

Supporting information

Ruthenium Porphyrin Catalyzed Diimination of Indoles with Aryl Azides as Nitrene Source

Jinhu Wei,^{†,a,b} Wenbo Xiao,^{†,b} Cong-Ying Zhou,^{a,b} Chi-Ming Che^{*,a,b}

^a HKU Shenzhen Institute of Research & Innovation, Shenzhen, China

^b State Key Laboratory of Synthetic Chemistry and Department of Chemistry, The University
of Hong Kong, Pokfulam Road, Hong Kong, China.

Fax: (852) 2857-1586; Tel: (852) 2859-2154; E-mail: cmche@hku.hk

Table of Contents

I. General Information.....	S2
II. General procedure for screening of catalysts and reaction conditions.....	S2
III. Table S1 Screening of catalysts and reaction conditions.....	S3
IV. General procedure for [Ru(TTP)CO] catalyzed diimination of indoles with 4-nitrophenyl azide or 3,5-bis(trifluoromethyl)phenyl azide.....	S3
V. Stoichiometric reaction of [Ru(TPP)(NAr) ₂] (Ar= 3,5-bis(trifluoromethyl)phenyl) with 1-methylindole.....	S4
VI. Control reaction of 1-methylindole with 3,5- bis(trifluoromethyl)phenyl azide and 4-nitroaniline.....	S4
VII. Figure S1 X-ray Crystal Structure of 3a	S5
VIII. Characterizations of Products.....	S6
IX. NMR Spectra of Products.....	S15

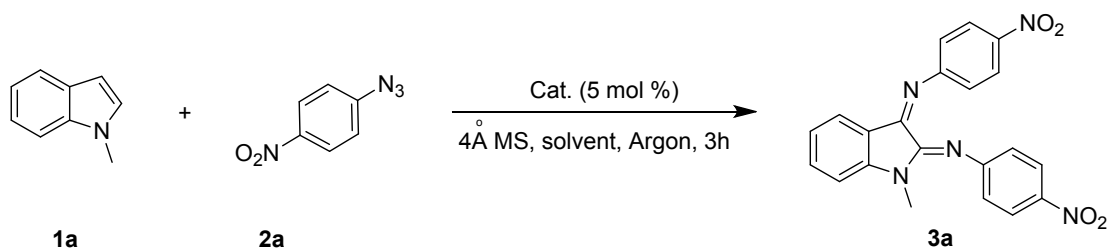
Experimental Section

General Information. All reactions were performed under argon atmosphere unless indicated otherwise. Molecular sieves were dried at 400°C for 3 h prior to use. All anhydrous solvents used in the reactions were dried and freshly distilled. All manipulations with air-sensitive reagents were carried out under a dry argon atmosphere. Metal porphyrin catalysts and organic azides were synthesized according to previously reported methods. All ¹H NMR and ¹³C NMR spectra were recorded on Bruker AV300 or AV400 NMR spectrometers with tetramethylsilane (TMS) as internal reference. Mass spectra were recorded on a Finnigan MAT 95 mass spectrometer. Mass spectra were obtained on a HP5989A spectrometer (EI), an IonSpec 4.7 Tesla FTMS spectrometer (MALDI). X-ray diffraction data were collected on Bruker SMART 1000 CCD diffractometer with graphite monochromatized MoK α radiation. Preparative thin layer chromatography was performed on pre-coated silica gel 60 F254 plates.

General procedure for screening of catalysts and reaction conditions

To an oven-dried Schlenk flask equipped with a rubber seal was added 1-methyl indole (0.2 mmol), 4-nitrophenyl azide (0.6 mmol), catalyst (5 mol %) and 200 mg of 4Å molecular sieve. The flask was evacuated and backfilled with argon three times. Then freshly distilled 1,2-dichloroethane (2 mL) was added via syringe. The reaction mixture was stirred at reflux for 3h. The mixture was cooled down to room temperature and filtered through a plug of celite. The filtrate was concentrated by rotary evaporator and the residue was purified by flash chromatography on a silica gel column (eluent: Hexane/EA = 4:1) to give the corresponding red solid product.

Table S1 Screening of catalysts and reaction conditions ^a



Entry	Catalyst	solvent	Temp.	Conv.(%) ^b	Yield(%) ^c
1	[Ru(TTP)(CO)]	DCE	85	78	80
2	[Ru(F ₂₀ -TPP)(CO)]	DCE	85	46	21
3	[Ru(TDCPP)(CO)]	DCE	85	81	47
4	[Rh ₂ (OAc) ₄]	DCE	85	NR ^d	
5	[Cu(OTf) ₂]	DCE	85	NR	
6	[Fe(TTP)Cl]	DCE	85	NR	
7	[Co(TTP)]	DCE	85	NR	
8	[Ru(TTP)(CO)]	CH ₂ Cl ₂	40	39	42
9	[Ru(TTP)(CO)]	DCE	25	34	33
11	[Ru(TTP)(CO)]	Toluene	85	94	70
12	[Ru(TTP)(CO)]	MeCN	85	82	45
13	none	DCE	85	NR	

^a Conditions: N-methylindole (0.2 mmol), 4-nitrophenylazide (0.6 mmol), catalyst (5 mol %), 200 mg of 4ÅMS, 2 mL of solvent, argon; ^b Conv. was based on N-methylindole by ¹H-NMR; ^c Isolated yield based on N-methylindole conversion. ^d No reaction.

General procedure for [Ru(TTP)CO]-catalyzed diimination of indoles with 4-nitrophenyl azide or 3,5-bis(trifluoromethyl)phenyl azide

To an oven-dried Schlenk flask equipped with a rubber seal was added indole (0.2 mmol), azide (0.4 mmol), [Ru(TTP)CO] (5 mol %) and 200 mg of 4Å molecular sieve. The flask was evacuated and backfilled with argon three times. Then freshly distilled

1,2-dichloroethane (2 mL) was added via syringe. The reaction mixture was stirred at reflux. When azide was completely consumed (monitored by TLC), another portion of azide (0.25 mmol) was added into the reaction mixture. The reaction mixture was continuously stirred until all of the azide was consumed. The mixture was cooled down to room temperature and filtered through a plug of celite. The filtrate was concentrated by rotary evaporator and the residue was purified by flash chromatography on a silica gel column (eluent: Hexane/EA = 5:1~3:1 or Hexane/DCM = 2:1~1:1) to give the corresponding red solid product.

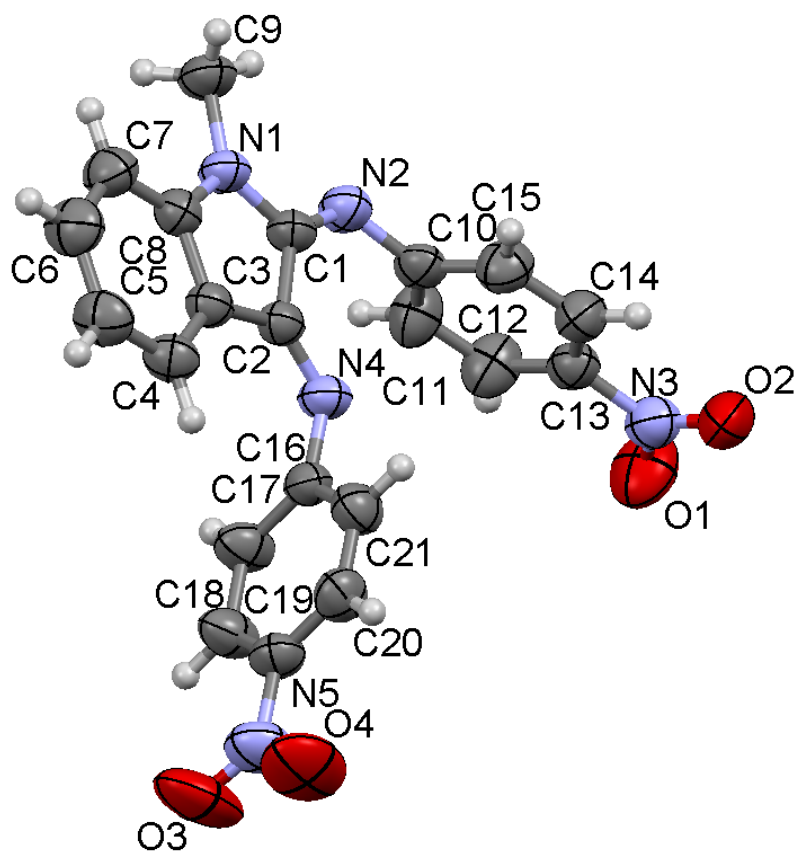
Stoichiometric reaction of [Ru(TPP)(NAr)₂] (Ar= 3,5-bis(trifluoromethyl)phenyl) **5 with 1-methylindole**

To an oven-dried Schlenk flask was added 0.05 mmol of 1-methylindole and 0.025 mmol of complex **5**. The flask was evacuated and backfilled with argon three times. Freshly distilled DCE (2 mL) was added via syringe. The mixture was stirred at reflux under argon atmosphere for 1.5h. After complex **5** was completely consumed, the reaction mixture was concentrated by rotary evaporator. The residue was purified by silica gel column chromatography (eluent: hexane/DCM = 5:1) to give the product **3b** in 35% yield.

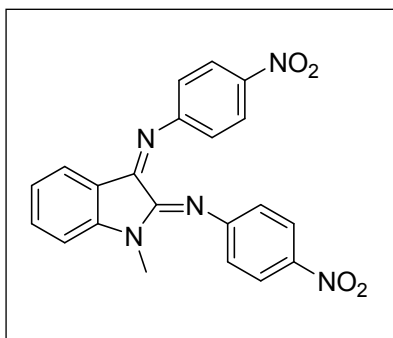
Control reaction of 1-methylindole with 3,5- bis(trifluoromethyl)phenyl azide and 4-nitroaniline

To an oven-dried Schlenk flask equipped with a rubber seal was added 1-methylindole (0.2 mmol), 3,5-bis(trifluoromethyl)phenyl azide (0.4 mmol), 4-nitroaniline (0.4 mmol) and [Ru(TTP)CO] (5mol %) and 200 mg of 4Å molecular sieve. The flask was evacuated and backfilled with argon three times. Then freshly distilled 2ml of 1,2-dichloroethane was added via syringe. The reaction mixture was stirred at reflux under atmosphere for 6h. After azide was completely consumed (monitored by TLC) the mixture was cooled down to room temperature and filtered through a plug of celite. The filtrate was concentrated by rotary evaporator and purified by silica gel column chromatography (eluent: Hexane/DCM = 5:1) to give the product **3b** in 65% yield based on 80% conversion of indole.

Figure S1 X-ray Crystal Structure of **3a** (Solvent is not included). CCDC 973563 for **3a** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif)



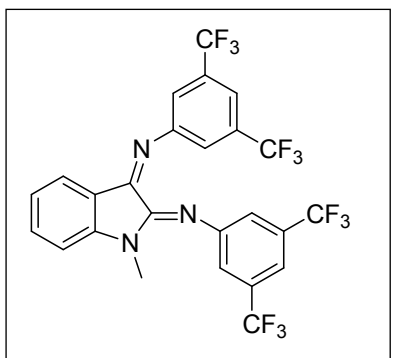
Characterizations of Products



1-Methyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine (3a)

^1H NMR (400 MHz, CDCl_3) δ 8.22(d, J = 8.72 Hz, 2H), 8.14(d, J = 8.80 Hz, 2H), 7.40(t, J = 7.78 Hz, 1H), 6.98(d, J = 8.60 Hz, 2H), 6.88(d, J = 8.04 Hz, 1H), 6.80(d, J = 7.52 Hz, 2H), 6.67(t, J = 7.58 Hz, 1H), 6.44(d, J = 7.52 Hz, 1H), 3.36(s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.4, 155.3, 150.8, 147.7, 144.7, 143.1, 135.2, 126.7, 125.7, 125.4, 125.1, 121.4, 120.3, 117.7, 115.8, 109.2, 27.9.

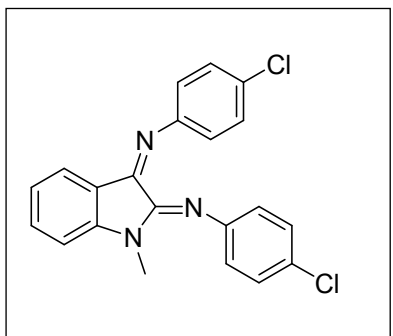
HRMS-EI (m/z), Calcd for, $\text{C}_{21}\text{H}_{15}\text{N}_5\text{O}_4$ $[\text{M}]^+$ 401.1124; found: 401.1076.



3-(3,5-Bis(trifluoromethyl)phenylimino)-1-methylindolin-2-ylidene)-3,5-bis(trifluoromethyl)benzenamine(3b)

^1H NMR (400 MHz, CDCl_3) δ 7.64(s, 1H), 7.46-7.38 (m, 4H), 7.14(s, 2H), 6.90(d, J = 8.03 Hz, 1H), 6.68(t, J = 7.32 Hz, 1H), 6.41(d, J = 6.88 Hz, 1H), 3.39(s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.62, 150.85, 150.53, 149.17, 135.45, 133.14(q, $J_{(\text{CF}_3)}$ = 33.40 Hz), 131.95(q, $J_{(\text{CF}_3)}$ = 32.70 Hz), 127.44(d, $J_{(\text{C-F})}$ = 57.90 Hz), 126.31, 124.74(d, $J_{(\text{C-F})}$ = 57.80 Hz), 122.03(d, $J_{(\text{C-F})}$ = 58.10 Hz), 121.44, 121.15, 119.29(d, $J_{(\text{C-F})}$ = 58.30 Hz), 118-117(m, C-F), 116.14, 115.74, 109.42, 27.66;

HRMS-EI (m/z), Calcd for, $\text{C}_{25}\text{H}_{13}\text{N}_3\text{F}_{12}$ $[\text{M}]^+$ 583.0918; found: 583.0898.

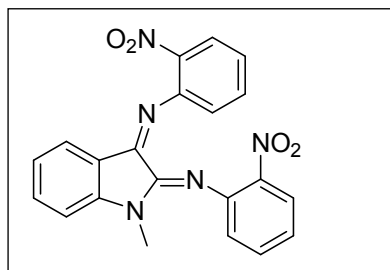


4-chloro-N-(3-(4-chlorophenylimino)-1-methylindolin-2-ylidene)benzenamine(3c)

^1H NMR (300 MHz, CD_2Cl_2) δ 7.33-7.29(m, 3H), 7.19 (d, J = 8.07 Hz, 2H), 6.89-6.82(m, 3H), 6.68-6.49(m, 4H), 3.32(s, 3H); ^{13}C NMR (75 MHz, CD_2Cl_2) δ 150.88, 149.11, 148.61, 138.21, 134.44, 129.88,

128.89, 127.40, 126.76, 122.20, 121.98, 121.62, 120.61, 119.03, 116.63, 108.95, 30.07;

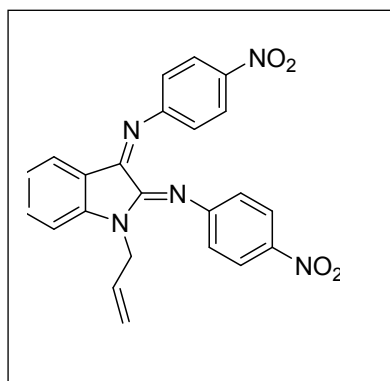
HRMS-EI (*m/z*), Calcd for, C₂₁H₁₅N₃Cl₂ [M]⁺ 379.0643; found: 379.0608.



1-Methyl-3-(2-nitrophenylimino)indolin-2-ylidene)-2-nitrobenzenamine(3e)

¹H NMR (400 MHz, CDCl₃) δ 8.04(dd, *J* = 8.31, 1.21 Hz, 1H), 7.93(dd, *J* = 8.30, 1.35 Hz, 1H), 7.50(td, *J* = 8.32, 1.30 Hz, 1H), 7.42(td, *J* = 8.36, 1.39 Hz, 1H), 7.37(td, *J* = 7.84, 1.07 Hz, 1H), 7.21(td, *J* = 8.44, 1.22 Hz, 1H), 7.05(dd, *J* = 8.10, 1.15 Hz, 1H), 6.99(td, *J* = 8.38, 1.25 Hz, 1H), 6.88(d, *J* = 8.03 Hz, 1H), 6.76(dd, *J* = 8.02, 1.10 Hz, 1H), 6.63(t, *J* = 7.67 Hz, 1H), 6.42(d, *J* = 7.42 Hz, 1H), 3.41(s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 153.02, 150.73, 148.39, 145.43, 144.94, 139.64, 138.10, 134.89, 134.65, 133.91, 125.96, 125.43, 124.95, 124.58, 123.84, 122.28, 121.02, 119.46, 116.32, 109.04, 29.69;

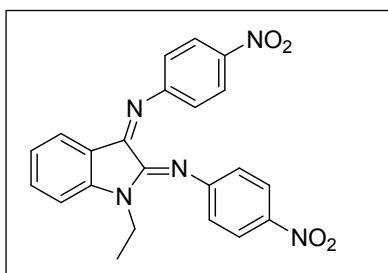
HRMS-EI (*m/z*), Calcd for, C₂₁H₁₅N₅O₄ [M]⁺ 401.1124; found: 401.1077.



1-Allyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4a)

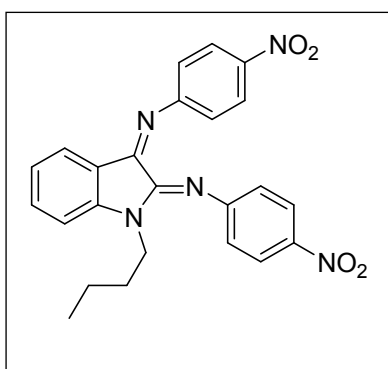
¹H NMR (400 MHz, CDCl₃) δ 8.21(d, *J* = 8.76 Hz, 2H), 8.12(d, *J* = 8.84 Hz, 2H), 7.36(t, *J* = 7.80 Hz, 1H), 6.97(d, *J* = 8.84 Hz, 2H), 6.87(d, *J* = 8.08 Hz, 1H), 6.81(d, *J* = 8.44 Hz, 2H), 6.66(t, *J* = 7.64 Hz, 1H), 6.46(d, *J* = 7.68 Hz, 1H), 5.95-5.89(m, 1H), 5.35-5.28(m, 2H), 4.49(s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 156.27, 155.32, 152.49, 150.05, 146.93, 144.60, 143.07, 135.16, 130.82, 126.69, 126.49, 125.66, 125.06, 121.42, 120.22, 117.87, 117.67, 115.78, 110.02, 43.70;

HRMS-EI (*m/z*), Calcd for, C₂₃H₁₇N₅O₄ [M]⁺ 427.1281; found: 427.1280.



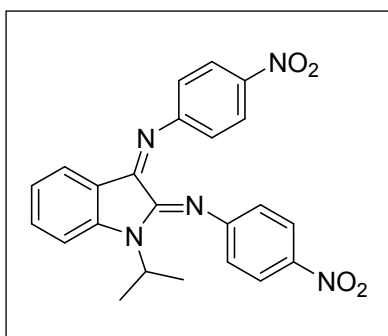
1-Ethyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4b)

^1H NMR (400 MHz, CDCl_3) δ 8.21(d, J = 8.80 Hz, 2H), 8.12(d, J = 8.92 Hz, 2H), 7.37(t, J = 7.88 Hz, 1H), 6.97(d, J = 8.80 Hz, 2H), 6.89(d, J = 8.04 Hz, 1H), 6.80(d, J = 8.56 Hz, 2H), 6.64(t, J = 7.68 Hz, 1H), 6.44(d, J = 7.68 Hz, 1H), 3.92-3.90(m, 2H), 1.35(t, J = 7.04 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.59, 155.37, 152.48, 149.92, 146.86, 144.61, 143.03, 135.21, 126.87, 125.68, 125.11, 121.20, 120.24, 117.66, 115.90, 109.28, 36.14, 12.11; HRMS-EI (m/z), Calcd for, $\text{C}_{22}\text{H}_{17}\text{N}_5\text{O}_4$ $[\text{M}]^+$ 415.1281; found: 415.1275.



1-Butyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4c)

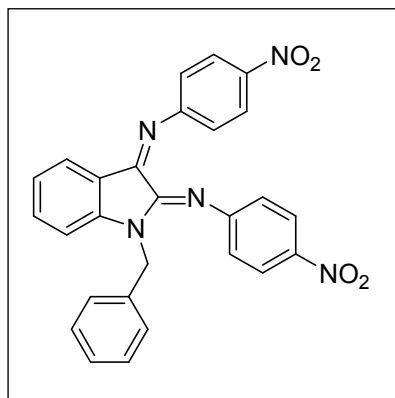
^1H NMR (400 MHz, CDCl_3) δ 8.21(d, J = 8.80 Hz, 2H), 8.12(d, J = 8.88 Hz, 2H), 7.37(t, J = 7.72 Hz, 1H), 6.96(d, J = 8.76 Hz, 2H), 6.88(d, J = 8.08 Hz, 1H), 6.80(d, J = 8.60 Hz, 2H), 6.64(t, J = 7.64 Hz, 1H), 6.44(d, J = 7.72 Hz, 1H), 3.84(t, J = 6.93 Hz, 2H), 1.80-1.72(m, 2H), 1.49-1.44(m, 2H), 1.00(t, J = 7.28 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.66, 155.38, 152.19, 150.36, 147.22, 144.61, 142.99, 135.17, 126.80, 125.67, 125.12, 121.14, 120.17, 117.66, 115.79, 109.46, 41.19, 29.22, 20.41, 13.96; HRMS-EI (m/z), Calcd for, $\text{C}_{24}\text{H}_{21}\text{N}_5\text{O}_4$ $[\text{M}]^+$ 443.1594; found: 443.1585.



