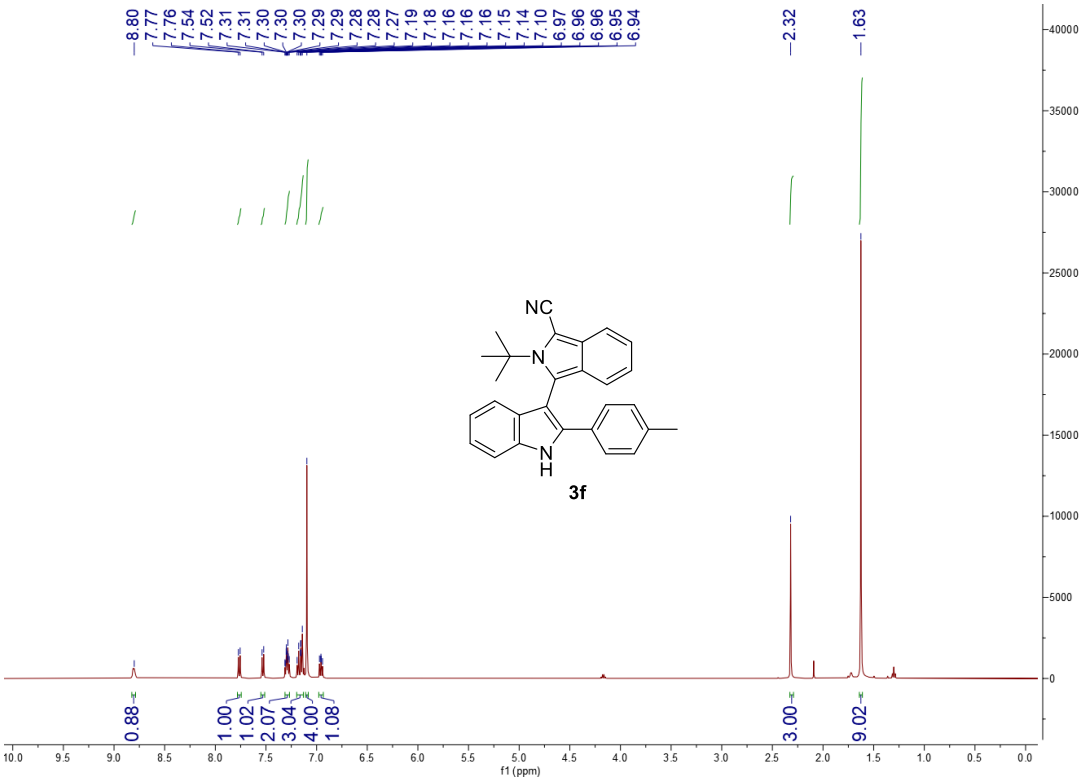
f1 (ppm)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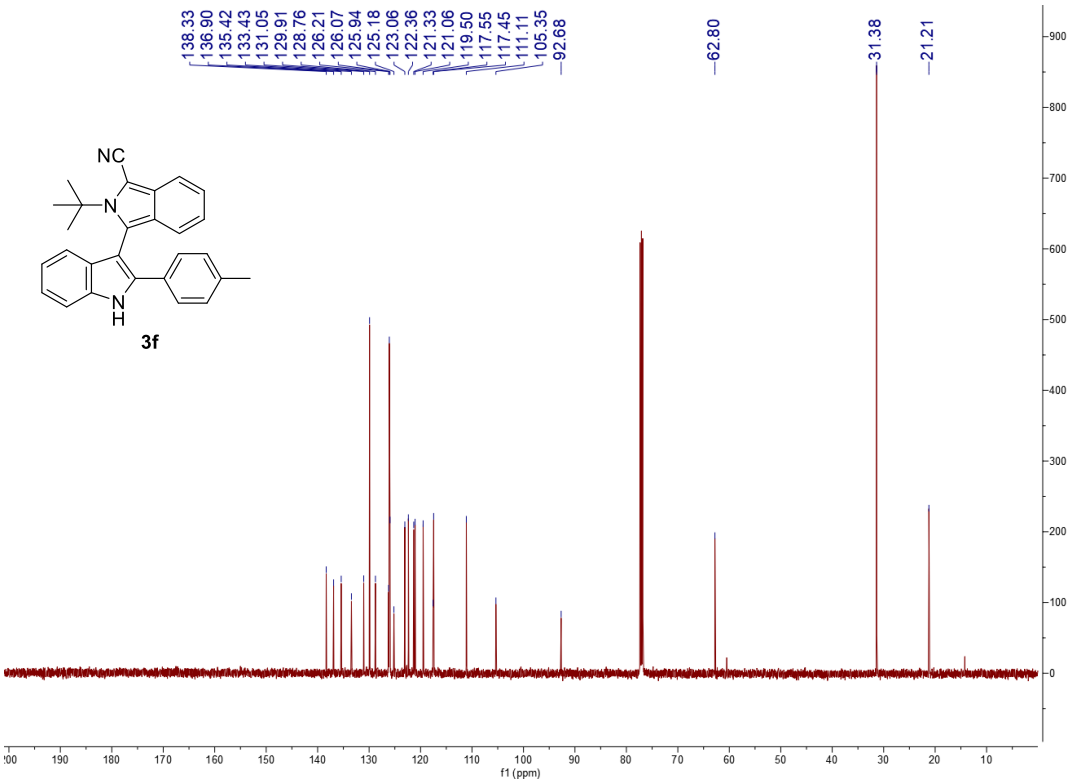
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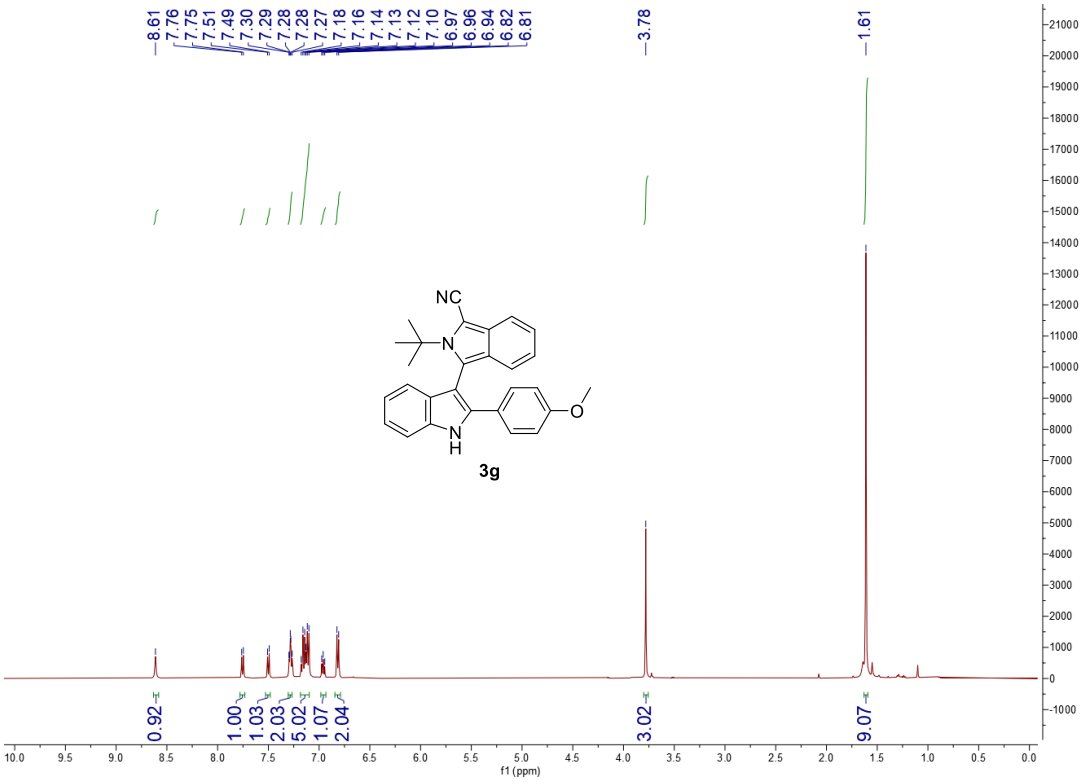
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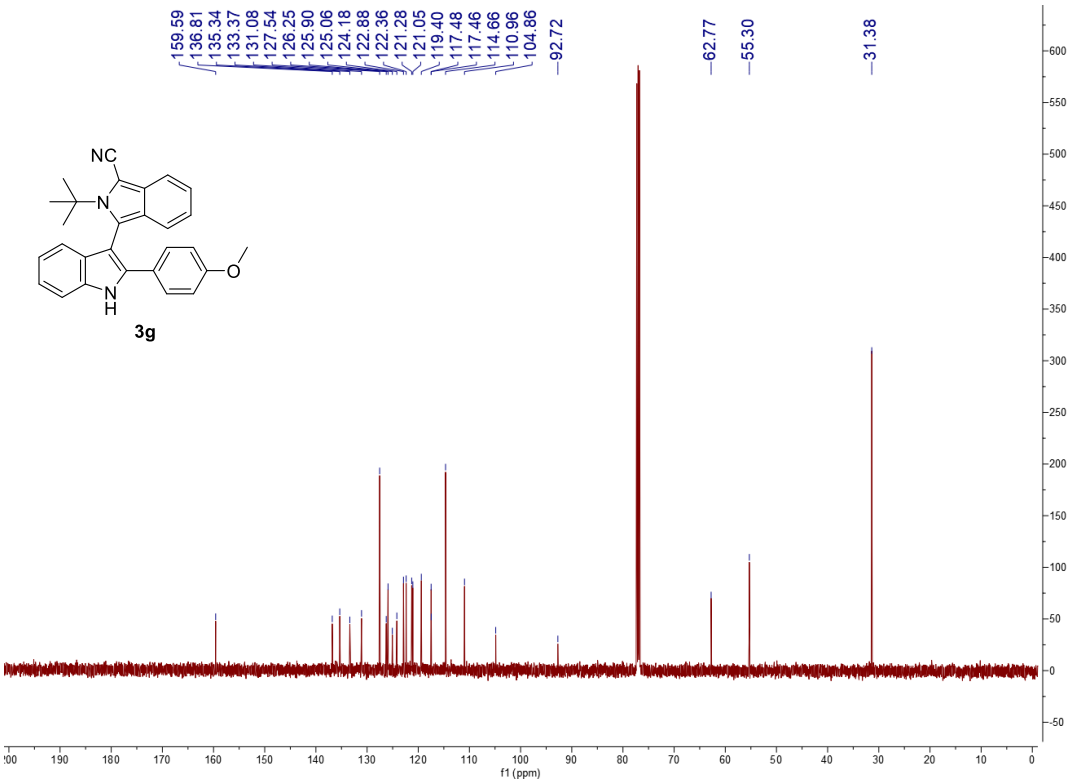
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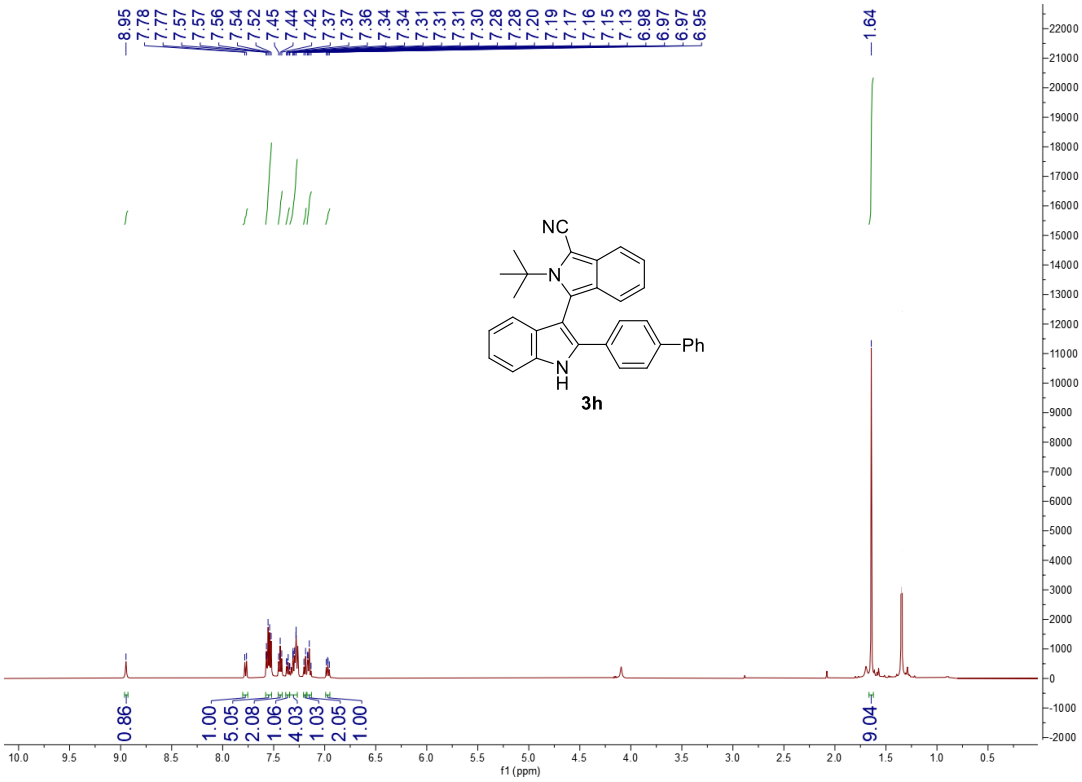
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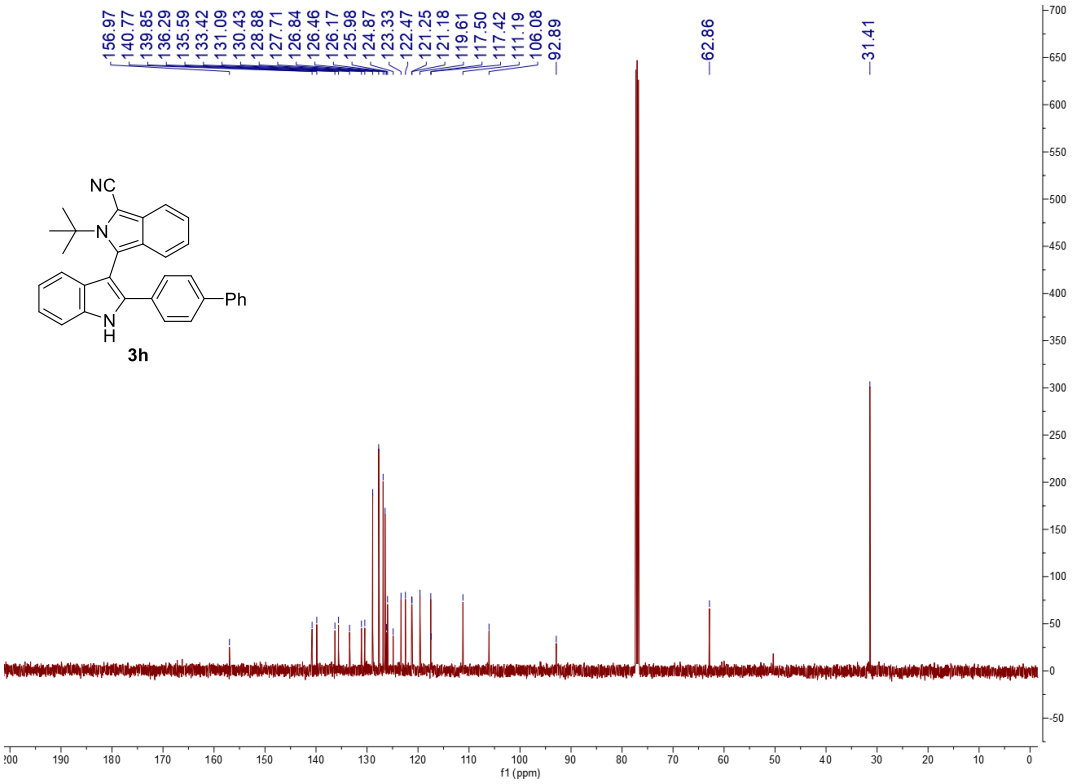
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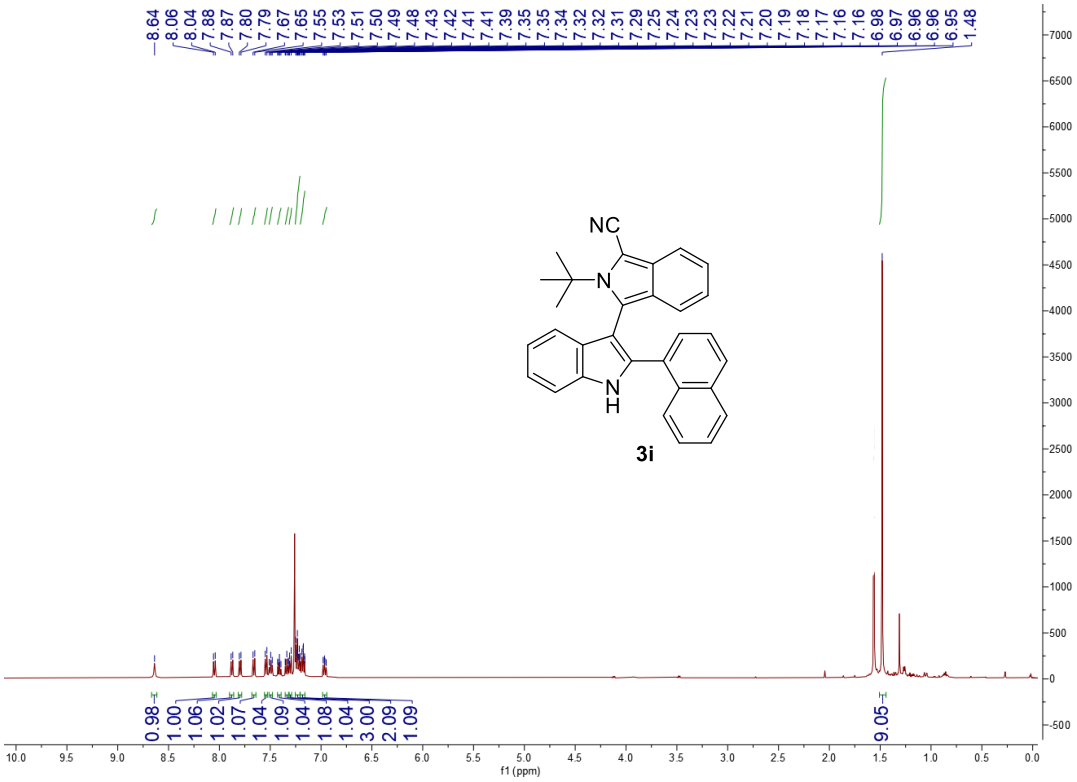
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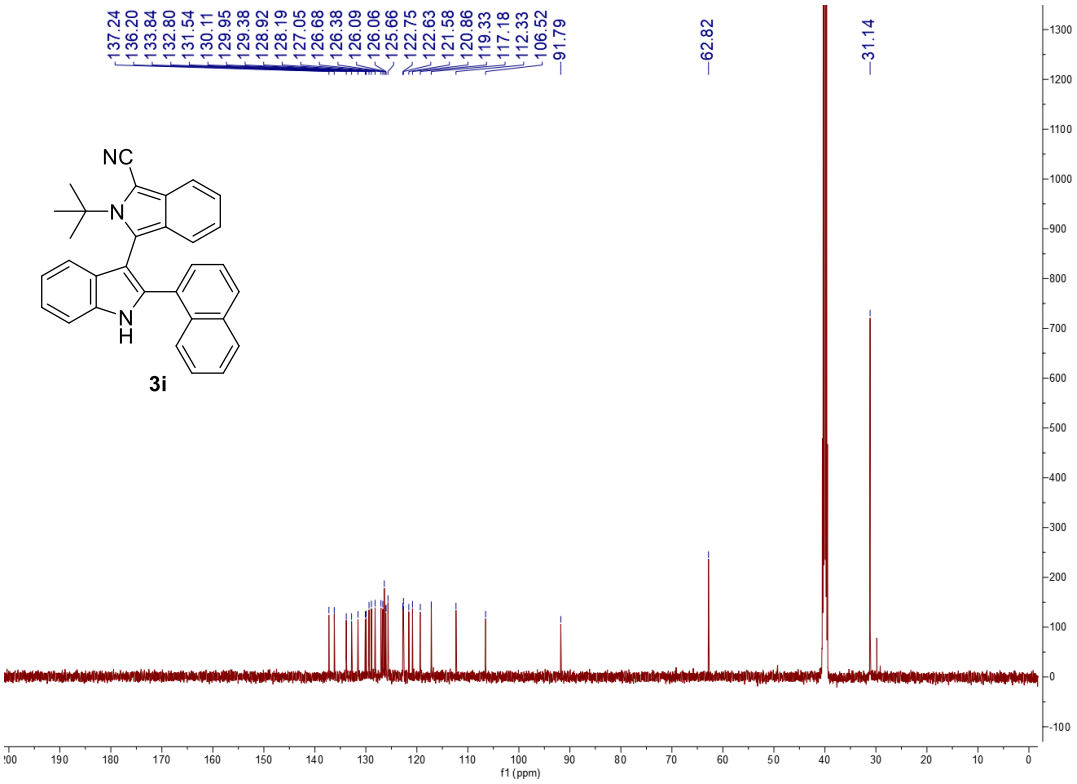
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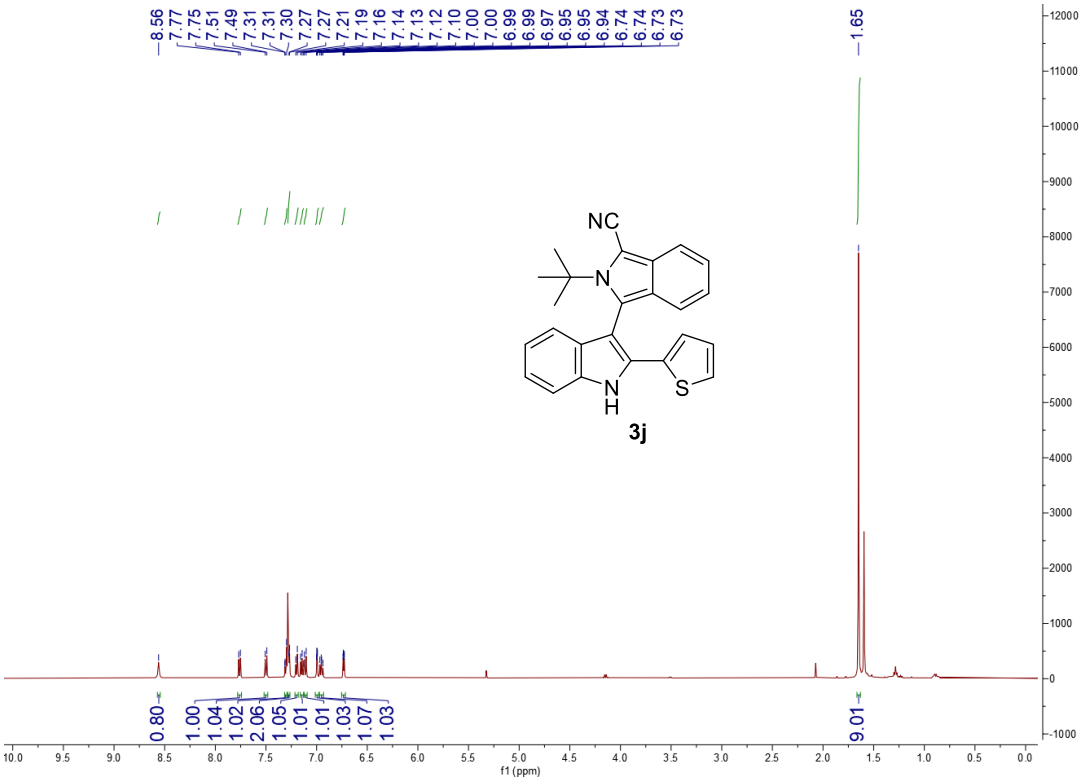
3i
f1 (ppm)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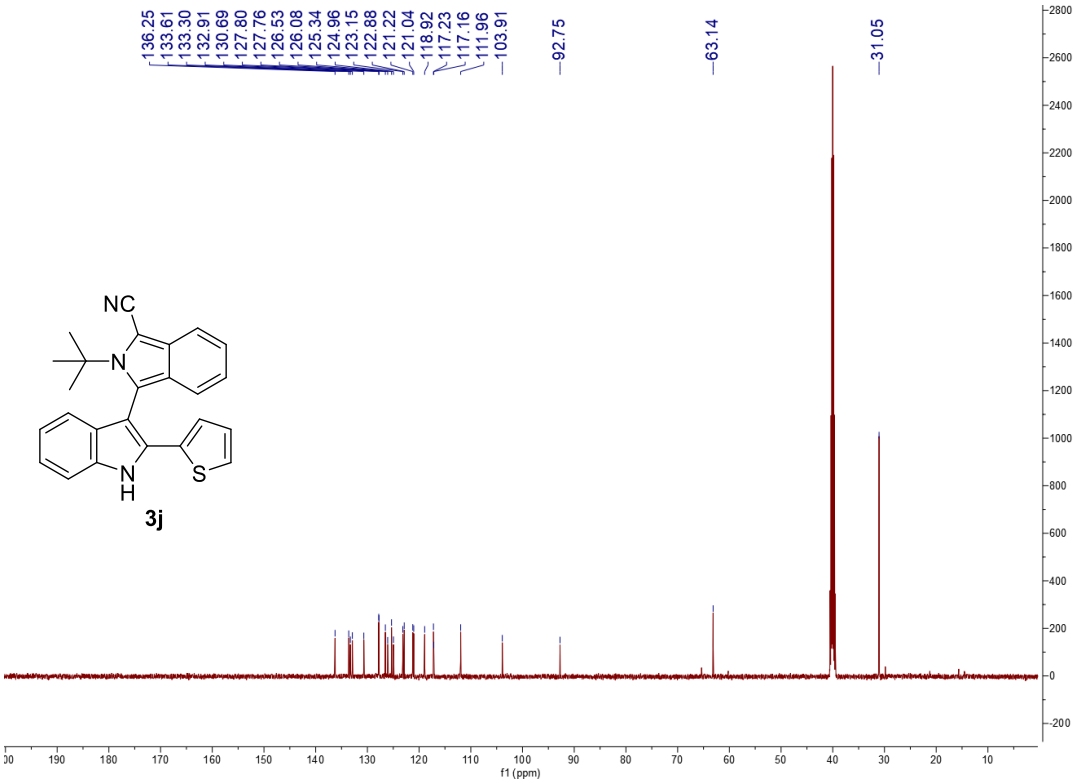
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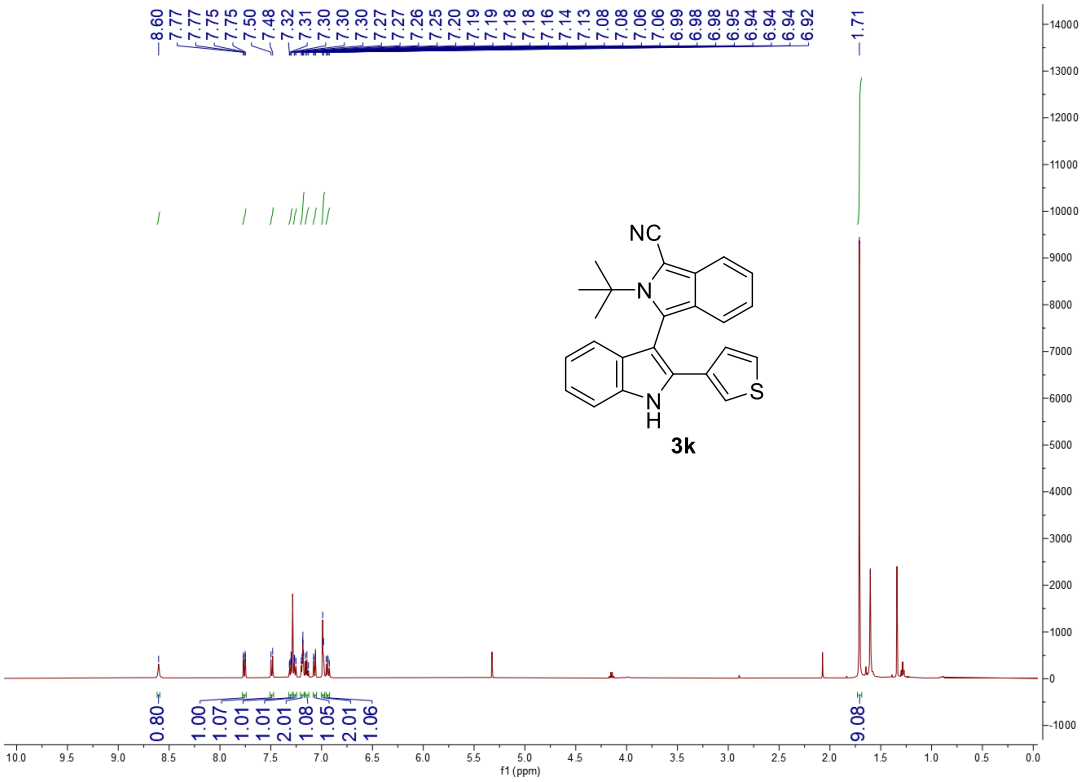
f1 (ppm)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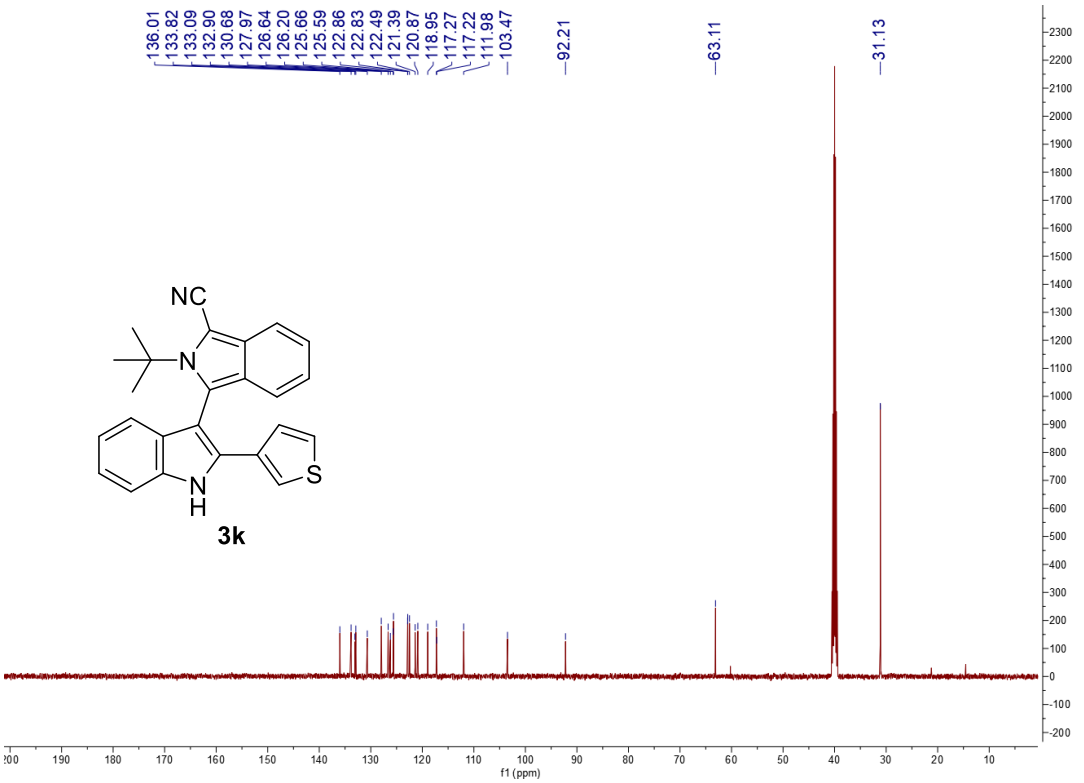
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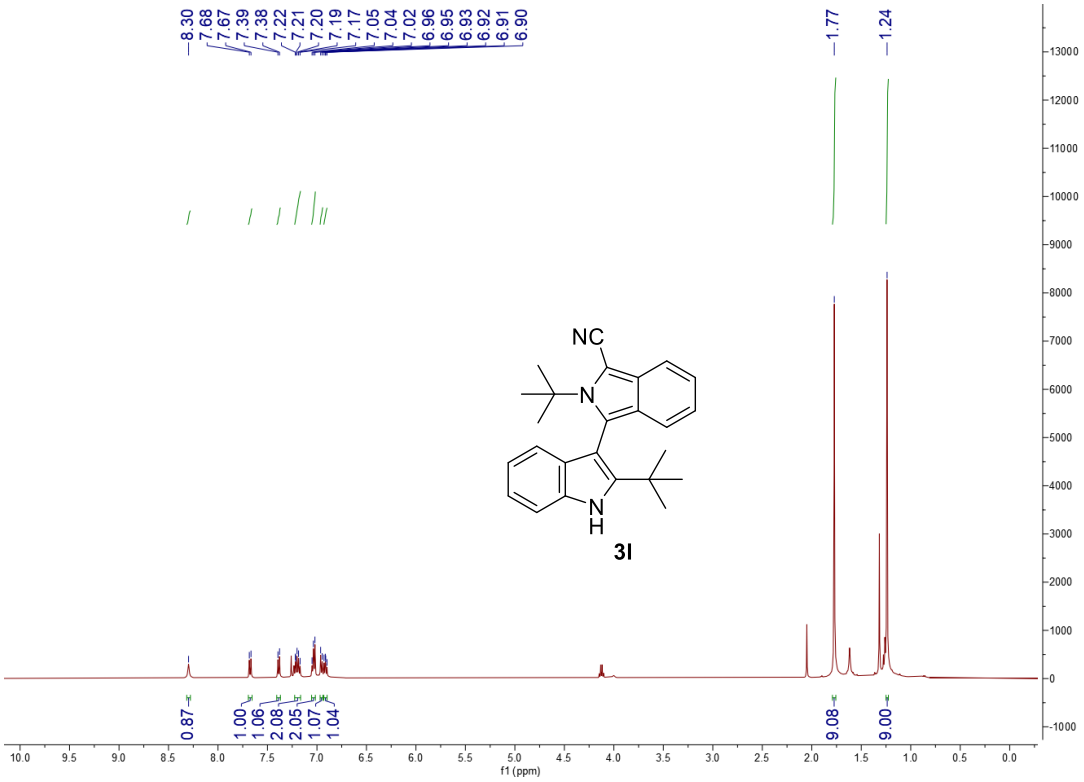
f1 (ppm)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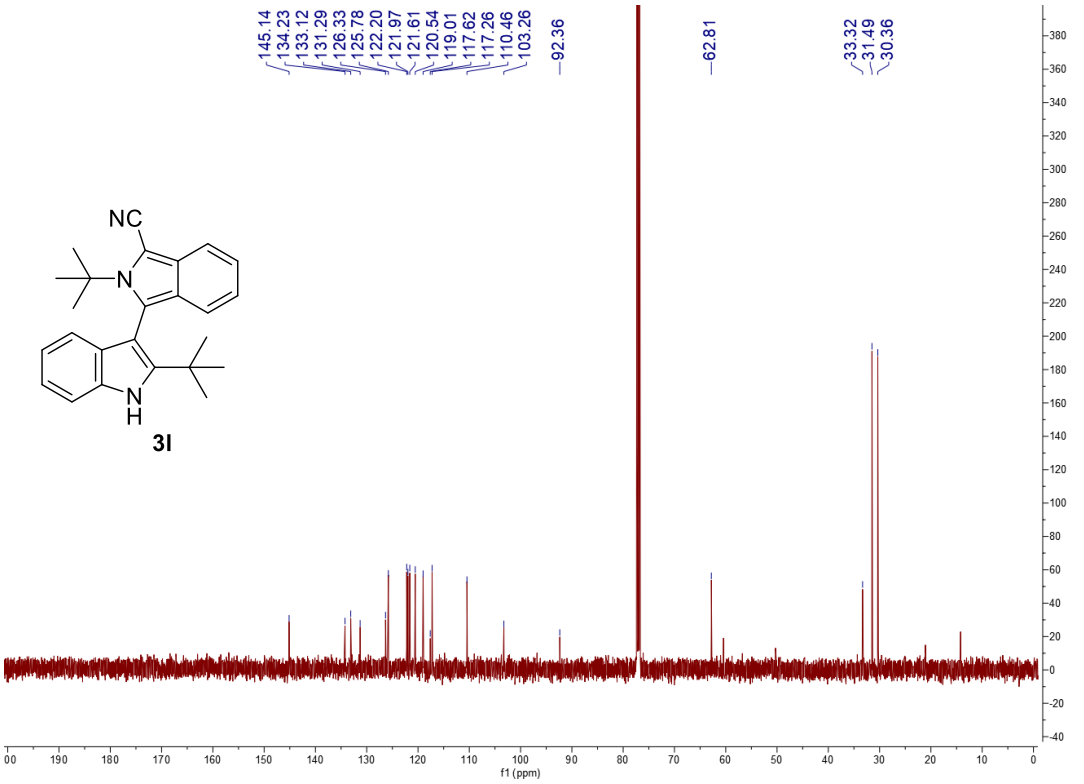
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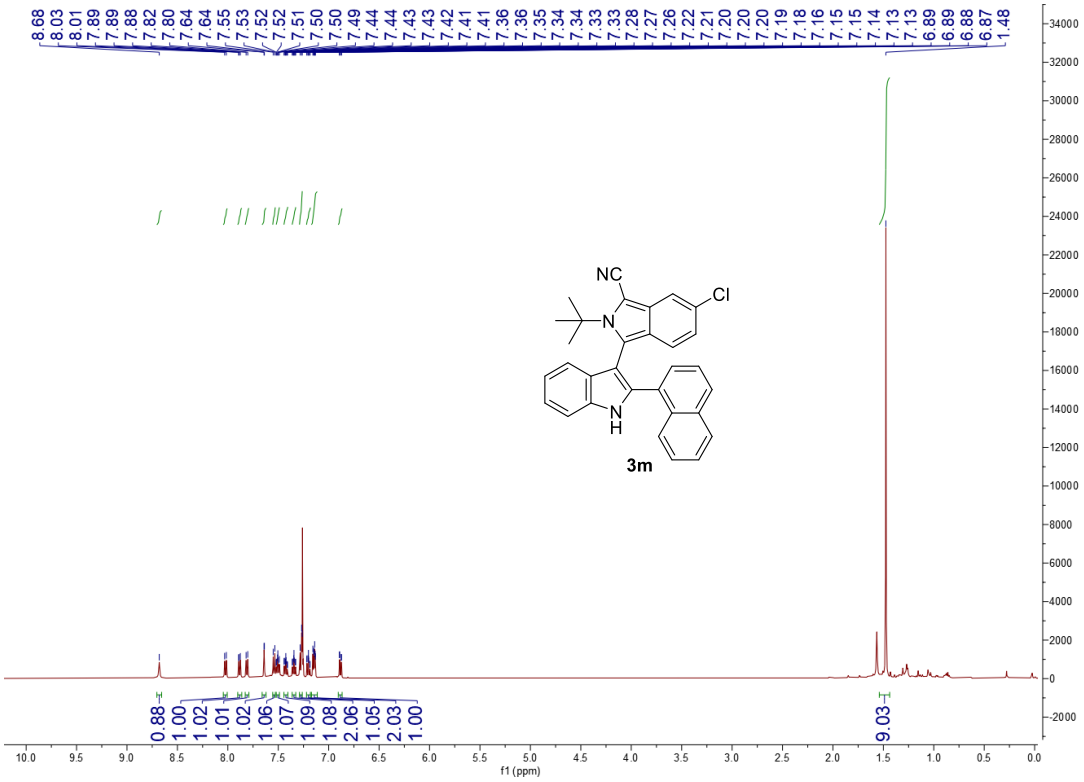
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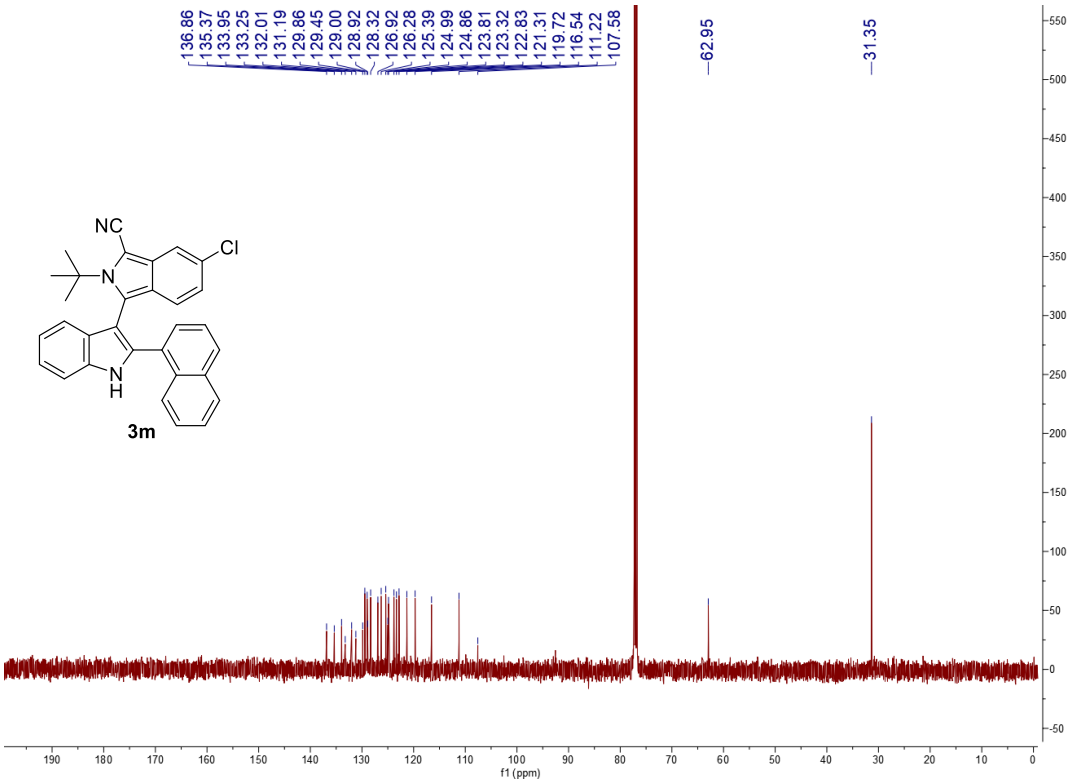
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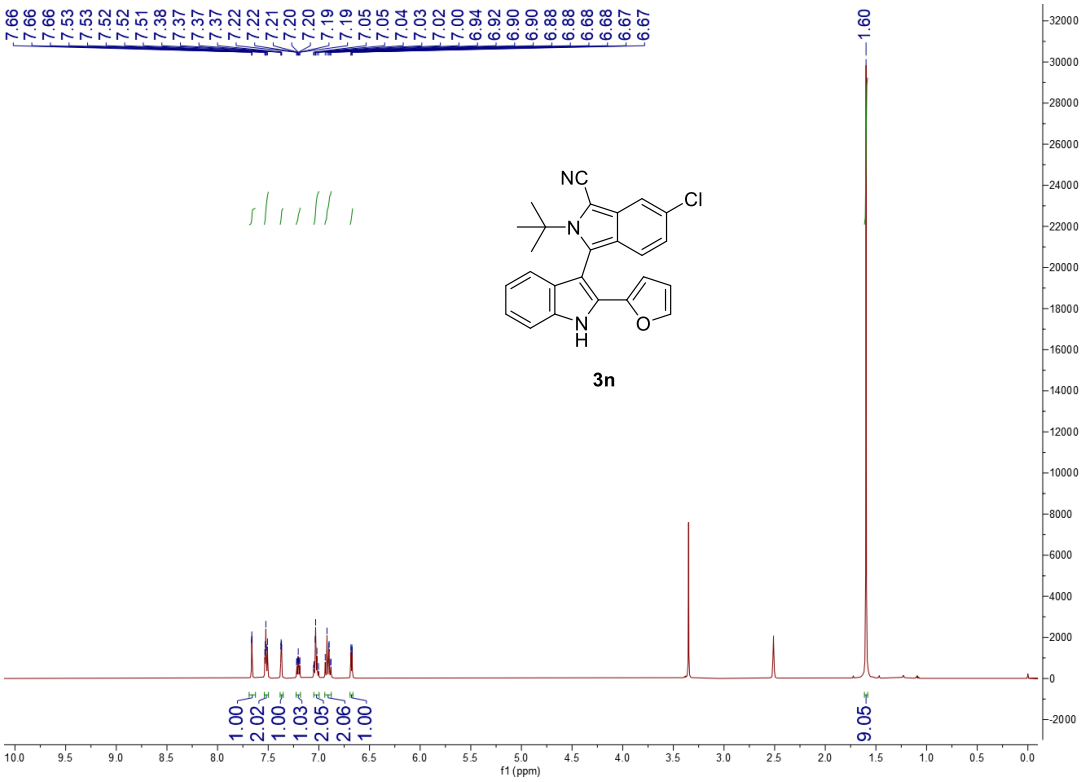
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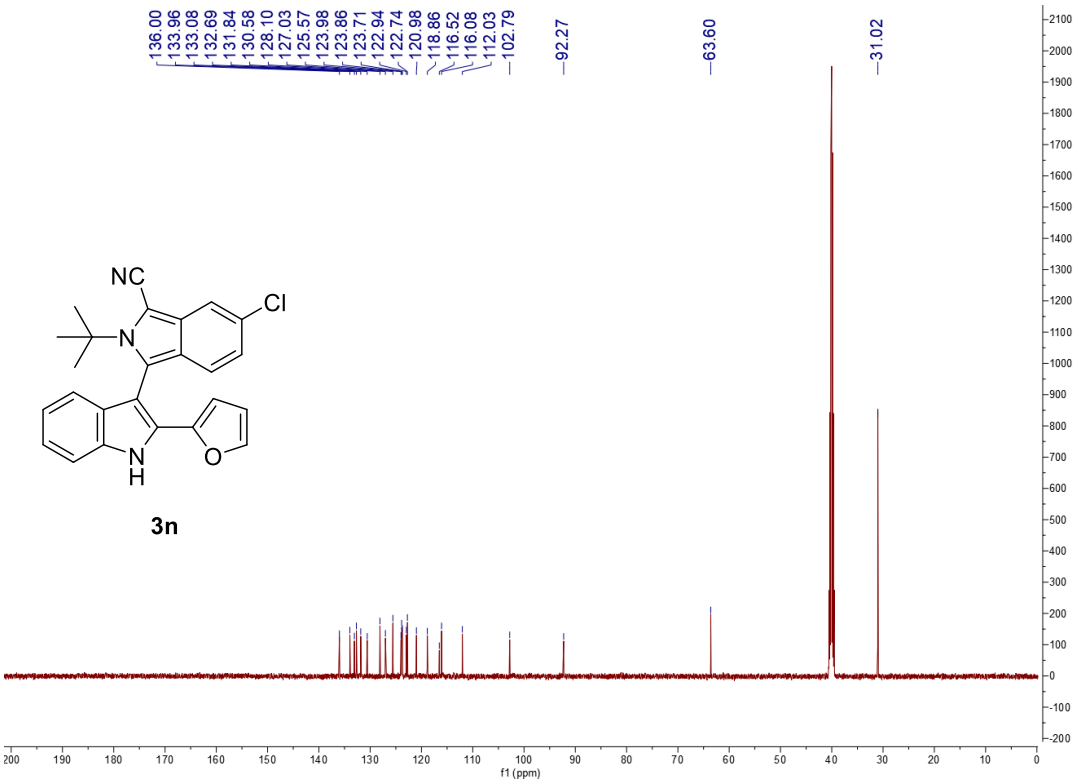
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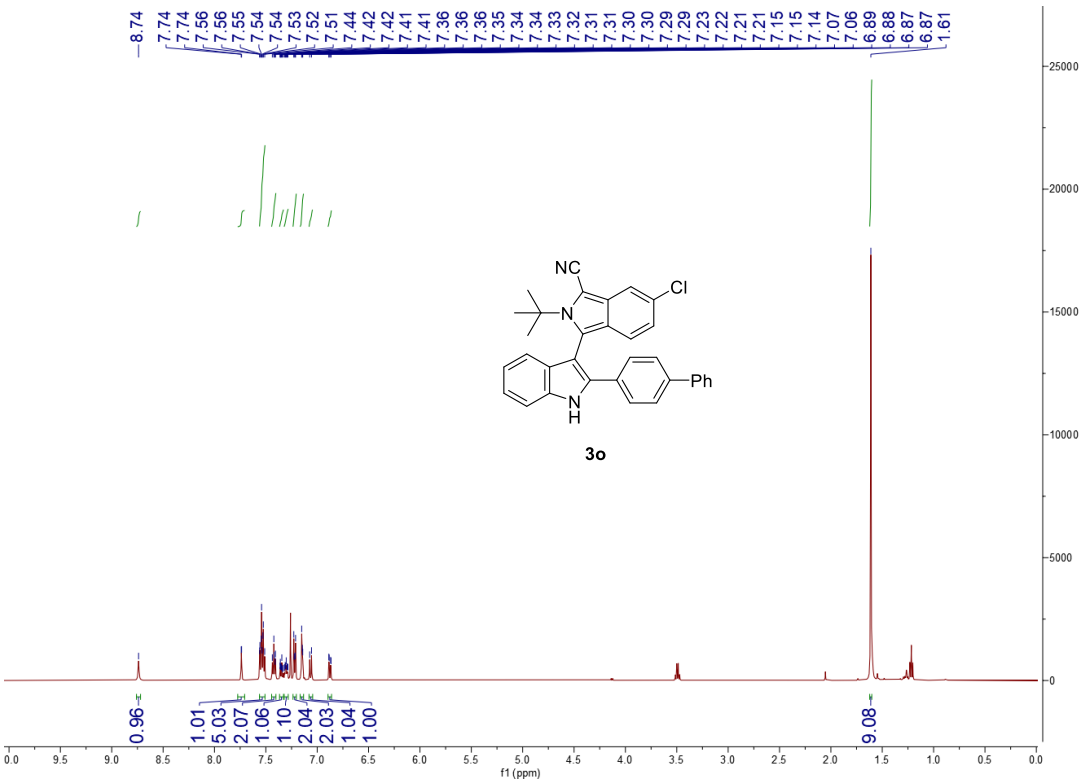
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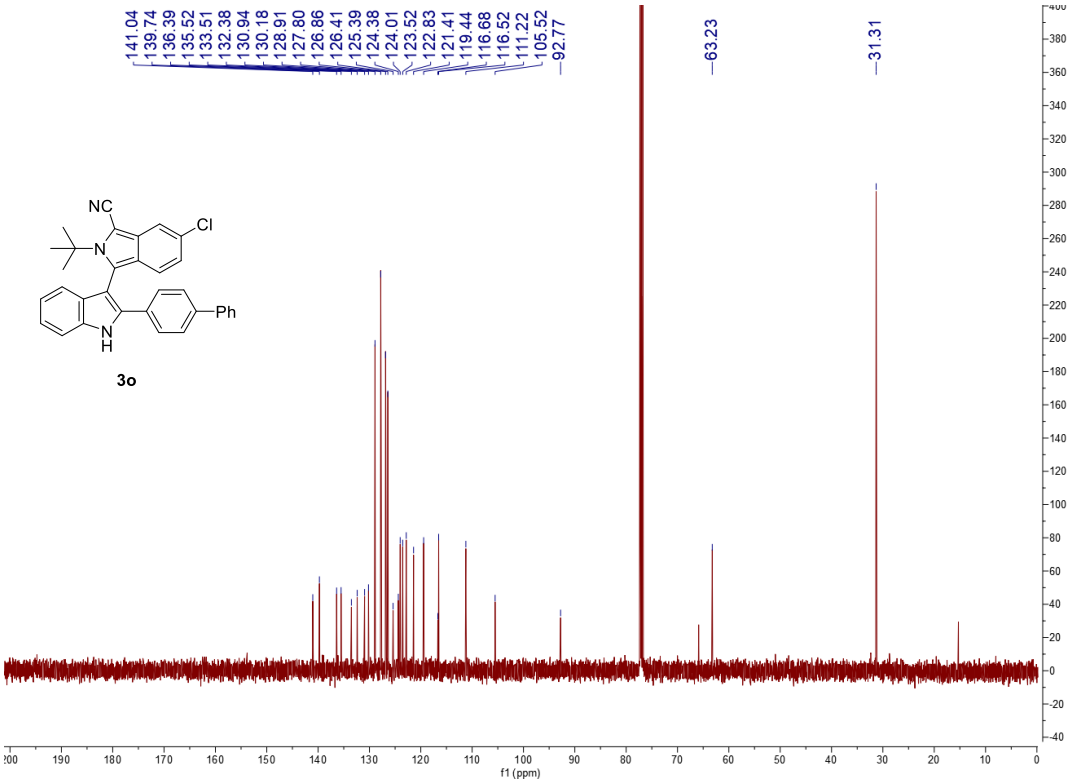
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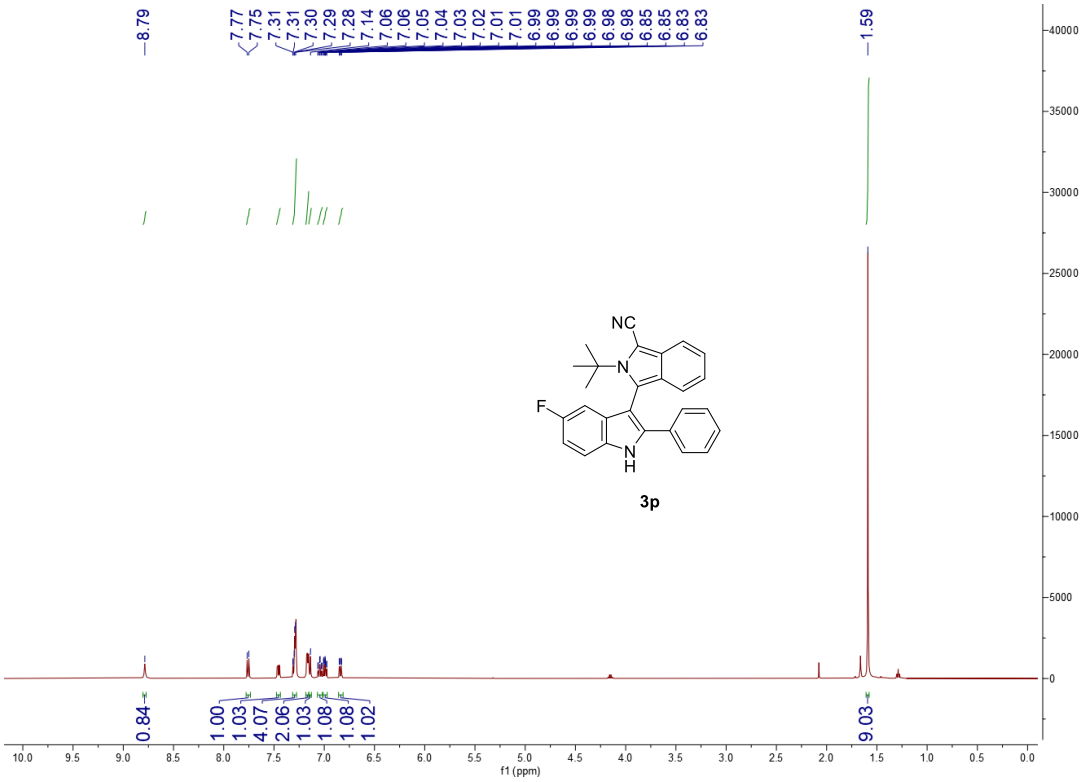
3o
f1 (ppm)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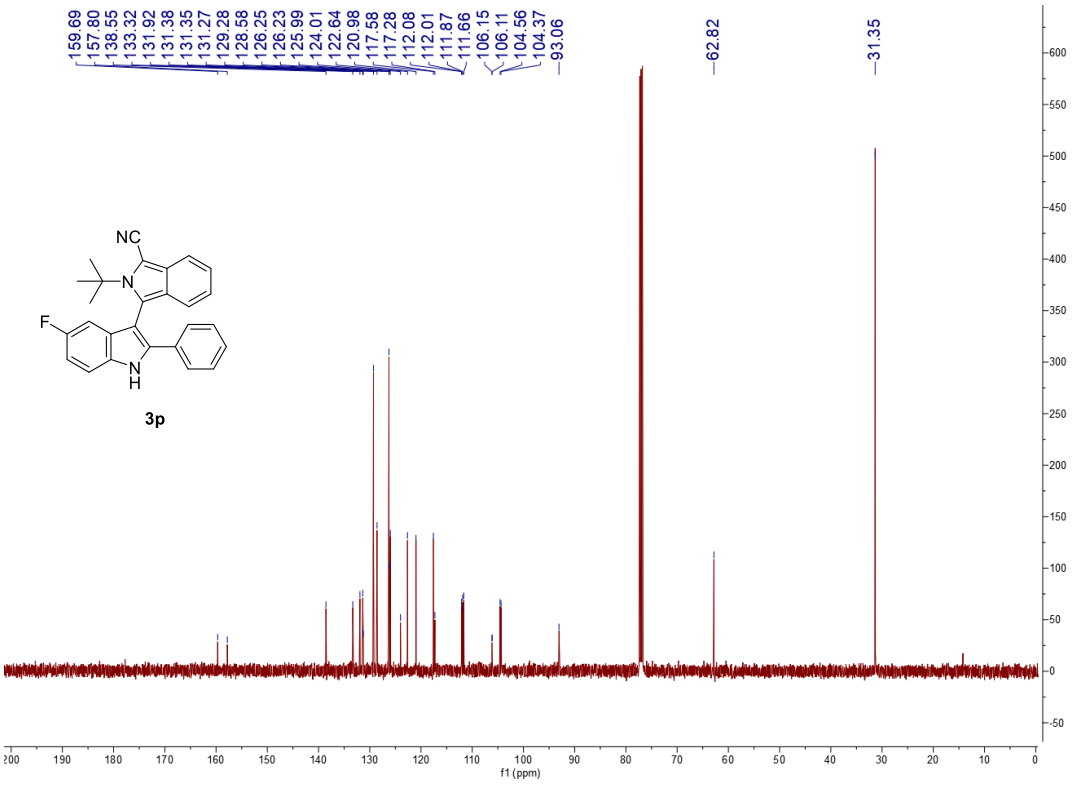
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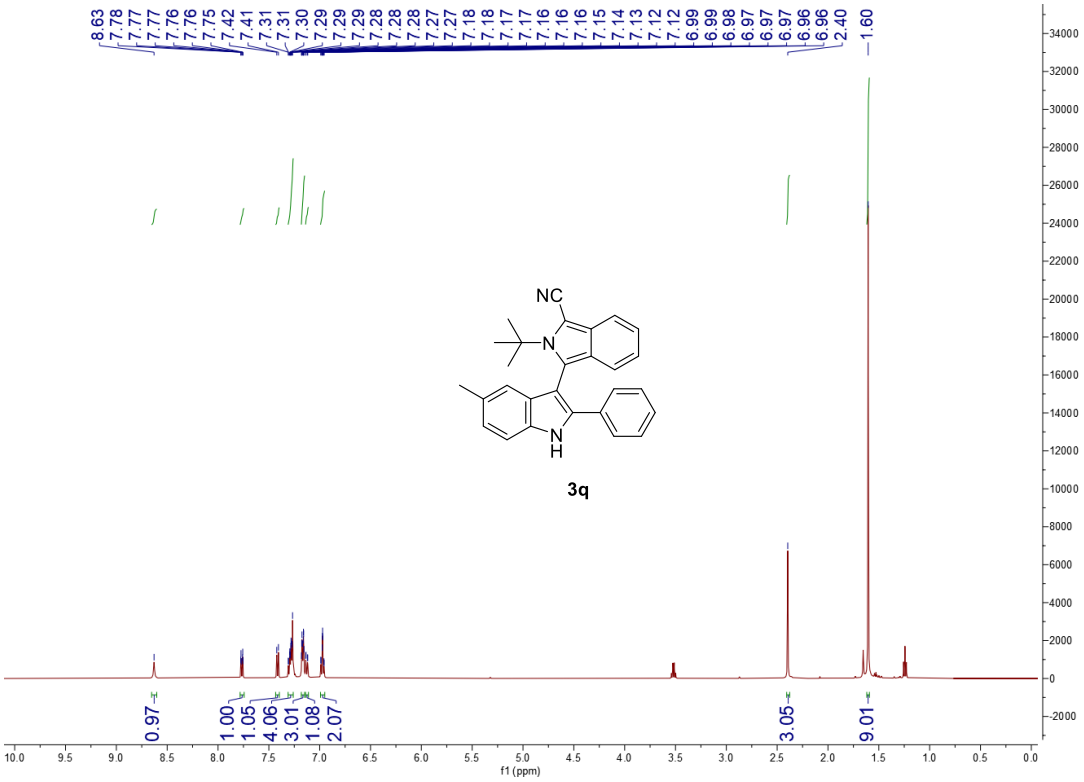
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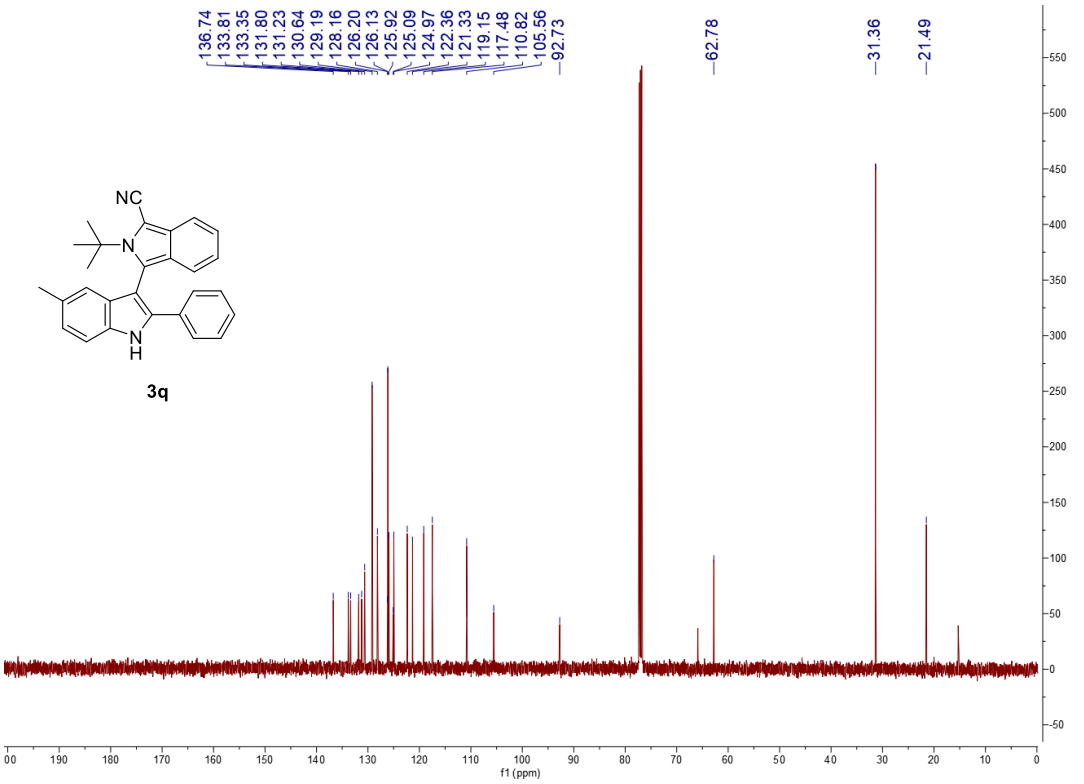
f1 (ppm)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NC
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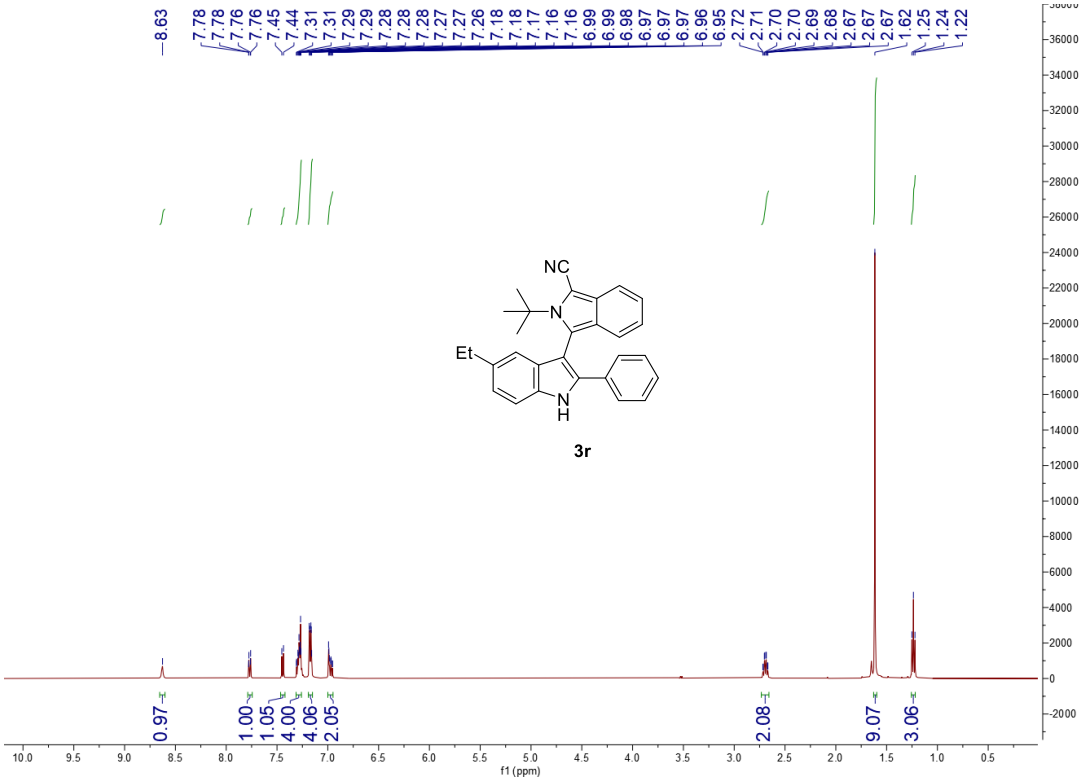
N
H
3q
f1 (ppm)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7.17
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7.16
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6.98
6.97
6.97
6.97
6.96
6.95
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2.68
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2.67
2.67
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1.25
1.24
1.22
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N
Et
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4.00
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2.08
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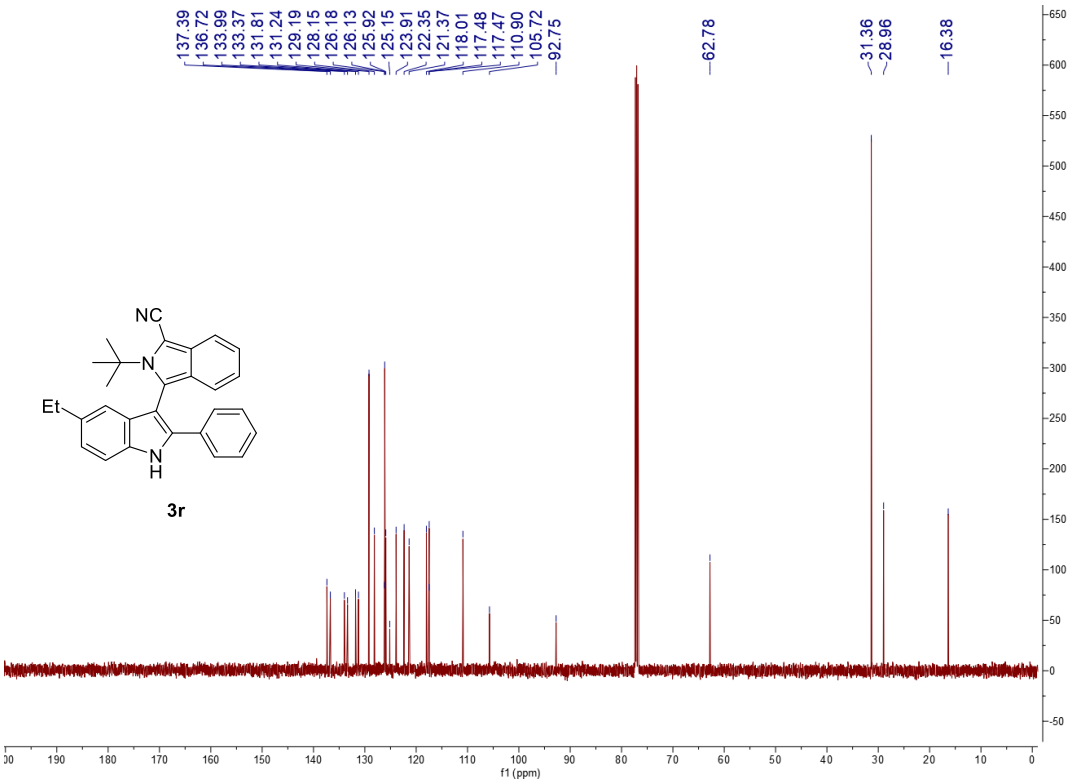
f1 (ppm)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118.01
117.48
117.47
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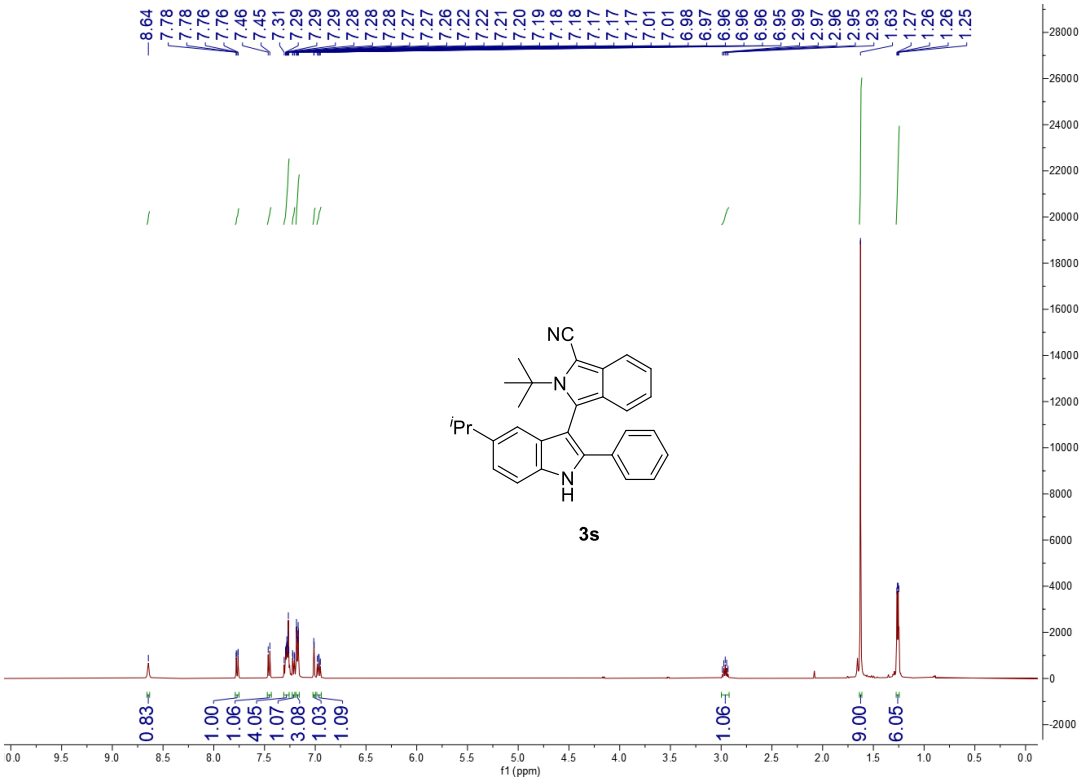
16.38
NC
N
Et
N
H
3r
f1 (ppm)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7.22
7.22
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7.18
7.18
7.17
7.17
7.17
7.01
7.01
6.98
6.97
6.96
6.96
6.96
6.95
2.99
2.97
2.96
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2.93
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1.26
1.26
1.25
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iPr
N
H
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1.03
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1.06
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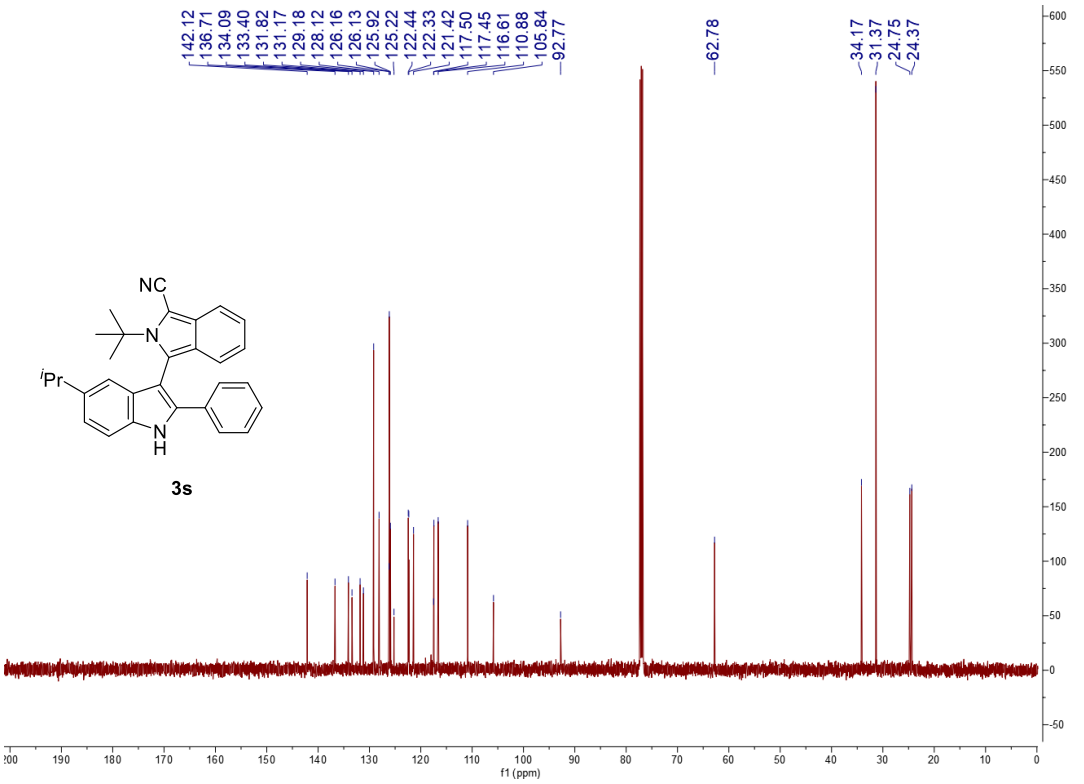
f1 (ppm)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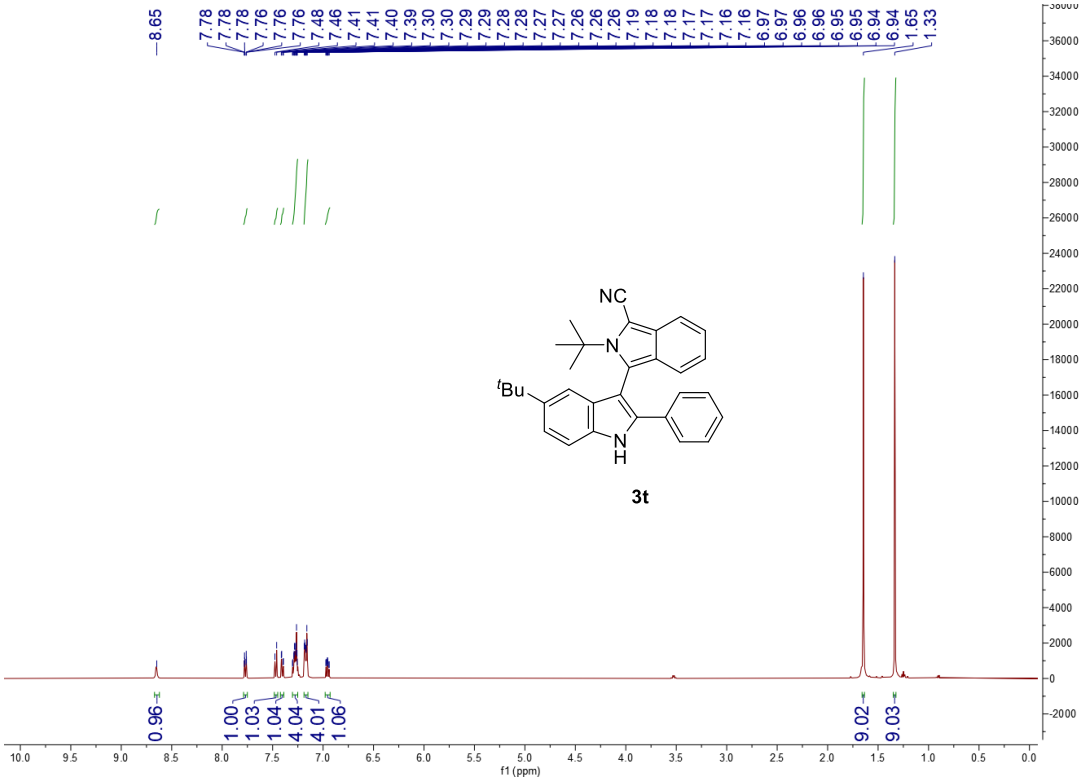
3s
f1 (ppm)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7.18
7.18
7.17
7.17
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6.97
6.96
6.96
6.95
6.95
6.94
6.94
1.65
1.33
NC
N
tBu
N
H
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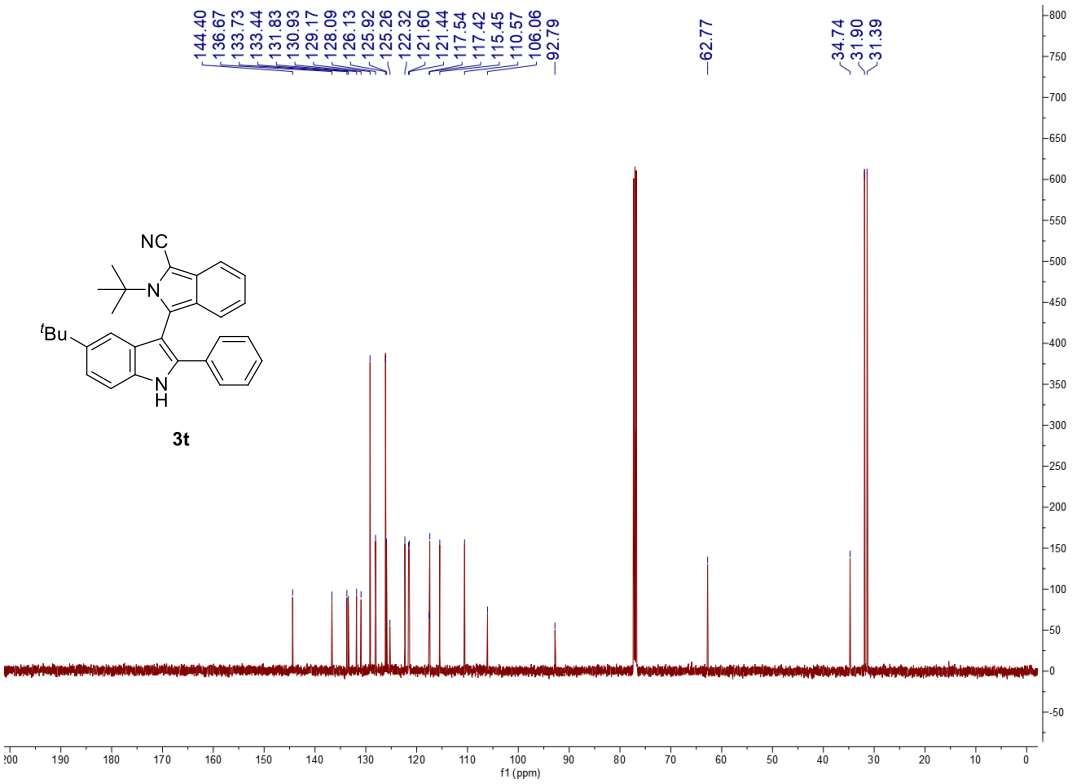
1.04
4.04
4.01
1.06
9.02
9.03
f1 (ppm)

