Traceless Directing Strategy: Efficient Synthesis of N-alkyl Indoles via Redox-neutral C-H Activation

Chengming Wang, Yong Huang*

Laboratory of Chemical Genomics, School of Chemical Biology and Biotechnology, Peking University, Shenzhen Graduate School, Shenzhen, China 518055
Email: huangyong@pkusz.edu.cn

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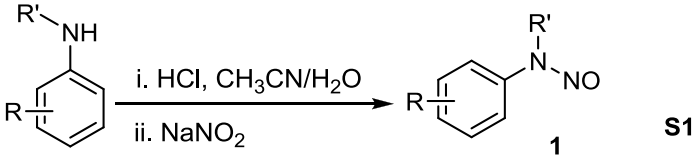
General Methods and Materials:

Unless specified, all reactions were carried out under air using commercial available solvents as received. Dichloro(η^5-pentamethylcyclopentadienyl)rhodium(III) dimer (99%) was purchased from Sinocompound Technology Co., Ltd. Alkyne substrates were purchased from Alfa Aesar and used directly. All other reagents were purchased and used without further purification unless specified otherwise. Solvents for chromatography were technical grade and distilled prior to use. Flash chromatography was performed using 200-300 mesh silica gel with the indicated solvent system according to standard techniques. Analytical thin-layer chromatography (TLC) was performed on pre-coated, glass-backed silica gel plates. Visualization of the developed chromatogram was performed by UV absorbance (254 nm). ^{1}H NMR and ^{13}C NMR data were recorded on Bruker 400 M nuclear resonance spectrometers unless otherwise specified, respectively. Chemical shifts (δ) in ppm are reported as quoted relative to the residual signals of chloroform (^{1}H 7.26 ppm or ^{13}C 77.16 ppm). Multiplicities are described as: s (singlet), bs (broad singlet), d (doublet), t (triplet), q (quartet), m (multiplet); and coupling constants (*J*) are reported in Hertz (Hz). ^{13}C NMR spectra were recorded with total proton decoupling. HRMS (ESI) analysis was performed by The Analytical Instrumentation Center at Peking University, Shenzhen Graduate School and (HRMS) data were reported with ion mass/charge (m/z) ratios as values in atomic mass units.

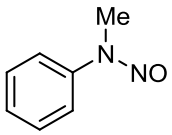
Synthesis and Characterization of Starting Materials

General procedure for preparation of N-nitroso aniline substrates 1 (eq S1)[1]

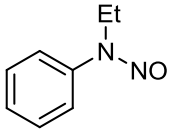
The aniline (0.05 mol, 1.0 equiv) was dissolved in a 1:2 mixture of acetonitrile and water (30 mL) and cooled to 0 °C (ice bath). Concentrated aqueous HCl (7.3 mL, 0.24 mol) was added dropwise. The mixture was stirred vigorously for half an hour, while maintained at 0 °C. To this mixture was added an aqueous solution (13 mL) of $NaNO_2$ (3.5 g, 0.05 mol) over the course of 10 min. The reaction was allowed to proceed for 1 h. The mixture was then extracted with EtOAc. The combined organic layer was washed with brine, dried over Na_2SO_4, concentrated under reduced pressure, and purified by flash silica gel column chromatography (petroleum ether / ethyl acetate = 20:1) to give the corresponding N-nitroso aniline substrates 1.



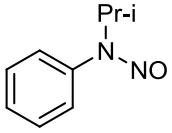
S1



N-methyl-N-phenylnitrous amide (**1a**)[2]: 96% yield, yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.47 (t, *J* = 8.4 Hz, 2H), 7.36 (td, *J* = 8.0, 0.8 Hz, 1H), 3.45 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.4, 129.6, 127.4, 119.3, 31.6. HRMS (ESI): found: 137.0709, calcd. for $C_7H_9N_2O$ ($[M+H]^+$): 137.0715.

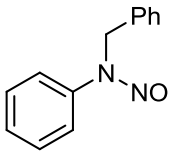


N-ethyl-N-phenylnitrous amide (**1b**)[1]: 99% yield, yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ; 7.54-7.52 (m, 2H), 7.48-7.44 (m, 2H), 7.37-7.33 (m, 1H), 4.10-4.04 (m, 2H), 1.18-1.124 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.5, 129.6, 127.4, 119.6, 39.3, 11.8. HRMS (ESI): found: 151.0865, calcd. for $C_8H_{11}N_2O$ ($[M+H]^+$): 151.0871.

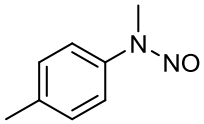


N-isopropyl-N-phenylnitrous amide (**1c**)[1]: 93% yield, as an inseparable rotameric mixture (1.8:1), yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) for the major rotamer: δ 7.49-7.40 (m, 3H), 7.39-7.33 (m, 2H), 6.97-6.94 (m, 1H), 5.27-5.17 (m, 1H), 1.45 (dd, *J* = 6.8, 1.6 Hz, 3H), 1.18 (dd, *J* = 6.8, 1.6 Hz, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) as a mixture: δ 139.5, 136.6, 129.4, 129.3, 129.2, 128.8, 127.8, 126.0, 56.2, 46.4, 22.1, 19.8. HRMS (ESI): found: 165.1026, calcd. for

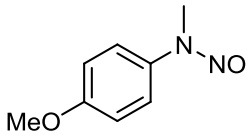
$C_9H_{13}N_2O$ ([M+H]$^+$): 165.1028.