1-Isopropyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4d)

^1H NMR (400 MHz, CDCl_3) δ 8.20(d, J = 8.76 Hz, 2H), 8.12(d, J = 8.84 Hz, 2H), 7.34(t, J = 7.84 Hz, 1H), 7.05(d, J = 8.16 Hz, 1H), 6.93(d, J = 8.88 Hz, 2H), 6.76(d, J = 8.72 Hz, 2H), 6.62(t, J = 7.64 Hz, 1H), 6.45(d, J = 7.76 Hz, 1H), 4.90-4.80(m, 1H), 1.60(d, J = 6.96 Hz, 6H); ^{13}C NMR

(100 MHz, CDCl₃) δ 156.83, 155.35, 151.96, 149.51, 146.86, 144.56, 142.87, 134.92, 126.98, 125.73, 125.21, 120.82, 119.92, 117.51, 116.16, 110.02, 45.05, 19.11;
HRMS-EI (m/z), Calcd for, C₂₃H₁₉N₅O₄ [M]⁺ 429.1437; found: 429.1325.

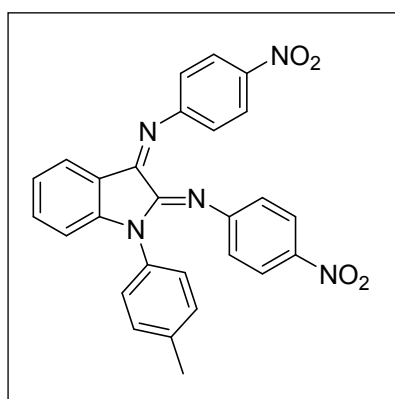


1-Benzyl-3-(4-nitrophenylimino)indolin-2-ylidene-4-nitrobenzenamine(4e)

¹H NMR (300 MHz, CDCl₃) δ 8.23(d, *J* = 8.91 Hz, 2H), 8.13(d, *J* = 8.91 Hz, 2H), 7.40-7.27(m, 7H), 6.97(d, *J* = 8.91 Hz, 2H), 6.82(d, *J* = 7.83 Hz, 2H), 6.65(t, *J* = 7.57 Hz, 1H), 6.46(d, *J* = 7.56 Hz, 1H), 5.09(s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 156.17,

155.31, 150.13, 147.38, 144.77, 143.25, 135.71, 135.23, 129.09, 128.04, 127.40, 126.83, 125.76, 125.16, 121.58, 120.23, 117.73, 115.95, 110.15, 45.14;

HRMS-EI (m/z), Calcd for, C₂₇H₁₉N₅O₄ [M]⁺ 477.1437; found: 477.1404.

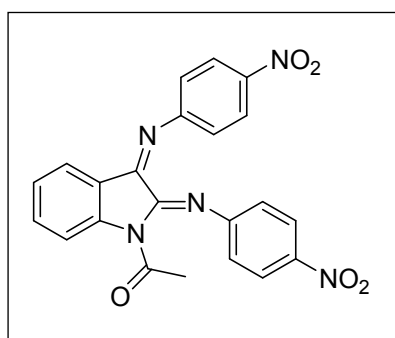


4-Nitro-N-(3-(4-nitrophenylimino)-1-p-tolylindolin-2-ylidene)benzenamine(4f)

¹H NMR (400 MHz, CDCl₃): δ 8.29(d, *J* = 5.72 Hz, 2H), 7.92(br, 2H), 7.40-6.90(br, 7H), 6.90-6.60(m, 4H), 6.57(br, 1H), 2.33(s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 151.26, 144.70, 142.85, 139.01, 138.08, 135.03, 132.26, 130.44, 127.51, 126.97, 126.52,

125.68, 124.35, 122.21, 120.36, 117.97, 115.91, 113.39, 110.88, 110.69, 21.18;

HRMS-EI (m/z), Calcd for, C₂₇H₁₉N₅O₄ [M]⁺ 477.1437; found: 477.1407.

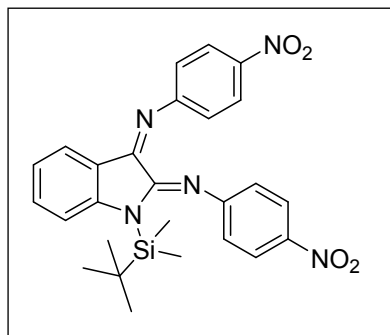


2,3-Bis(4-nitrophenylimino)indolin-1-yl)ethanone(4g)

¹H NMR (400 MHz, CDCl₃) δ 8.52(d, *J* = 8.36 Hz, 1H), 8.22(d, *J* = 8.88 Hz, 2H), 8.18(d, *J* = 8.92 Hz, 2H), 7.52-7.51(m, 1H), 6.97-6.93(m, 3H), 6.75(d, *J* = 8.84 Hz, 2H), 6.63(d, *J* = 7.84 Hz, 1H), 2.84(s, 3H);

^{13}C NMR (100 MHz, CDCl_3) δ 170.62, 154.50, 154.46, 150.18, 146.99, 146.38, 144.89, 143.64, 135.54, 125.97, 125.93, 125.33, 124.92, 118.56, 118.41, 117.44, 117.27, 28.19;

HRMS-EI (m/z), Calcd for, $\text{C}_{22}\text{H}_{15}\text{N}_5\text{O}_5$ $[\text{M}]^+$ 429.1073; found: 429.1044.

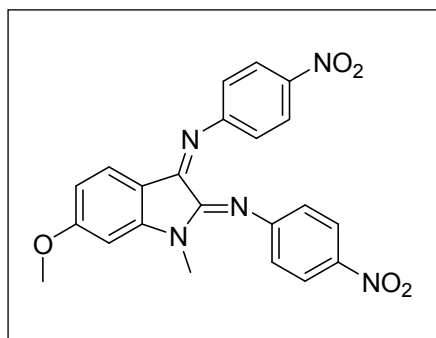


1-(*tert*-Butyldimethylsilyl)-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine (4h)

^1H NMR (400 MHz, CDCl_3) δ 8.19(d, J = 7.92 Hz, 2H), 8.12(d, J = 7.96 Hz, 2H), 7.29(t, J = 7.80 Hz, 1H), 7.10(d, J = 7.10 Hz, 1H), 6.85(d, J = 8.04 Hz, 2H), 6.76(d, J = 8.00 Hz, 2H), 6.64(t, J = 7.54 Hz,

1H), 6.48(d, J = 7.76 Hz, 1 H), 1.10(s, 9H), 0.61(s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.3, 155.4, 154.2, 152.7, 152.3, 144.4, 142.7, 134.8, 126.7, 125.7, 125.2, 121.2, 118.9, 118.5, 117.5, 114.4, 31.6, 27.0, - 1.9;

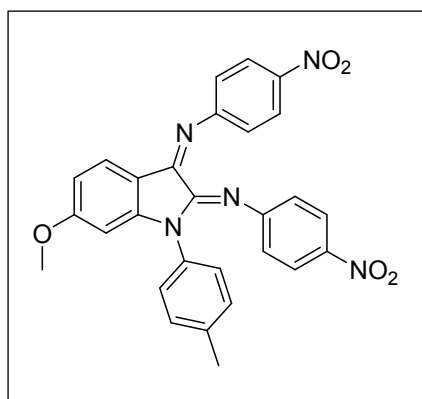
HRMS-EI (m/z), Calcd for, $\text{C}_{26}\text{H}_{27}\text{N}_5\text{O}_4\text{Si}$ $[\text{M}]^+$ 501.1832; found: 501.1799.



6-Methoxy-1-methyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4i)

^1H NMR (400 MHz, CDCl_3) δ 8.20(d, J = 8.72 Hz, 2H), 8.13(d, J = 8.88 Hz, 2H), 6.97(d, J = 8.72 Hz, 2H), 6.78(d, J = 6.68 Hz, 2H), 6.38-6.34(m, 2H), 6.15(d, J = 8.52 Hz, 1H), 3.83(s, 3H), 3.32(s, 3H);

^{13}C NMR (100 MHz, CDCl_3) δ 165.63, 155.97, 152.99, 148.63, 144.41, 143.11, 128.47, 125.68, 125.08, 120.72, 120.37, 118.11, 109.19, 107.71, 106.46, 95.75, 55.96, 29.83; HRMS-EI (m/z), Calcd for, $\text{C}_{22}\text{H}_{17}\text{N}_5\text{O}_5$ $[\text{M}]^+$ 431.1230; found: 431.1178.

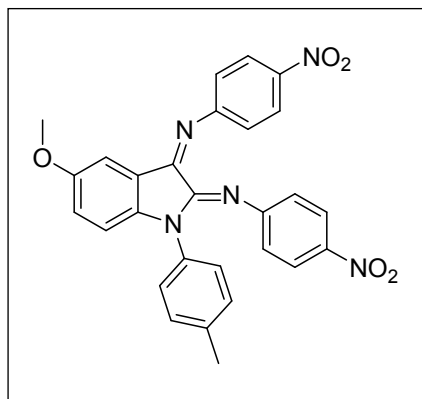


N-(6-methoxy-3-(4-nitrophenylimino)-1-p-tolyindolin-2-ylidene)-4-nitrobenzenamine(4j)

^1H NMR (400 MHz, CDCl_3) δ 8.25(br, 2H), 7.93(br, 2H), 7.60-6.60(m/br, 8H), 6.48(br, 1H),

6.22(d, $J = 8.28$ Hz, 1H), 6.13(br, 1H), 3.70(s, 3H), 2.32(s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 165.43, 156.82, 153.55, 147.48, 144.43, 142.78, 139.04, 132.24, 130.50, 128.35, 127.63, 125.68, 124.30, 120.41, 118.44, 113.12, 109.28, 107.92, 96.72, 55.87, 21.25;

HRMS-EI (m/z), Calcd for, $\text{C}_{28}\text{H}_{21}\text{N}_5\text{O}_5$ $[\text{M}]^+$ 507.1543; found: 507.1499.

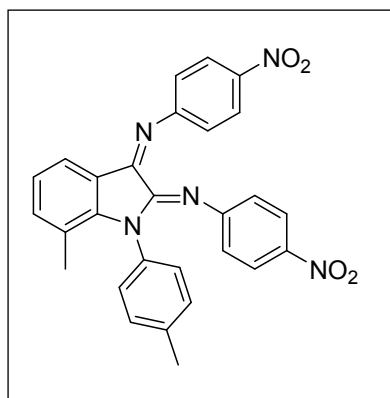


N-(5-methoxy-3-(4-nitrophenylimino)-1-p-tolyldolin-2-ylidene)-4-nitrobenzenamine(4k)

^1H NMR (400 MHz, CDCl_3) δ 8.27(d, $J = 8.76$ Hz, 2H), 7.91(d, $J = 8.36$ Hz, 2H), 7.14(br, 4H), 6.99(d, $J = 8.16$ Hz, 2H), 6.87(dd, $J = 8.80, 2.52$ Hz, 1H), 6.77(d, $J = 8.00$ Hz, 2H), 6.60(d, $J = 8.76$ Hz, 1H), 6.22(br, 1H), 3.49(s, 3H), 2.32(s, 3H); ^{13}C NMR

(100 MHz, CDCl_3): δ 155.10, 145.54, 144.73, 142.86, 138.93, 132.64, 131.03, 130.47, 127.49, 126.92, 126.49, 125.71, 124.31, 121.10, 120.55, 118.23, 113.51, 111.70, 111.49, 55.79, 21.27;

HRMS-EI (m/z), Calcd for, $\text{C}_{28}\text{H}_{21}\text{N}_5\text{O}_5$ $[\text{M}]^+$ 507.1543; found: 507.1507.

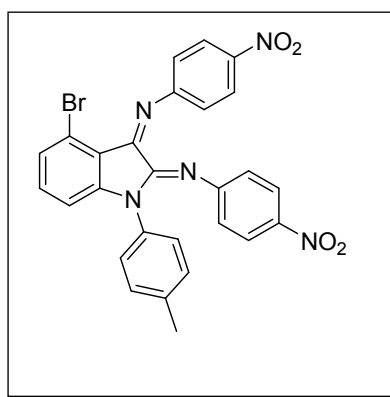


7-Methyl-3-(4-nitrophenylimino)-1-p-tolyldolin-2-ylidene)-4-nitrobenzenamine(4l)

^1H NMR (400 MHz, CDCl_3) δ 8.22(d, $J = 8.80$ Hz, 2H), 8.01(d, $J = 6.76$ Hz, 2H), 7.30(br, 4H), 7.08(d, $J = 7.60$ Hz, 1H), 6.86(br, 4H), 6.61(t, $J = 7.70$ Hz, 1H), 6.43(br, 1H), 2.41(s, 3H), 1.68(s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.94, 148.77, 144.59, 142.78,

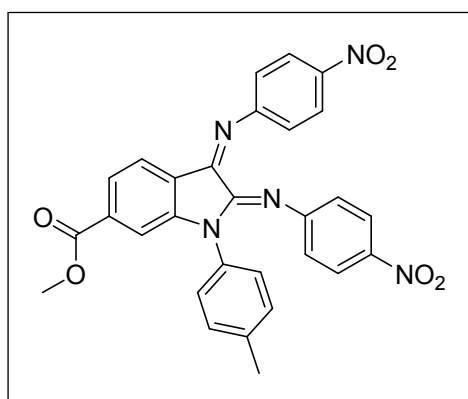
139.44, 138.87, 135.38, 130.11, 129.50, 126.47, 125.81, 124.56, 123.70, 122.59, 122.10, 119.93, 117.71, 113.50, 21.39, 19.07.

HRMS-EI (m/z), Calcd for, $\text{C}_{28}\text{H}_{21}\text{N}_5\text{O}_4$ $[\text{M}]^+$ 491.1594; found: 491.1550.



4-Bromo-3-(4-nitrophenylimino)-1-p-tolyldolin-2-ylidene)-4-nitrobenzenamine(4m)

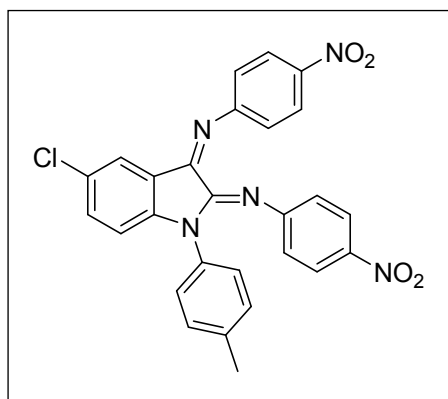
^1H NMR (400 MHz, CDCl_3) δ 8.14(d, J = 8.96 Hz, 2H), 7.61(d, J = 8.94 Hz, 2H), 7.27(d, J = 8.15 Hz, 1H), 7.17(t, J = 8.01 Hz, 1H), 6.96(d, J = 8.95 Hz, 2H), 6.91(d, J = 8.09 Hz, 2H), 6.80(d, J = 8.22 Hz, 2H), 6.50(d, J = 7.93 Hz, 1H), 6.22(d, J = 8.91 Hz, 2H), 2.17(s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.25, 152.77, 152.26, 152.02, 143.30, 142.43, 139.43, 139.38, 134.68, 131.96, 130.24, 128.18, 127.73, 124.97, 123.62, 119.92, 119.63, 118.88, 117.03, 109.03, 21.00;
HRMS-EI (m/z), Calcd for, $\text{C}_{27}\text{H}_{18}\text{BrN}_5\text{O}_4$ $[\text{M}]^+$ 555.0542; found: 555.0539.



Methyl 1-methyl-2,3-bis(4-nitrophenylimino)indoline-6-carboxylate(4n)

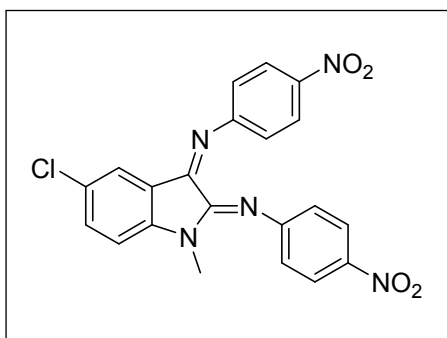
^1H NMR (400 MHz, CDCl_3) δ 8.30(br, 2H), 7.96(br, 2H), 7.5-6.7(br/m, 10H), 6.60(br/m, 1H), 3.84(s, 3H), 2.35(s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 165.57, 151.29, 145.00, 143.05, 139.40, 135.80, 131.95, 130.75, 127.52, 127.03, 126.44, 125.82, 124.60, 123.45, 120.38, 118.99, 117.85, 113.46, 111.76, 111.37, 52.79, 21.31;

HRMS-EI (m/z), Calcd for, $\text{C}_{29}\text{H}_{21}\text{N}_5\text{O}_6$ $[\text{M}]^+$ 535.1492; found: 535.1462.



5-Chloro-3-(4-nitrophenylimino)-1-p-tolyldolin-2-ylidene)-4-nitrobenzenamine(4o)

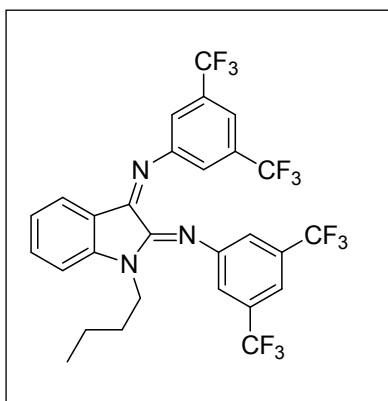
^1H NMR (400 MHz, CDCl_3) δ 8.26(d, J = 8.84 Hz, 2H), 7.93(d, J = 8.64 Hz, 2H), 7.25-7.15(m, 5H), 6.95(d, J = 8.56 Hz, 2H), 6.77(d, J = 8.28 Hz, 2H), 6.68(br, 1H), 6.62(d, J = 8.56 Hz, 1H), 2.34(s, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 155.11, 149.79, 144.92, 143.04, 139.35, 134.81, 132.02, 130.65, 127.47, 126.97, 126.05, 125.84, 125.31, 124.48, 120.22, 117.86, 113.45, 112.27, 111.88, 21.27;
HRMS-EI (m/z), Calcd for, $\text{C}_{27}\text{H}_{18}\text{N}_5\text{O}_4\text{Cl}$ $[\text{M}]^+$ 511.1047; found: 511.1011.



N-(5-chloro-1-methyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4p)

^1H NMR (400 MHz, CDCl_3) δ 8.24(d, J = 8.68 Hz, 2H), 8.13(d, J = 8.76 Hz, 2H), 7.36(dd, J = 8.52, 1.76 Hz, 1H), 6.96(d, J = 8.60 Hz, 2H), 6.83(d, J = 8.52 Hz, 2H), 6.79(d, J = 7.96 Hz, 1H), 6.42(s, 1H), 3.35(s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.99, 154.49, 152.52, 149.26, 147.30, 144.90, 143.28, 134.95, 126.57, 126.30, 125.82, 125.17, 120.17, 117.57, 116.58, 110.33, 28.01;

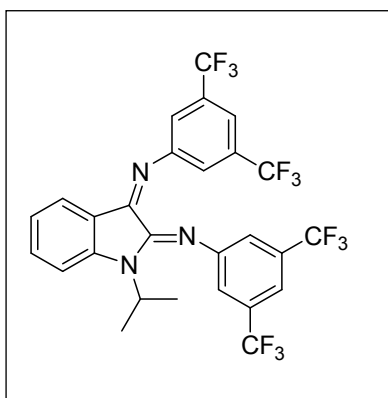
HRMS-EI (m/z), Calcd for, $\text{C}_{21}\text{H}_{14}\text{N}_5\text{O}_4\text{Cl}$ $[\text{M}]^+$ 435.0734; found: 435.0704.



3-(3,5-Bis(trifluoromethyl)phenylimino)-1-butyrylindolin-2-ylidene)-3,5-bis(trifluoromethyl)benzenamine(4q)

^1H NMR (400 MHz, CDCl_3) δ 7.64(s, 1H), 7.46-7.37 (m, 4H), 7.16(s, 2H), 6.90(d, J = 8.07 Hz, 1H), 6.66(t, J = 7.49 Hz, 1H), 6.41(d, J = 6.88 Hz, 1H), 3.88(s, 2H), 1.79(t, J = 6.68 Hz, 2H), 1.57-1.47 (m, 2H), 1.03(t, J = 7.08 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.68, 150.71, 150.63, 150.51, 148.68, 135.36, 133.15(q, $J_{(\text{CF}_3)}$ = 33.40 Hz), 131.96(q, $J_{(\text{CF}_3)}$ = 32.70 Hz), 127.49(d, $J_{(\text{C-F})}$ = 58.40 Hz), 126.44, 124.78(d, $J_{(\text{C-F})}$ = 58.90 Hz), 122.07(d, $J_{(\text{C-F})}$ = 59.20 Hz), 121.22, 121.06, 119.31(d, $J_{(\text{C-F})}$ = 59.50 Hz), 118.24-117.93(m, C-F), 116.01-115.80(m, C-F), 109.62, 41.18, 29.27, 20.50, 13.96;

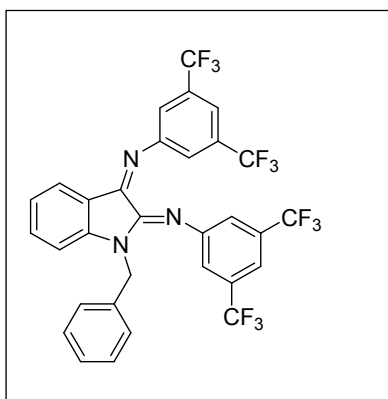
HRMS-EI (m/z), Calcd for, $\text{C}_{28}\text{H}_{19}\text{N}_3\text{F}_{12}$ $[\text{M}]^+$ 625.1387; found: 625.1356.