3t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125.26
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121.44
117.54
117.42
115.45
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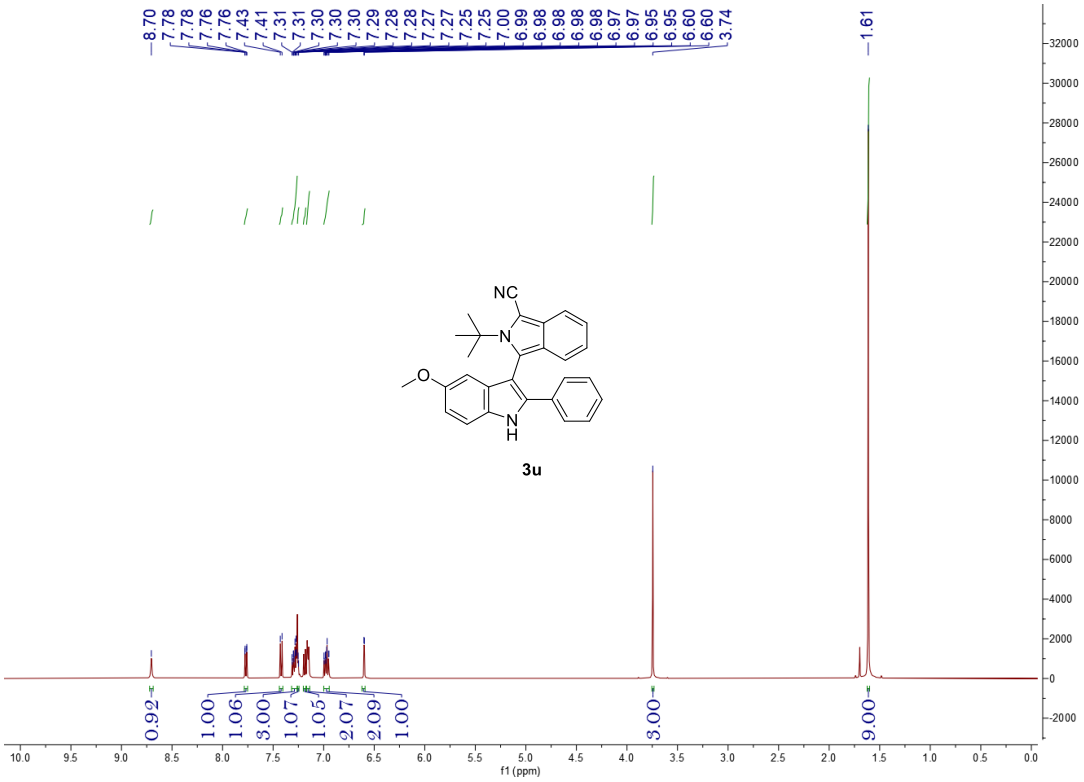
N
tBu
N
H
f1 (ppm)