3-(3,5-Bis(trifluoromethyl)phenylimino)-1-isopropylindolin-2-ylidene)-3,5-bis(trifluoromethyl)benzenamine(4r)

^1H NMR (400 MHz, CDCl_3) δ 7.63(s, 1H), 7.44(s, 1H), 7.39-7.34(m, 3H), 7.13(s, 2H), 7.08(d, J = 8.18

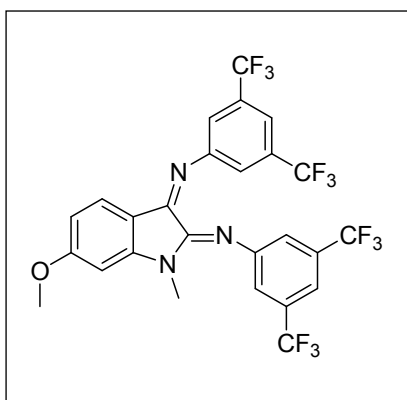
Hz, 1H), 6.65(t, $J = 7.62$ Hz, 1H), 6.42(d, $J = 7.22$ Hz, 1H), 4.93- 4.89(m, 1H), 1.61(d, $J = 7.05$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.55, 150.87, 150.67, 149.62, 148.33, 135.10, 133.15(q, $J_{(\text{CF}_3)} = 33.40$ Hz), 131.98(q, $J_{(\text{CF}_3)} = 32.80$ Hz), 127.51(d, $J_{(\text{C-F})} = 60.40$ Hz), 126.62, 124.79(d, $J_{(\text{C-F})} = 60.80$ Hz), 122.08(d, $J_{(\text{C-F})} = 61.10$ Hz), 120.89, 120.81, 119.37(d, $J_{(\text{C-F})} = 61.60$ Hz), 118.13-117.78(m, C-F), 116.18-115.77(m, C-F), 111.16, 45.04, 19.06; HRMS-EI (m/z), Calcd for, $\text{C}_{27}\text{H}_{17}\text{N}_3\text{F}_{12}$ $[\text{M}]^+$ 611.1231; found: 611.1221



3-(3,5-Bis(trifluoromethyl)phenylimino)-1-benzylindolin-2-ylidene)-3,5-bis(trifluoromethyl)benzenamine(4s)

^1H NMR (400 MHz, CDCl_3) δ 7.67(s, 1H), 7.49-7.39 (m, 7H), 7.36-7.31(m, 2H), 7.20(s, 2H), 6.85(d, $J = 8.06$ Hz, 1H), 6.68(t, $J = 7.50$ Hz, 1H), 6.46(d, $J = 6.99$ Hz, 1H), 5.14(s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.51, 150.53, 150.29, 150.19, 148.90,

135.72, 135.42, 133.17(q, $J_{(\text{CF}_3)} = 33.50$ Hz), 131.95(q, $J_{(\text{CF}_3)} = 32.80$ Hz), 129.13, 128.03, 127.46(d, $J_{(\text{C-F})} = 56.40$ Hz), 127.36, 126.40, 124.76(d, $J_{(\text{C-F})} = 56.90$ Hz), 122.04(d, $J_{(\text{C-F})} = 57.10$ Hz), 121.63, 121.11, 119.29(d, $J_{(\text{C-F})} = 57.60$ Hz), 118.36-117.97(m, C-F), 116.29-115.86(m, C-F), 110.32, 45.00; HRMS-EI (m/z), Calcd for, $\text{C}_{31}\text{H}_{17}\text{N}_3\text{F}_{12}$ $[\text{M}]^+$ 659.1231; found: 659.1216.



3-(3,5-Bis(trifluoromethyl)phenylimino)-6-methoxy-1-methylindolin-2-ylidene)-3,5-bis(trifluoromethyl)benzenamine(4t)

^1H NMR (400 MHz, CDCl_3) δ 7.60(s, 1H), 7.45(s, 1H), 7.41(s, 2H), 7.12(s, 2H), 6.36-6.32(m, 2H), 6.17(d, $J = 8.32$ Hz, 1H), 3.84(s, 3H), 3.35(s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 165.76, 153.08, 152.60, 151.04, 150.43, 150.06, 133.03(q, $J_{(\text{CF}_3)} =$

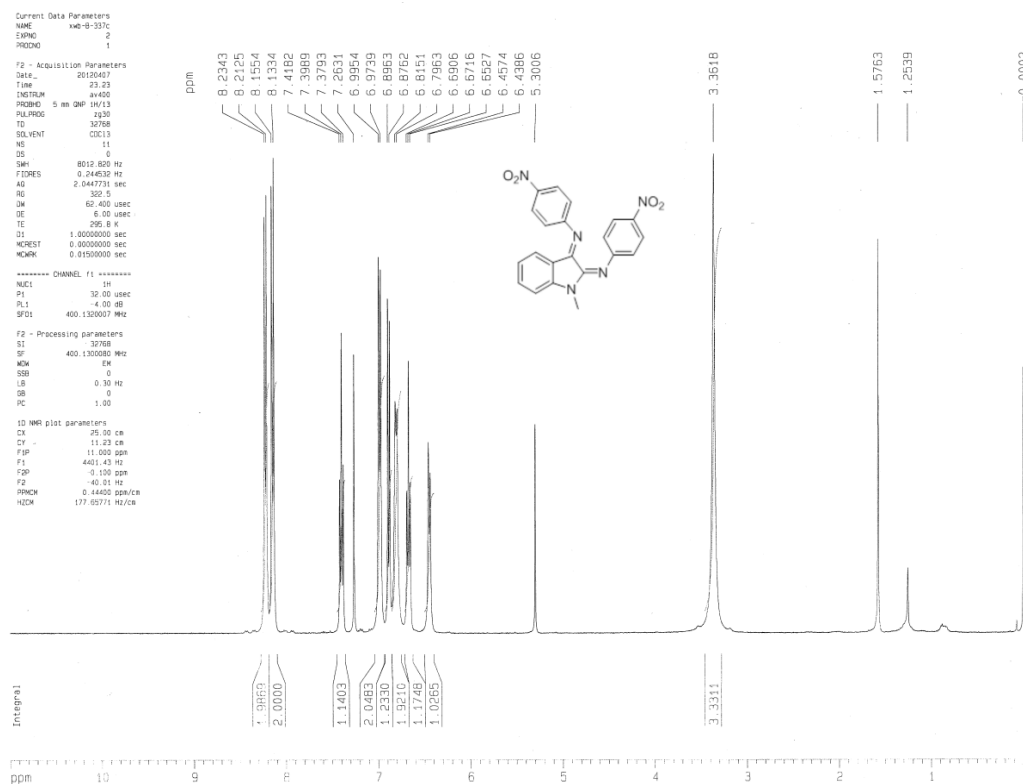
33.20 Hz), 131.84(q, $J_{(\text{CF}_3)} = 32.80$ Hz), 128.10, 127.52(d, $J_{(\text{C-F})} = 52.90$ Hz),

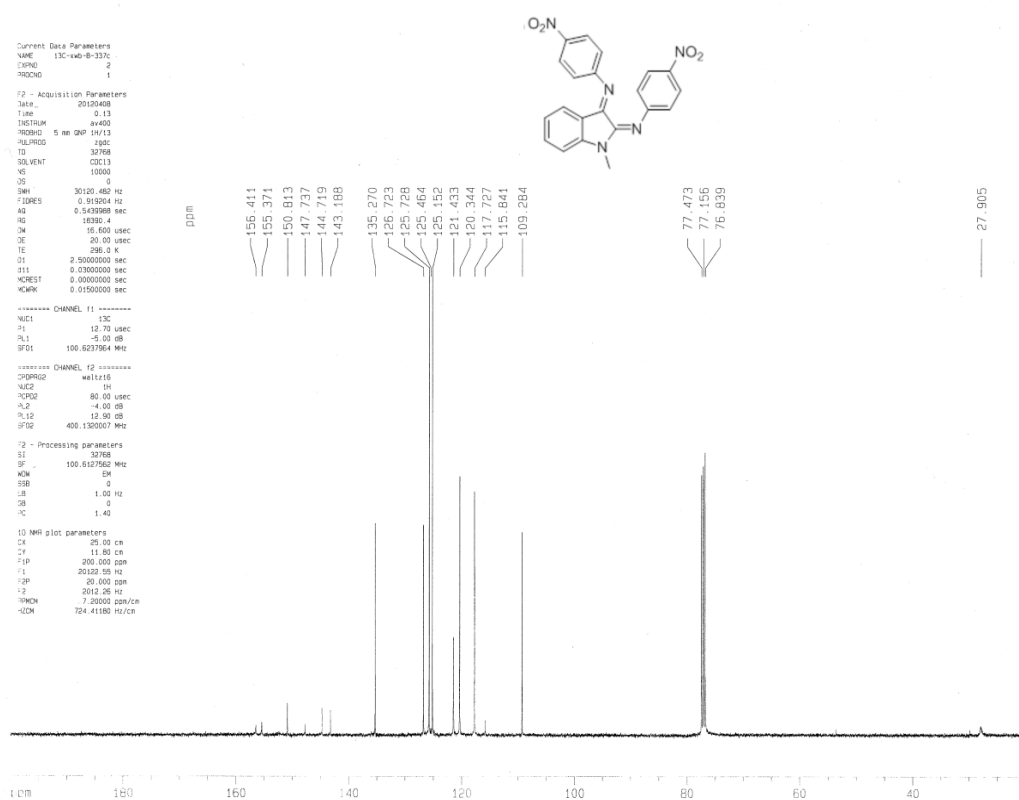
124.78(d, $J_{(C-F)} = 53.40$ Hz), 122.06(d, $J_{(C-F)} = 53.70$ Hz), 121.17, 119.37(d, $J_{(C-F)} = 53.60$ Hz), 118.31, 116.11, 106.49, 95.89, 55.98, 29.87;

HRMS-EI (m/z), Calcd for, $C_{26}H_{15}N_3OF_{12}[M]^+$ 613.1024; found: 613.0994.

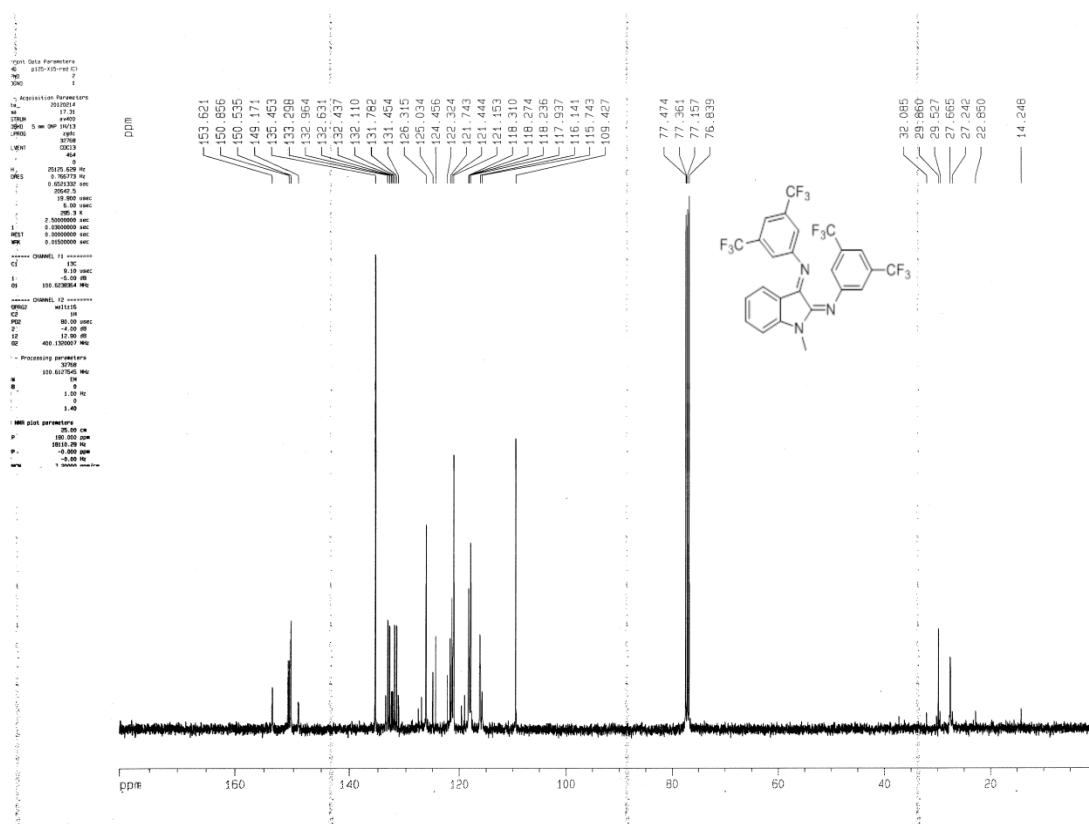
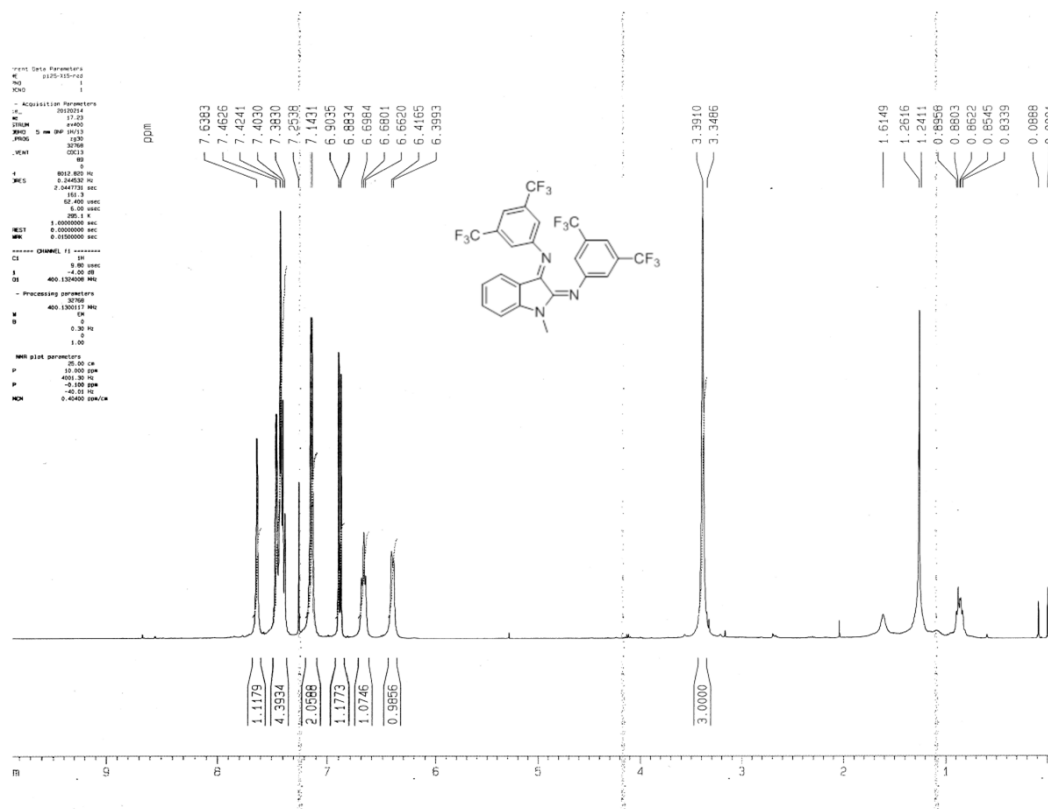
NMR Spectra of products

1-Methyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine (3a)

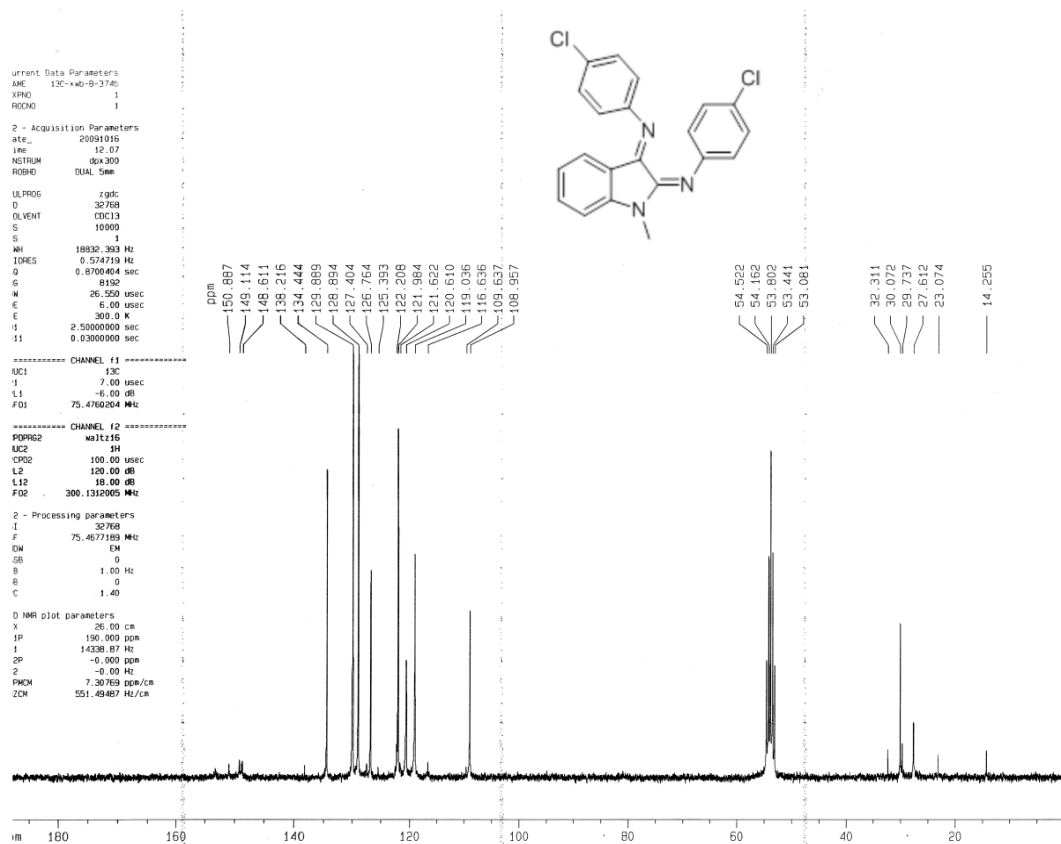
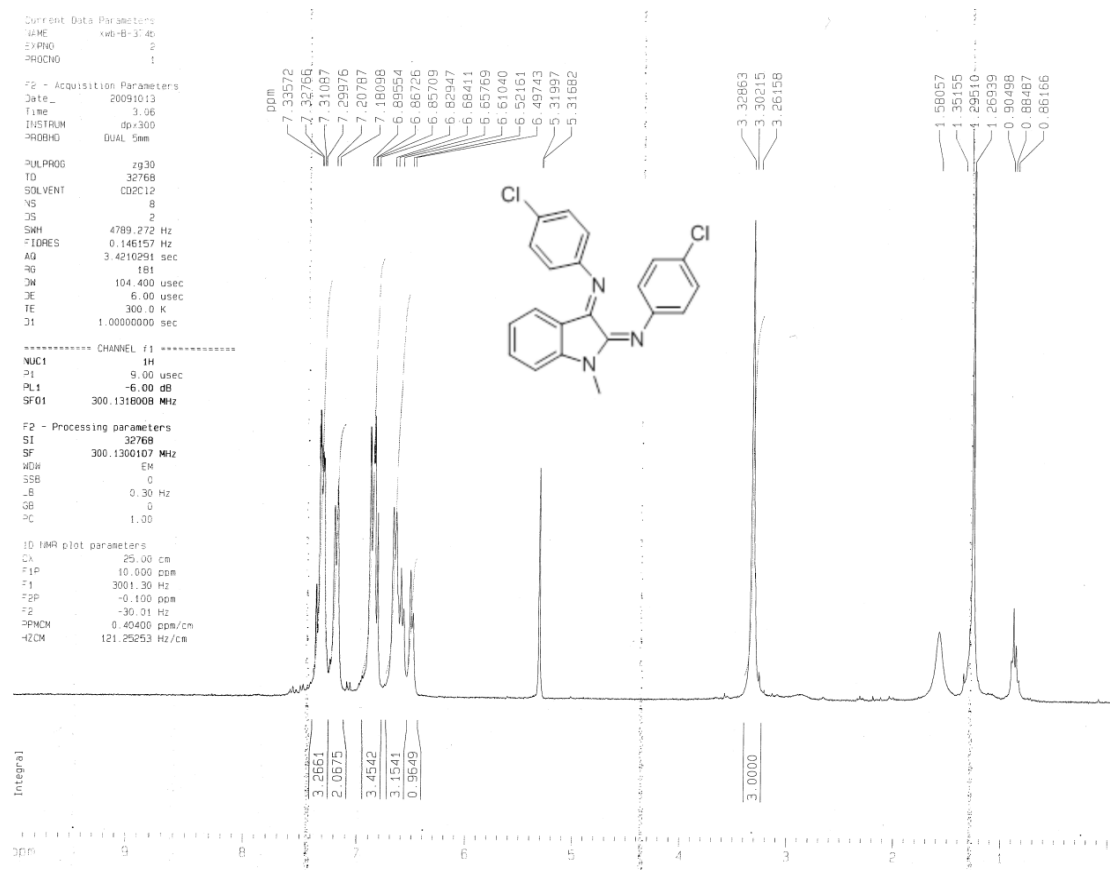


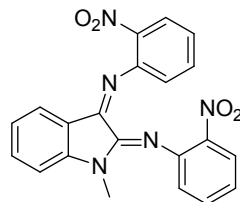


3-(3,5-Bis(trifluoromethyl)phenylimino)-1-methylindolin-2-ylidene)-3,5-bis(trifluoromethyl)benzenamine(3b)



4-chloro-N-(3-(4-chlorophenylimino)-1-methylindolin-2-ylidene)benzenamine(3c)



[illegible]