3t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7.25
7.25
7.00
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6.97
6.97
6.95
6.95
6.60
6.60
3.74
1.61
NC
N
O
N
H
3u
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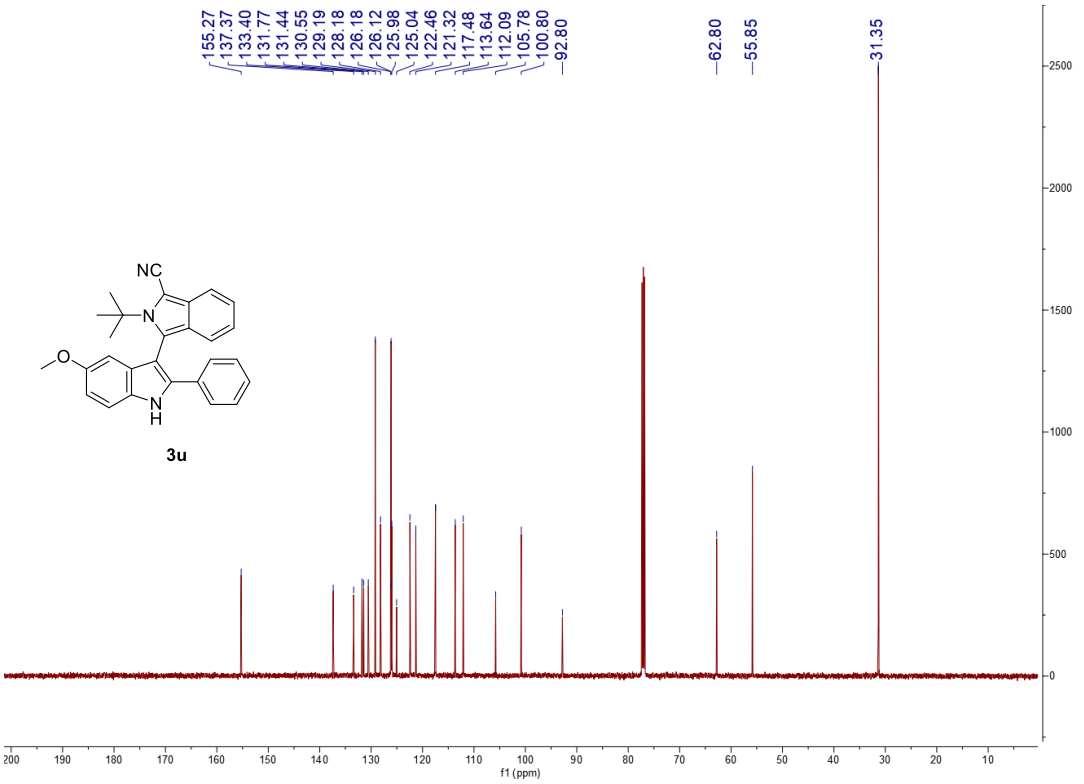
1.07
1.05
2.07
2.09
1.00
3.00
9.00
f1 (ppm)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117.48
113.64
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31.35
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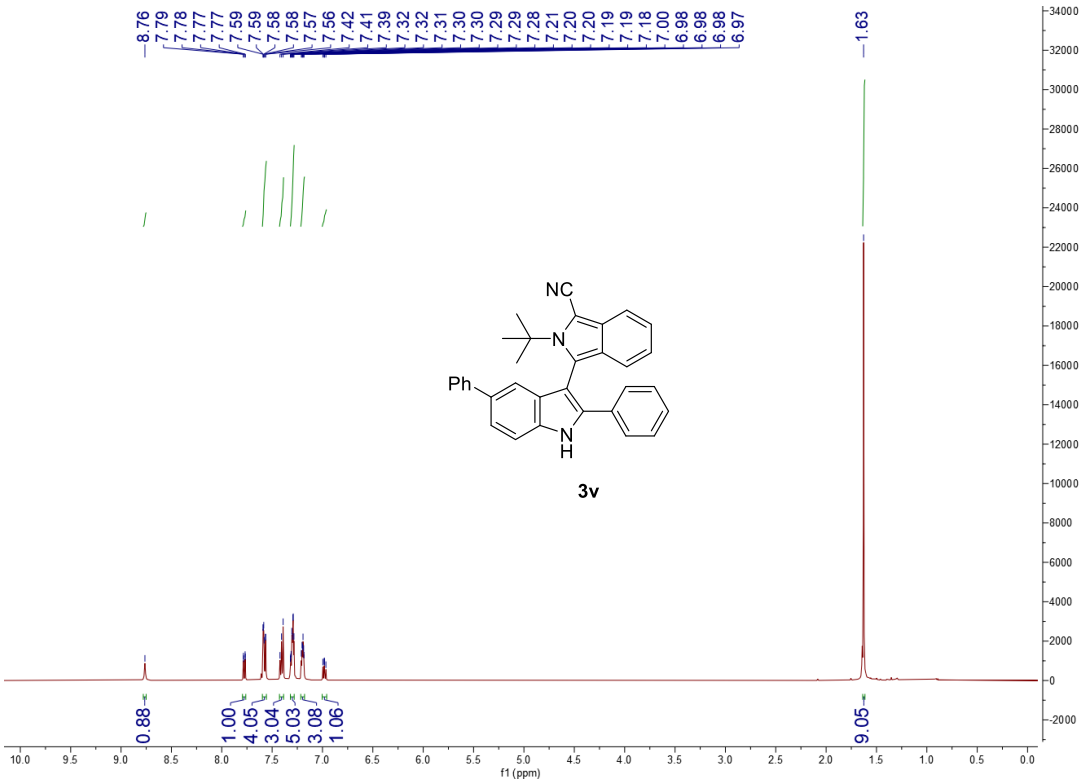
N
O
N
H
3u
f1 (ppm)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7.32
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7.30
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7.29
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7.28
7.21
7.20
7.20
7.19
7.19
7.18
7.00
6.98
6.98
6.97
1.63
NC
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Ph
N
H
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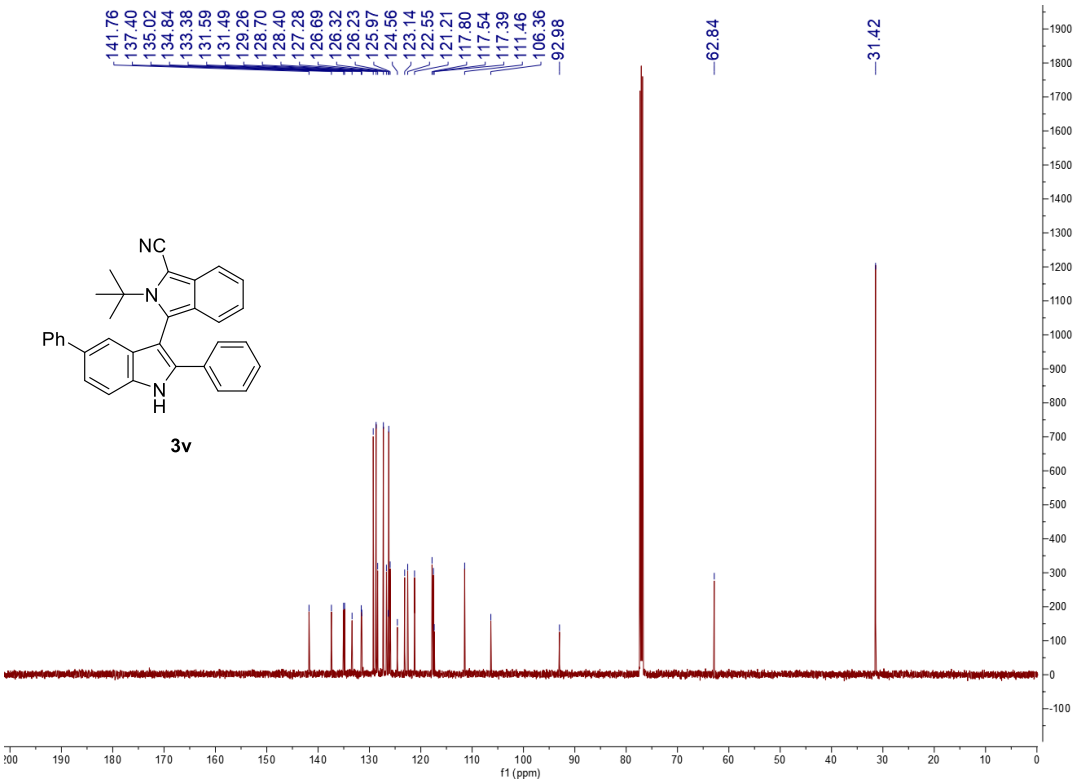
3.04
5.03
3.08
1.06
9.05
f1 (ppm)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123.14
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121.21
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31.42
NC
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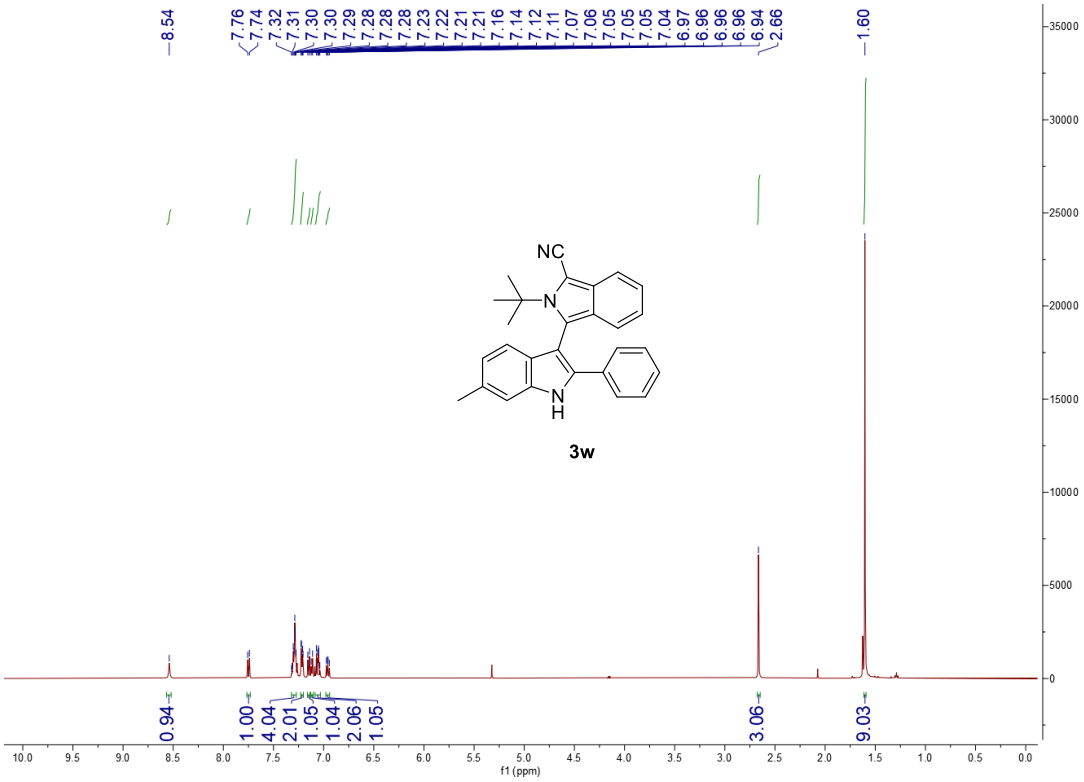
Ph
N
H
3v
f1 (ppm)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7.21
7.21
7.16
7.14
7.12
7.11
7.07
7.06
7.05
7.05
7.05
7.04
6.97
6.96
6.96
6.96
6.94
2.66
1.60
NC
N
N
H
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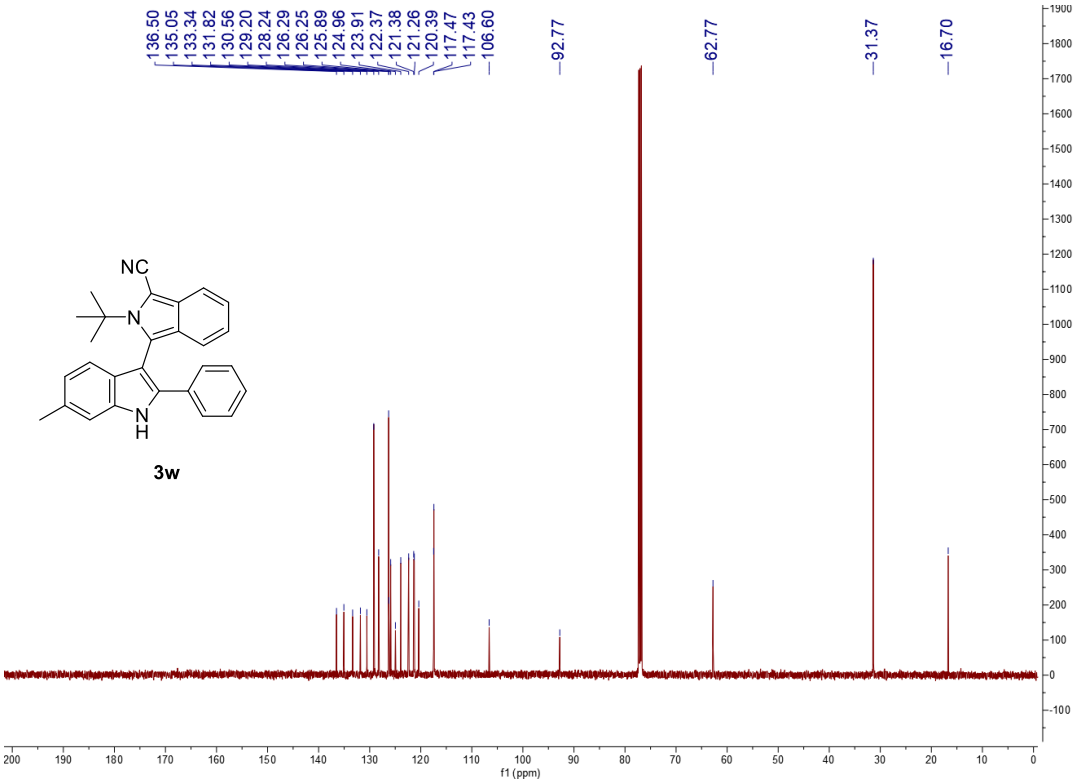
2.01
1.05
1.04
2.06
1.05
3.06
9.03
f1 (ppm)

3w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122.37
121.38
121.26
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62.77
31.37
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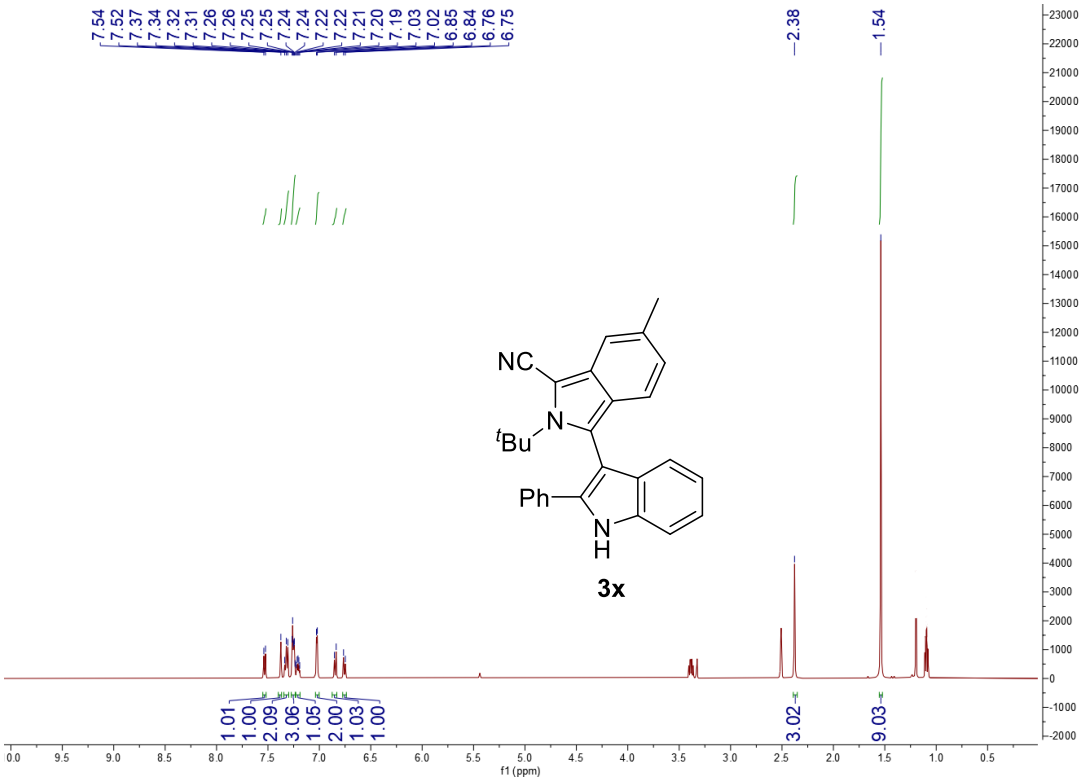
NC
N
N
H
f1 (ppm)