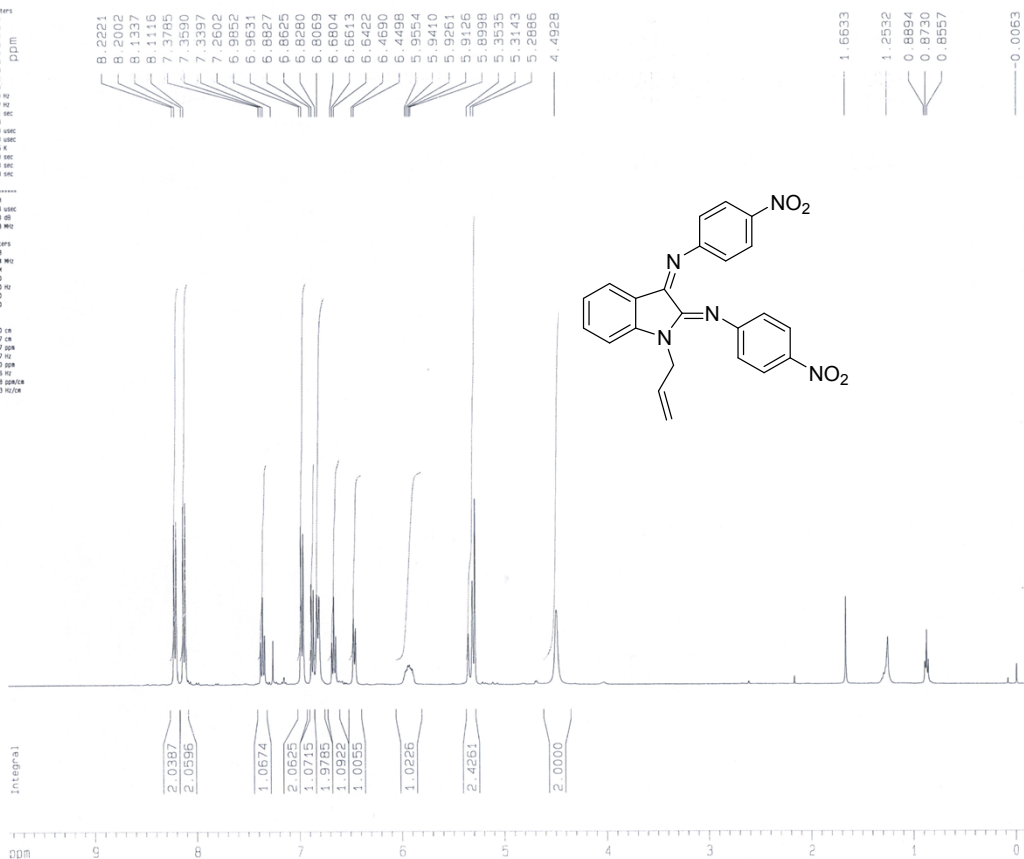
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EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
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Time: 11.29
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
SOLVENT: DMSO
NS: 400
DS: 4
SWH: 8532.820 Hz
F2RES: 2.344332 Hz
AQ: 2.5447733 sec
RG: 328
DQ: 62.400 uSec
DE: 6.00 uSec
TE: 300.4 K
D1: 1.50000000 sec
WDECT: 0.00000000 sec
WDMR: 0.01500000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 9.80 uSec
PL1: 4.00 dB
SFO1: 400.1324080 MHz

F2 - Processing parameters
SI: 32768
SF: 400.1324080 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

===== CHANNEL f2 =====
Date_: 20130303
Time: 11.29
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
SOLVENT: DMSO
NS: 400
DS: 4
SWH: 8532.820 Hz
F2RES: 2.344332 Hz
AQ: 2.5447733 sec
RG: 328
DQ: 62.400 uSec
DE: 6.00 uSec
TE: 300.4 K
D1: 1.50000000 sec
WDECT: 0.00000000 sec
WDMR: 0.01500000 sec

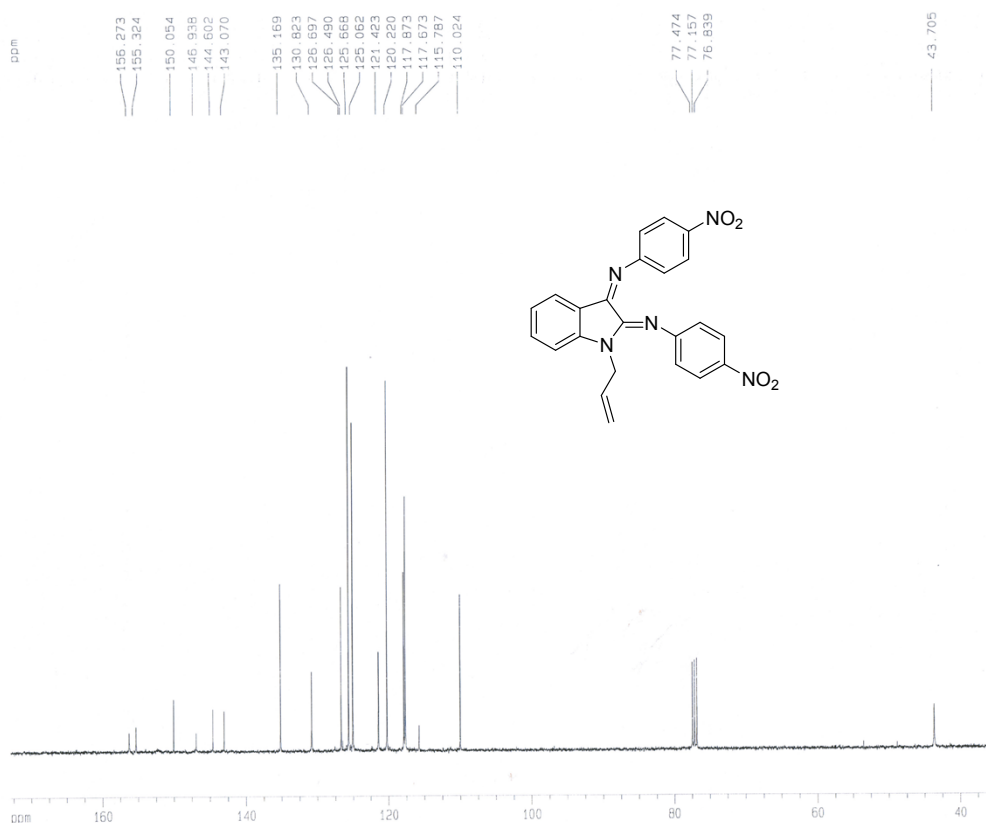


Current Data Parameters
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PROCNO: 1

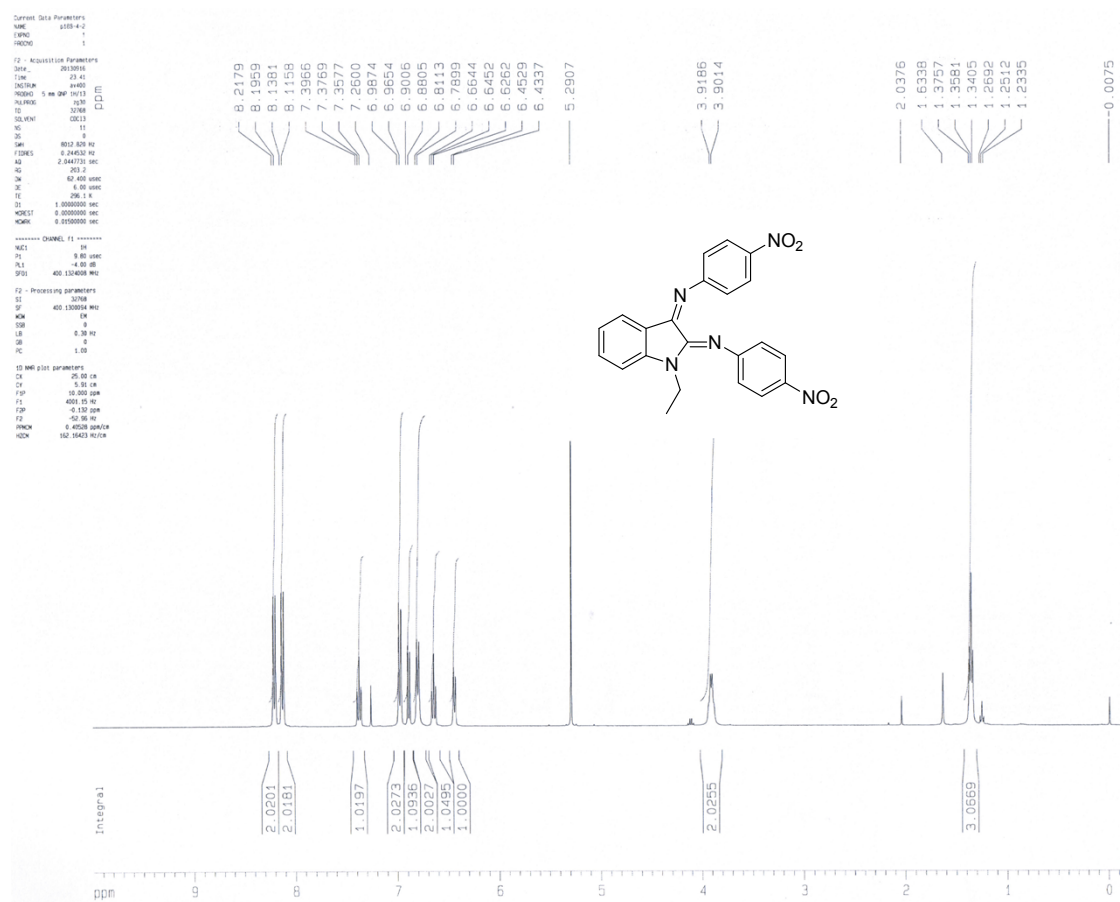
F2 - Acquisition Parameters
Date_: 20130303
Time: 16.41
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
SOLVENT: DMSO
NS: 548
DS: 4
SWH: 25075.820 Hz
F2RES: 6.366773 Hz
AQ: 6.602332 sec
RG: 328
DQ: 19.900 uSec
DE: 6.00 uSec
TE: 300.4 K
D1: 2.50000000 sec
WDECT: 0.00000000 sec
WDMR: 0.01500000 sec

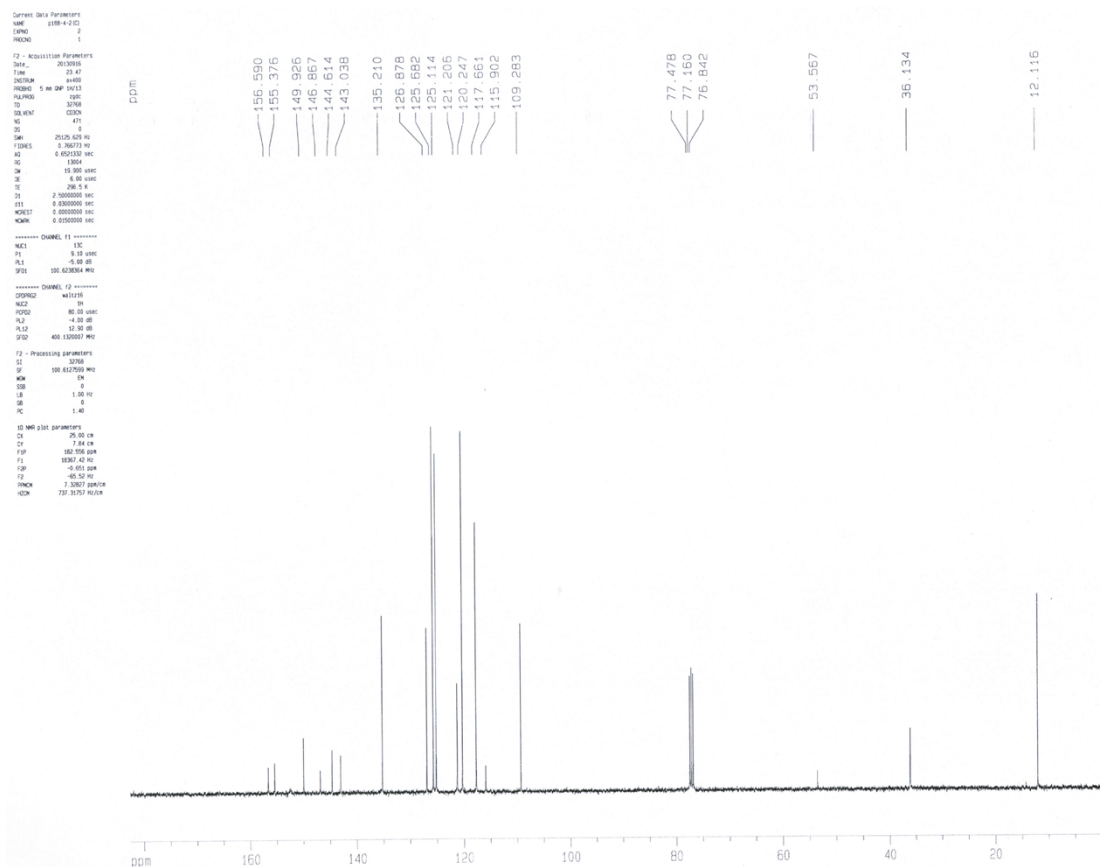
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NUC1: 13C
P1: 9.30 uSec
PL1: 5.00 dB
SFO1: 100.6260540 MHz

===== CHANNEL f2 =====
Date_: 20130303
Time: 16.41
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
SOLVENT: DMSO
NS: 548
DS: 4
SWH: 25075.820 Hz
F2RES: 6.366773 Hz
AQ: 6.602332 sec
RG: 328
DQ: 19.900 uSec
DE: 6.00 uSec
TE: 300.4 K
D1: 2.50000000 sec
WDECT: 0.00000000 sec
WDMR: 0.01500000 sec

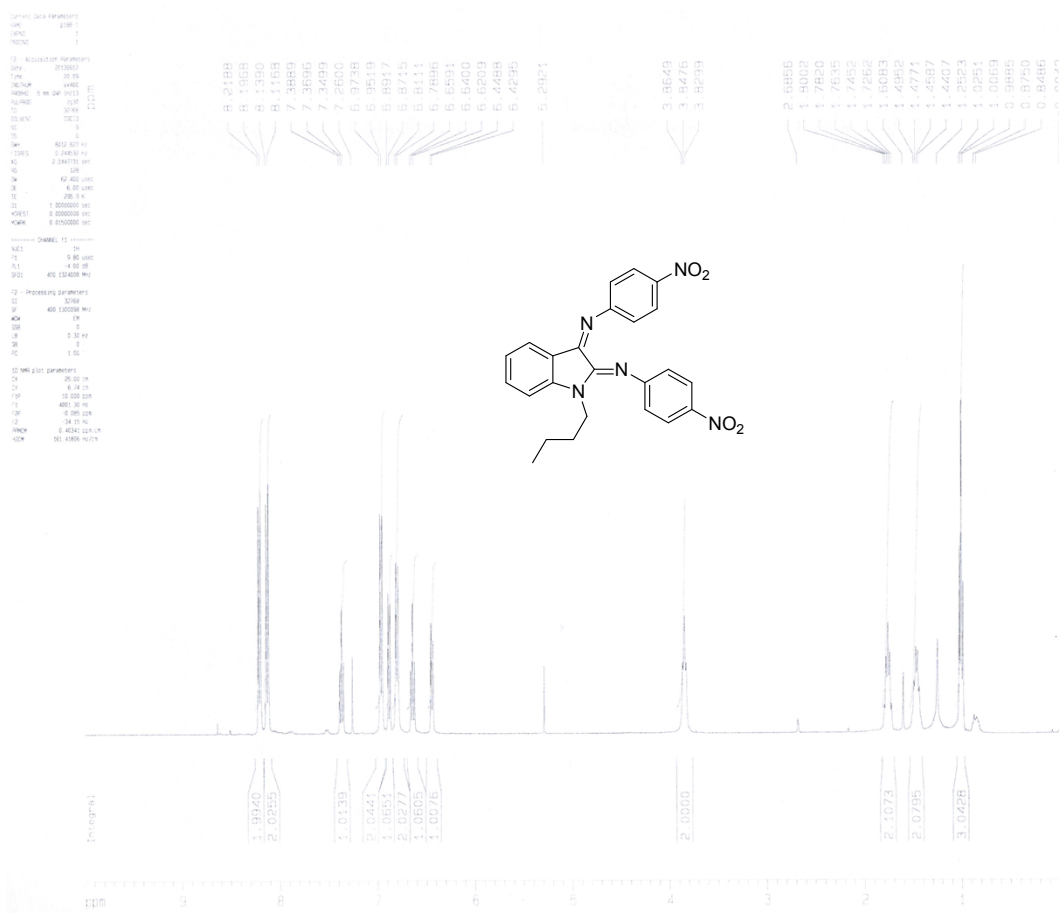


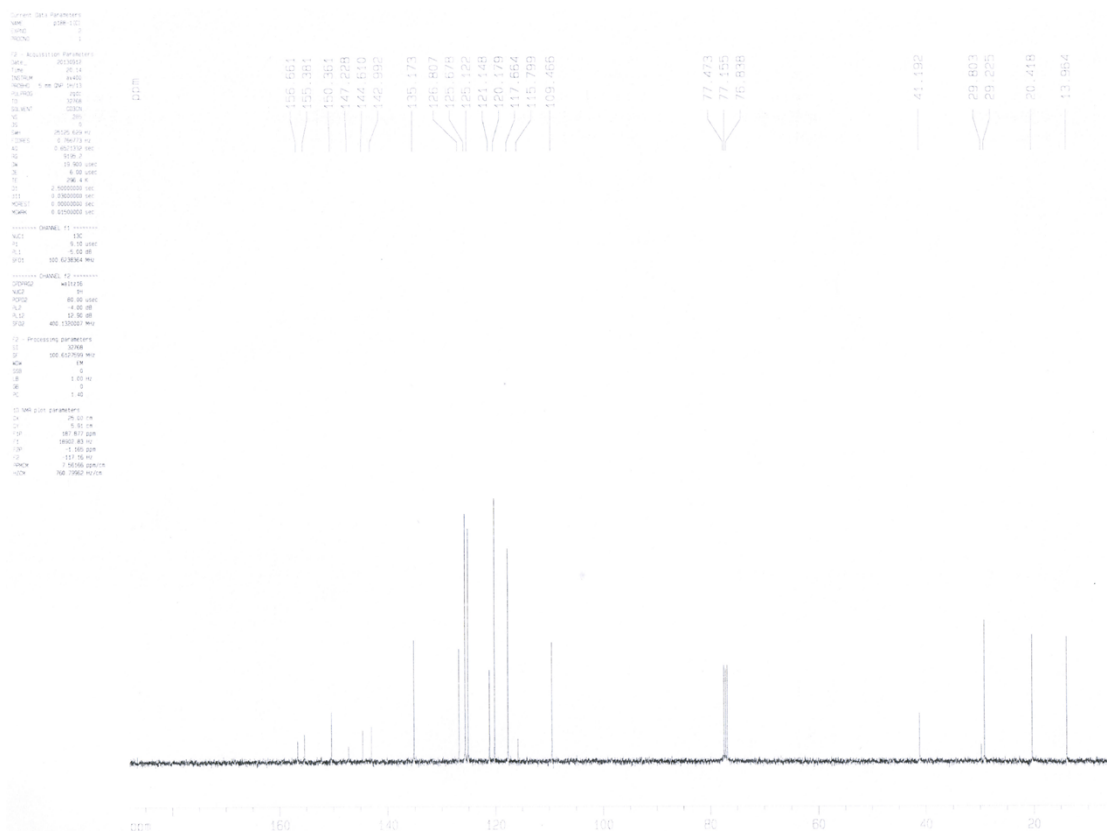
1-Ethyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4b)



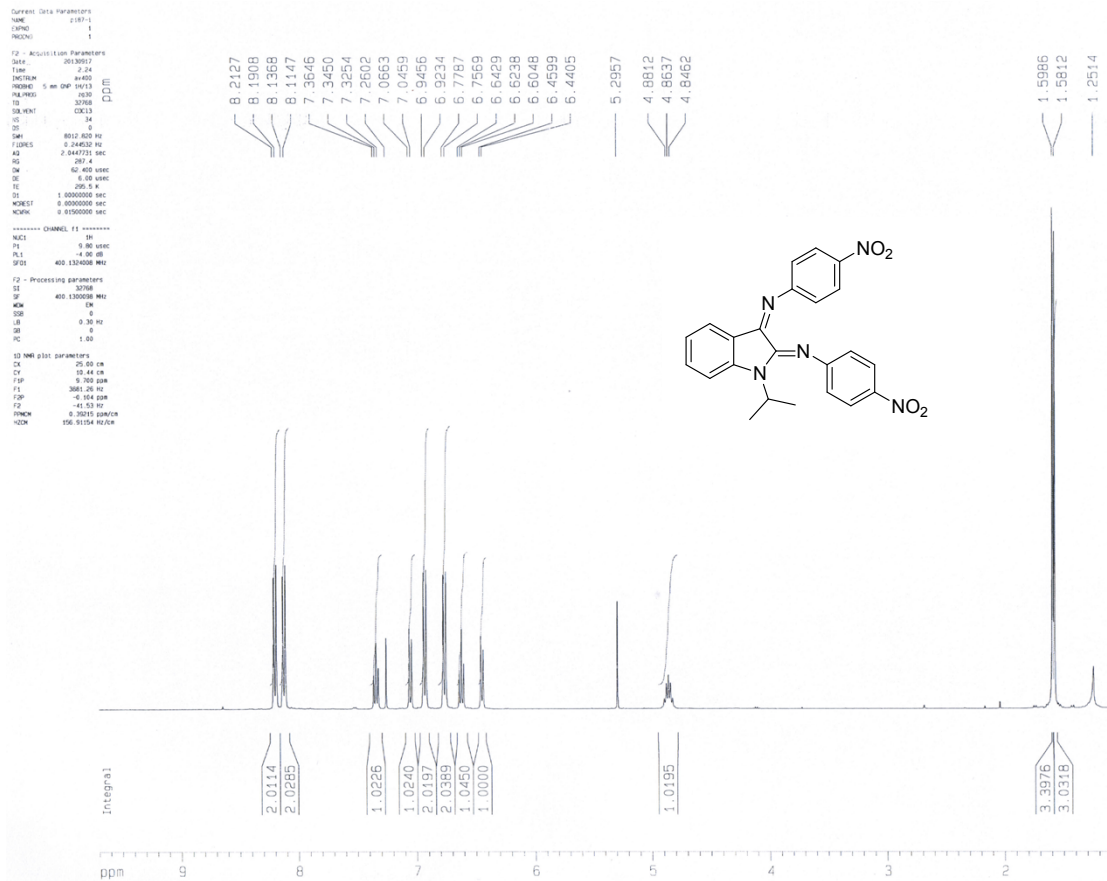


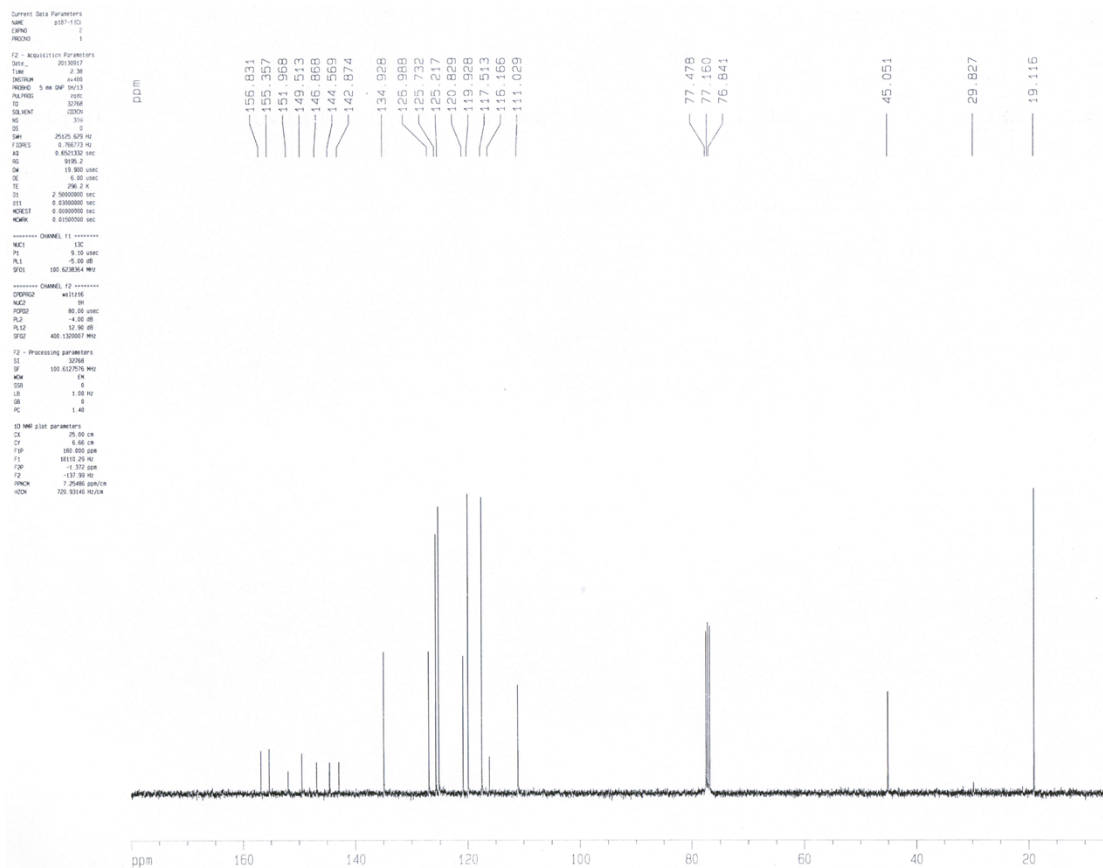
1-Butyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4c)



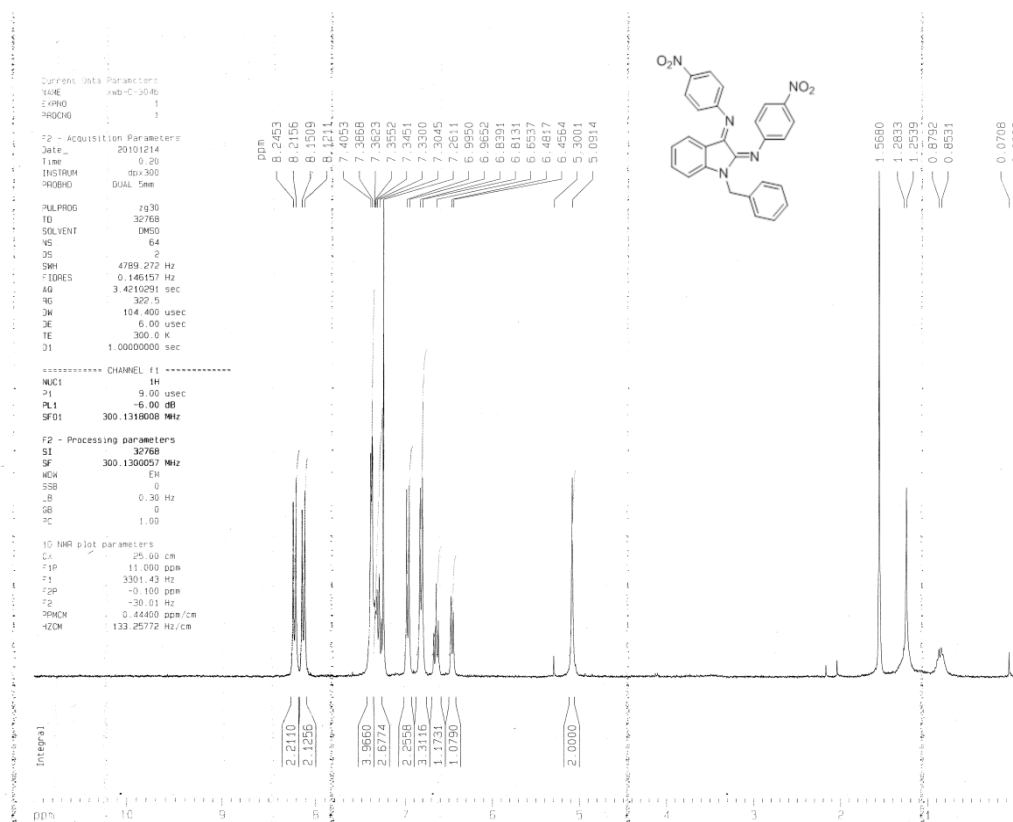


1-Isopropyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4d)





1-Benzyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine(4e)



Current Data Parameters
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 (PNO) 1
 (NOCHO) 1

2 - Acquisition Parameters
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 Time 0.26
 INSTRUM dxt300
 PROBHD DUAL 5mm

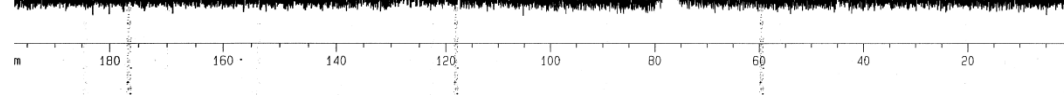
ALPROG zgpgc
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 ALVENT C0C13
 S 9573
 S 1
 MH 19832.393 Hz
 TDRES 0.574719 Hz
 J 0.8700404 sec
 S 8192
 S 26.550 usec
 S 6.00 usec
 S 300.0 K
 S1 2.50000000 sec
 S11 0.03000000 sec

===== CHANNEL f1 =====
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 J1 7.00 usec
 L1 -6.00 dB
 F01 75.4760204 MHz

===== CHANNEL f2 =====
 JC2 1H
 JPC2 100.00 usec
 L2 -2.00 dB
 F02 300.1312005 MHz

2 - Processing parameters
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 S 75.4677376 MHz
 SN EM
 SB 0
 S 1.00 Hz
 S 0
 S 1.40

3 NMR plot parameters
 S 20.00 cm
 SP 200.000 ppm
 S1 15093.55 Hz
 SP -0.000 ppm
 S2 -0.00 Hz
 S 7.69235 ppm/cm
 S2M 580.52108 Hz/cm



4-Nitro-N-(3-(4-nitrophenylimino)-1-p-tolylindolin-2-ylidene)benzenamine(4f)

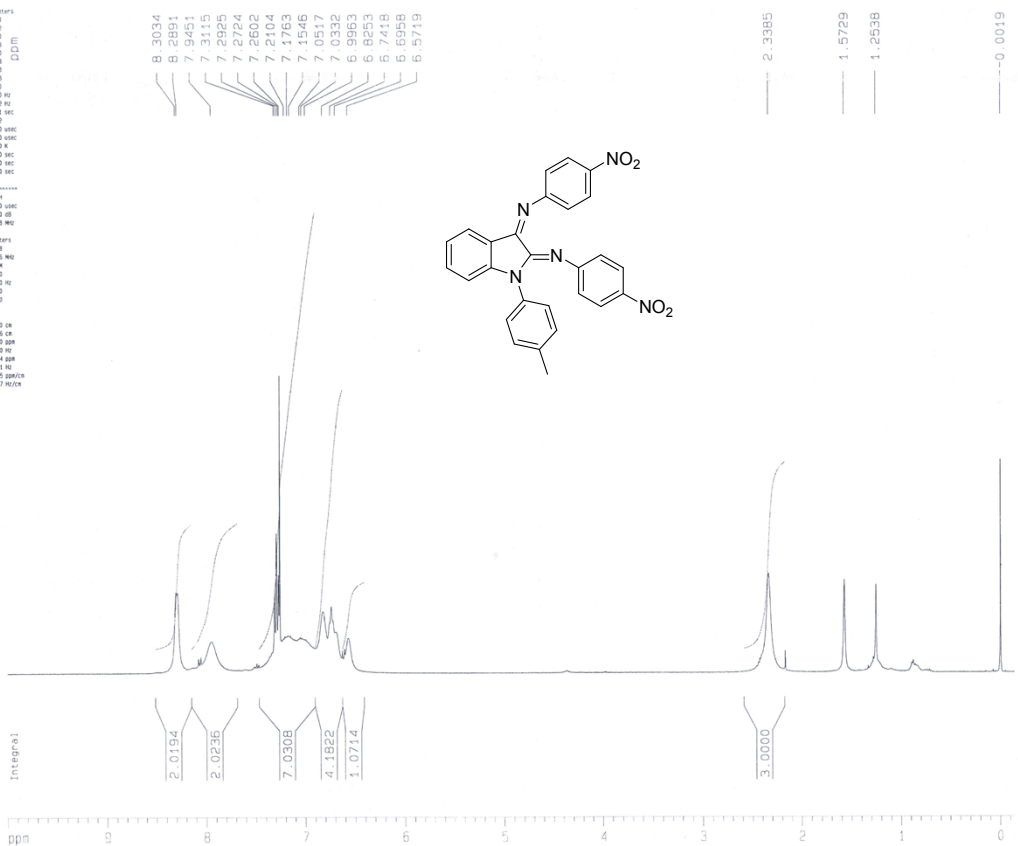
Current Data Parameters
NAME p111-3-1
EXPNO 1
PROCNO 1

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PD 0.00
PC 0.00
SOLVENT dms
NS 2000
DS 4
SWH 8002.800 MHz
FIDRES 0.244632 Hz
AQ 2.6447722 sec
RG 512
DA 62.400 usec
DE 0.00 usec
TE 300.2 K
D1 1.0000000 sec
DECST 0.0000000 sec
KORR 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1504000 MHz

F2 - Processing parameters
SI 32768
SF 400.1504000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 6.25 cm
FAP 15.0000000 Hz
F1 400.150 MHz
F2 101.625 MHz
F3 51.512 MHz
IRACK 0.0000000 Hz
AQ 162.35217 MHz



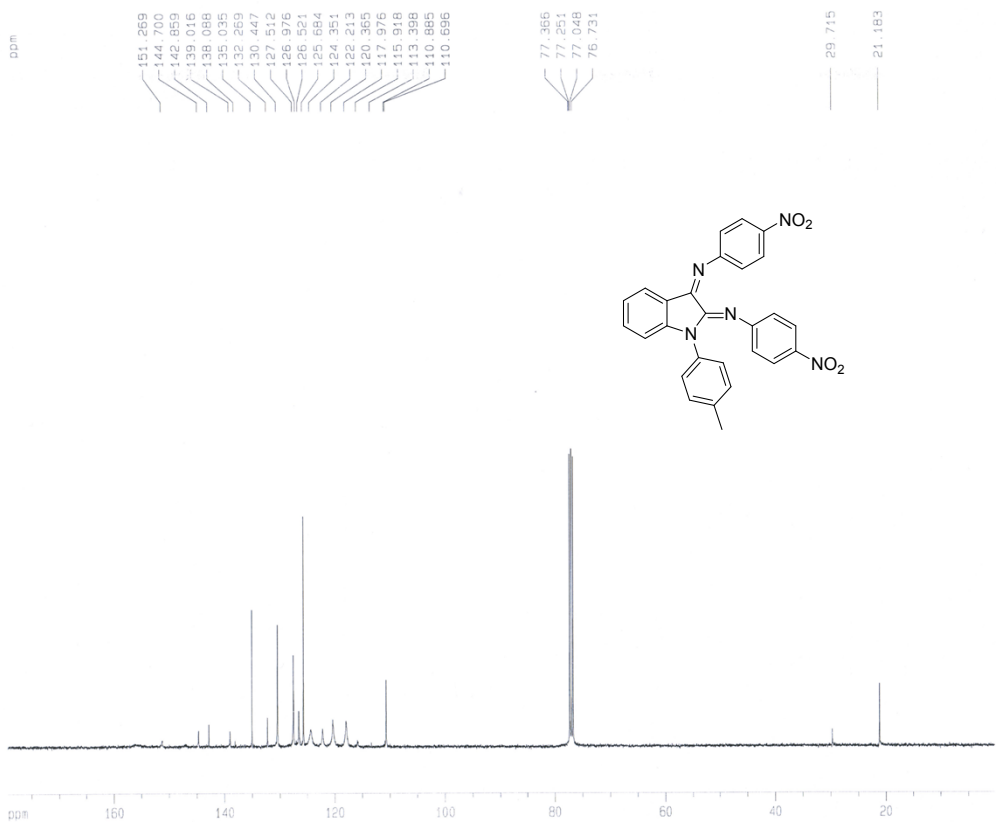
Current Data Parameters
NAME p111-3-1-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130305
Time 23.40
INSTRUM waltz
PULPROG zgpg30
PROBHD 5 mm QNP 1H/13
P1 12.00
PD 0.00
PC 0.00
SOLVENT dms
NS 2000
DS 4
SWH 8002.800 MHz
FIDRES 0.244632 Hz
AQ 2.6447722 sec
RG 512
DA 62.400 usec
DE 0.00 usec
TE 300.2 K
D1 1.0000000 sec
DECST 0.0000000 sec
KORR 0.0150000 sec

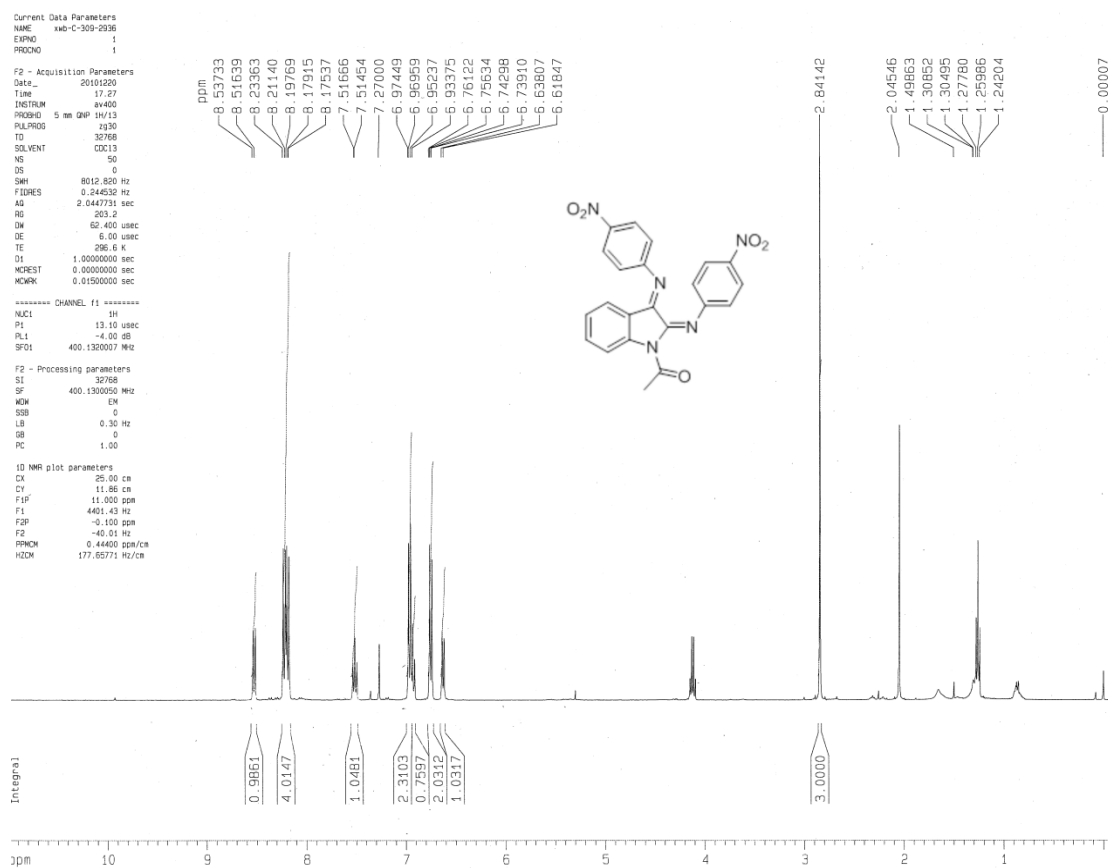
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1504000 MHz

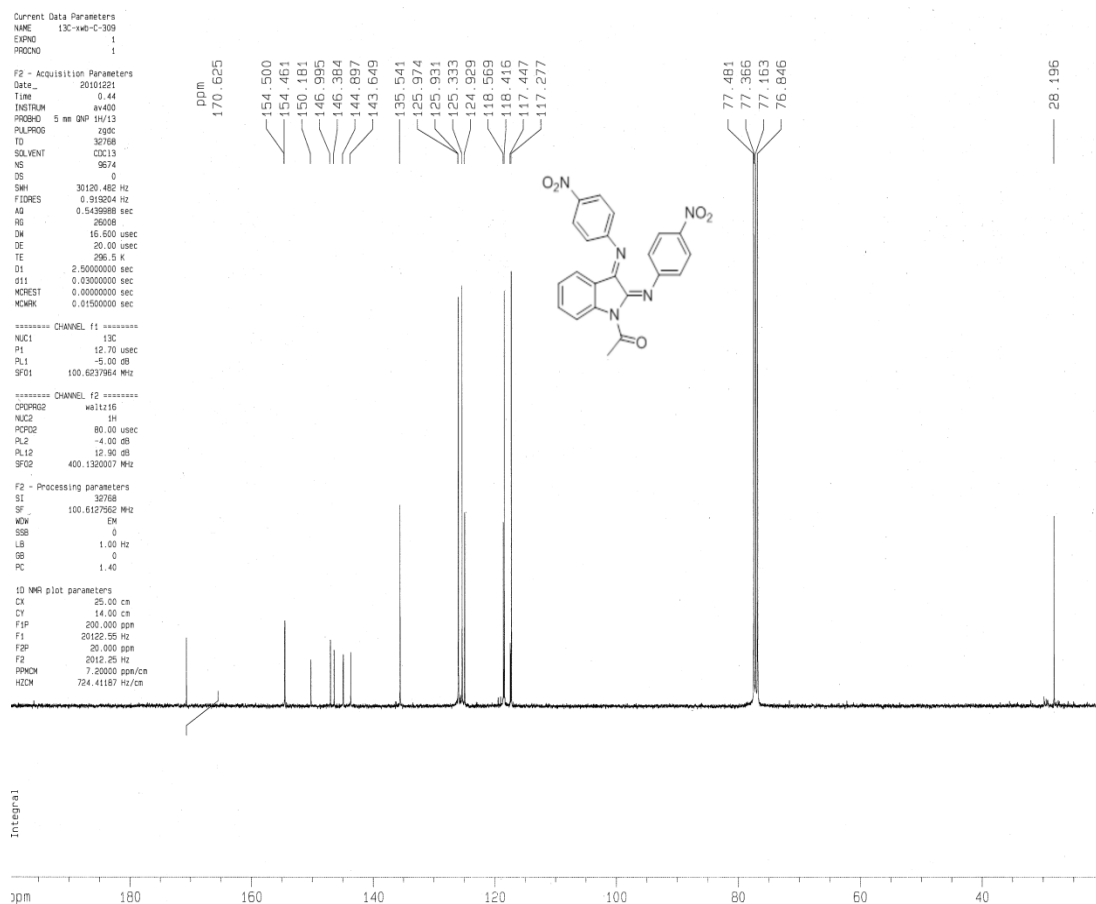
F2 - Processing parameters
SI 32768
SF 400.1504000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 6.25 cm
FAP 15.0000000 Hz
F1 400.150 MHz
F2 101.625 MHz
F3 51.512 MHz
IRACK 0.0000000 Hz
AQ 162.35217 MHz