3w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7.24
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7.22
7.22
7.21
7.20
7.19
7.03
7.02
6.85
6.84
6.76
6.75
2.38
1.54
NC
tBu
N
Ph
N
H
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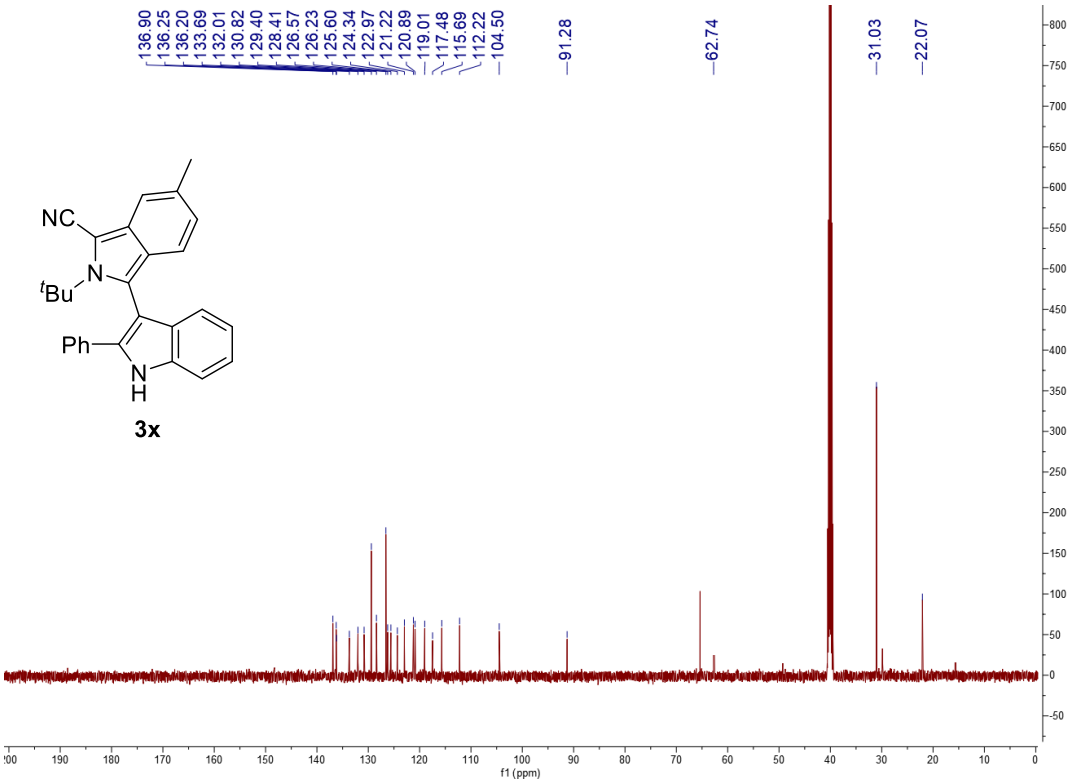
2.09
3.06
1.05
2.00
1.03
1.00
3.02
9.03
f1 (ppm)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120.89
119.01
117.48
115.69
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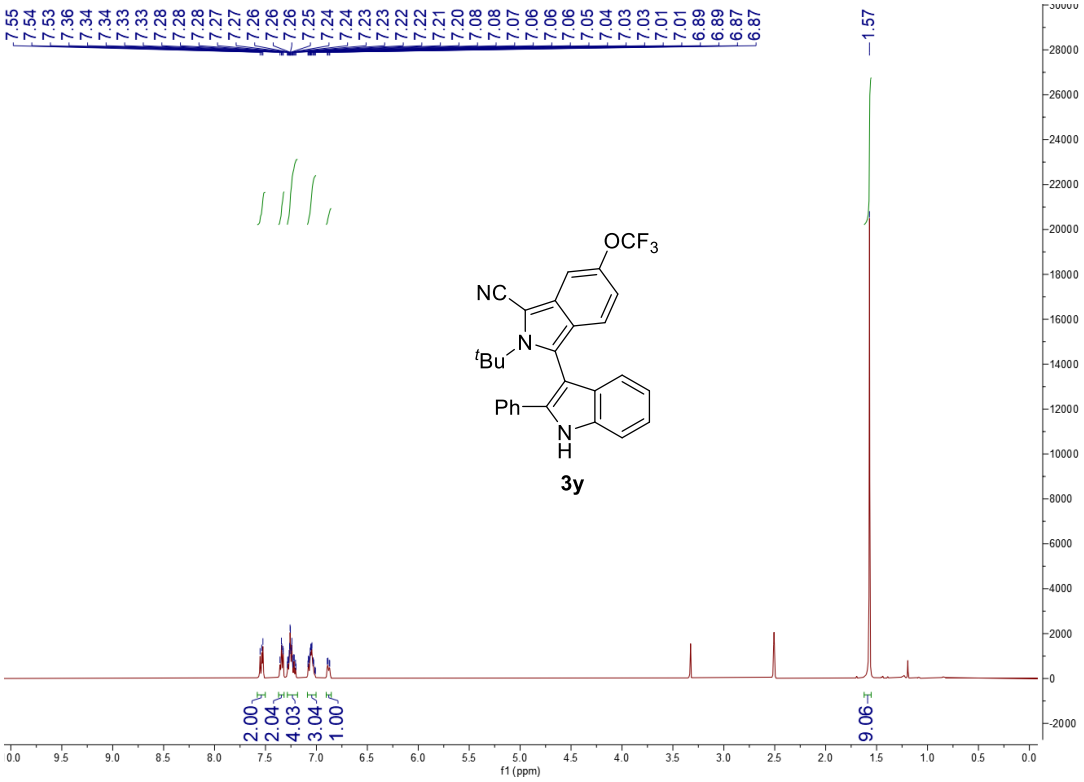
NC
tBu
N
Ph
N
H
3x
f1 (ppm)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7.06
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7.06
7.05
7.04
7.03
7.03
7.01
7.01
6.89
6.89
6.87
6.87
1.57
OCF3
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Ph
N
H
3y
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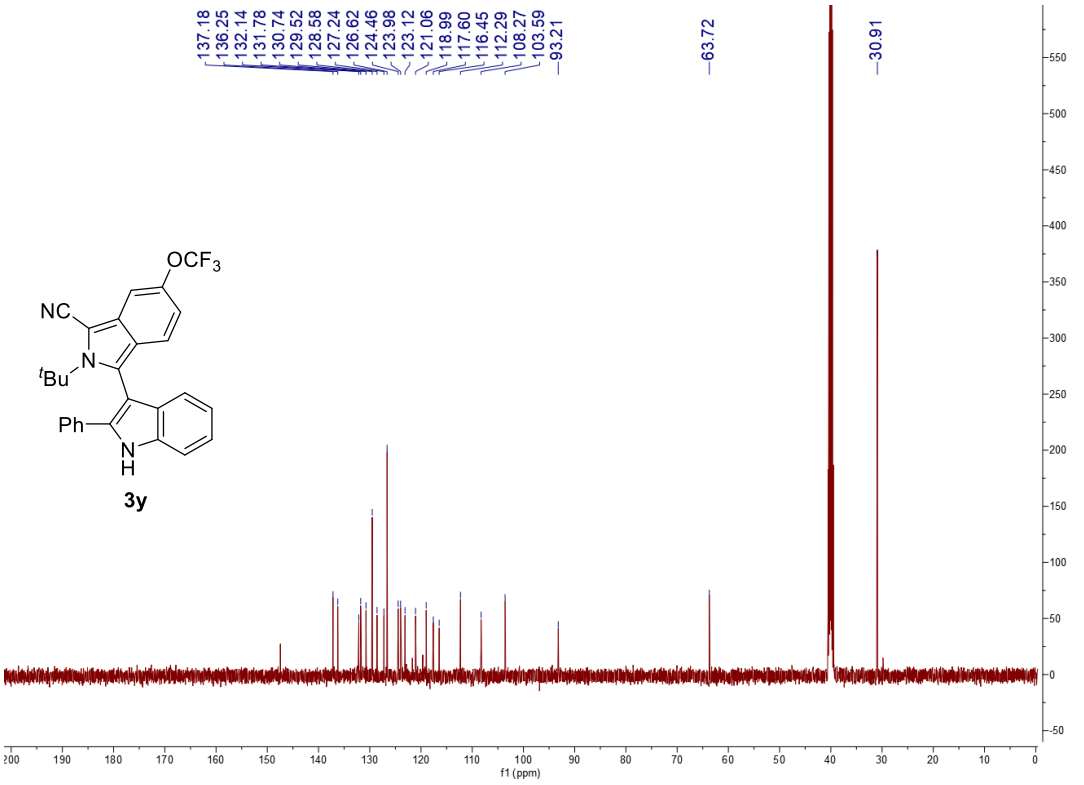
2.04
4.03
3.04
1.00
9.06
f1 (ppm)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118.99
117.60
116.45
112.29
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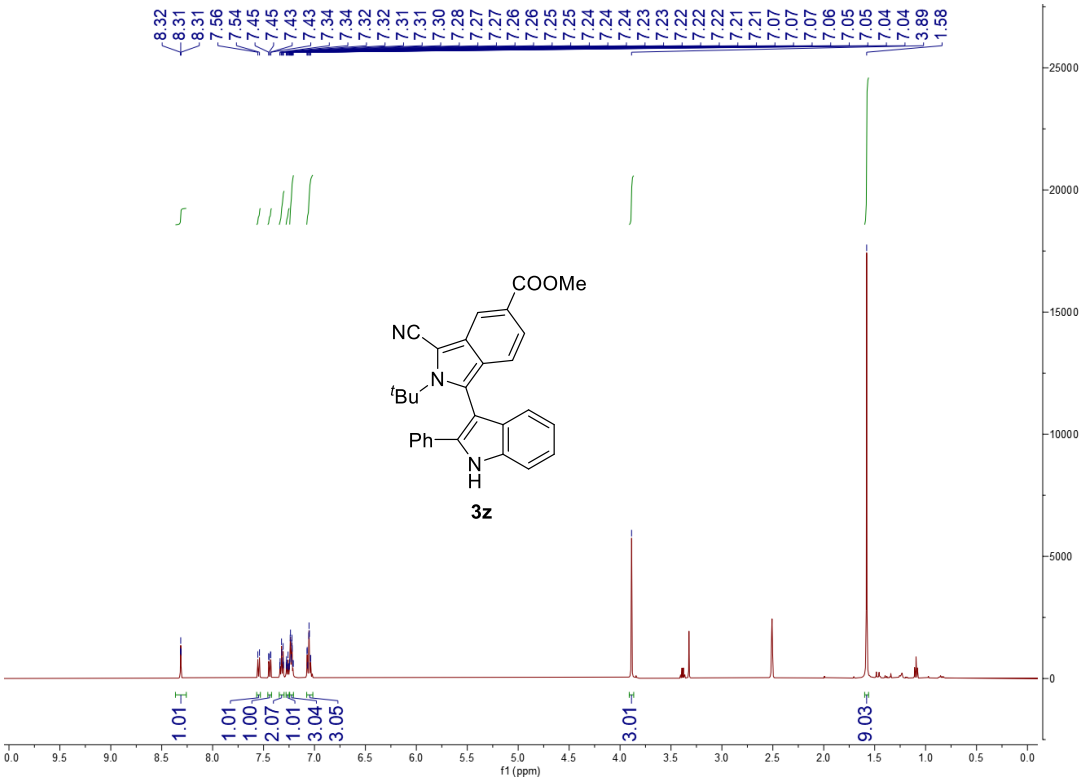
30.91
OCF3
NC
tBu
N
Ph
N
H
3y
f1 (ppm)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7.07
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7.06
7.05
7.05
7.04
7.04
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N
Ph
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3.05
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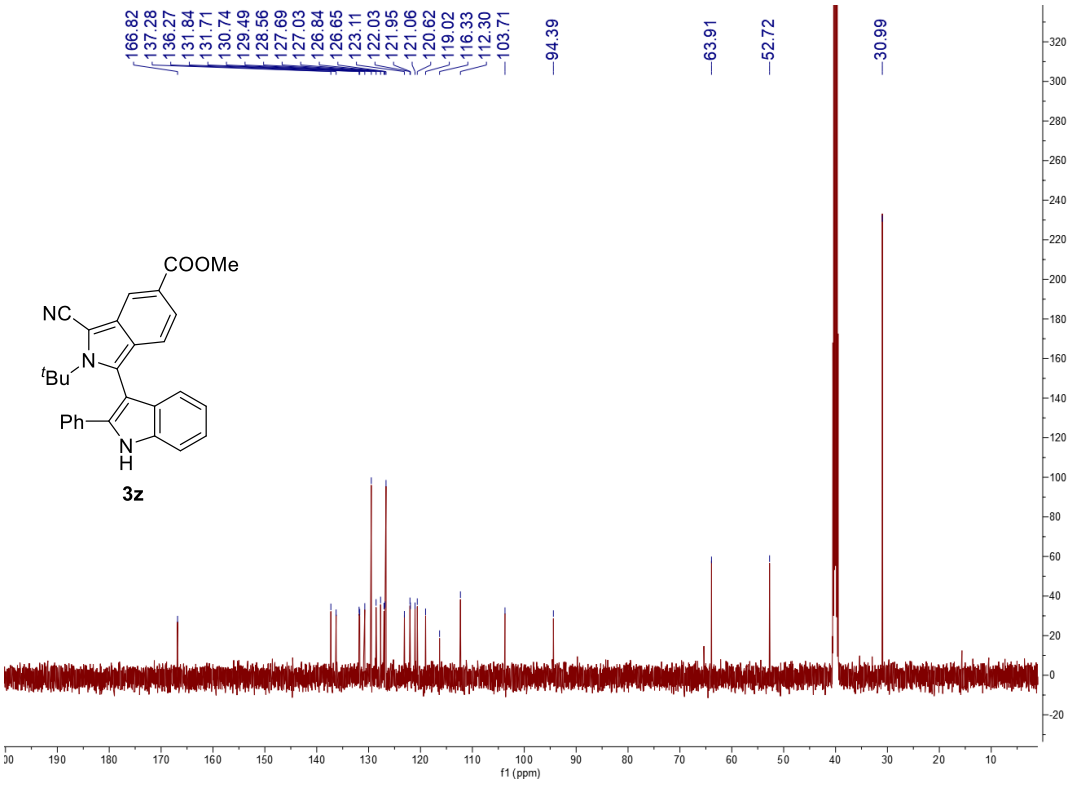
9.03
f1 (ppm)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123.11
122.03
121.95
121.06
120.62
119.02
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112.30
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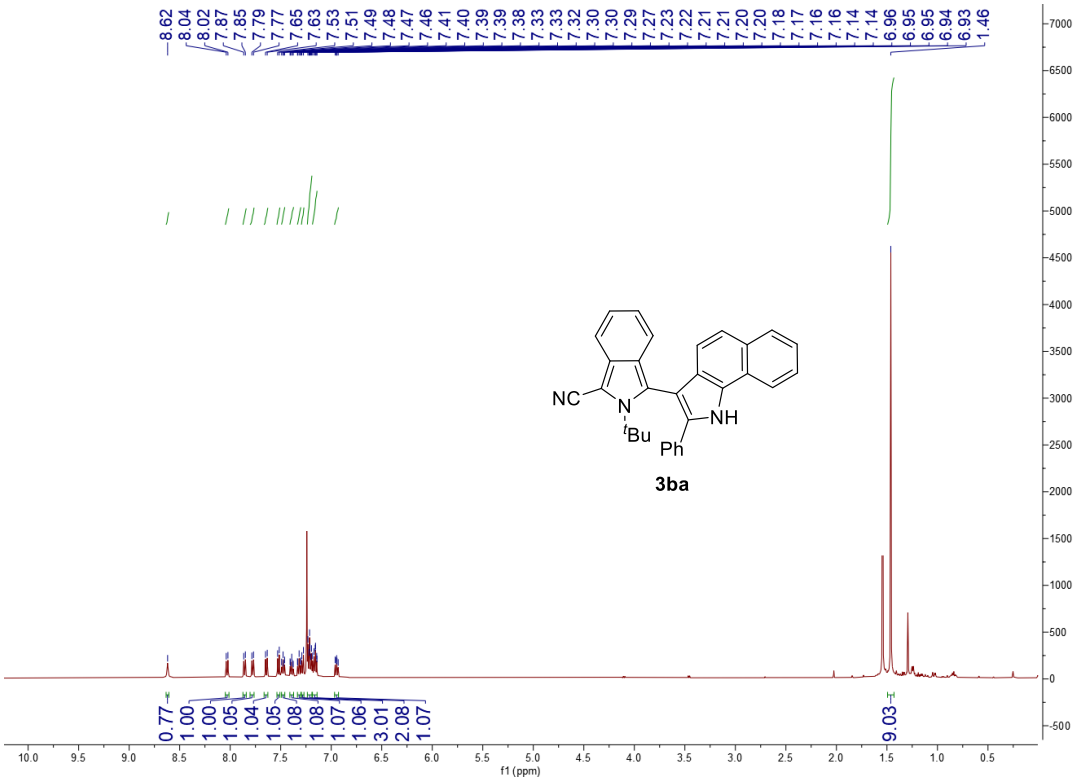
tBu
N
Ph
N
H
3z
f1 (ppm)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7.16
7.14
7.14
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6.95
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6.94
6.93
1.46
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N
tBu
NH
Ph
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1.00
1.05
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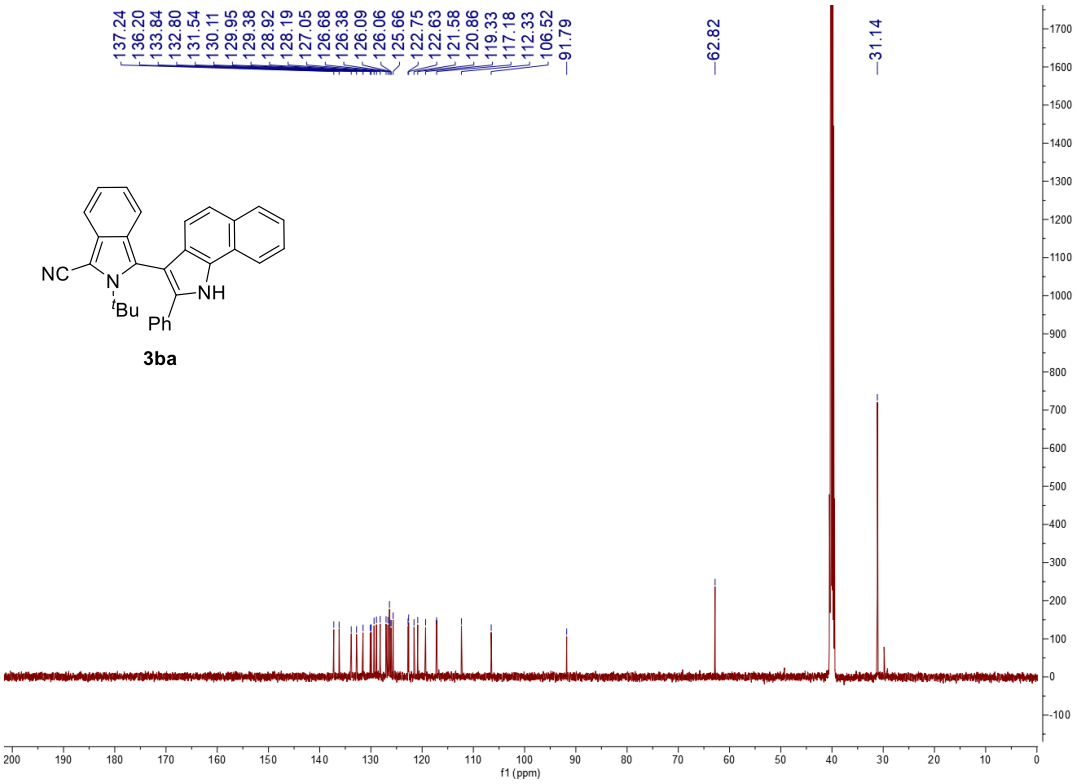
1.08
1.07
1.06
3.01
2.08
1.07
9.03
f1 (ppm)

3ba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62.82
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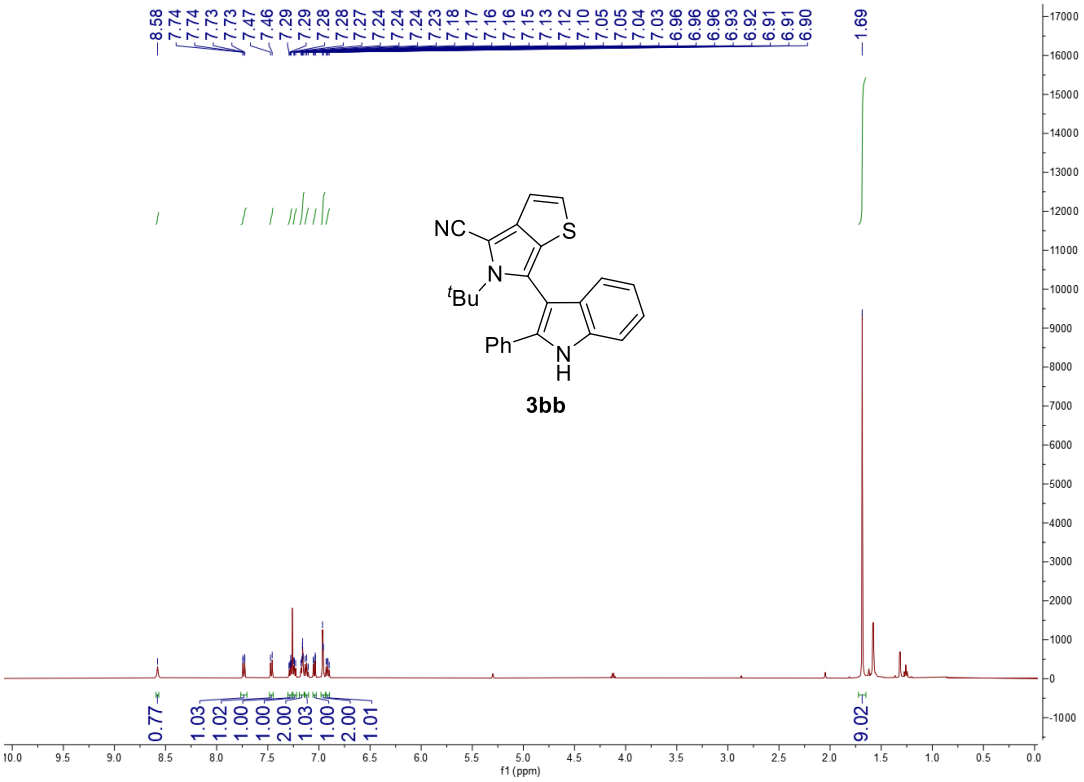
N
tBu
NH
Ph
f1 (ppm)

3ba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7.05
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7.04
7.03
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6.96
6.96
6.93
6.92
6.91
6.91
6.90
1.69
NC
S
N
tBu
Ph
N
H
0.77
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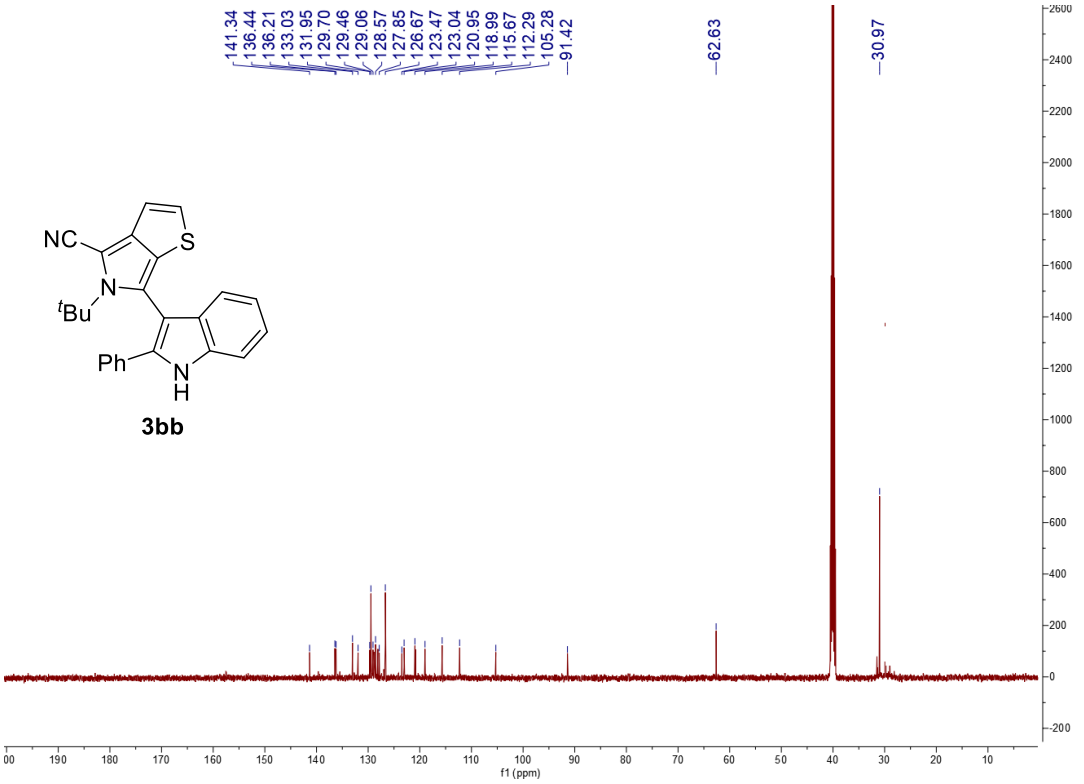
1.00
2.00
1.03
1.00
2.00
1.01
9.02
f1 (ppm)

3bb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123.04
120.95
118.99
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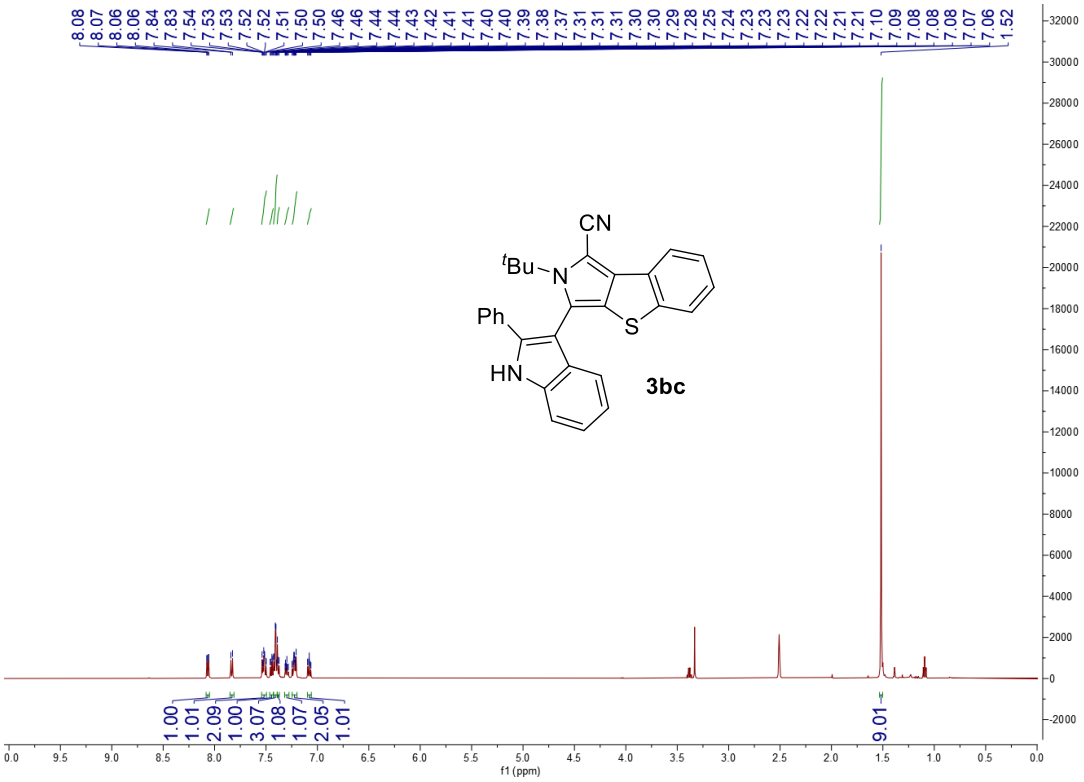
30.97
NC
S
N
tBu
Ph
N
H
f1 (ppm)

3bb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CN
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HN
S
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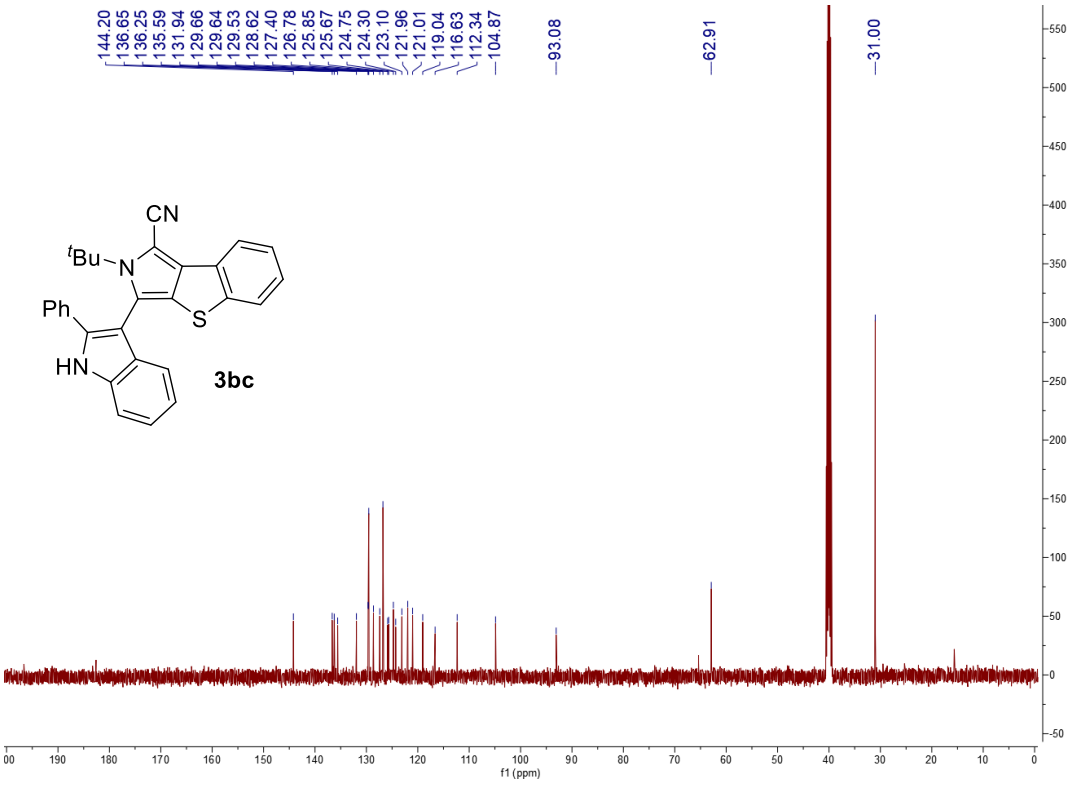
9.01
f1 (ppm)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93.08
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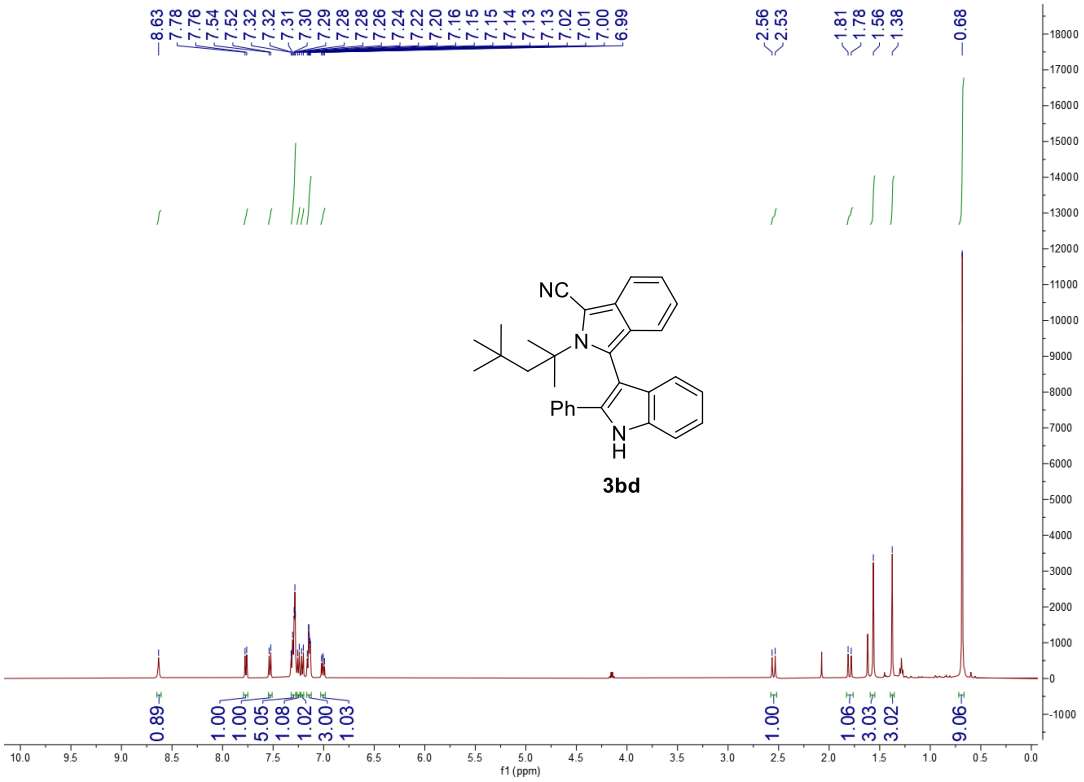
tBu
N
Ph
HN
S
3bc
f1 (ppm)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7.24
7.22
7.20
7.16
7.15
7.15
7.14
7.13
7.13
7.02
7.01
7.00
6.99
2.56
2.53
1.81
1.78
1.56
1.38
0.68
NC
N
Ph
N
H
0.89
1.00
1.00
5.05
1.08
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1.00
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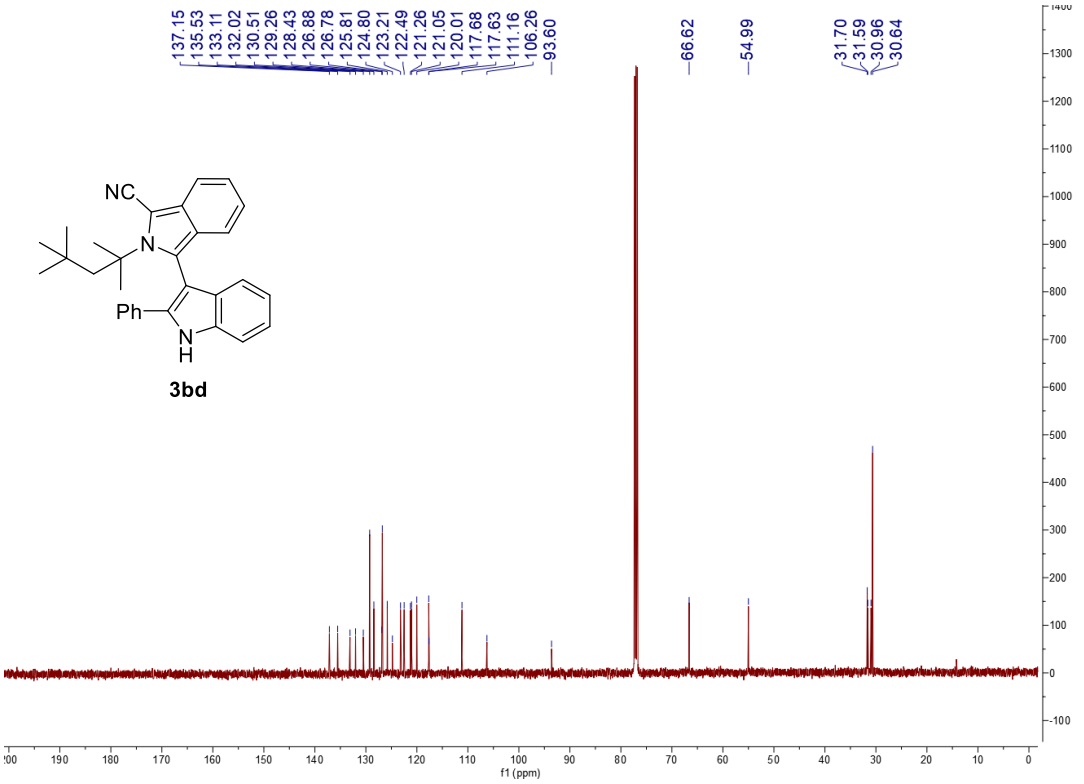
3.02
9.06
f1 (ppm)

3bd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121.05
120.01
117.68
117.63
111.16
106.26
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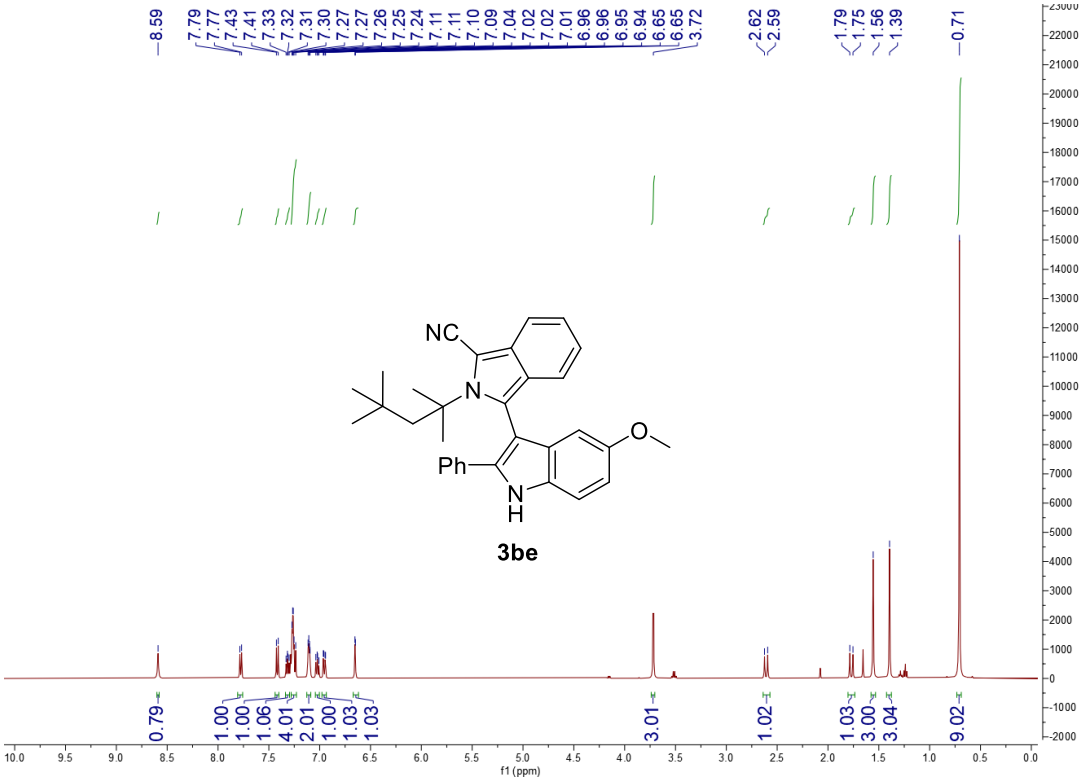
N
Ph
N
H
f1 (ppm)