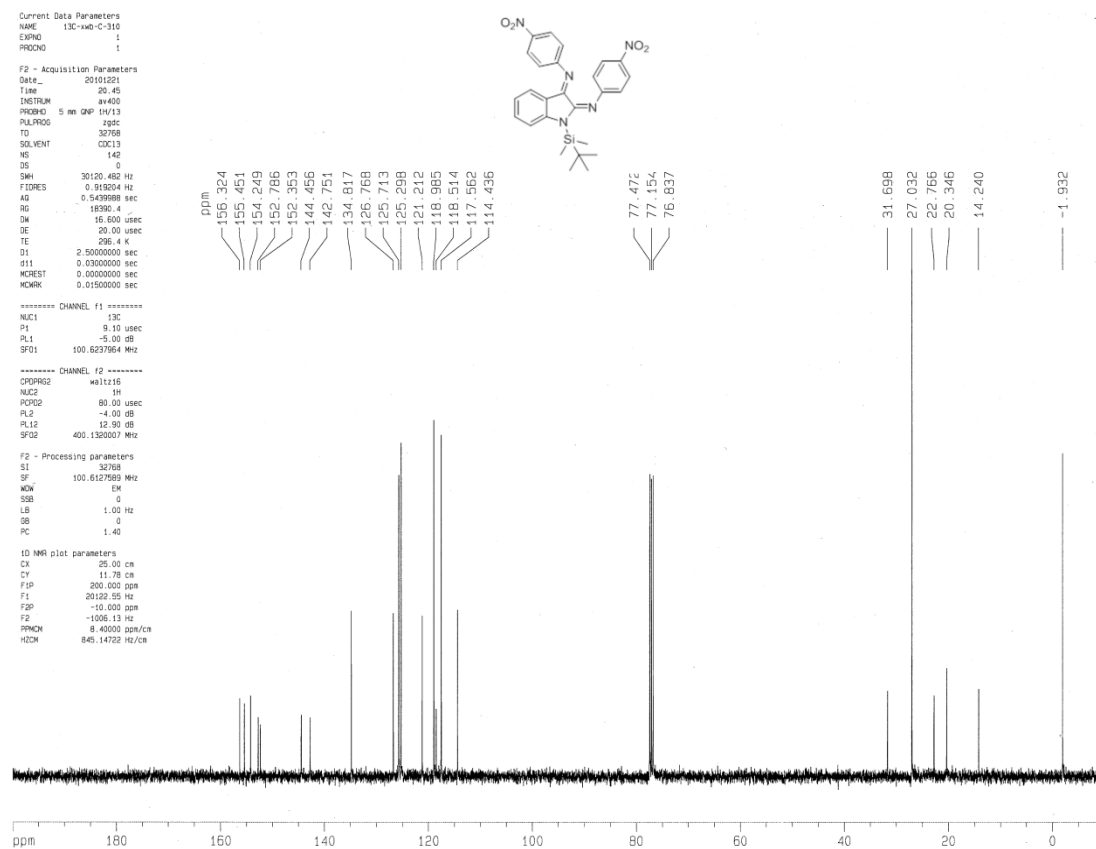
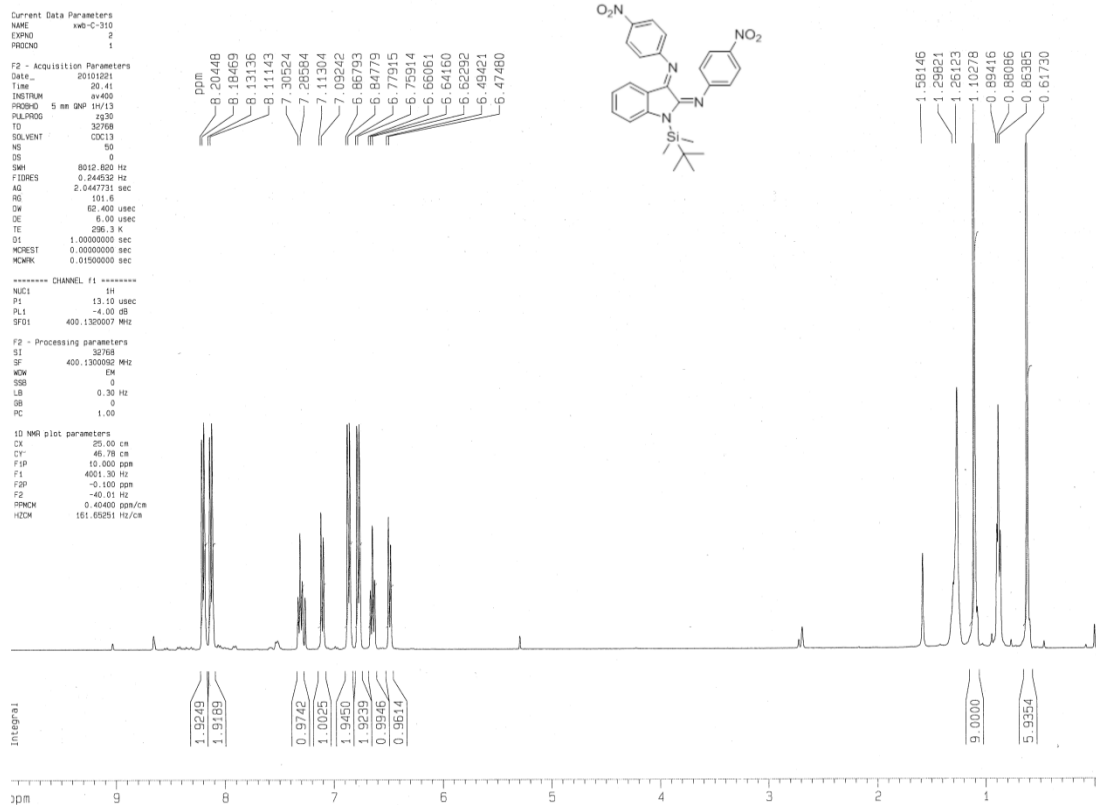


2,3-Bis(4-nitrophenylimino)indolin-1-yl)ethanone(4g)

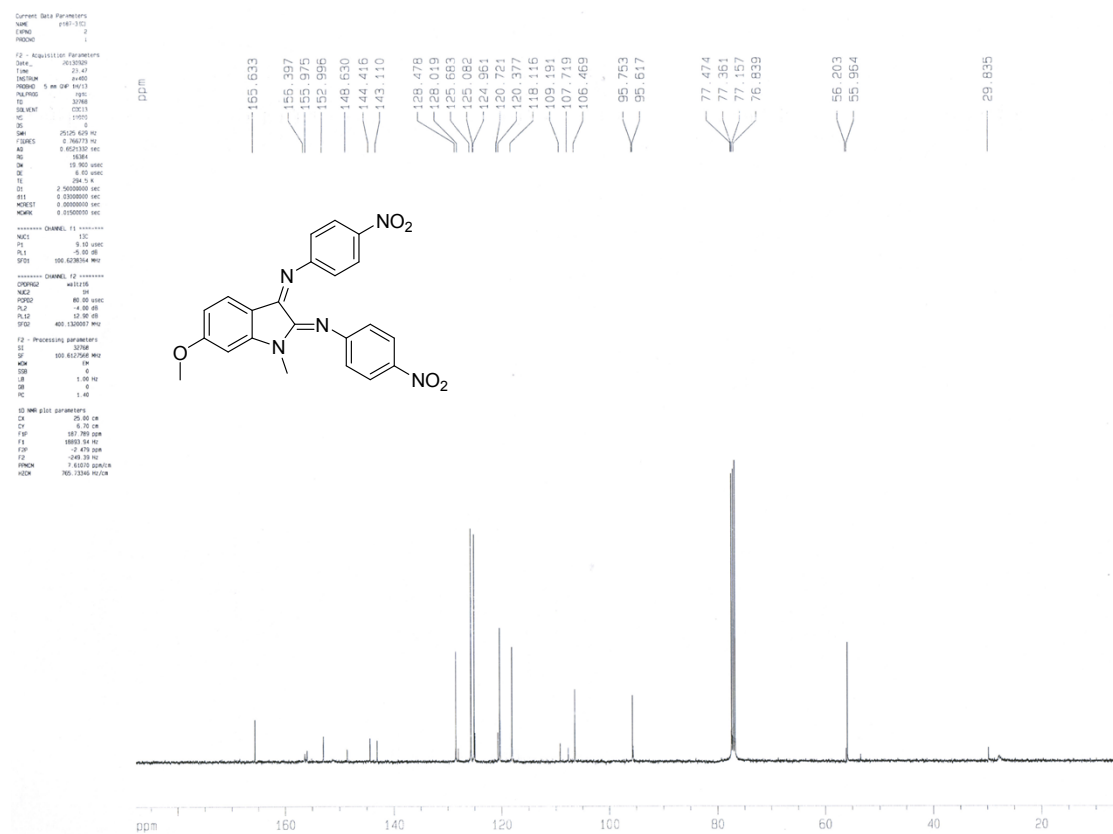
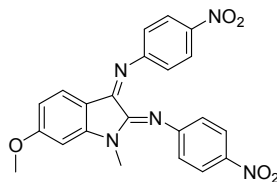
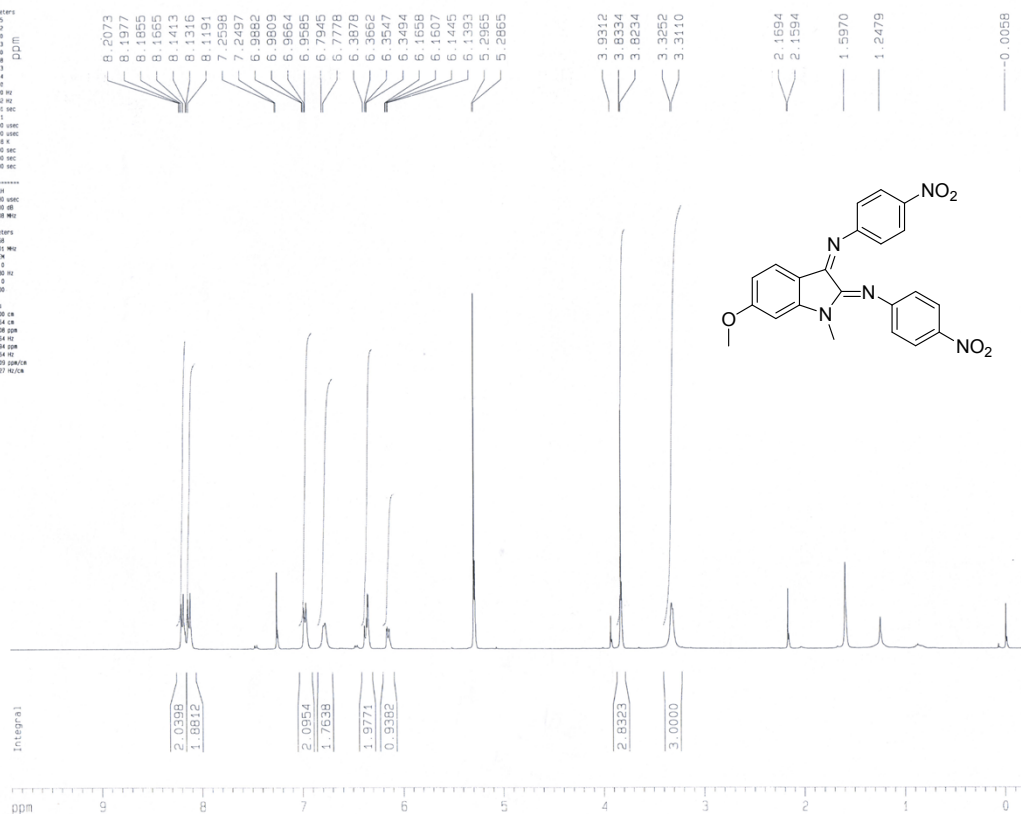




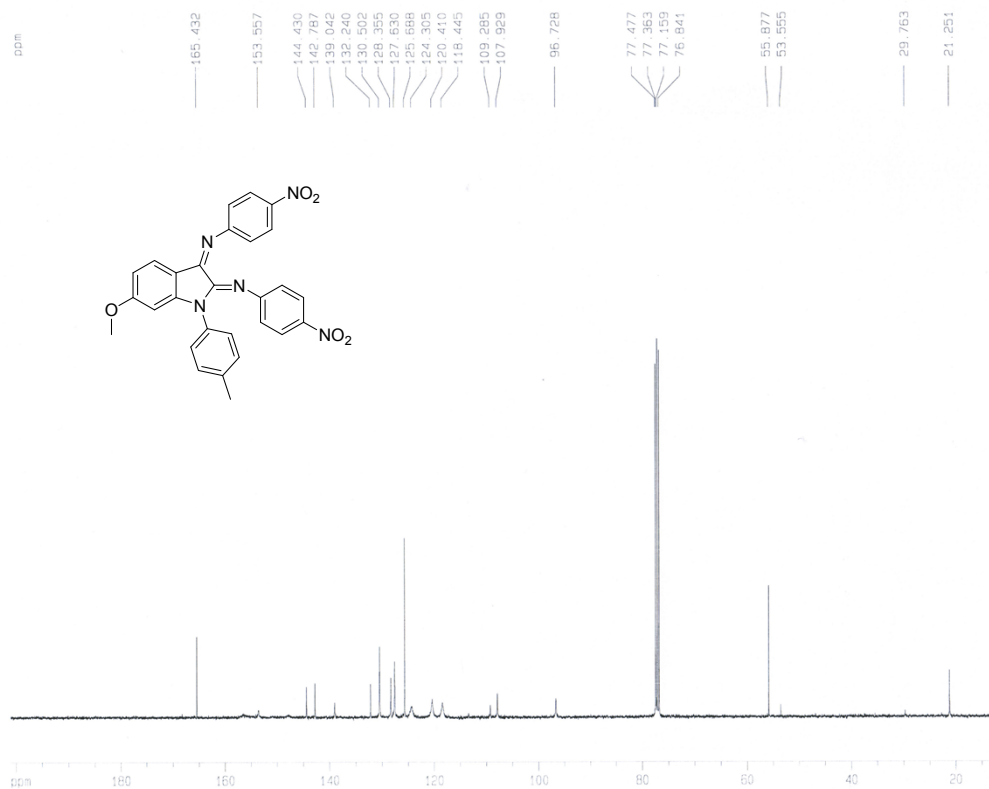
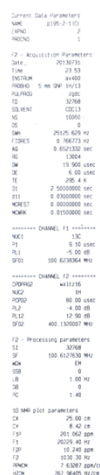
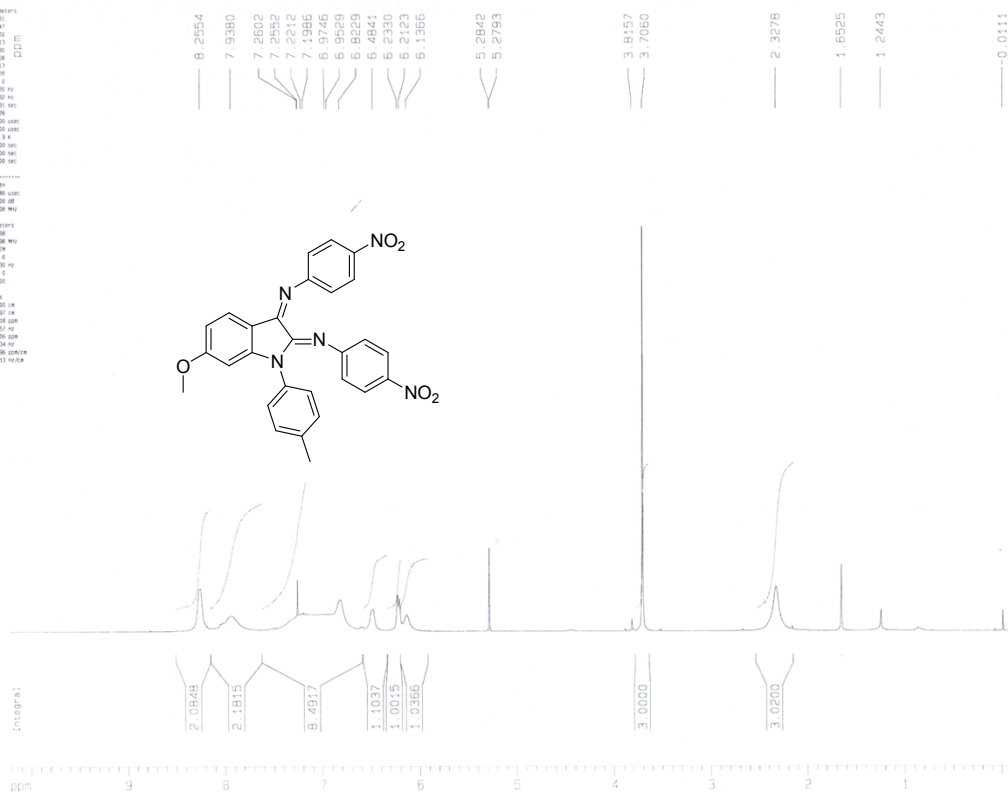
1-(*tert*-Butyldimethylsilyl)-3-(4-nitrophenylimino)indolin-2-ylidene)-4-nitrobenzenamine (4h)



6-Methoxy-1-methyl-3-(4-nitrophenylimino)indolin-2-ylidene)-4-

[illegible]

Current Data Parameters	
NAME	ATPS-1
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
DATE_	20100701
TIME	23:47
INSTRUM	topcon
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
VS	20
DS	4
SWH	8052.880 MHz
F2 - 13C	125.76177 MHz
NUC1	13
NUC2	13
JE	6.00 MHz
TE	294.2 K
DELTA	1.0000000000 sec
NUC1ST	0.0000000000 sec
NUC2ST	0.0000000000 sec
===== CHANNEL f1 =====	
NUC1	13
PA	9.00 MHz
PL	0.00 dB
PC	400.1330000 MHz
F2 - Processing parameters	
SI	32768
SD	400.1330000 MHz
SR	0
SB	0
LC	1.00
GB	0.30
1D NMR list parameters	
WDW	20.00 sec
SSB	0.00 sec
YF0	10.2128 dB
YF1	40.88515 dB
YF2	-9.350000 dB
YF3	42.3434 dB
SNOW	1.4200000000 sec
NO	100.0000000000 sec



Current Data Parameters

NAME kwb-c-26
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

DATE_ 20091218
TIME 0.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
FIDRES 0.0013
SOLVENT DMS
NS 16
DS 3
SWH 6012.820 Hz
F2RES 0.244532 Hz
AQ 2.044773 sec
RG 324.7
ZG 62.450 usec
TE 8.50 usec
TE 308.2 K
Z1 1.0000000 sec
VDELTA 0.0000000 sec
VDELTA 0.0150000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 13.10 usec
PL1 -4.00 dB
SFO1 400.130027 MHz

F2 - Processing Parameters

SI 32768
SF 400.1300141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CH 25.00 cm
CH 11.31 cm
FID 16.000 ppm
F1 4001.30 Hz
F2 100.625 MHz
F3 40.01 Hz
F4 0.4040 ppm/cm
F5 161.6250 Hz/cm

Chemical structure of the compound is shown, featuring a central benzimidazole core substituted with a 4-nitrophenyl group, a 4-methoxyphenyl group, and a 4-nitrophenyl group.

Integration values are provided for the peaks:

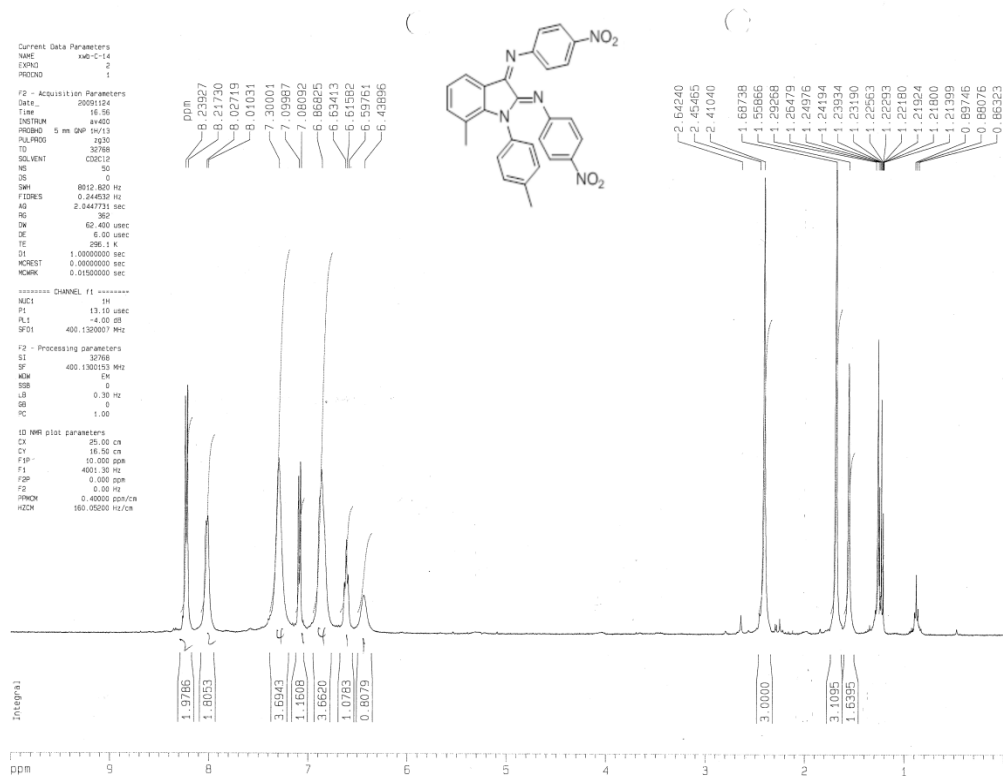
- 1.9592
- 1.8328
- 3.6930
- 1.9559
- 1.1484
- 1.8530
- 1.1561
- 0.6932
- 2.9538
- 3.0000

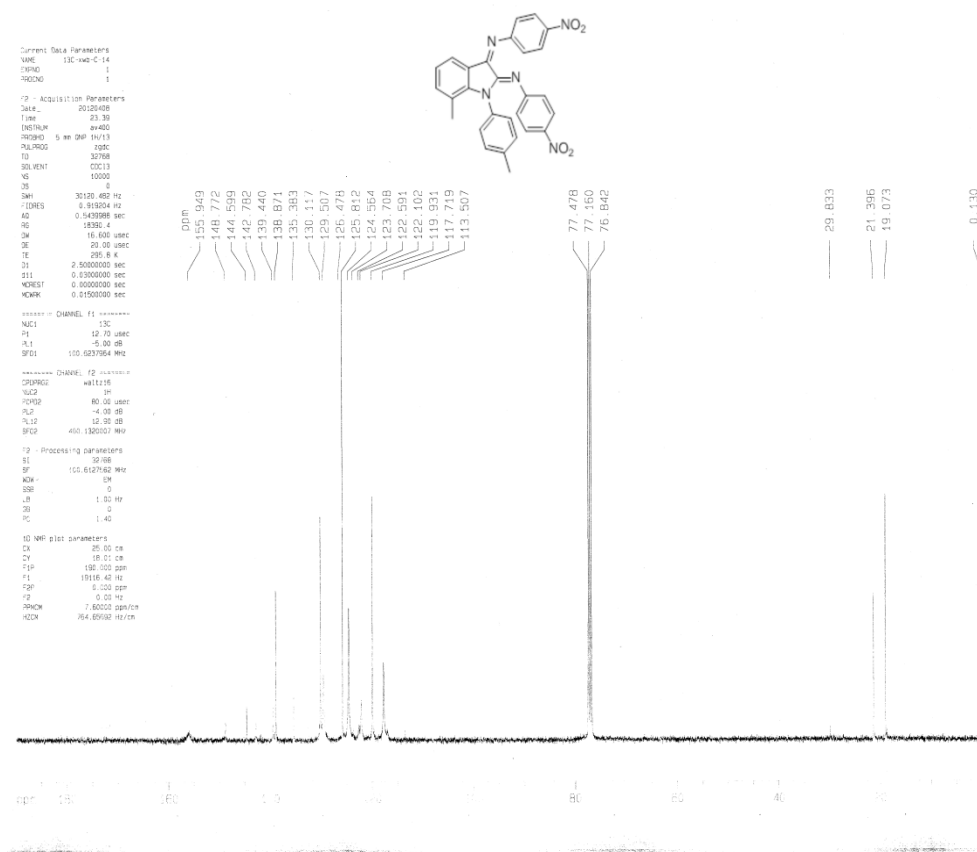
Peak chemical shifts (ppm) are listed on the right:

- 8.28013
- 8.25821
- 8.05765
- 7.92413
- 7.90320
- 7.24514
- 7.14657
- 7.00538
- 6.98437
- 6.88156
- 6.87526
- 6.85962
- 6.85334
- 6.78207
- 6.76210
- 6.61279
- 6.59090
- 6.22323
- 5.27384
- 3.78922
- 3.49853
- 2.37895
- 2.32262
- 1.43965
- 1.26785
- 0.92616
- 0.00036



7-Methyl-3-(4-nitrophenylimino)-1-p-tolylindolin-2-ylidene)-4-nitrobenzenamine(4l)





4-Bromo-3-(4-nitrophenylimino)-1-p-tolylindolin-2-ylidene)-4-nitrobenzenamine (4m)

Current Data Parameters
NAME 1000-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130424
Time 21:15
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
SOLVENT dms
DS 13
SW 18.800 MHz
F2FRES 6.246330 MHz
AQ 2.044732 sec
RG 314
CH 62.400 usec
JE 6.00 usec
TE 300.7 K
D1 0.0000000 sec
dWST 0.0000000 sec
dWPR 0.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 0.00 dB
SFO1 100.626050 MHz

F2 - Processing parameters
SI 32768
SF 400.1300500 MHz
WDW EM
SS 0
LB 0.30 Hz
GB 0
PC 1.00

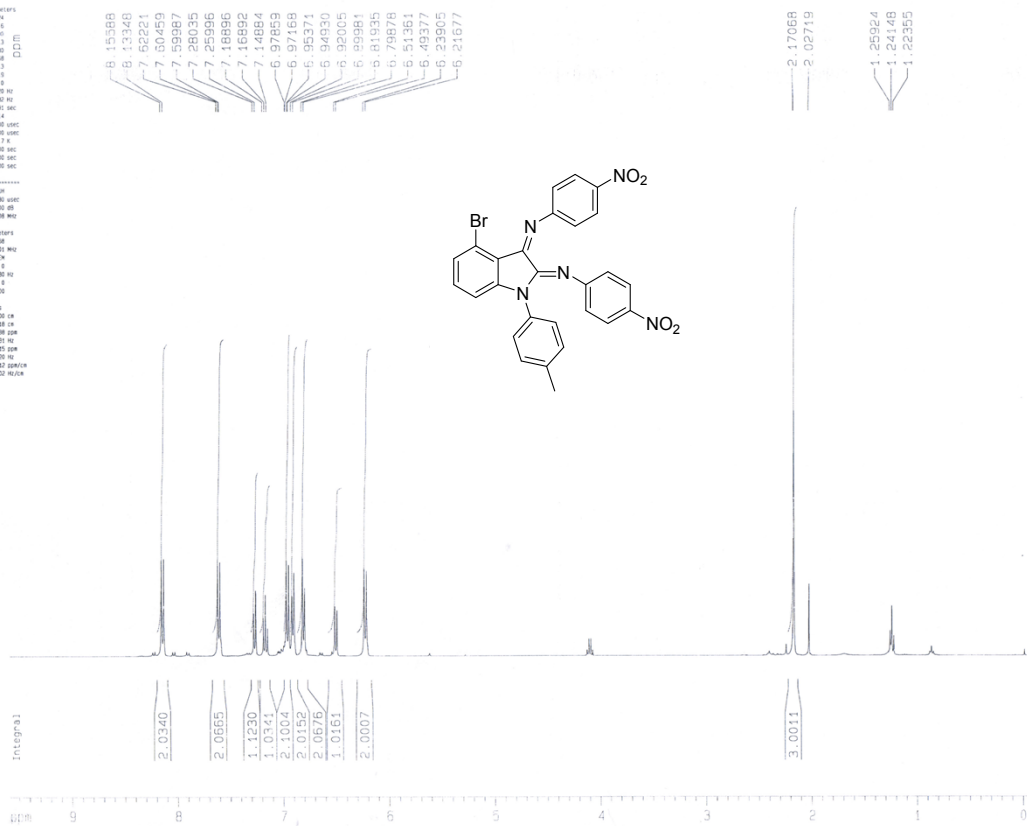
===== CHANNEL f2 =====
Date_ 20130424
Time 21:23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
SOLVENT dms
DS 13
SW 18.800 MHz
F2FRES 6.246330 MHz
AQ 2.044732 sec
RG 314
CH 62.400 usec
JE 6.00 usec
TE 300.7 K
D1 0.0000000 sec
dWST 0.0000000 sec
dWPR 0.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 0.00 dB
SFO1 100.626050 MHz

===== CHANNEL f2 =====
Date_ 20130424
Time 21:23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
SOLVENT dms
DS 13
SW 18.800 MHz
F2FRES 6.246330 MHz
AQ 2.044732 sec
RG 314
CH 62.400 usec
JE 6.00 usec
TE 300.7 K
D1 0.0000000 sec
dWST 0.0000000 sec
dWPR 0.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 0.00 dB
SFO1 100.626050 MHz

===== CHANNEL f2 =====
Date_ 20130424
Time 21:23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
SOLVENT dms
DS 13
SW 18.800 MHz
F2FRES 6.246330 MHz
AQ 2.044732 sec
RG 314
CH 62.400 usec
JE 6.00 usec
TE 300.7 K
D1 0.0000000 sec
dWST 0.0000000 sec
dWPR 0.0000000 sec



Current Data Parameters
NAME 1000-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130424
Time 21:23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
SOLVENT dms
DS 13
SW 18.800 MHz
F2FRES 6.246330 MHz
AQ 2.044732 sec
RG 314
CH 62.400 usec
JE 6.00 usec
TE 300.7 K
D1 0.0000000 sec
dWST 0.0000000 sec
dWPR 0.0000000 sec

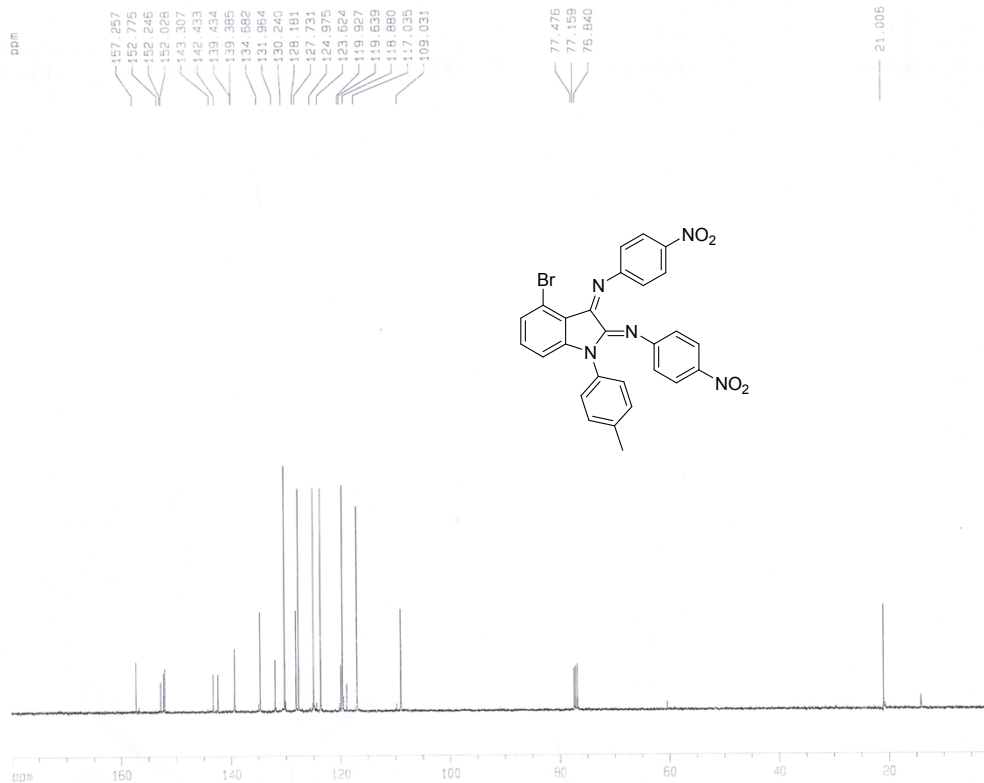
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 0.00 dB
SFO1 100.626050 MHz

F2 - Processing parameters
SI 32768
SF 400.1300500 MHz
WDW EM
SS 0
LB 0.30 Hz
GB 0
PC 1.00

===== CHANNEL f2 =====
Date_ 20130424
Time 21:23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
SOLVENT dms
DS 13
SW 18.800 MHz
F2FRES 6.246330 MHz
AQ 2.044732 sec
RG 314
CH 62.400 usec
JE 6.00 usec
TE 300.7 K
D1 0.0000000 sec
dWST 0.0000000 sec
dWPR 0.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 0.00 dB
SFO1 100.626050 MHz

===== CHANNEL f2 =====
Date_ 20130424
Time 21:23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
SOLVENT dms
DS 13
SW 18.800 MHz
F2FRES 6.246330 MHz
AQ 2.044732 sec
RG 314
CH 62.400 usec
JE 6.00 usec
TE 300.7 K
D1 0.0000000 sec
dWST 0.0000000 sec
dWPR 0.0000000 sec



Methyl 1-methyl-2,3-bis(4-nitrophenylimino) indoline-6-carboxylate(4n)

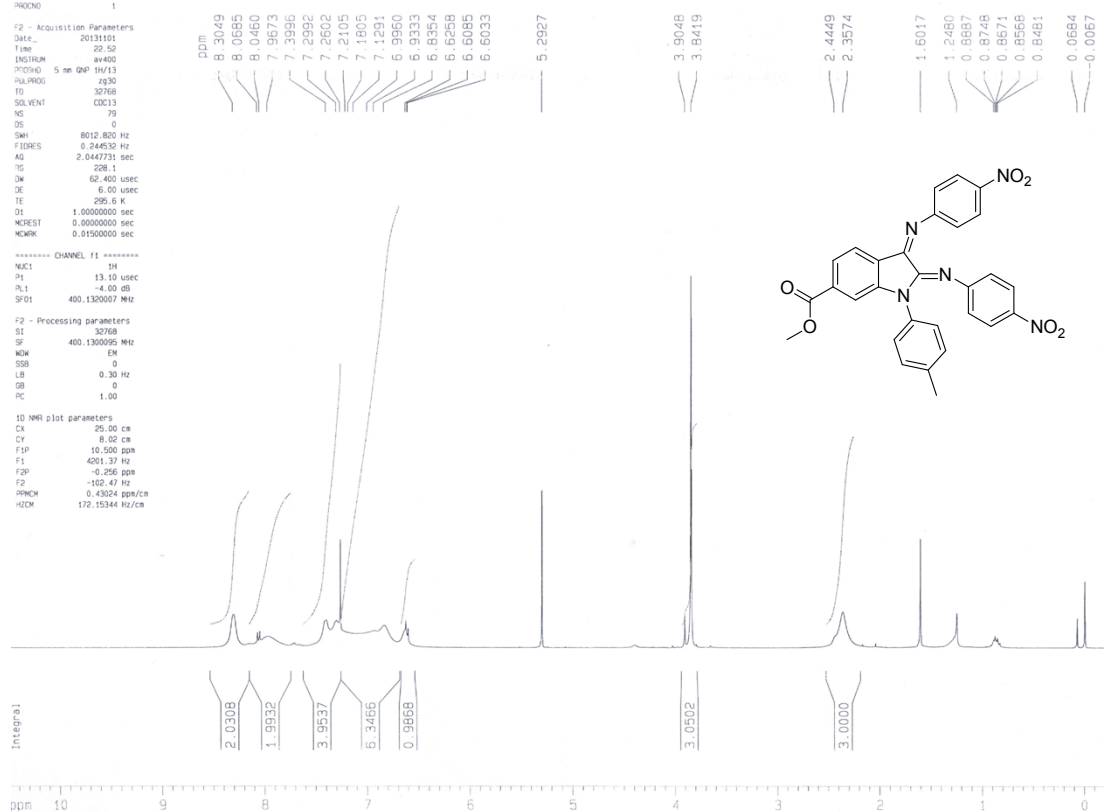
Current Data Parameters
NAME p196-2-3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131001
Time 22:52
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 79
DS 0
SWH 8012.850 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 228.1
DQ 62.400 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
dCREST 0.00000000 sec
dCMR 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 13.10 usec
PL1 -4.00 dB
SFO1 400.1300000 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 25.00 cm
CY 6.00 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.256 ppm
F2 -102.47 Hz
PRMCM 0.43024 ppm/cm
dCCK 172.15344 Hz/cm



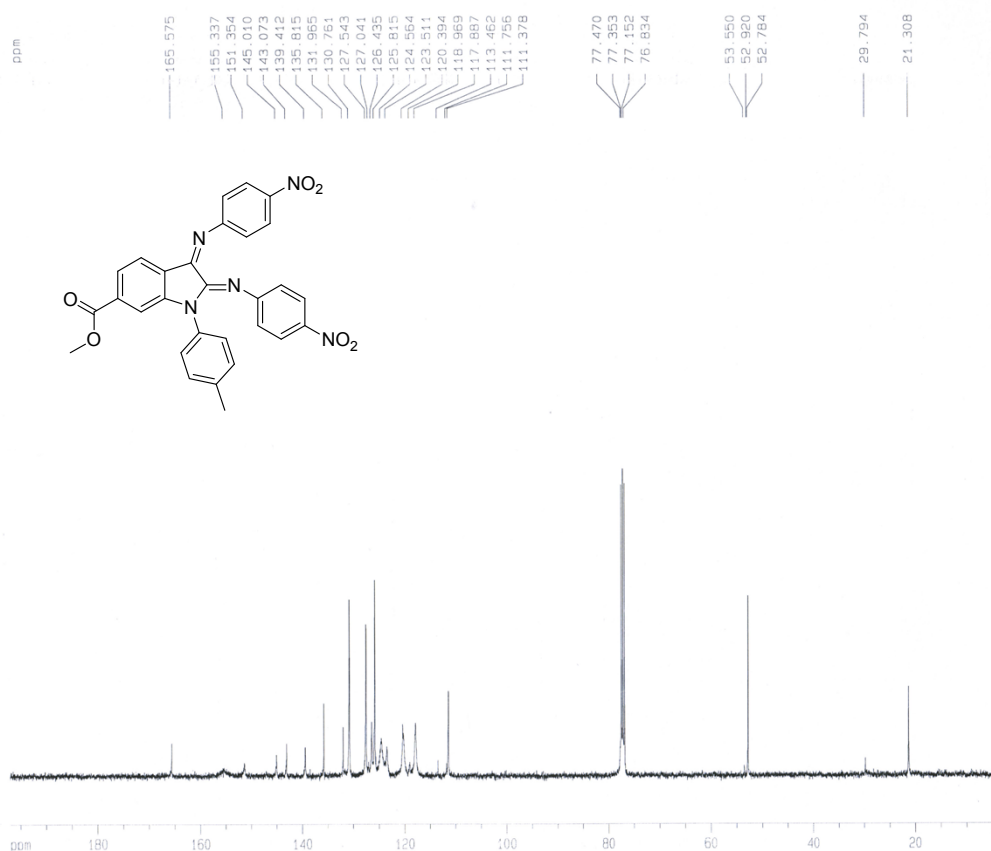
Current Data Parameters
NAME p196-2-3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131001
Time 22:52
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 79
DS 0
SWH 8012.850 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 228.1
DQ 62.400 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
dCREST 0.00000000 sec
dCMR 0.01500000 sec

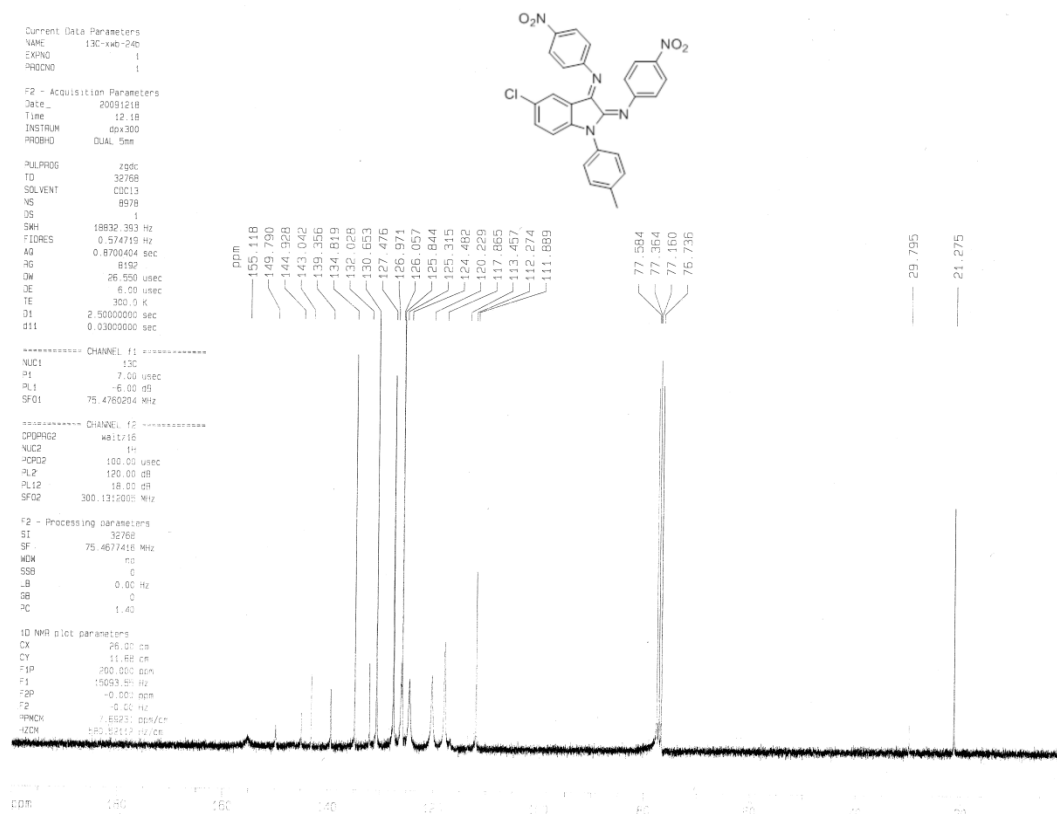
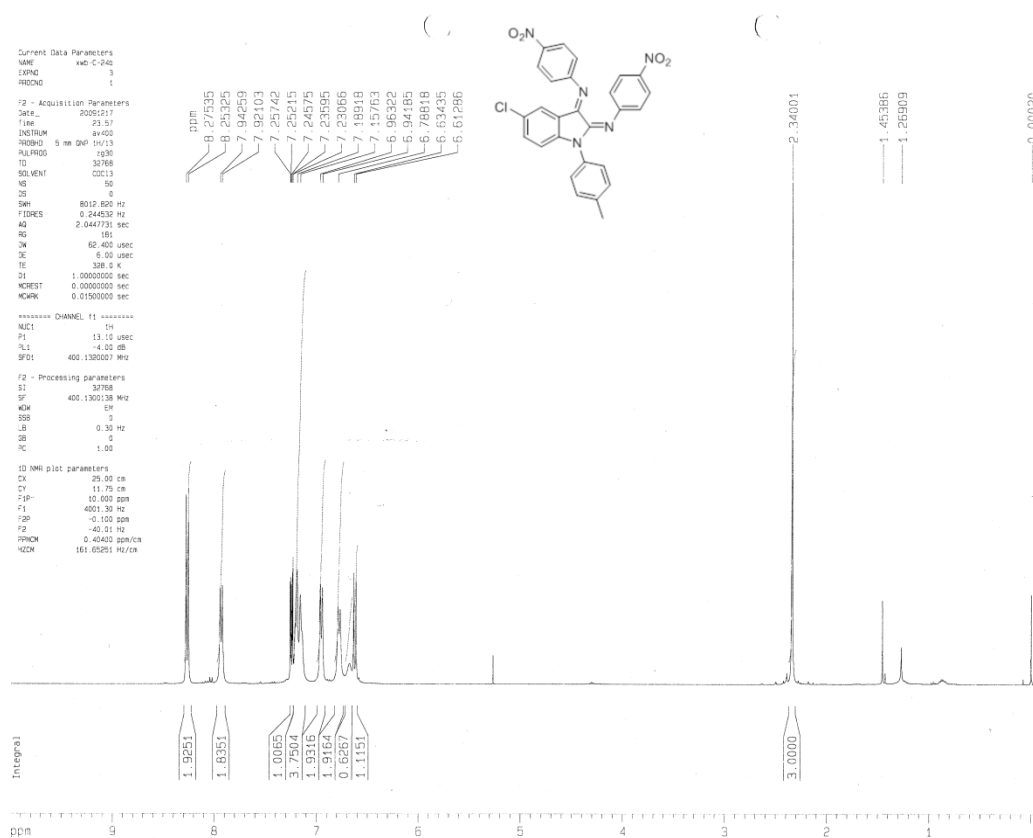
***** CHANNEL f1 *****
NUC1 13C
P1 13.10 usec
PL1 -4.00 dB
SFO1 400.1300000 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 25.00 cm
CY 6.00 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.256 ppm
F2 -102.47 Hz
PRMCM 0.43024 ppm/cm
dCCK 172.15344 Hz/cm