3bd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7.24
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7.11
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7.02
7.02
7.01
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6.96
6.95
6.94
6.65
6.65
3.72
2.62
2.59
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1.75
1.56
1.39
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Ph
N
H
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1.00
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4.01
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1.03
3.01
1.02
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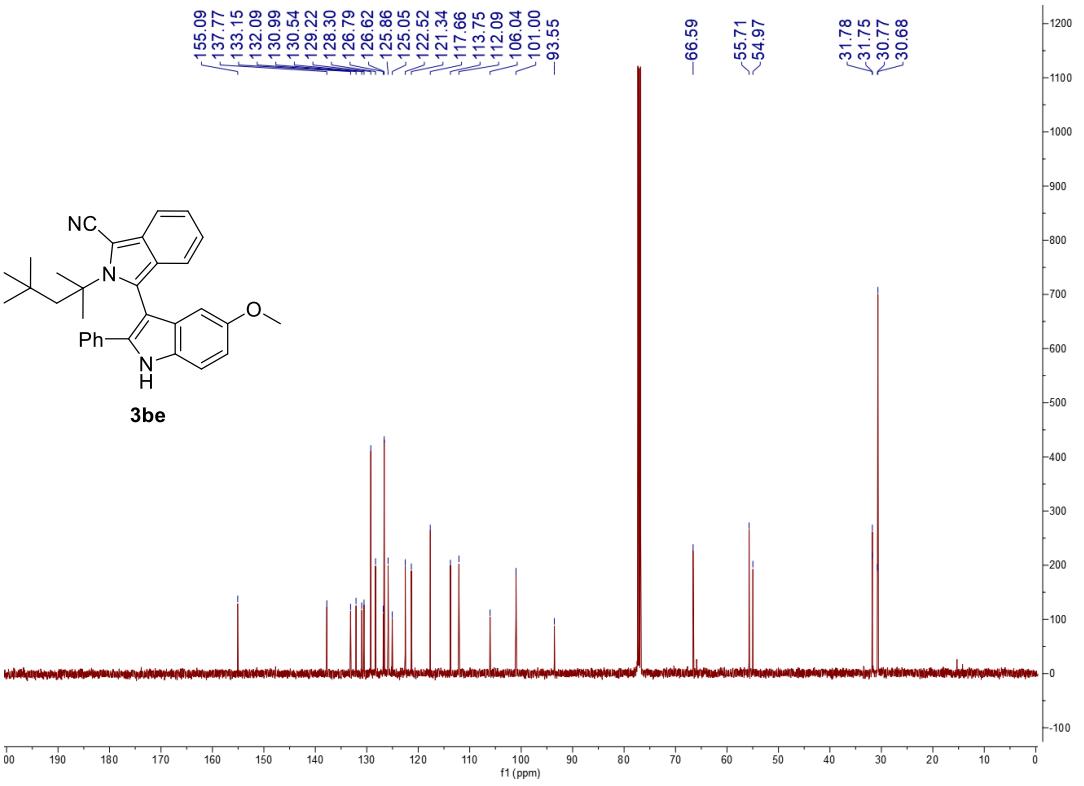
9.02
f1 (ppm)

3be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125.05
122.52
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113.75
112.09
106.04
101.00
93.55
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31.75
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30.68
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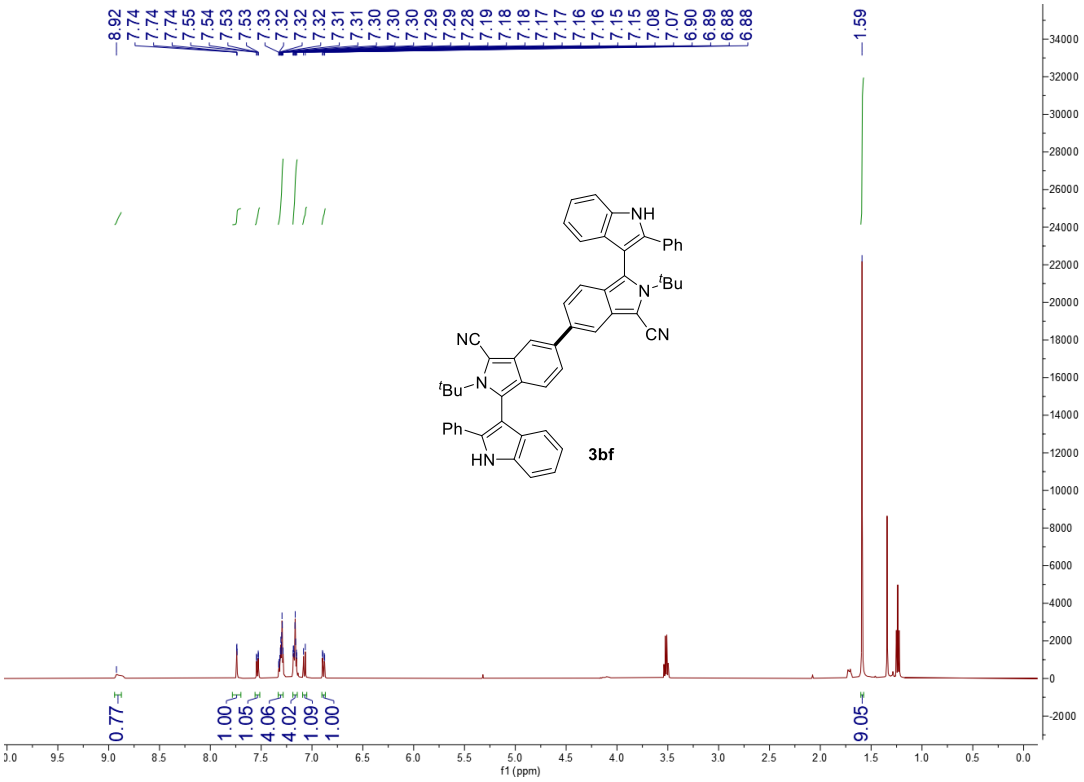
N
Ph
N
H
O
f1 (ppm)

3be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7.30
7.30
7.29
7.29
7.28
7.19
7.18
7.18
7.17
7.17
7.16
7.16
7.15
7.15
7.08
7.07
6.90
6.89
6.88
6.88
1.59
NH
Ph
N
tBu
CN
NC
tBu
N
Ph
HN
3bf
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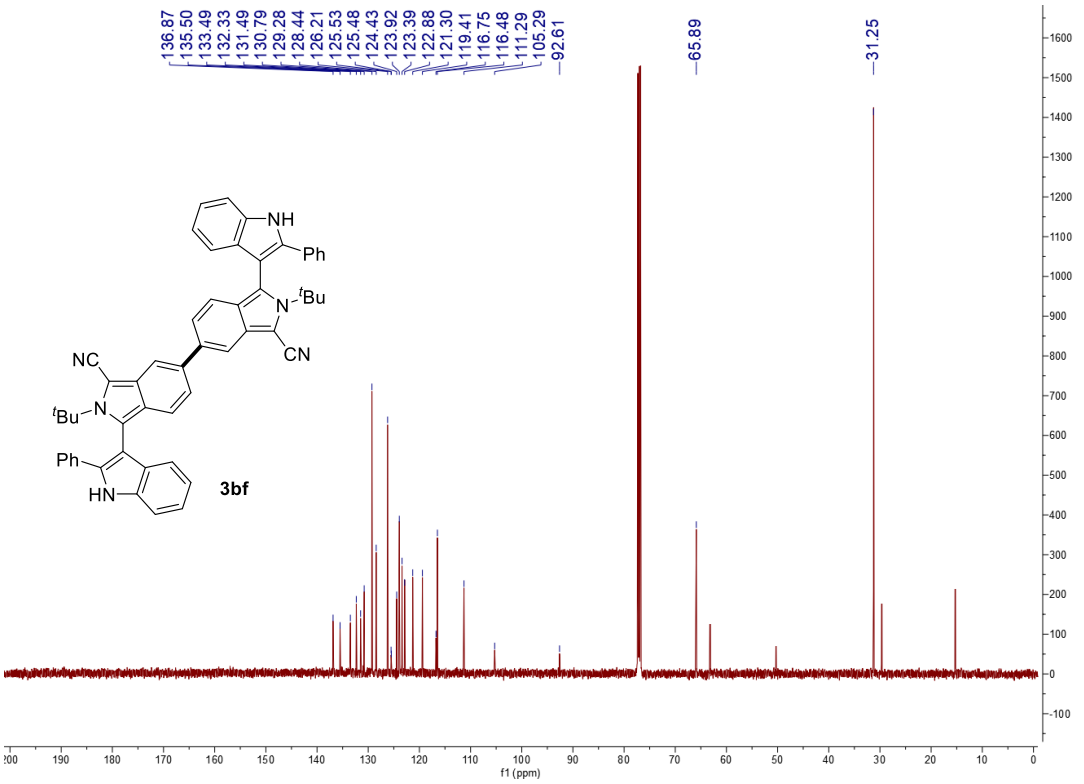
1.05
4.06
4.02
1.09
1.00
9.05
f1 (ppm)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123.92
123.39
122.88
121.30
119.41
116.75
116.48
111.29
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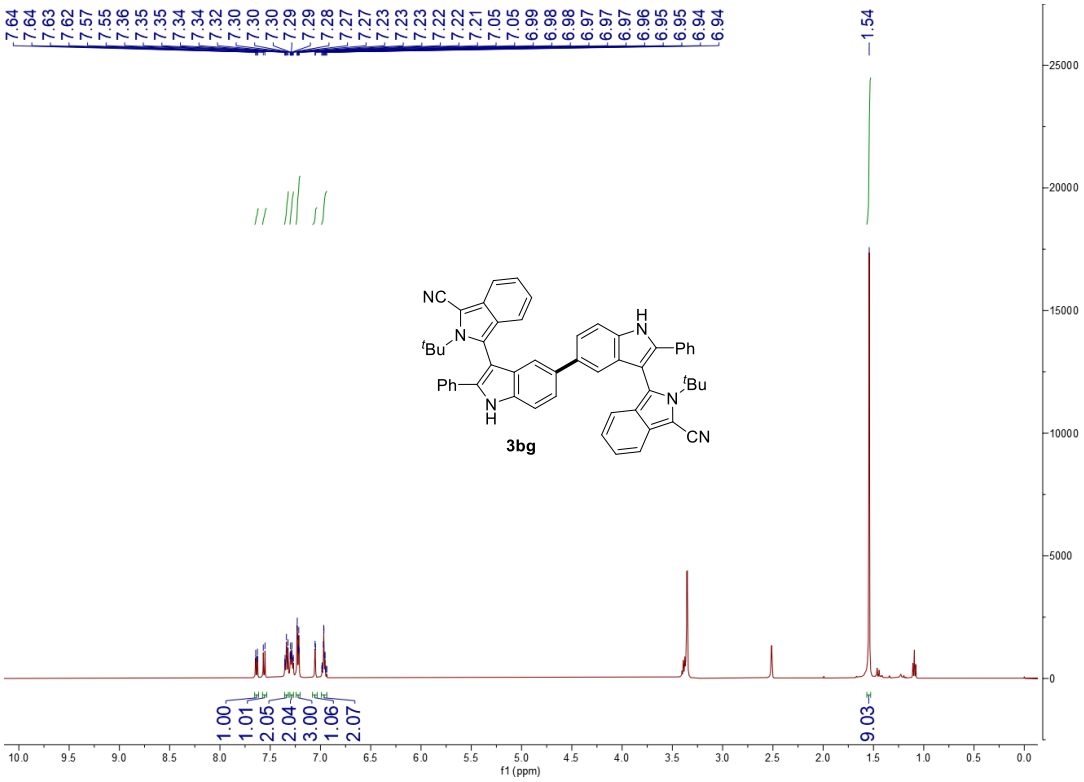
31.25
NH
Ph
N
tBu
CN
NC
tBu
N
Ph
HN
3bf
f1 (ppm)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6.97
6.97
6.96
6.95
6.95
6.94
6.94
1.54
NC
tBu
N
Ph
N
H
H
N
Ph
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N
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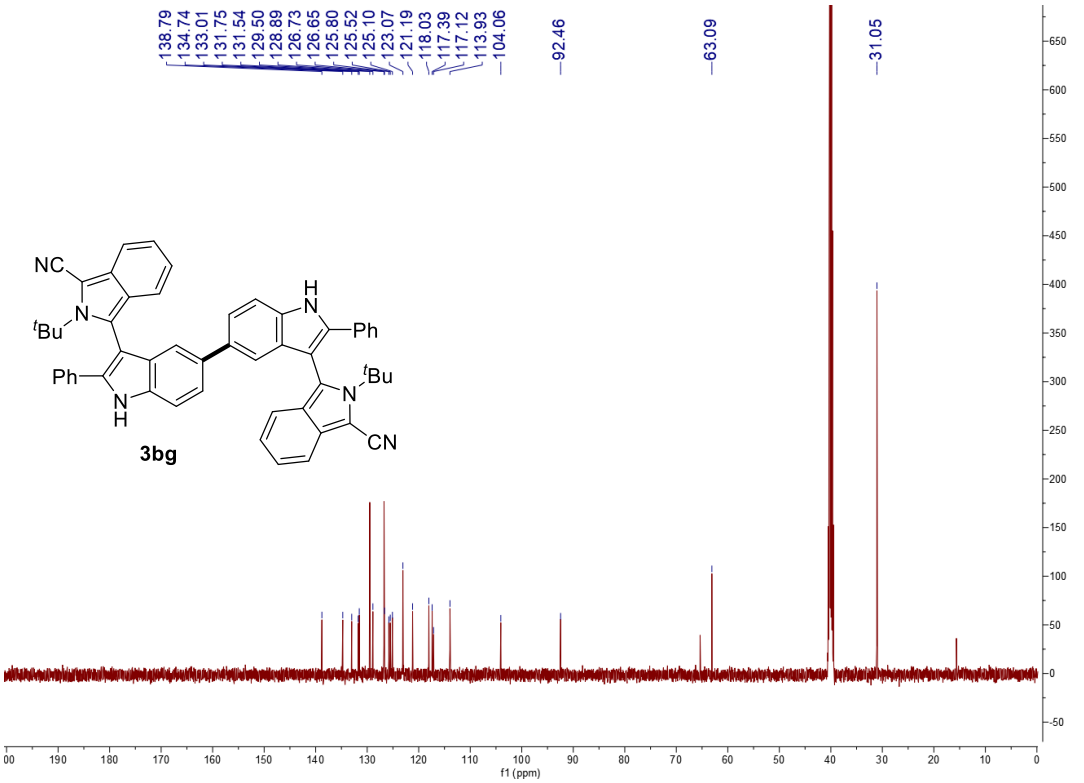
1.01
2.05
2.04
3.00
1.06
2.07
9.03
f1 (ppm)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125.52
125.10
123.07
121.19
118.03
117.39
117.12
113.93
104.06
92.46
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Ph
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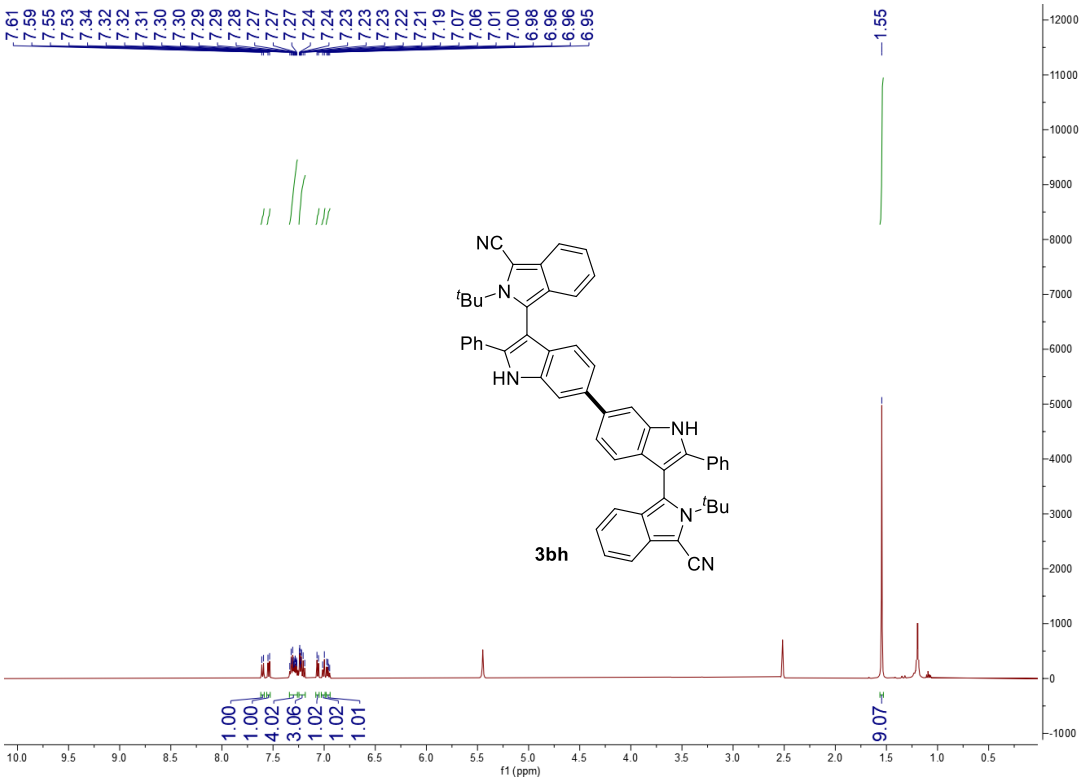
H
N
Ph
tBu
N
CN
3bg
f1 (ppm)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7.24
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7.23
7.23
7.22
7.21
7.19
7.07
7.06
7.01
7.00
6.98
6.96
6.96
6.95
1.55
NC
tBu
N
Ph
HN
NH
Ph
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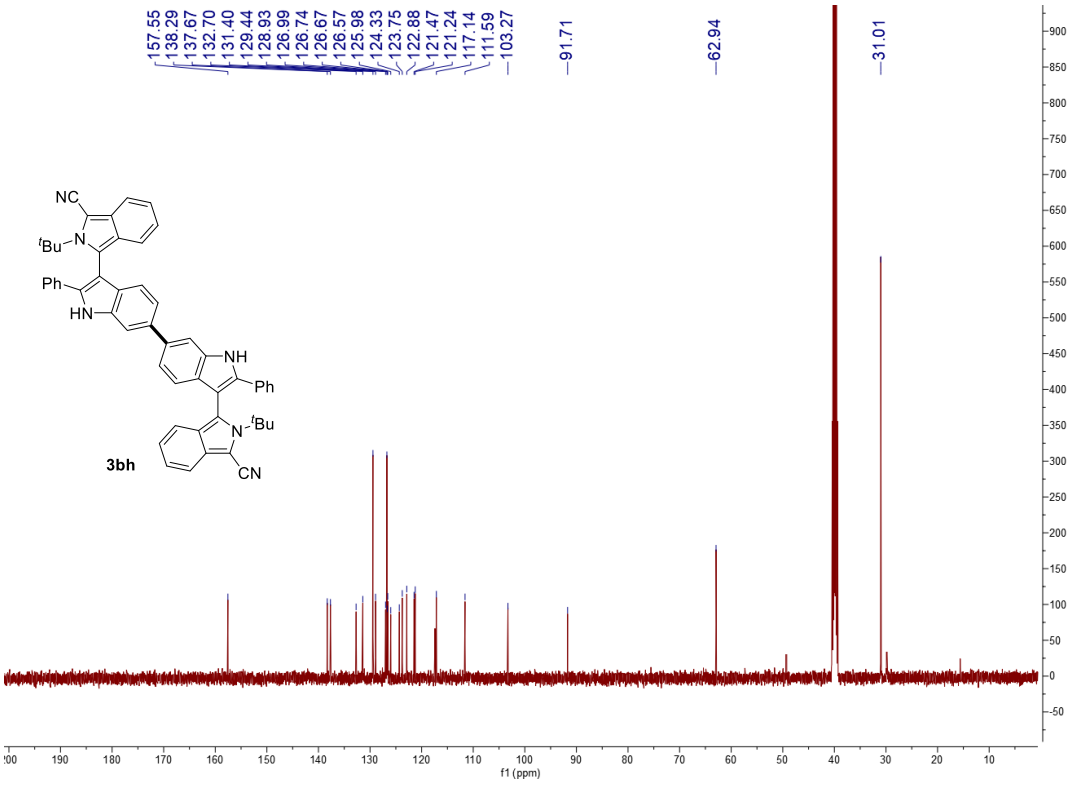
1.00
4.02
3.06
1.02
1.02
1.01
9.07
f1 (ppm)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124.33
123.75
122.88
121.47
121.24
117.14
111.59
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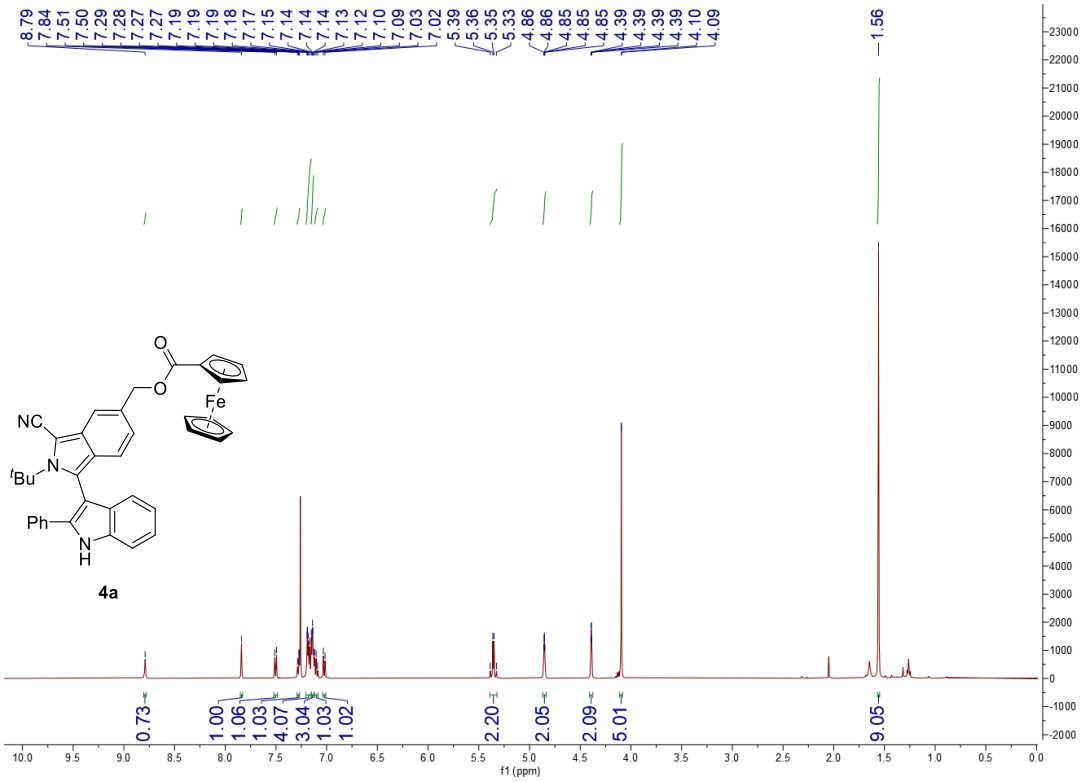
31.01
NC
tBu
N
Ph
HN
NH
Ph
tBu
N
CN
3bh
f1 (ppm)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5.33
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4.39
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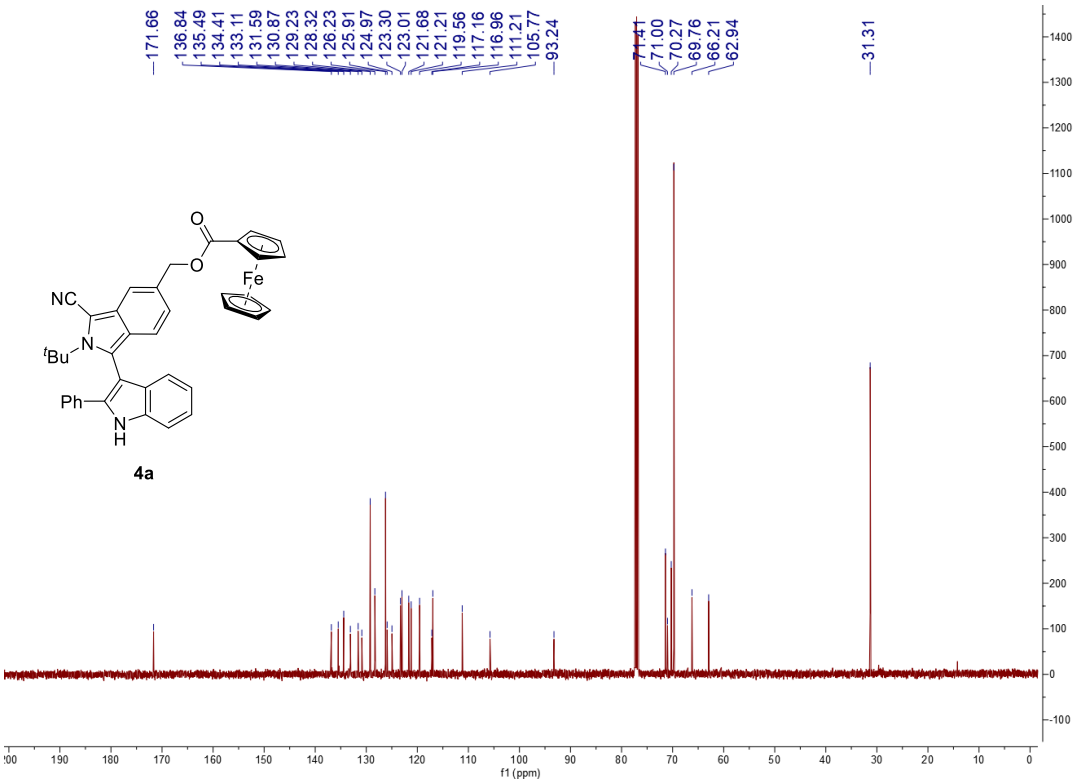
4.39
4.10
4.09
1.56
0.73
1.00
1.06
1.03
4.07
3.04
1.03
1.02
2.20
2.05
2.09
5.01
9.05
f1 (ppm)
NC
tBu
N
Ph
N
H
O
O
Fe
4a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123.30
123.01
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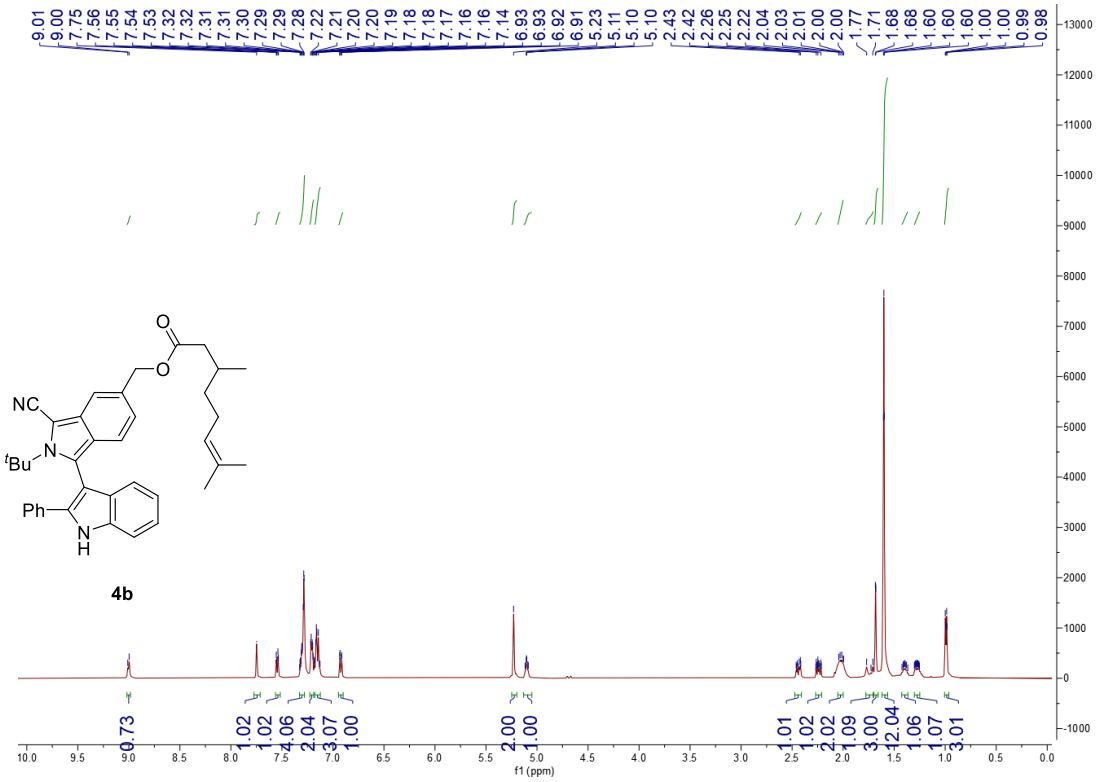
121.21
119.56
117.16
116.96
111.21
105.77
93.24
71.41
71.00
70.27
69.76
66.21
62.94
31.31
f1 (ppm)
NC
tBu
N
Ph
N
H
O
O
Fe
4a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NC
tBu
N
Ph
N
H
O
O
4b
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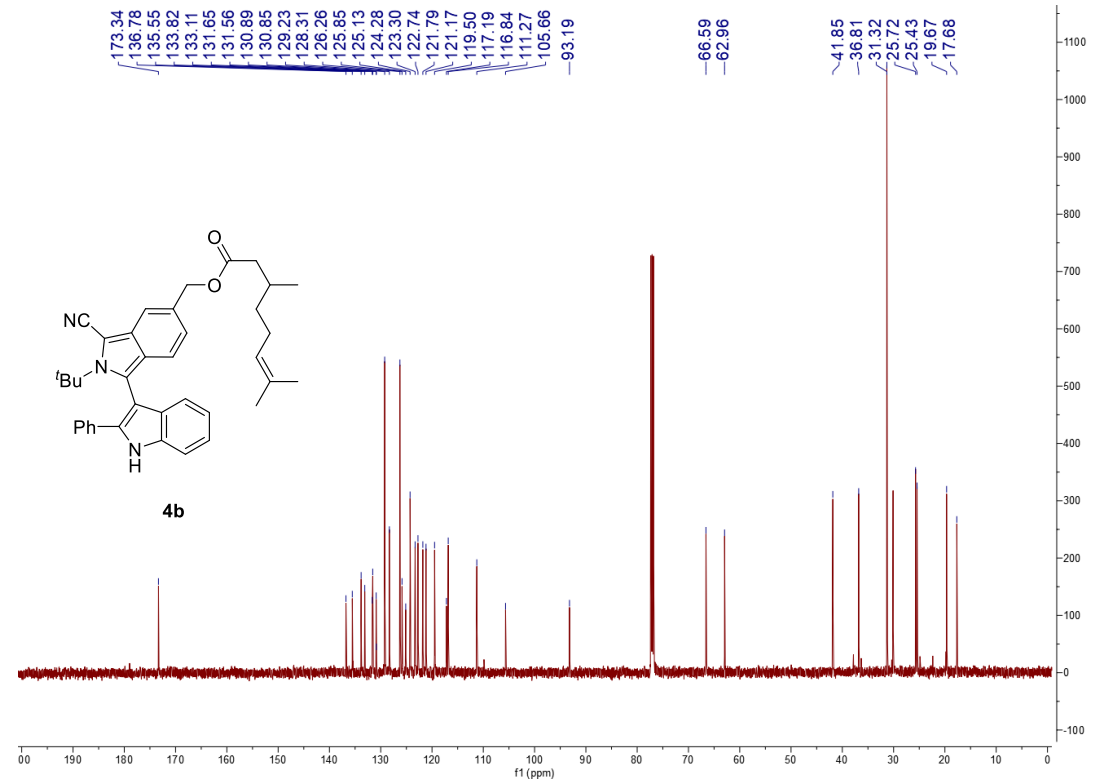
f1 (ppm)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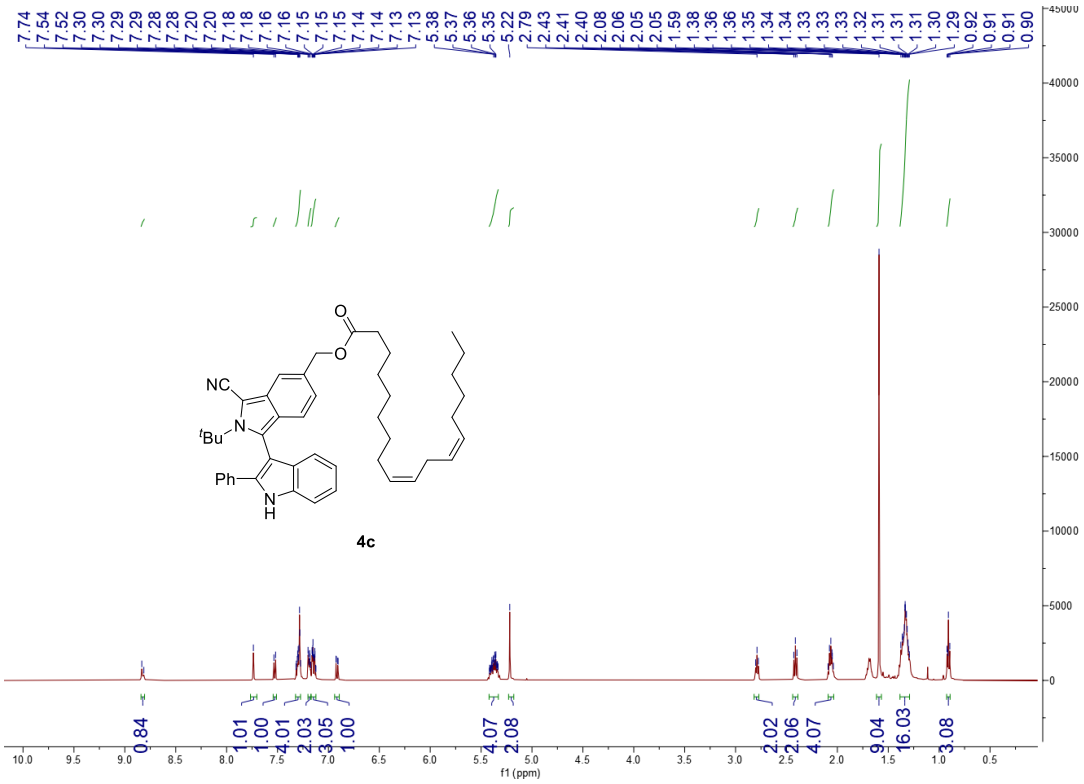
NC
tBu
N
Ph
N
H
O
O
4b
f1 (ppm)


7.74 7.54 7.52 7.30 7.30 7.29 7.29 7.28 7.28 7.20 7.20 7.18 7.18 7.16 7.16 7.15 7.15 7.15 7.14 7.14 7.13 7.13 5.38 5.37 5.36 5.35 5.22 2.79 2.43 2.41 2.40 2.08 2.06 2.05 2.05 1.59 1.38 1.36 1.36 1.35 1.34 1.34 1.33 1.33 1.32 1.31 1.31 1.31 1.30 1.29 0.92 0.91 0.91 0.90
NC
tBu
N
Ph
N
H
O
O
4c
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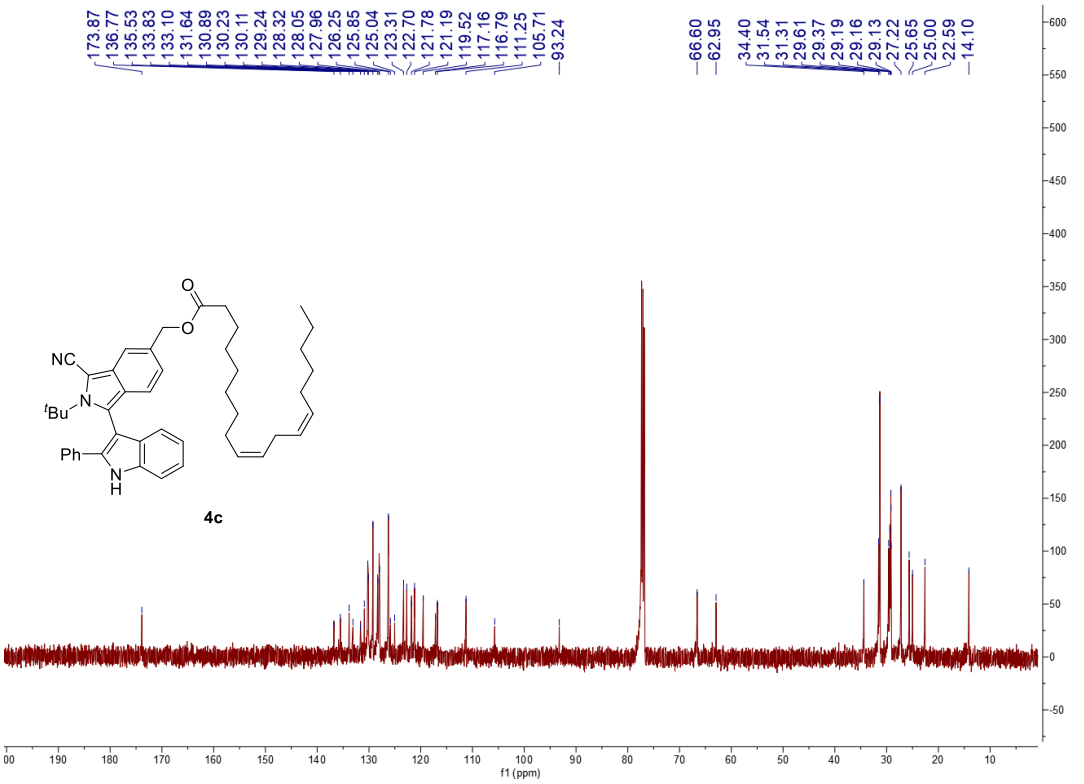
f1 (ppm)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66.60 62.95 34.40 31.54 31.31 29.61 29.37 29.19 29.16 29.13 27.22 25.65 25.00 22.59 14.10
NC
tBu
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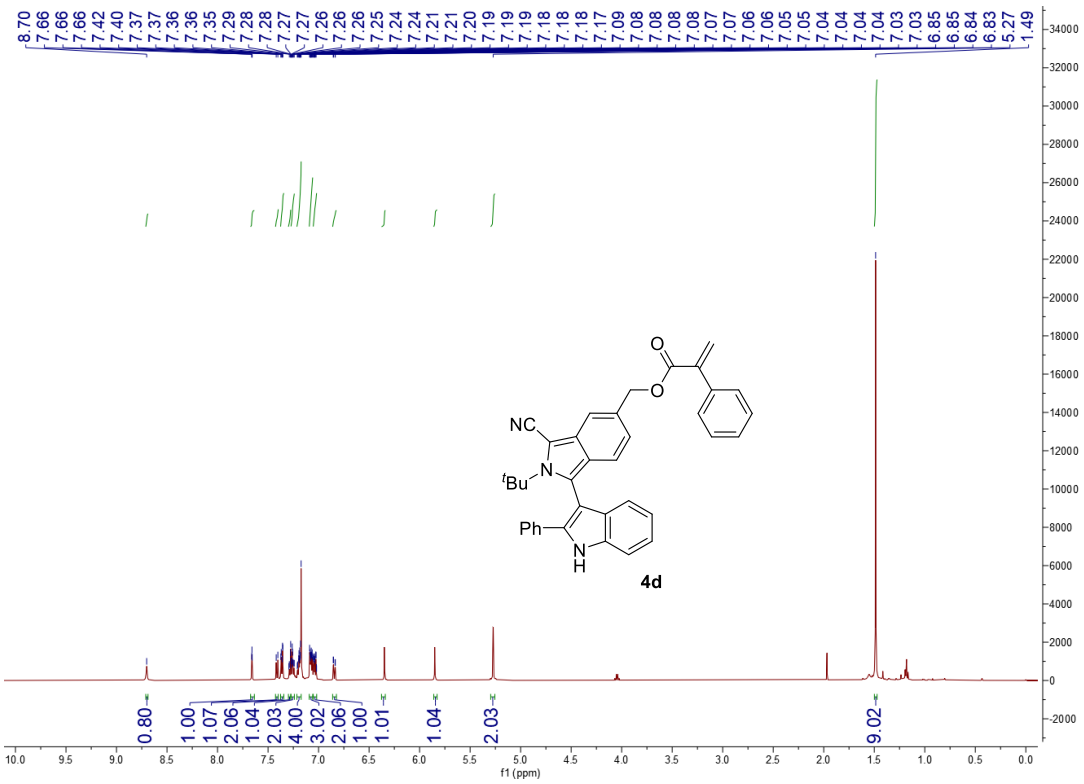
Ph
N
H
O
O
4c
f1 (ppm)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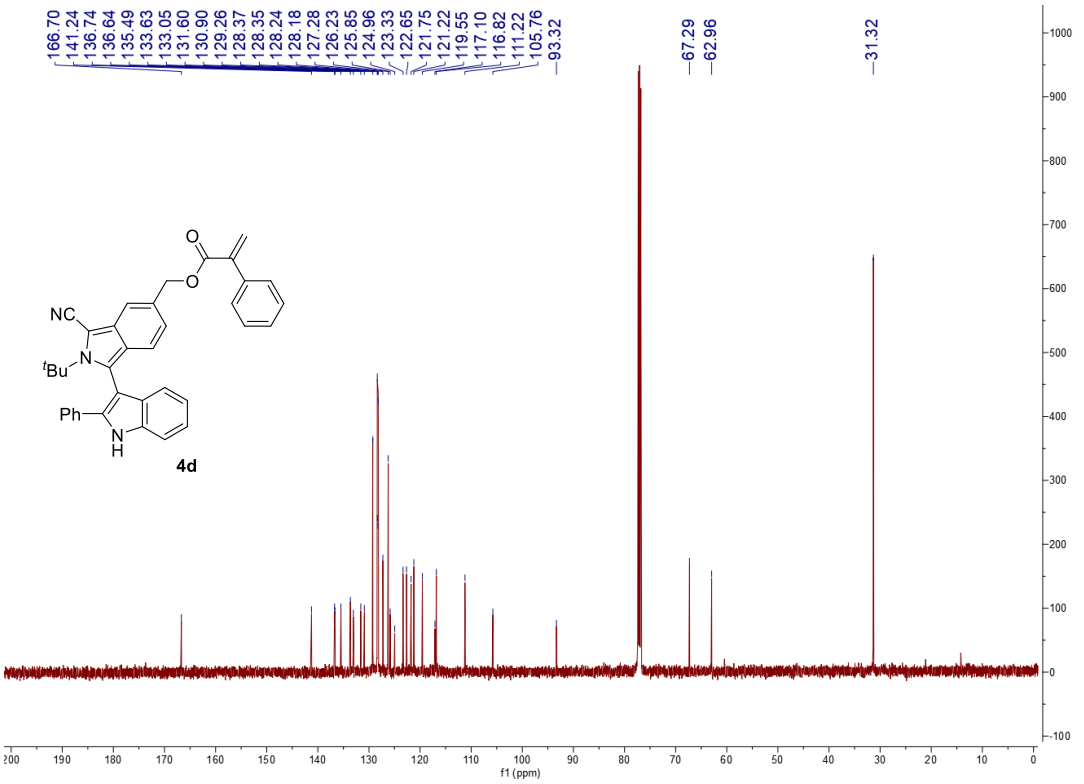
0.80 1.00 1.07 2.06 1.04 2.03 4.00 3.02 2.06 1.00 1.01 1.04 2.03 9.02
f1 (ppm)
4d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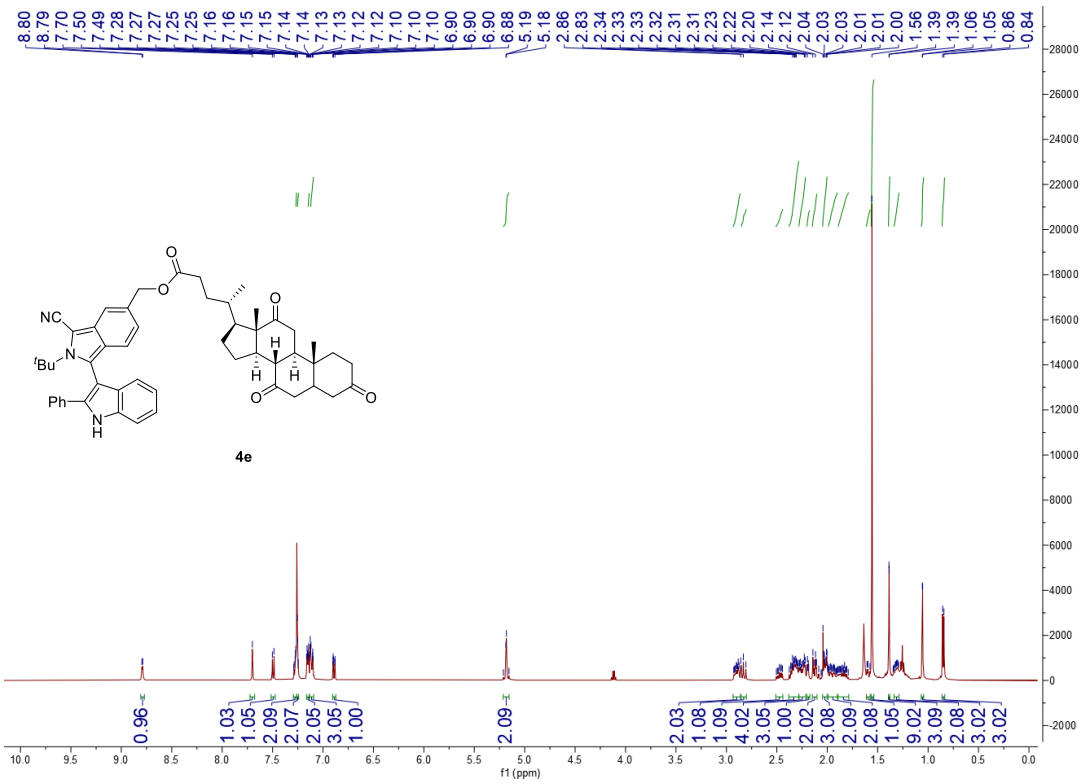
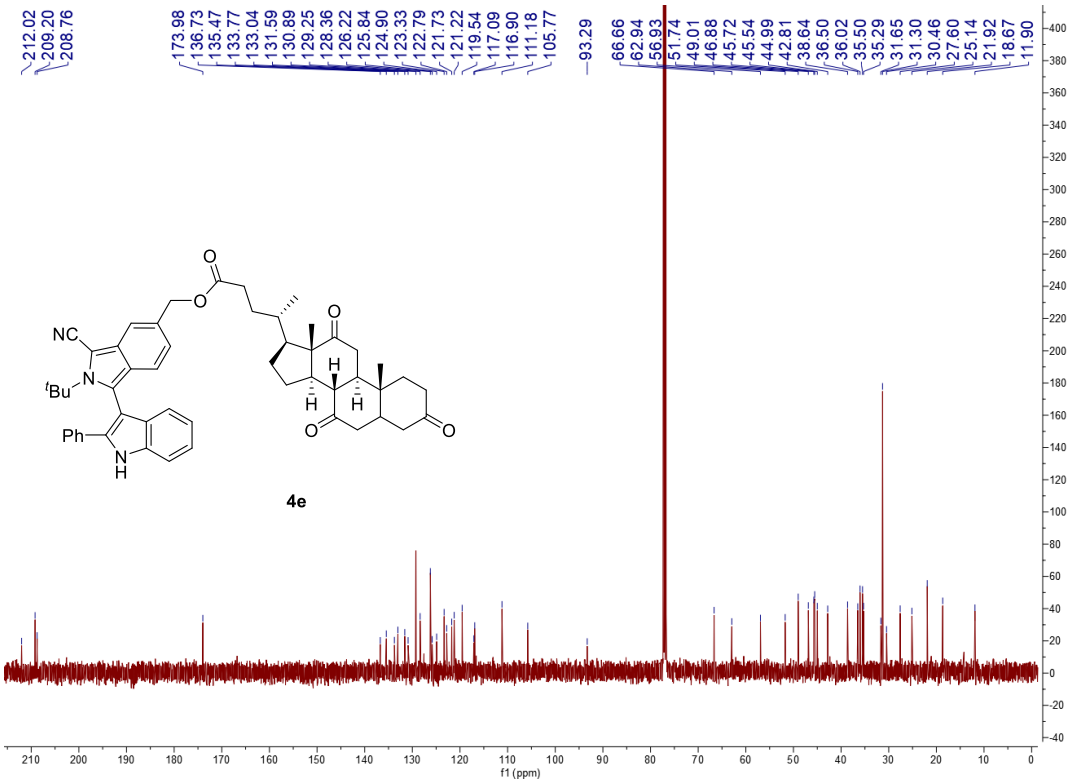
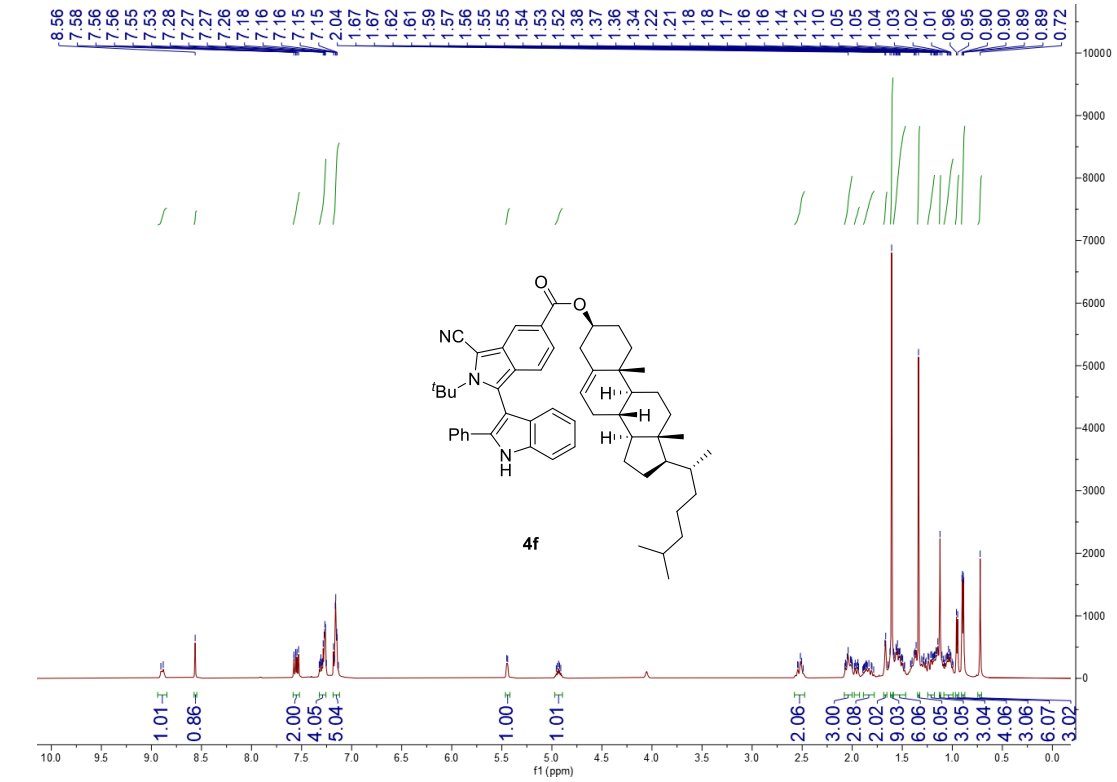
67.29 62.96
31.32
f1 (ppm)
4d


4e
f1 (ppm)


4e
f1 (ppm)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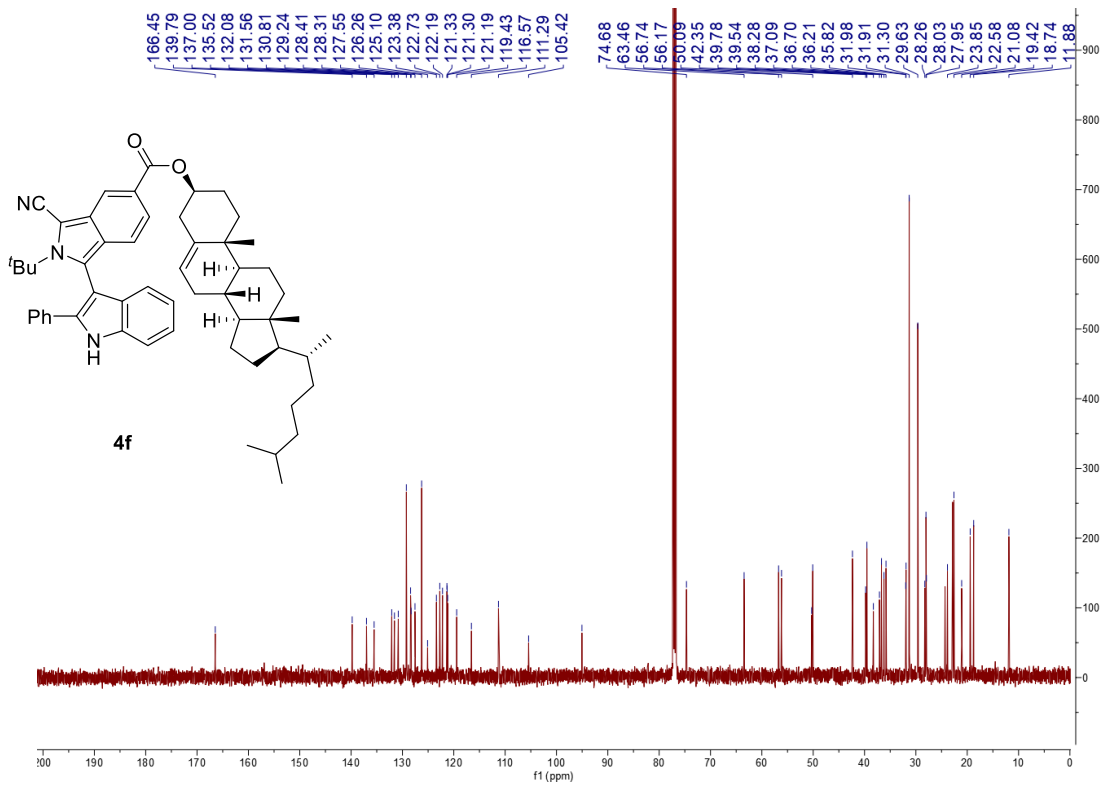
NC
tBu
N
Ph
N
H
O
O
H
H
H
4f
1.01 0.86 2.00 4.05 5.04 1.00 1.01 2.06 3.00 2.08 2.02 9.03 6.06 6.05 3.05 3.04 4.06 3.06 6.07 3.02
f1 (ppm)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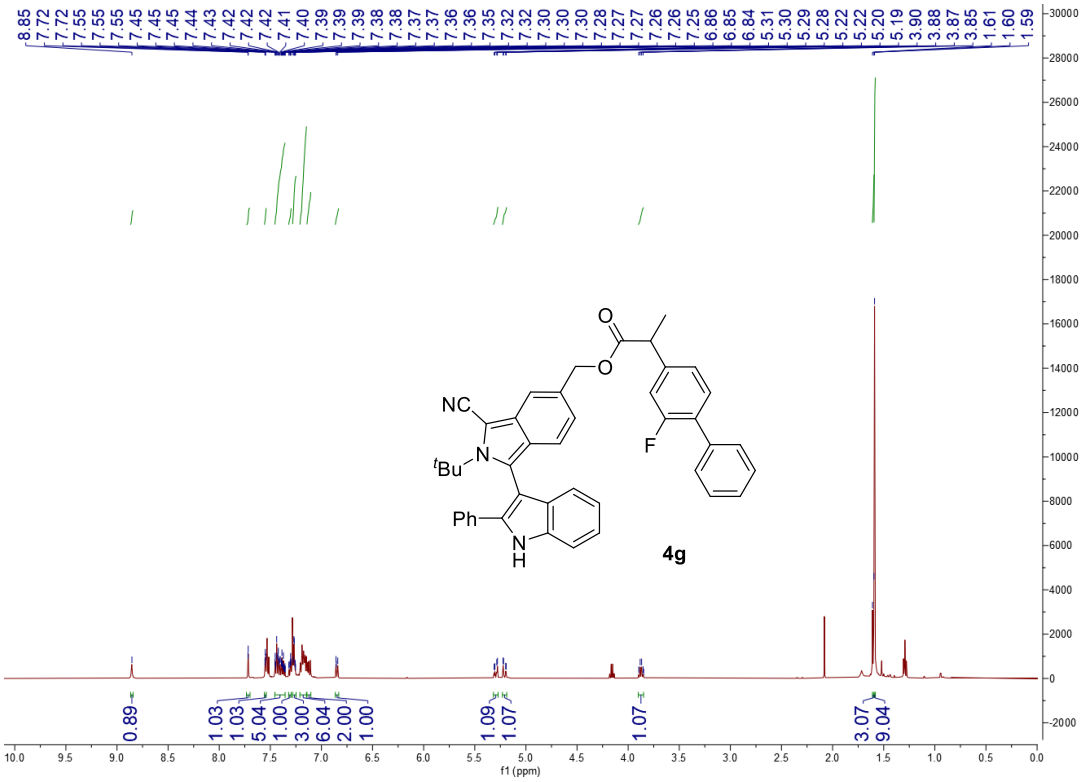
74.68 63.46 56.74 56.17 50.09 42.35 39.78 39.54 38.28 37.09 36.70 36.21 35.82 31.98 31.91 31.30 29.63 28.26 28.03 27.95 23.85 22.58 21.08 19.42 18.74 11.88
NC
tBu
N
Ph
N
H
O
O
H
H
H
4f
f1 (ppm)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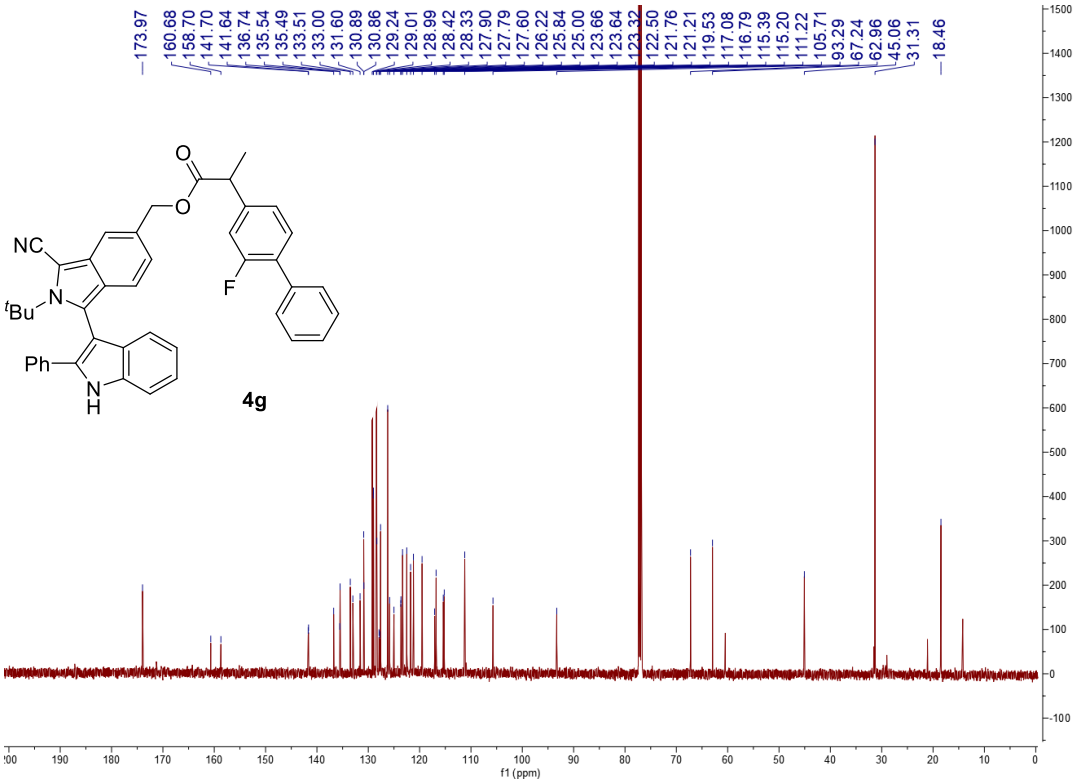
0.89 1.03 1.03 5.04 1.00 3.00 6.04 2.00 1.00 1.09 1.07 1.07 3.07 9.04
f1 (ppm)
4g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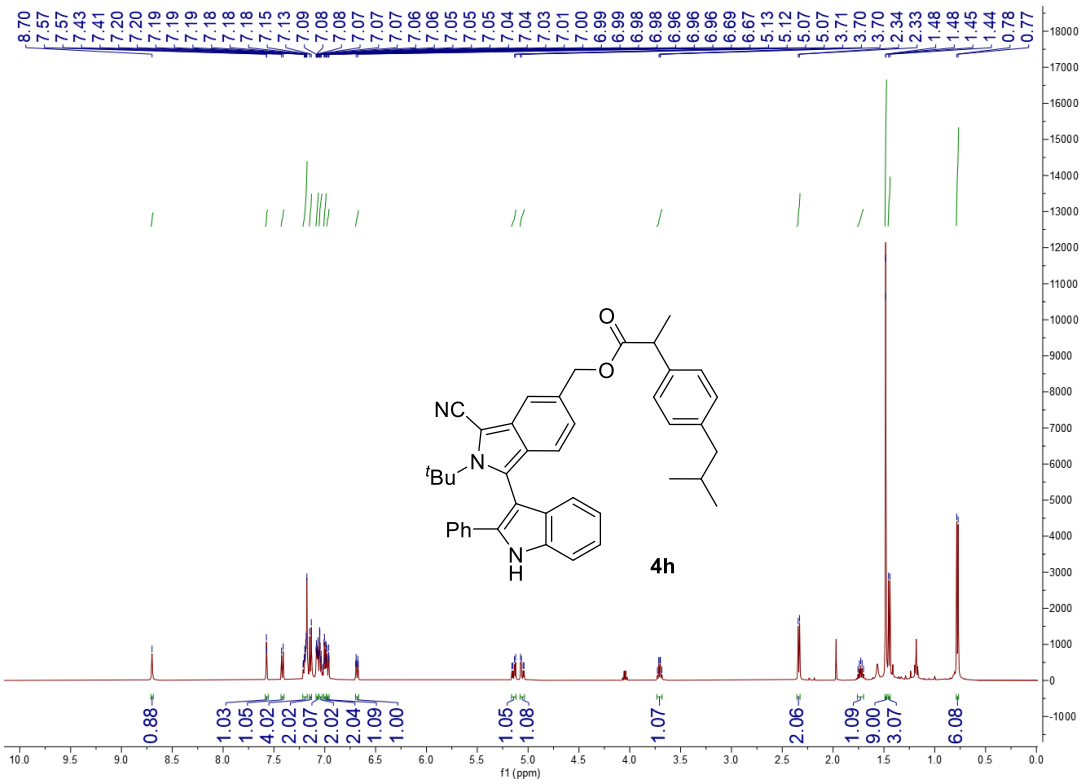
4g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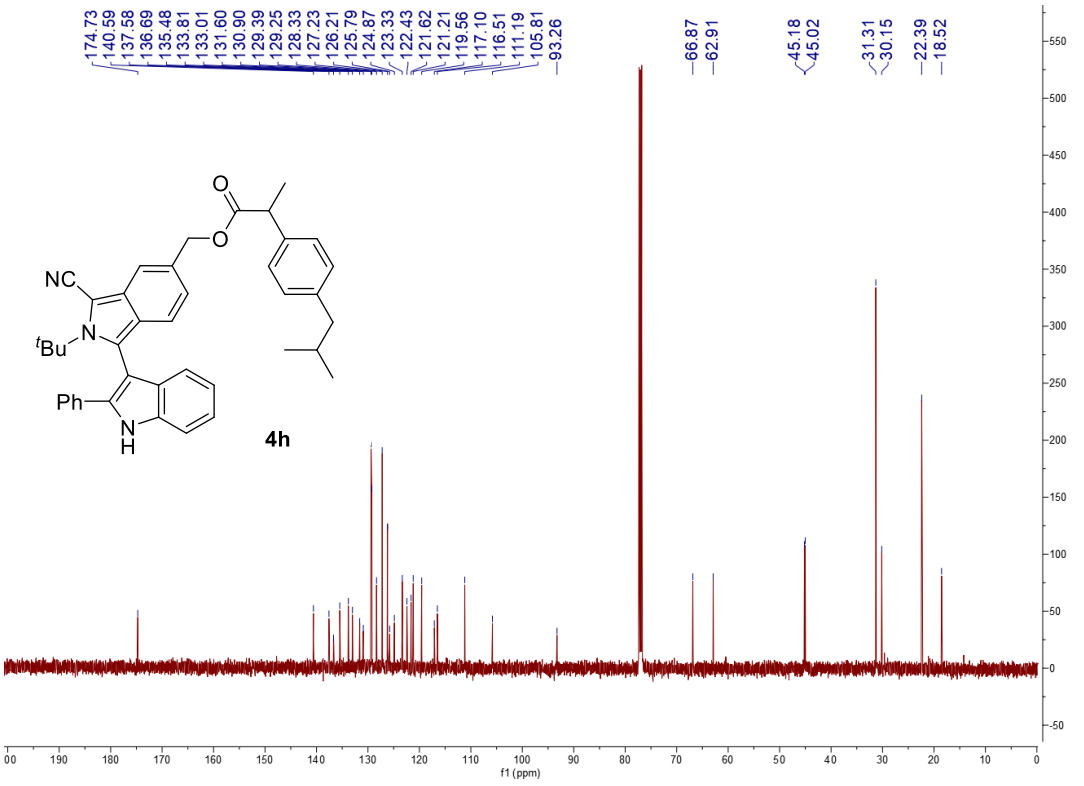
NC
tBu
N
Ph
N
H
O
O
4h
0.88 1.03 1.05 4.02 2.02 2.07 2.02 2.04 1.09 1.00 1.05 1.08 1.07 2.06 1.09 9.00 3.07 6.08
f1 (ppm)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66.87 62.91 45.18 45.02 31.31 30.15 22.39 18.52
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tBu
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Ph
N
H
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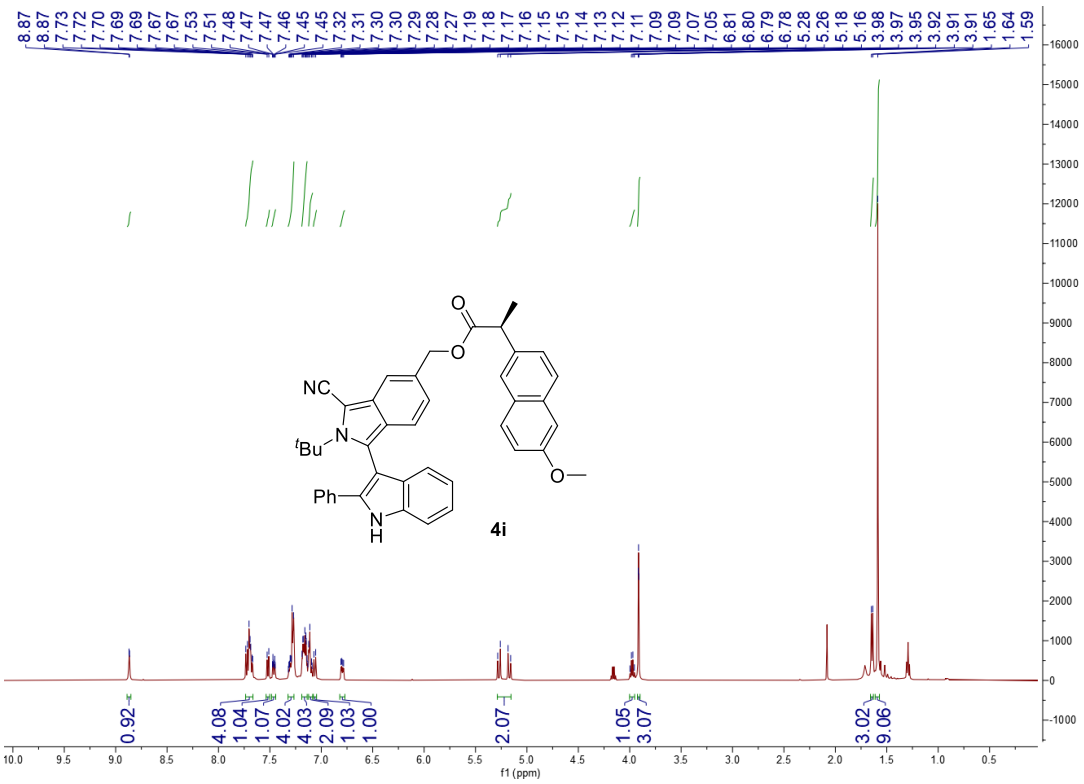
O
4h
f1 (ppm)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7.67
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7.18
7.17
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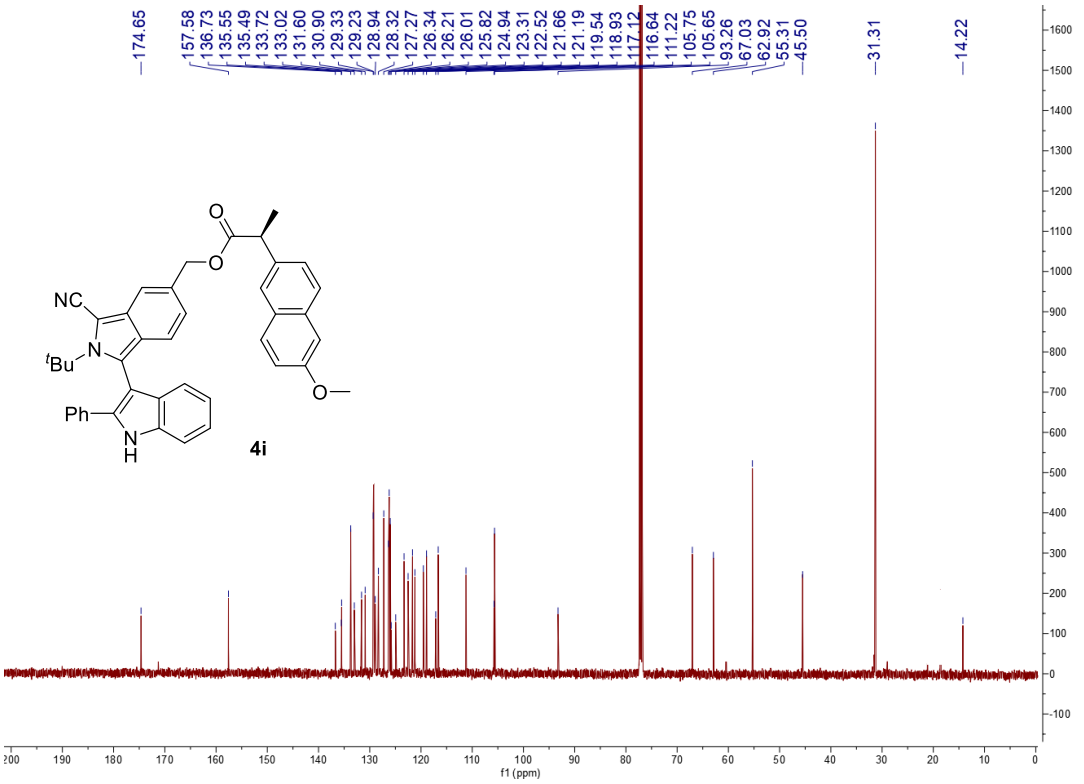
7.15
7.14
7.13
7.12
7.11
7.09
7.09
7.07
7.05
6.81
6.80
6.79
6.78
5.28
5.26
5.18
5.16
3.98
3.97
3.95
3.92
3.91
3.91
1.65
1.64
1.59
NC
tBu
N
Ph
N
H
O
O
O
O
4i
0.92
4.08
1.04
1.07
4.02
4.03
2.09
1.03
1.00
2.07
1.05
3.07
3.02
9.06
f1 (ppm)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129.23
128.94
128.32
127.27
126.34
126.21
126.01
125.82
124.94
123.31
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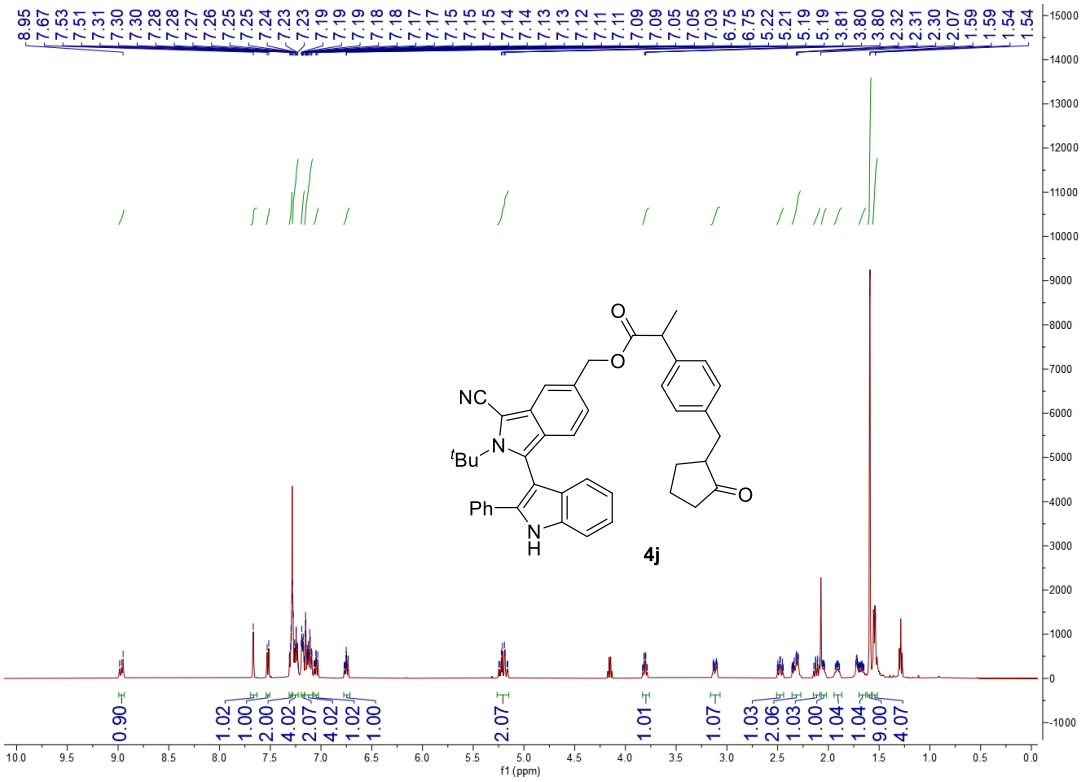
121.66
121.19
119.54
118.93
117.12
116.64
111.22
105.75
105.65
93.26
67.03
62.92
55.31
45.50
31.31
14.22
NC
tBu
N
Ph
N
H
O
O
O
O
4i
f1 (ppm)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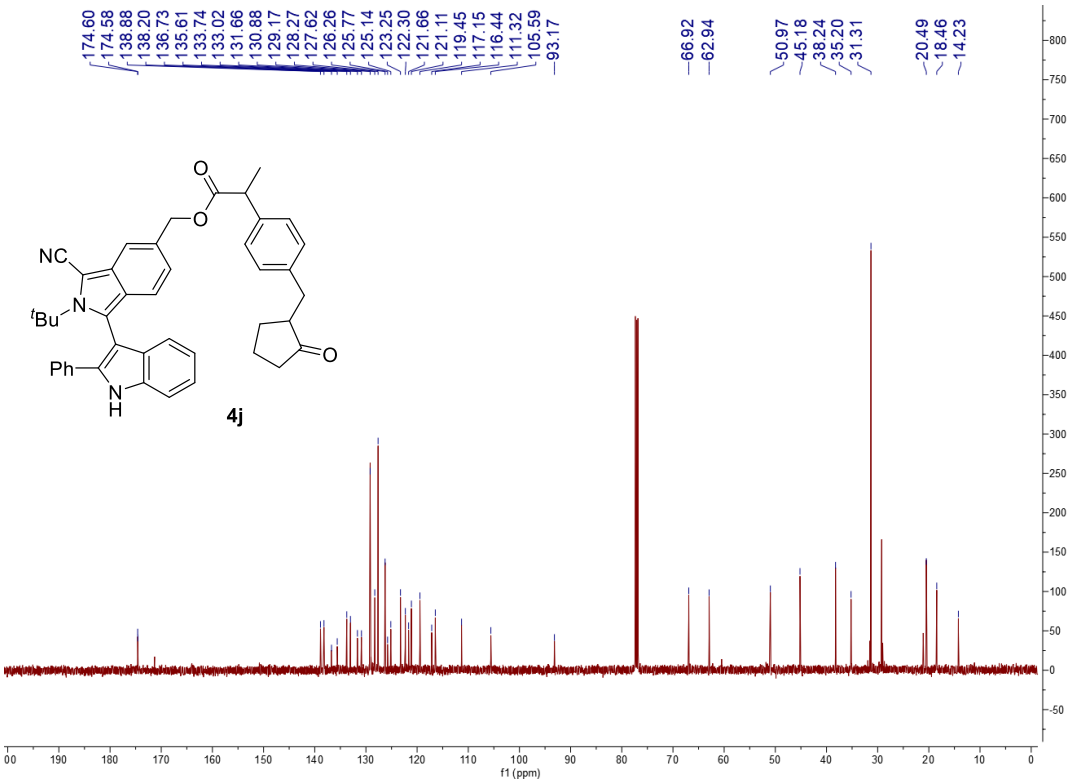
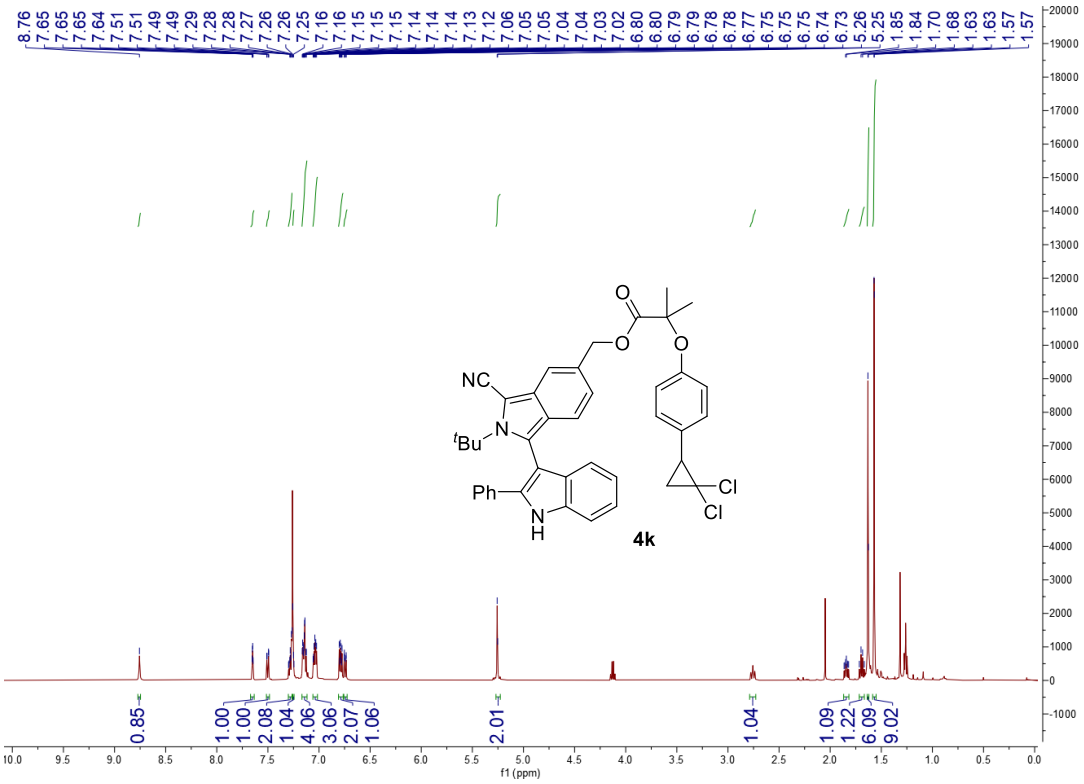
0.90 1.02 1.00 2.00 4.02 2.07 4.02 1.02 1.00 2.07 1.01 1.07 1.03 2.06 1.03 1.00 1.04 1.04 9.00 4.07
f1 (ppm)
4j