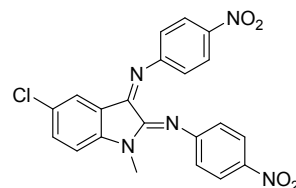
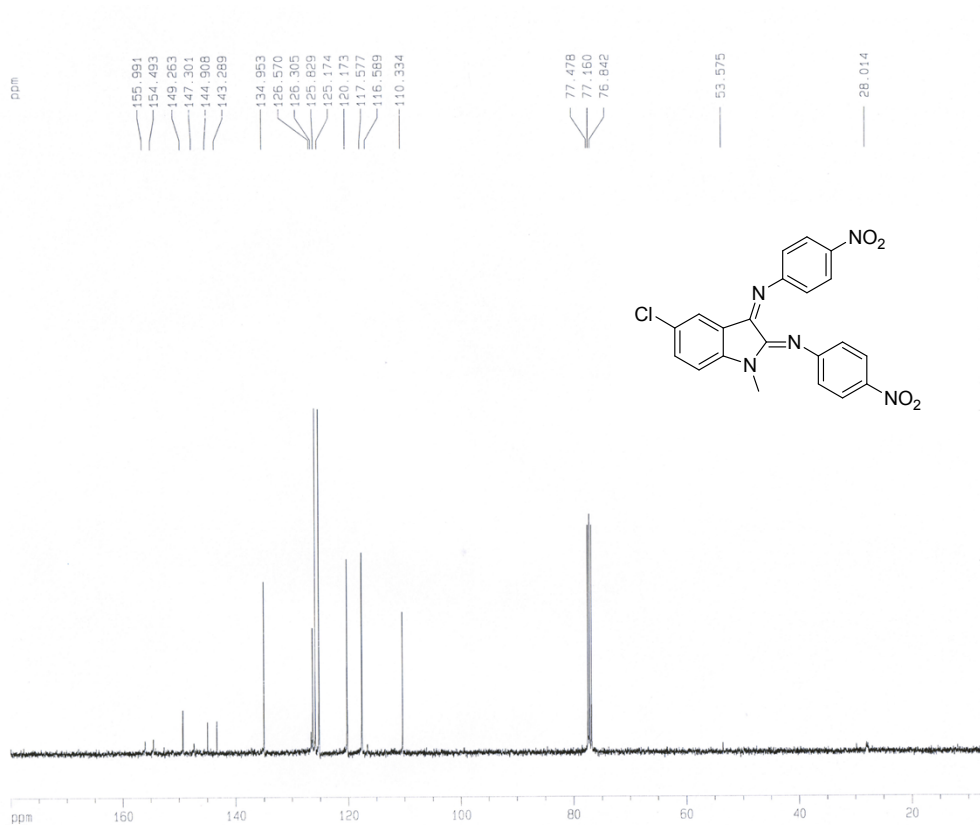
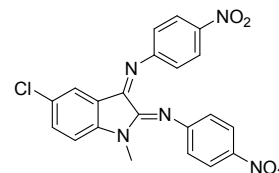
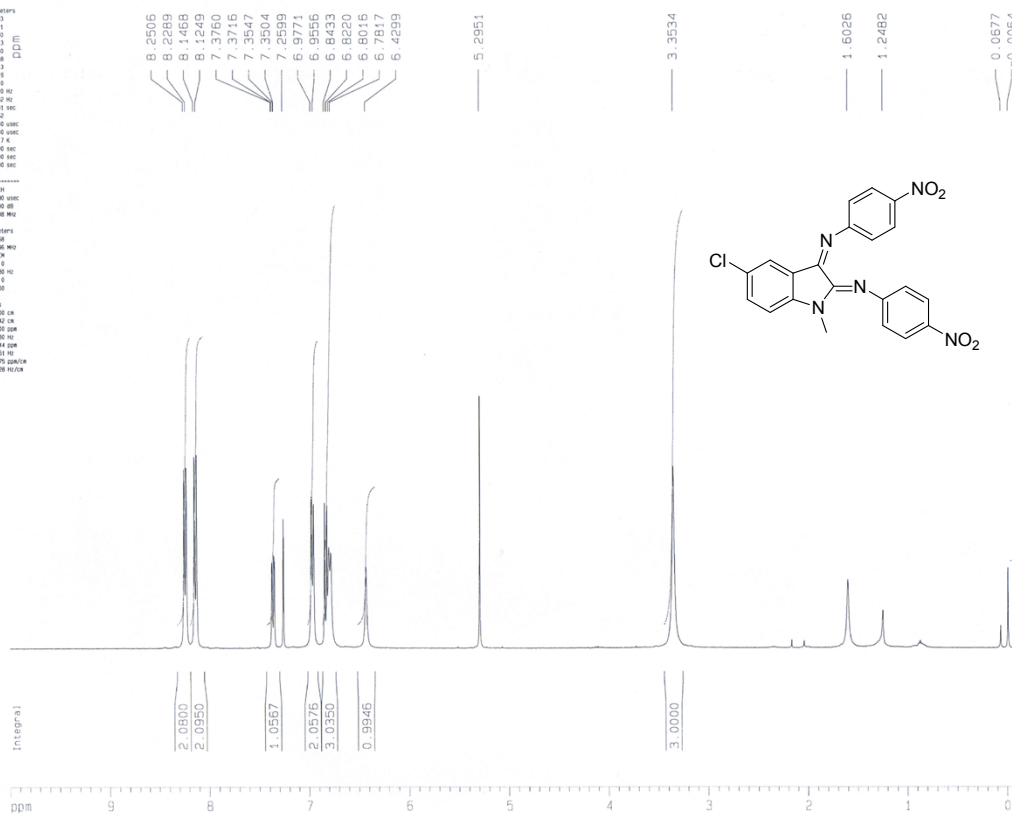


5-Chloro-3-(4-nitrophenylimino)-1-p-tolylindolin-2-ylidene)-4-nitrobenzenamine(4o)

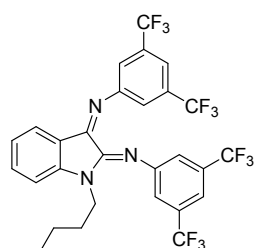
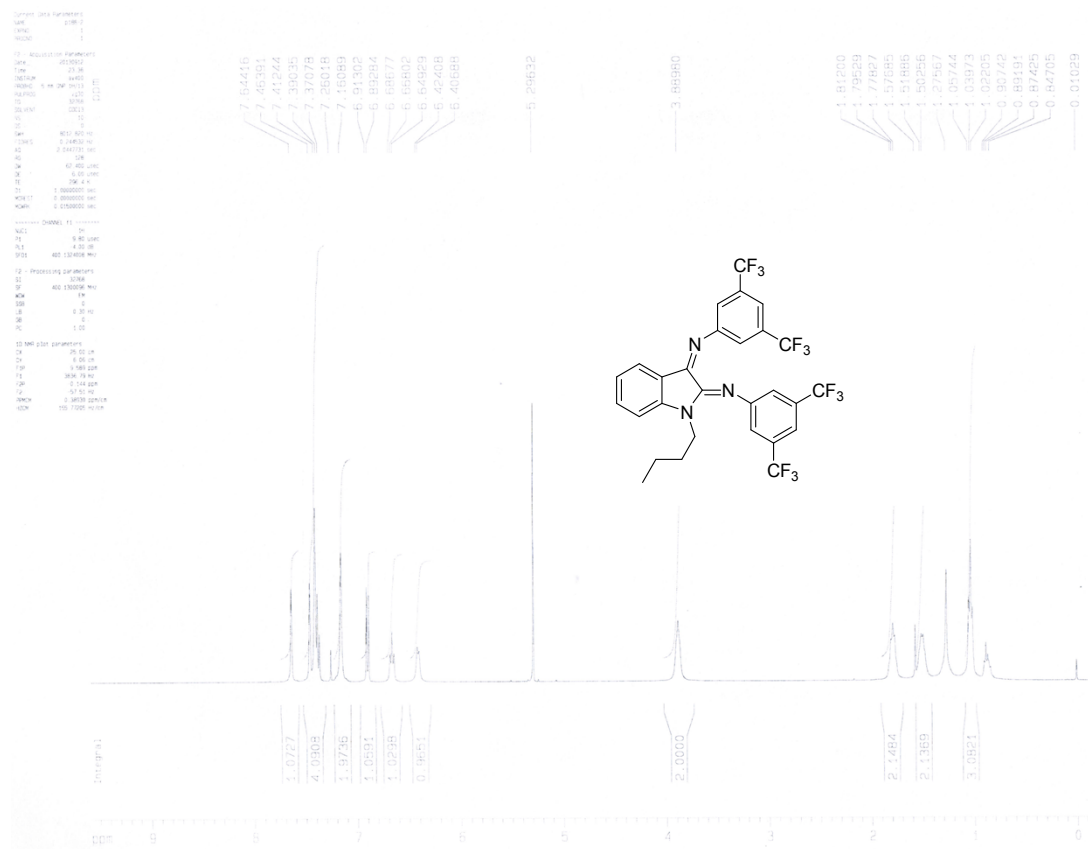


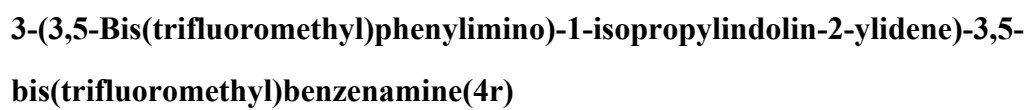
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Current Data Parameters
NAME          1386-1
EXPNO         1
PROCNO        1

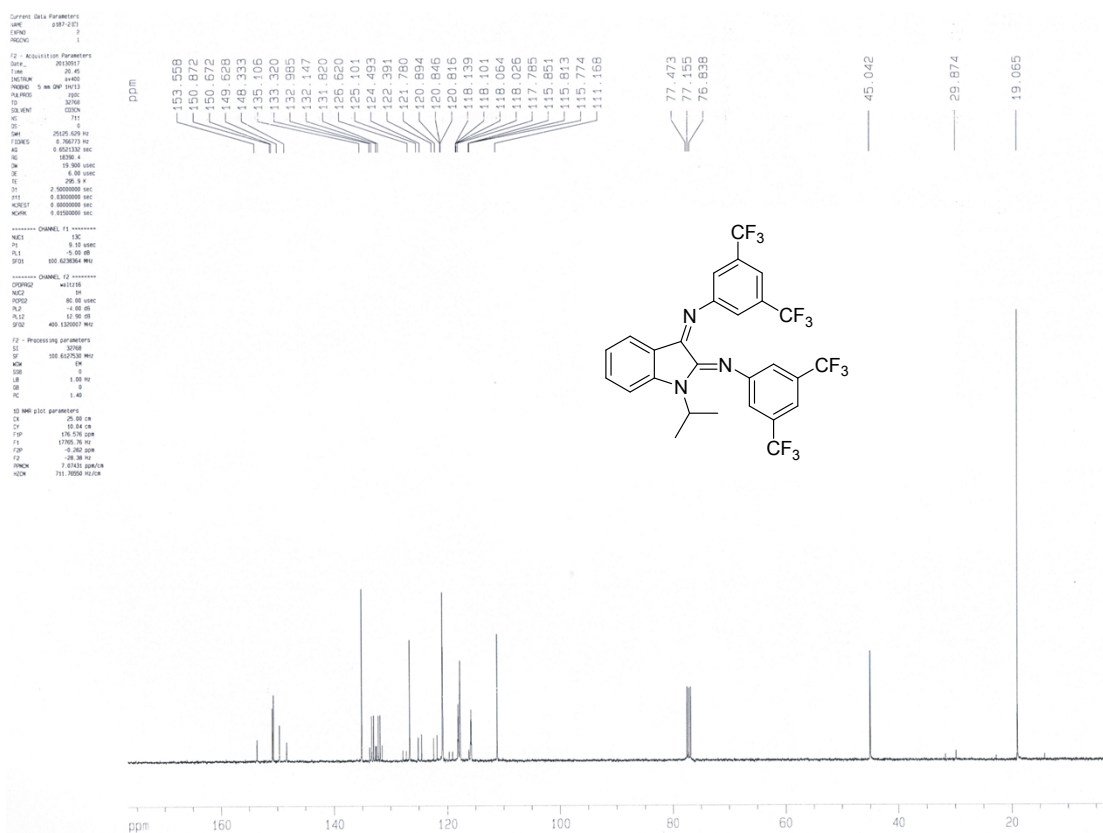
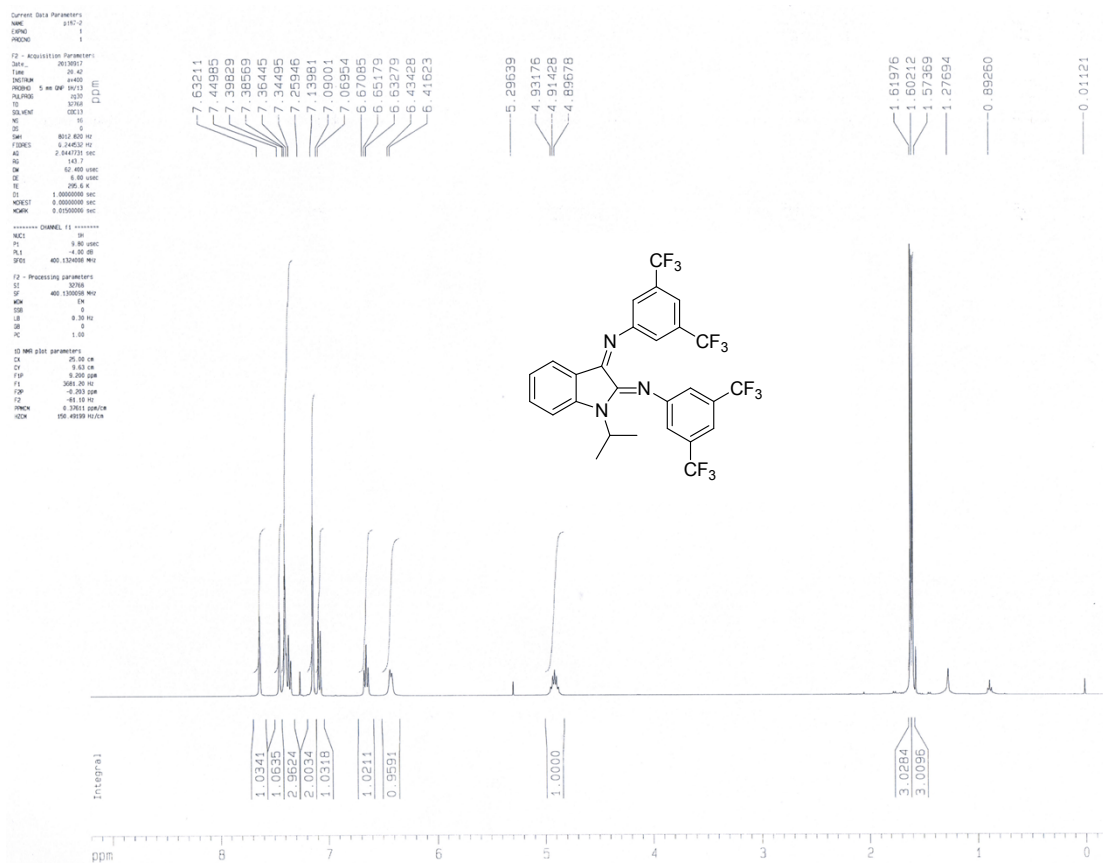
F2 - Acquisition Parameters
Date_         20030903
Time          20.21
INSTRUM       spect
PROBHD50      5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
AQ            0.10000000
RG            327.68
SD            0.00100000
SOLVENT       CDCl3
NS            512
DS            4
SWH            8532.840 Hz
FIDRES        0.20000000
AQRES         0.00100000
NUC1           13
NUC2           1H
PC            2.00000000
RG1            64
RG2            362
RG3            64
RG4            64
RG5            64
RG6            64
RG7            64
RG8            64
RG9            64
RG10           64
RG11           64
RG12           64
RG13           64
RG14           64
RG15           64
RG16           64
RG17           64
RG18           64
RG19           64
RG20           64
RG21           64
RG22           64
RG23           64
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RG25           64
RG26           64
RG27           64
RG28           64
RG29           64
RG30           64
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RG32           64
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RG34           64
RG35           64
RG36           64
RG37           64
RG38           64
RG39           64
RG40           64
RG41           64
RG42           64
RG43           64
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RG295          64
RG296          64
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3-(3,5-Bis(trifluoromethyl)phenylimino)-1-butylindolin-2-ylidene)-3,5-bis(trifluoromethyl)benzenamine(4q)

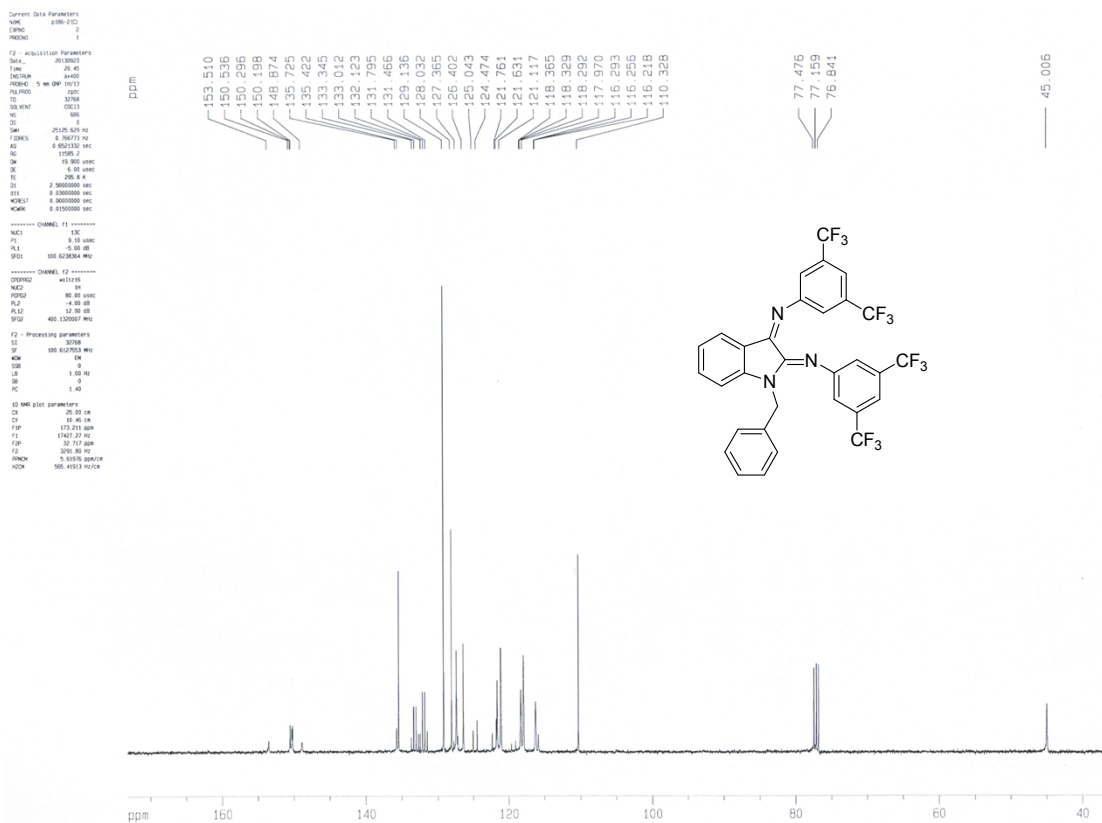
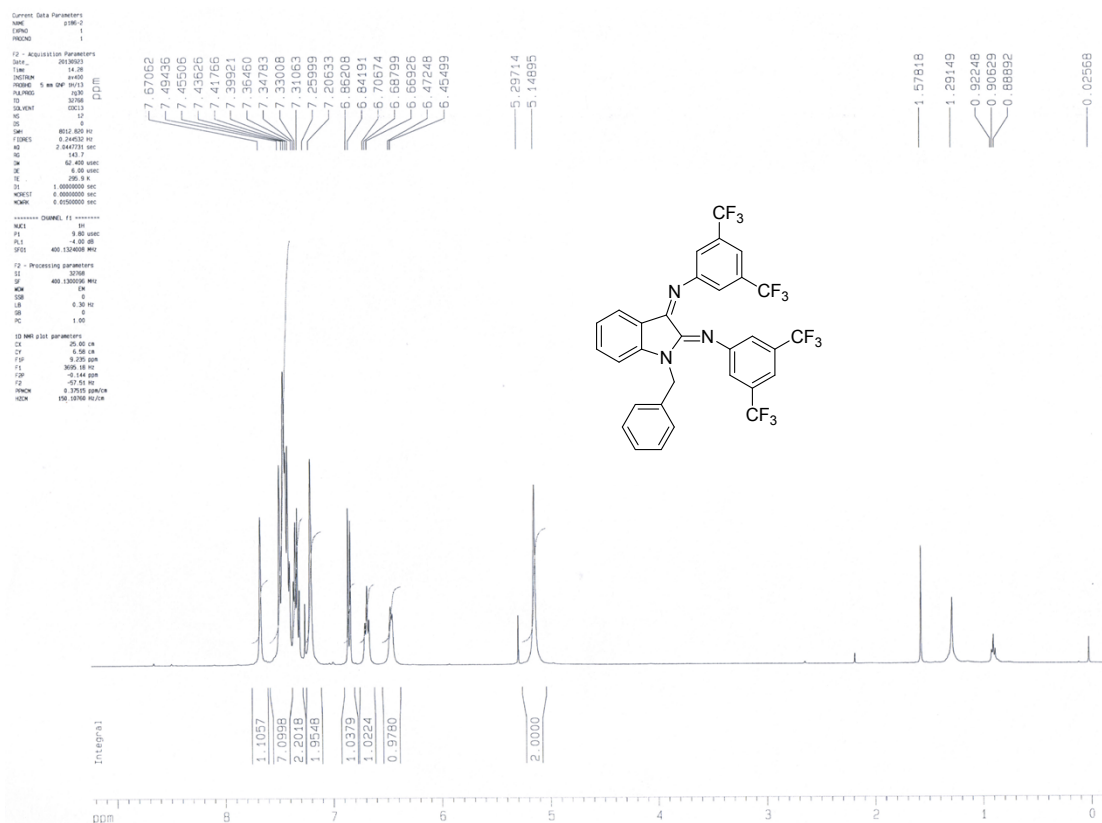






3-(3,5-Bis(trifluoromethyl)phenylimino)-1-benzylindolin-2-ylidene-3,5-

bis(trifluoromethyl)benzenamine(4s)



3-(3,5-Bis(trifluoromethyl)phenylimino)-6-methoxy-1-methylindolin-2-ylidene)- 3,5-bis(trifluoromethyl)benzenamine(4t)