174.60 174.58 138.88 138.20 136.73 135.61 133.74 133.02 131.66 130.88 129.17 128.27 127.62 126.26 125.77 125.14 123.25 122.30 121.66 121.11 119.45 117.15 116.44 111.32 105.59 93.17
66.92 62.94
50.97 45.18 38.24 35.20 31.31
20.49 18.46 14.23
f1 (ppm)
4j


8.76 7.65 7.65 7.65 7.64 7.51 7.51 7.49 7.49 7.29 7.28 7.28 7.27 7.26 7.26 7.25 7.16 7.16 7.15 7.15 7.15 7.14 7.14 7.14 7.13 7.12 7.06 7.05 7.05 7.04 7.04 7.03 7.02 6.80 6.80 6.79 6.79 6.78 6.78 6.77 6.75 6.75 6.75 6.74 6.73 5.26 5.25 1.85 1.84 1.70 1.68 1.63 1.63 1.57 1.57
NC
tBu
N
Ph
N
H
O
O
O
O
Cl
Cl
4k
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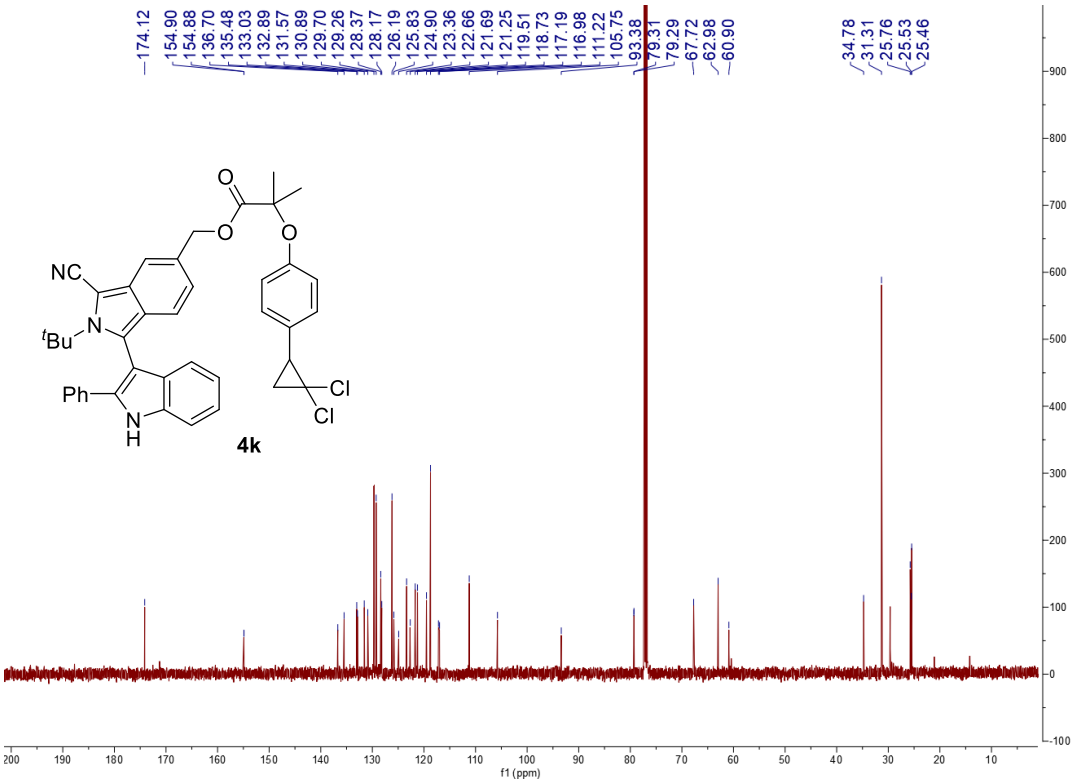
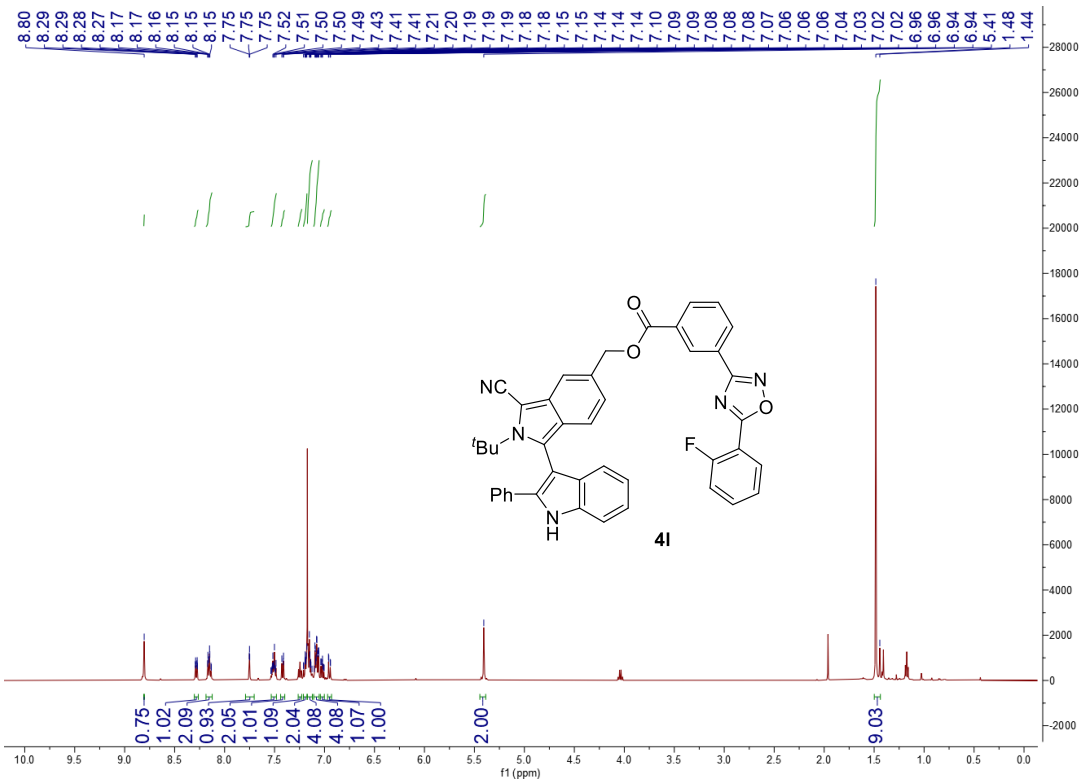
f1 (ppm)


174.12 154.90 154.88 136.70 135.48 133.03 132.89 131.57 130.89 129.70 129.26 128.37 128.17 126.19 125.83 124.90 123.36 122.66 121.69 121.25 119.51 118.73 117.19 116.98 111.22 105.75 93.38 79.31 79.29 67.72 62.98 60.90 34.78 31.31 25.76 25.53 25.46
NC
tBu
N
Ph
N
H
O
O
O
O
Cl
Cl
4k
f1 (ppm)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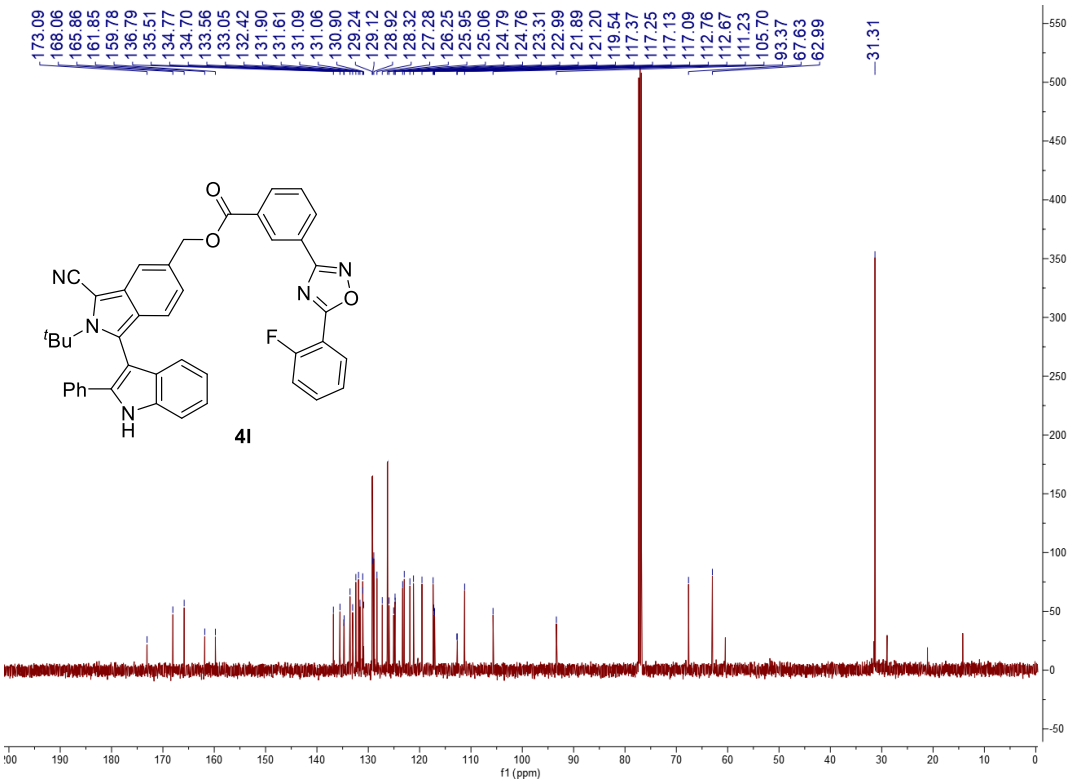
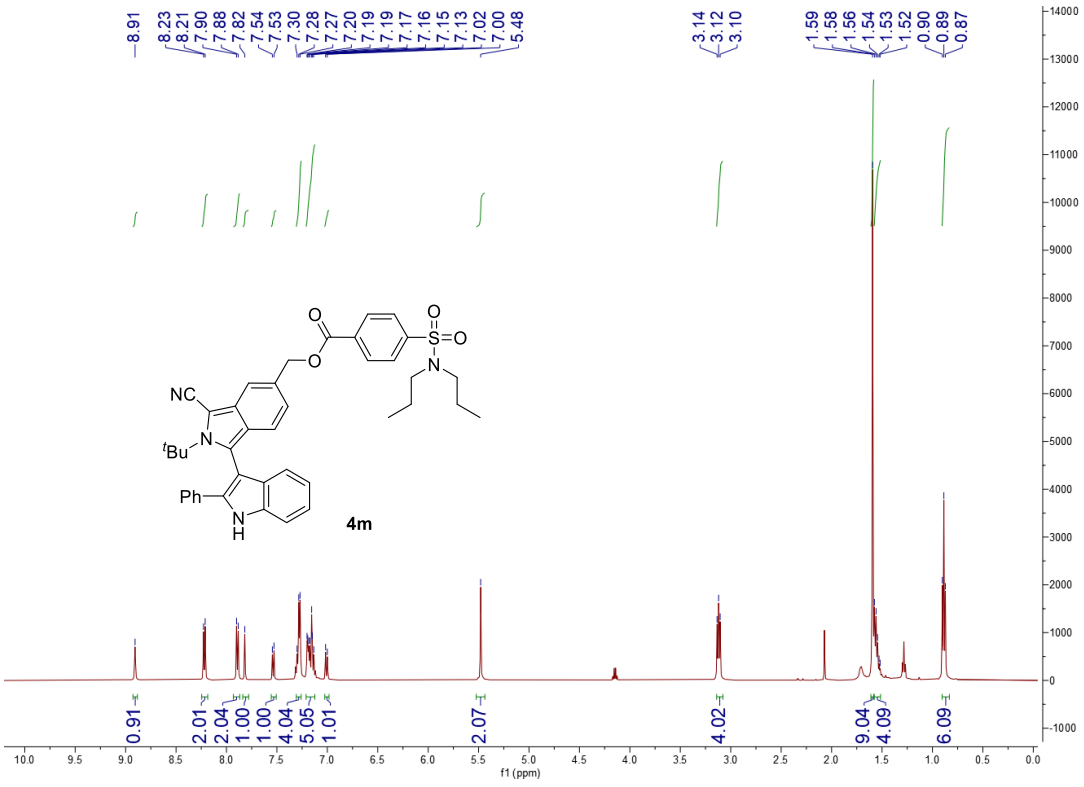
0.75 1.02 2.09 0.93 2.05 1.01 1.09 2.04 4.08 4.08 1.07 1.00 2.00 9.03
f1 (ppm)
4l


173.09 168.06 165.86 161.85 159.78 136.79 135.51 134.77 134.70 133.56 133.05 132.42 131.90 131.61 131.09 131.06 130.90 129.24 129.12 128.92 128.32 127.28 126.25 125.95 125.06 124.79 124.76 123.31 122.99 121.89 121.20 119.54 117.37 117.25 117.13 117.09 112.76 112.67 111.23 105.70 93.37 67.63 62.99 31.31
f1 (ppm)
4l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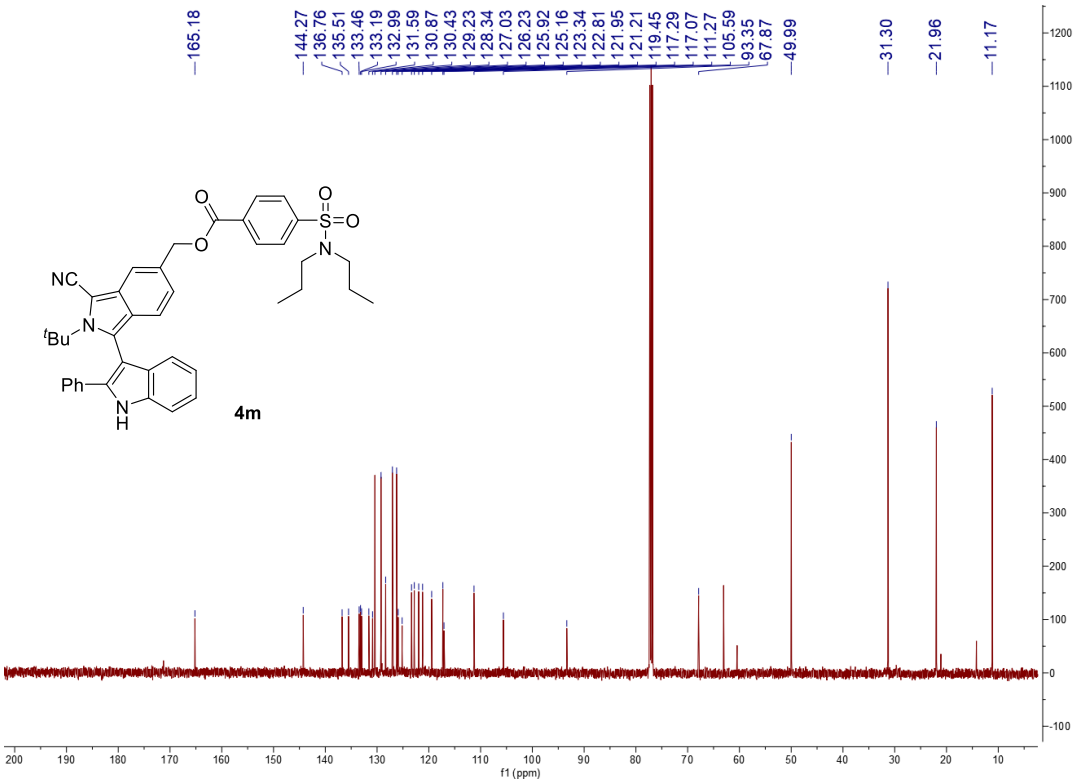
7.30
7.28
7.27
7.20
7.19
7.19
7.17
7.16
7.15
7.13
7.02
7.00
5.48
3.14
3.12
3.10
1.59
1.58
1.56
1.54
1.53
1.52
0.90
0.89
0.87
NC
tBu
N
Ph
N
H
O
O
S
O
N
4m
0.91
2.01
2.04
1.00
1.00
4.04
5.05
1.01
2.07
4.02
9.04
4.09
6.09
f1 (ppm)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131.59
130.87
130.43
129.23
128.34
127.03
126.23
125.92
125.16
123.34
122.81
121.95
121.21
119.45
117.29
117.07
111.27
105.59
93.35
67.87
49.99
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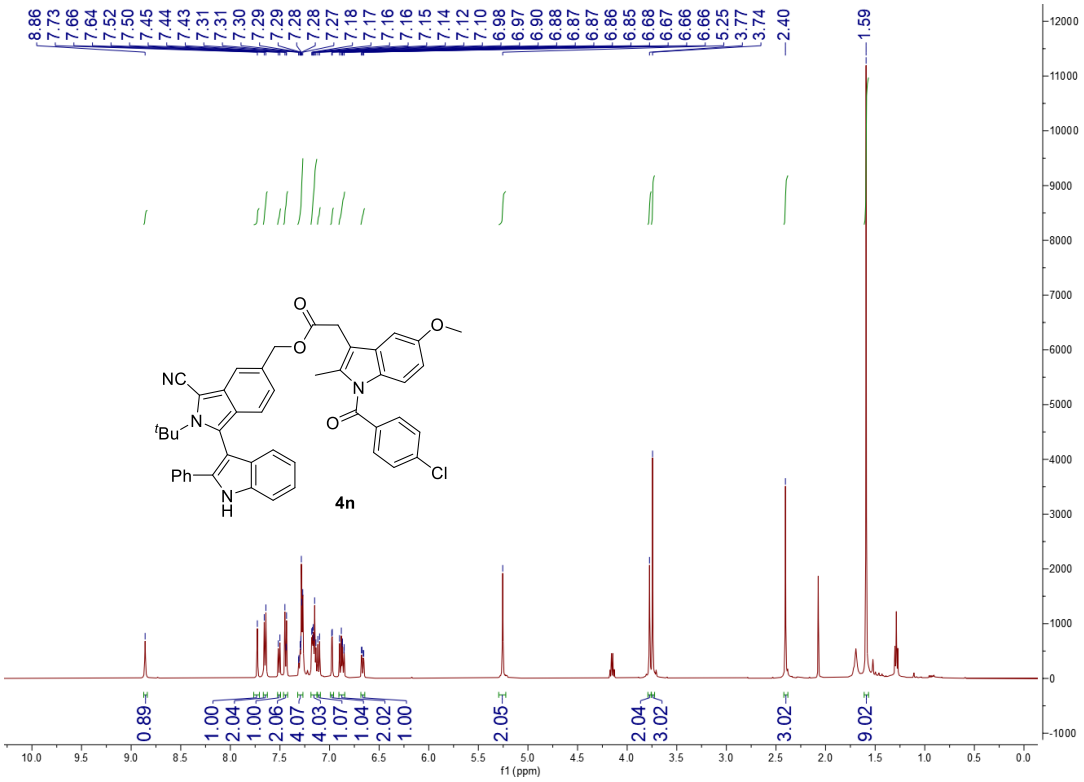
NC
tBu
N
Ph
N
H
O
O
S
O
N
4m
f1 (ppm)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7.29
7.28
7.28
7.27
7.18
7.17
7.16
7.16
7.15
7.14
7.12
7.10
6.98
6.97
6.90
6.88
6.87
6.87
6.86
6.85
6.68
6.67
6.66
6.66
5.25
3.77
3.74
2.40
1.59
NC
tBu
N
Ph
N
H
O
O
O
N
O
Cl
4n
0.89
1.00
2.04
1.00
2.06
4.07
4.03
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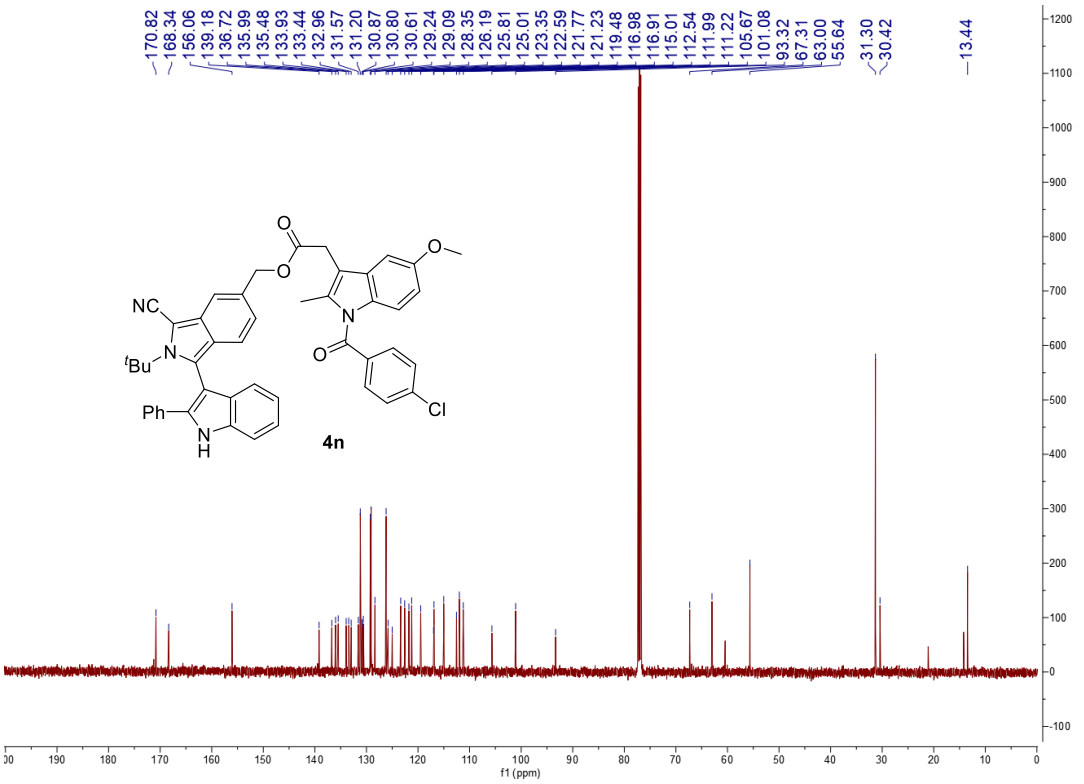
1.04
2.02
1.00
2.05
2.04
3.02
3.02
9.02
f1 (ppm)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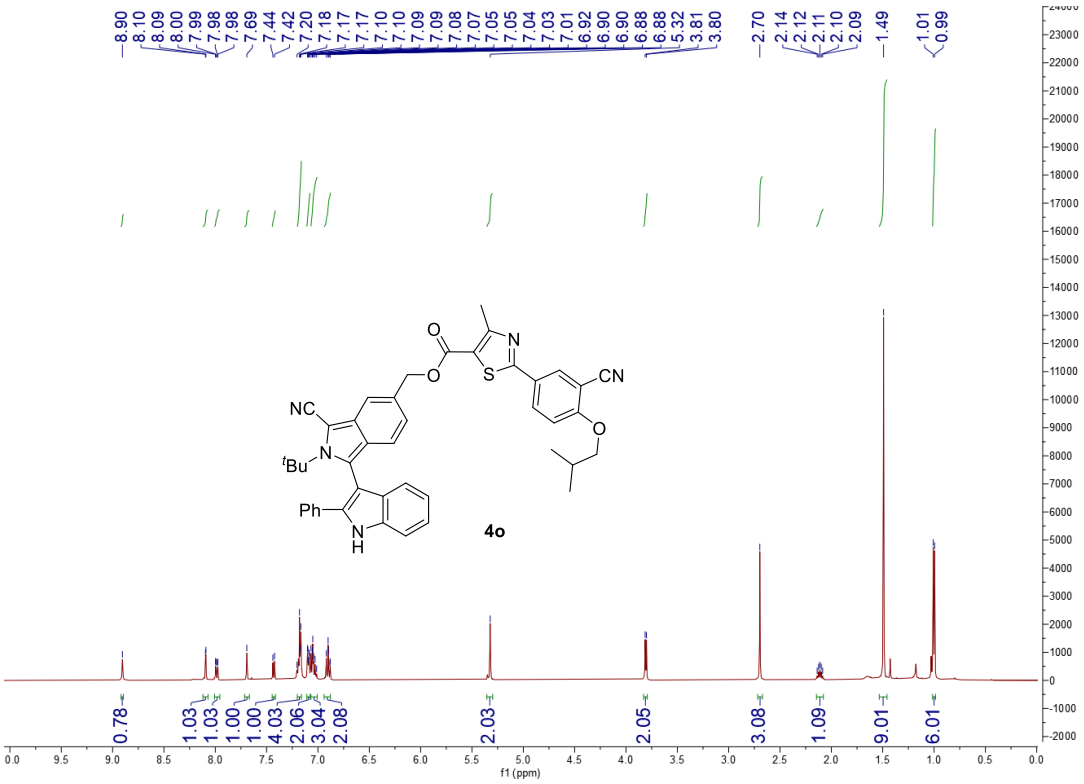
131.57
131.20
130.87
130.80
130.61
129.24
129.09
128.35
126.19
125.81
125.01
123.35
122.59
121.77
121.23
119.48
116.98
116.91
115.01
112.54
111.99
111.22
105.67
101.08
93.32
67.31
63.00
55.64
31.30
30.42
13.44
NC
tBu
N
Ph
N
H
O
O
O
N
O
Cl
4n
f1 (ppm)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7.98
7.69
7.44
7.42
7.20
7.18
7.17
7.17
7.10
7.10
7.09
7.09
7.08
7.07
7.05
7.05
7.04
7.03
7.01
6.92
6.90
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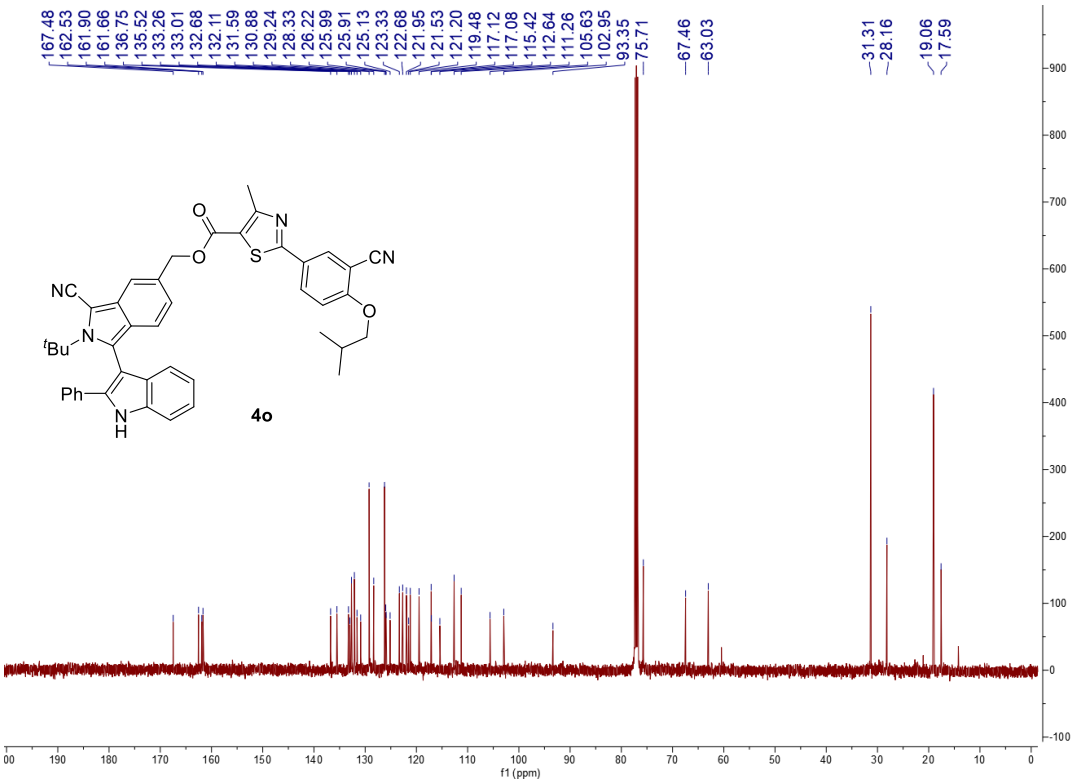
6.88
6.88
5.32
3.81
3.80
2.70
2.14
2.12
2.11
2.10
2.09
1.49
1.01
0.99
4o
0.78
1.03
1.03
1.00
1.00
4.03
2.06
3.04
2.08
2.03
2.05
3.08
1.09
9.01
6.01
f1 (ppm)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133.01
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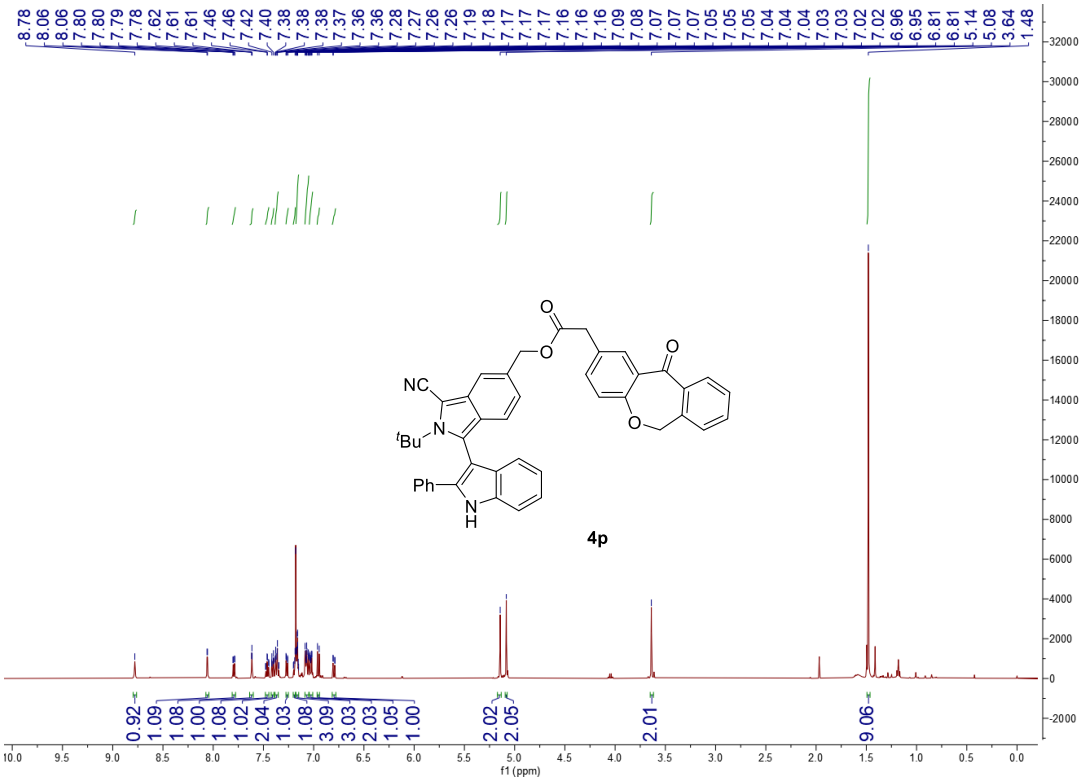
130.88
129.24
128.33
126.22
125.99
125.91
125.13
123.33
122.68
121.95
121.53
121.20
119.48
117.12
117.08
115.42
112.64
111.26
105.63
102.95
93.35
75.71
67.46
63.03
31.31
28.16
19.06
17.59
4o
f1 (ppm)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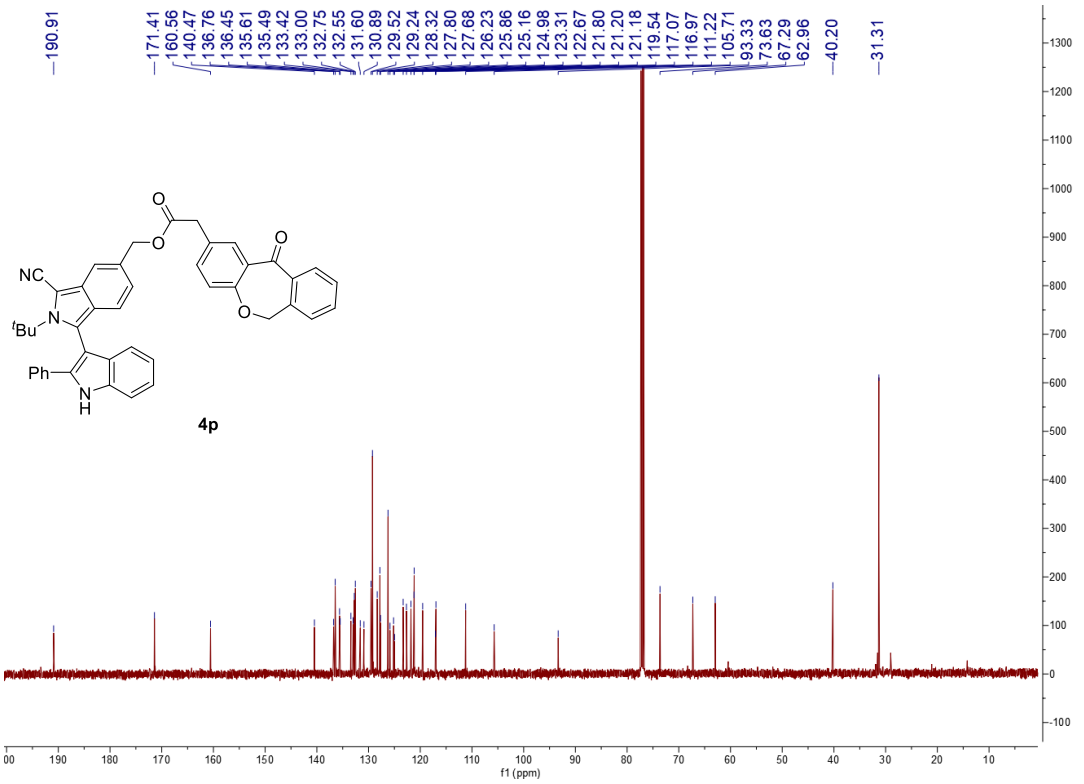
NC
tBu
N
Ph
N
H
O
O
O
O
4p
0.92 1.09 1.08 1.00 1.08 1.02 2.04 1.03 1.08 3.09 3.03 2.03 1.05 1.00 2.02 2.05 2.01 9.06
f1 (ppm)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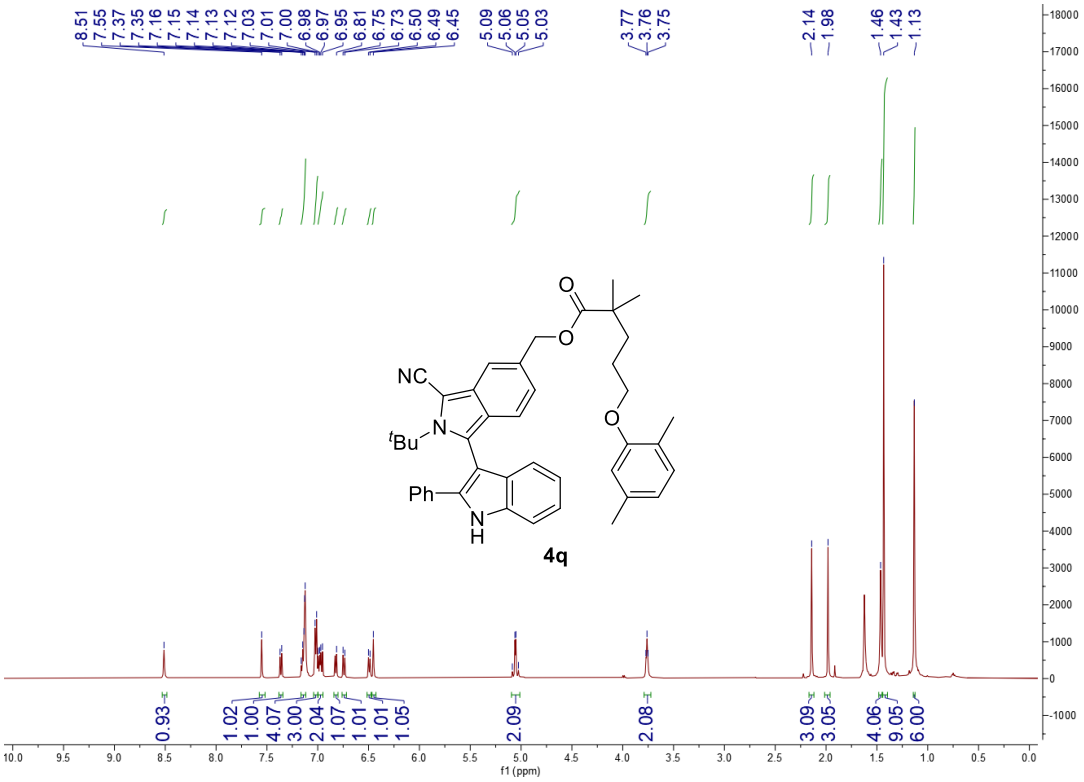
NC
tBu
N
Ph
N
H
O
O
O
O
4p
f1 (ppm)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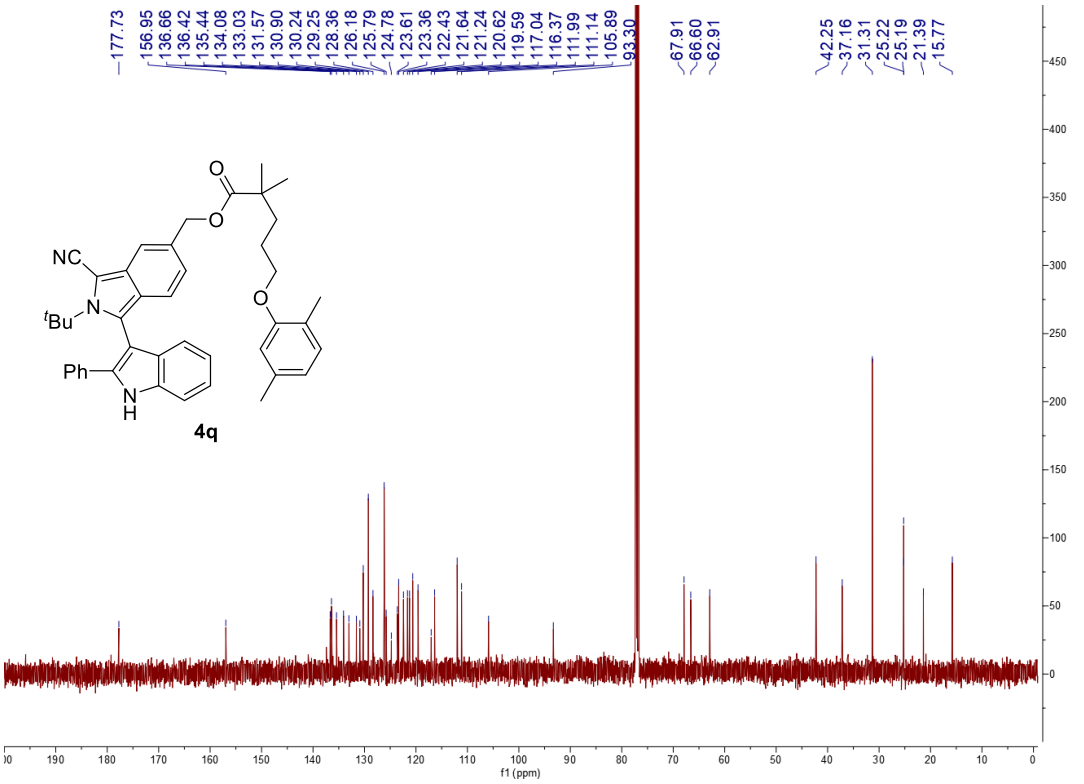
5.09
5.06
5.05
5.03
3.77
3.76
3.75
2.14
1.98
1.46
1.43
1.13
0.93
1.02
1.00
4.07
3.00
2.04
1.07
1.01
1.05
2.09
2.08
3.09
3.05
4.06
9.05
6.00
f1 (ppm)
NC
tBu
N
Ph
N
H
O
O
O
4q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131.57
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129.25
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124.78
123.61
123.36
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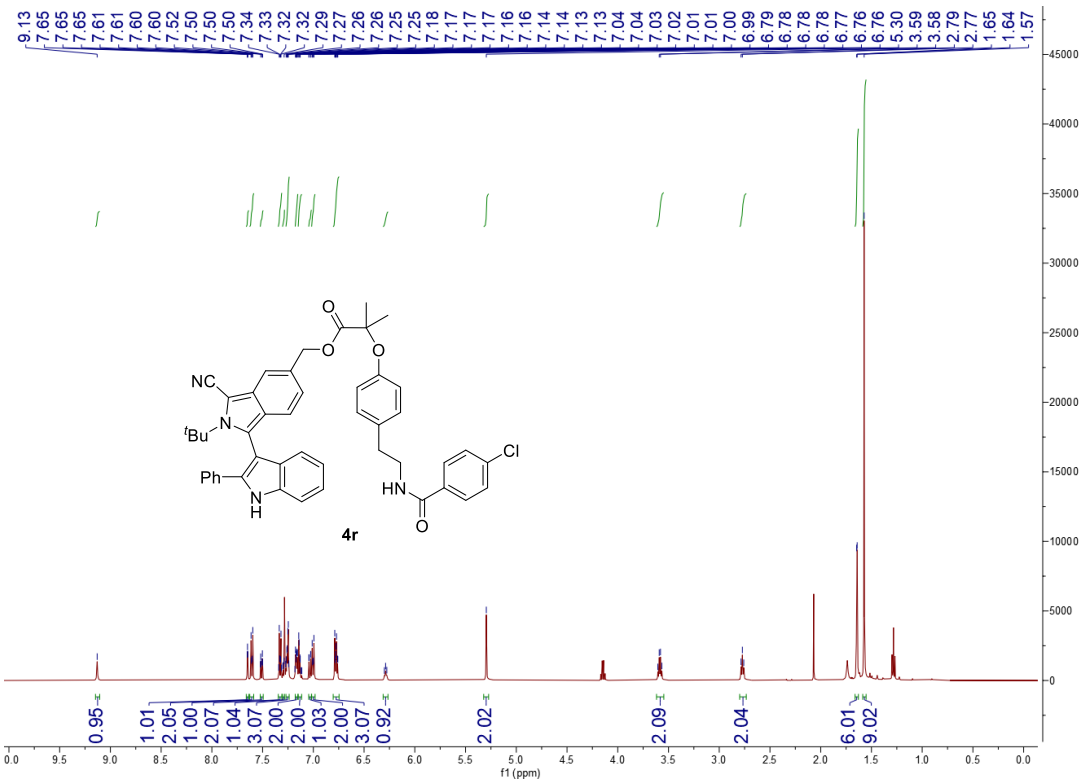
121.24
120.62
119.59
117.04
116.37
111.99
111.14
105.89
93.30
67.91
66.60
62.91
42.25
37.16
31.31
25.22
25.19
21.39
15.77
f1 (ppm)
NC
tBu
N
Ph
N
H
O
O
O
4q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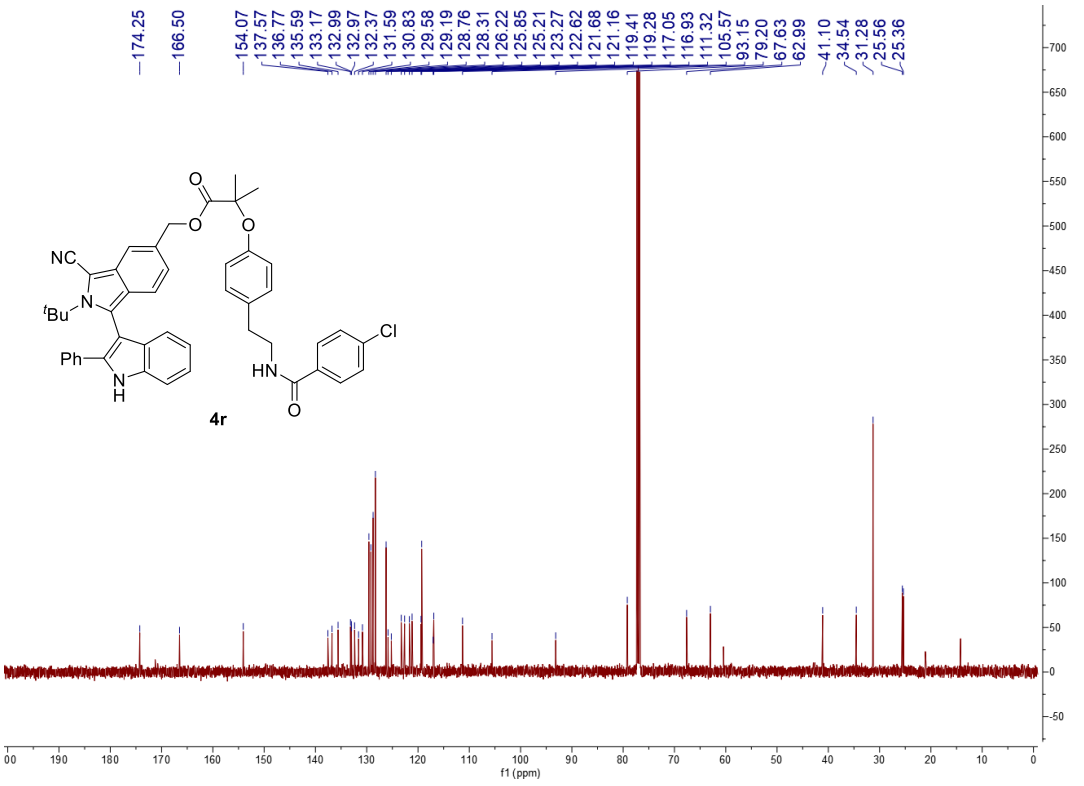
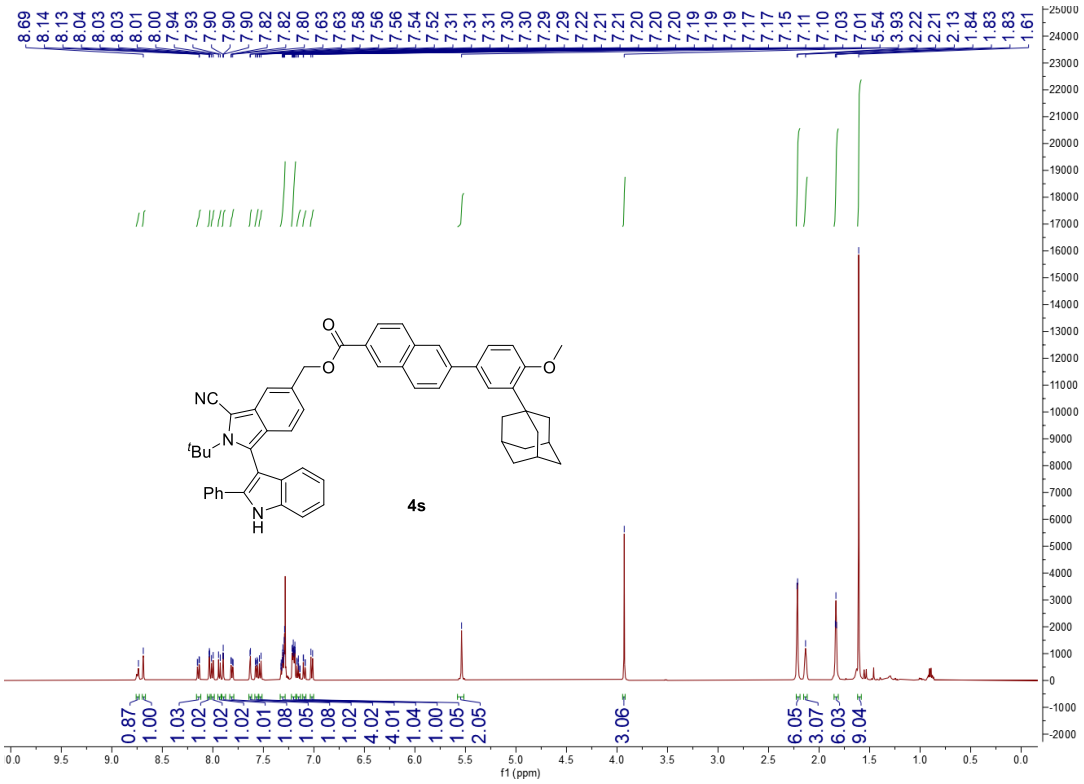
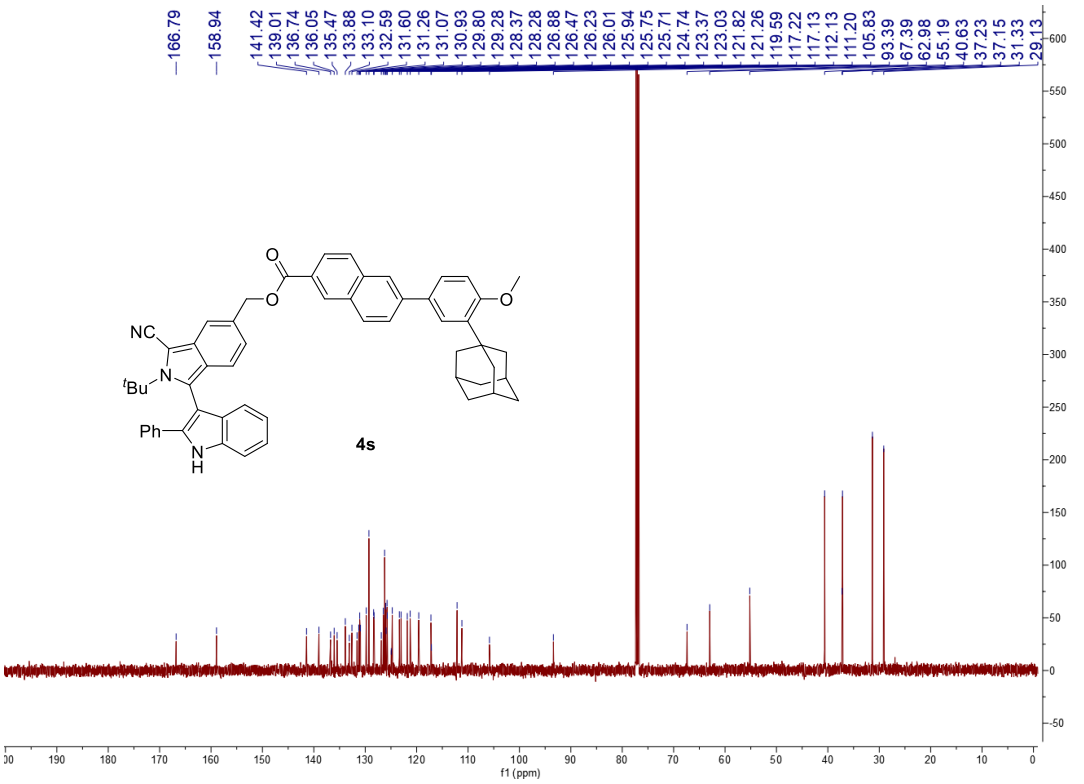
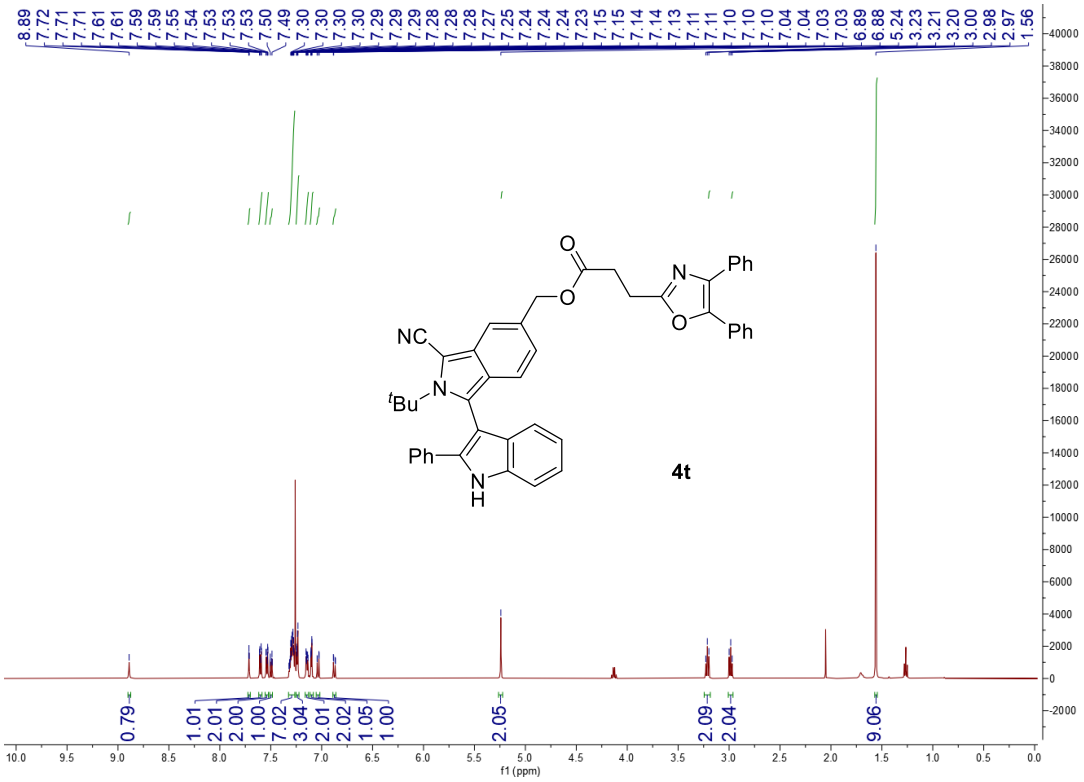
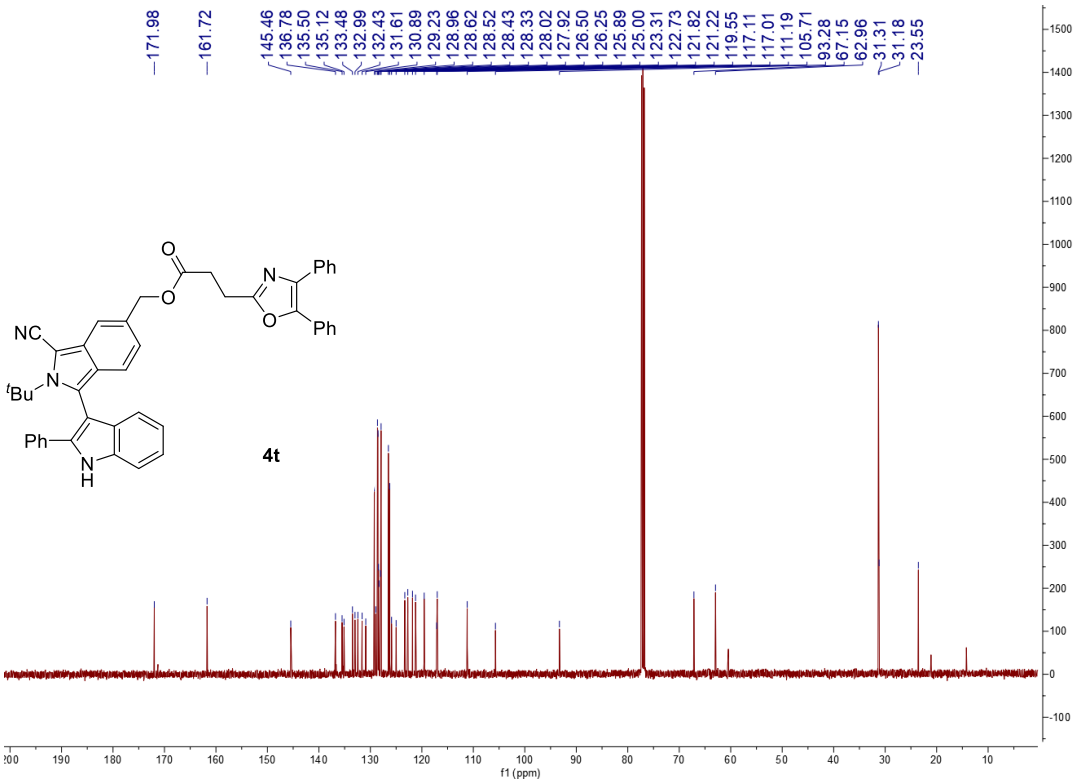
NC
tBu
N
Ph
N
H
O
O
O
HN
O
Cl
4r
0.95 1.01 2.05 1.00 2.07 1.04 3.07 2.00 2.00 1.03 2.00 3.07 0.92 2.02 2.09 2.04 6.01 9.02
f1 (ppm)


174.25 166.50 154.07 137.57 136.77 135.59 133.17 132.99 132.97 132.37 131.59 130.83 129.58 129.19 128.76 128.31 126.22 125.85 125.21 123.27 122.62 121.68 121.16 119.41 119.28 117.05 116.93 111.32 105.57 93.15 79.20 67.63 62.99 41.10 34.54 31.28 25.56 25.36
NC
tBu
N
Ph
N
H
O
O
O
HN
O
Cl
4r
f1 (ppm)


8.69 8.14 8.13 8.04 8.03 8.03 8.01 8.00 7.94 7.93 7.90 7.90 7.90 7.82 7.82 7.80 7.63 7.63 7.58 7.56 7.56 7.54 7.52 7.31 7.31 7.31 7.30 7.29 7.29 7.22 7.21 7.21 7.20 7.20 7.20 7.19 7.19 7.19 7.17 7.17 7.15 7.11 7.10 7.03 7.01 5.54 3.93 2.22 2.21 2.13 1.84 1.83 1.83 1.61
NC
tBu
N
Ph
N
H
O
O
O
4s
0.87 1.00 1.03 1.02 1.02 1.02 1.01 1.08 1.05 1.08 1.02 4.02 4.01 1.04 1.00 1.05 2.05 3.06 6.05 3.07 6.03 9.04
f1 (ppm)


166.79 158.94 141.42 139.01 136.74 136.05 135.47 133.88 133.10 132.59 131.60 131.26 131.07 130.93 129.80 129.28 128.37 128.28 126.88 126.47 126.23 126.01 125.94 125.75 125.71 124.74 123.37 123.03 121.82 121.26 119.59 117.22 117.13 112.13 111.20 105.83 93.39 67.39 62.98 55.19 40.63 37.23 37.15 31.33 29.13
NC
tBu
N
Ph
N
H
O
O
O
4s
f1 (ppm)


8.89 7.72 7.71 7.71 7.61 7.61 7.59 7.59 7.55 7.54 7.53 7.53 7.50 7.49 7.30 7.30 7.30 7.30 7.29 7.29 7.28 7.28 7.28 7.27 7.25 7.24 7.24 7.24 7.23 7.15 7.15 7.14 7.14 7.13 7.11 7.11 7.10 7.10 7.10 7.04 7.04 7.03 7.03 6.89 6.88 5.24 3.23 3.21 3.20 3.00 2.98 2.97 1.56
0.79 1.01 2.01 2.00 1.00 7.02 3.04 2.01 2.02 1.05 1.00 2.05 2.09 2.04 9.06
f1 (ppm)
4t


171.98 161.72 145.46 136.78 135.50 135.12 133.48 132.99 132.43 131.61 130.89 129.23 128.96 128.62 128.52 128.43 128.33 128.02 127.92 126.50 126.25 125.89 125.00 123.31 122.73 121.82 121.22 119.55 117.11 117.01 111.19 105.71 93.28 67.15 62.96 31.31 31.18 23.55
f1 (ppm)
4t