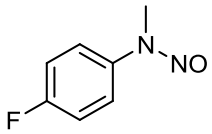
N-benzyl-N-phenylnitrous amide (**1e**)[3]: 66% yield, pale yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.54 (dd, J = 7.6, 0.8 Hz, 2H), 7.44-7.40 (m, 2H), 7.35-7.31 (m, 1H), 7.29-7.22 (m, 3H), 7.09 (d, J = 7.2 Hz, 2H), 5.25 (s, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 141.8, 134.4, 129.5, 128.9, 127.7, 127.4, 127.1, 119.6, 112.9, 47.4. HRMS (ESI): found: 213.1020, calcd. for $C_{13}H_{13}N_2O$ ([M+H]$^+$): 213.1028.



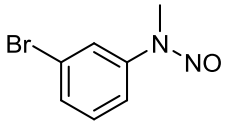
N-methyl-N-p-tolylnitrous amide (**1f**)[1]: 96% yield, yellowish brown solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.41 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.0, 2H), 3.44 (s, 3H), 2.40 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.1, 137.4, 130.1, 119.4, 31.9, 21.1. HRMS (ESI): found: 151.0867, calcd. for $C_8H_{11}N_2O$ ([M+H]$^+$): 151.0871.



N-(4-methoxyphenyl)-N-methylnitrous amide (**1g**)[1]: 83% yield, yellowish solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.44-7.40(m, 2H), 6.99-6.96 (m, 2H), 3.84-3.83 (m, 3H), 3.43-3.42 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.0, 135.8, 121.2, 114.7, 55.7, 32.4. HRMS (ESI): found: 167.0814, calcd. for $C_8H_{11}N_2O_2$ ([M+H]$^+$): 167.0821.

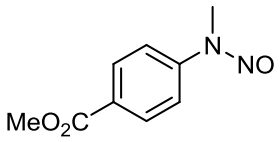


N-(4-fluorophenyl)-N-methylnitrous amide (**1h**)[1]: 89% yield, brown yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.50-7.46 (m, 2H), 7.17-7.12 (m, 2H), 3.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.7(J_{F1}=246.0), 138.6 (J_{F4}=3.0), 121.2 (J_{F3}=7.0), 116.4 (J_{F2}=23.0), 31.9. HRMS (ESI): found: 155.0614, calcd. for $C_7H_8FN_2O$ ([M+H]$^+$): 155.0621.

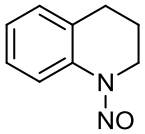


N-(3-bromophenyl)-N-methylnitrous amide (**1i**)[1]: 93% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.73 (d, *J* = 2.0 Hz, 1H), 7.50-7.47 (m, 2H), 7.37-7.32 (m, 1H), 3.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.5, 130.9, 130.2, 123.3, 122.0, 117.5, 31.1. HRMS (ESI): found:

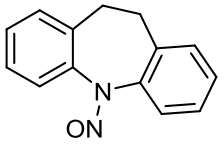
214.9817, calcd. for $C_7H_8BrN_2O$ ([M+H]$^+$): 214.9820.



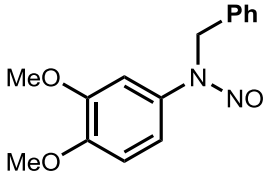
methyl 4-(methyl(nitroso)amino)benzoate (**1j**)[4]: 72% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.6 Hz, 2H), 3.93 (s, 3H), 3.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.3, 145.7, 131.1, 128.6, 117.9, 52.4, 30.6. HRMS (ESI): found: 195.0763, calcd. for $C_9H_{11}N_2O_3$ ([M+H]$^+$): 195.0770.



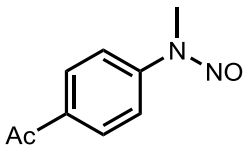
1-nitroso-1,2,3,4-tetrahydroquinoline (**1k**)[5]: 94% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.01 (d, *J* = 8.0 Hz, 1H), 7.27-7.22 (m, 1H), 7.18-7.17 (m, 2H), 3.85 (t, *J* = 6.4 Hz, 2H), 2.77 (t, *J* = 6.0 Hz, 2H), 1.99-1.95 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.4, 129.1, 127.6, 126.9, 126.2, 116.2, 42.4, 27.1, 20.7. HRMS (ESI): found: 163.0865, calcd. for $C_9H_{11}N_2O$ ([M+H]$^+$): 163.0871.



5-nitroso-10,11-dihydro-5H-dibenzo[b,f]azepine (**1l**)[6]: 92% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.61 (t, *J* = 4.4 Hz, 1H), 7.35-7.22 (m, 6H), 7.06 (d, *J* = 6.4 Hz, 1H), 3.3-3.14 (m, 2H), 2.97-2.77 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.8, 138.3, 136.5, 133.2, 131.2, 129.8, 129.5, 128.8, 127.3, 127.2, 127.0, 125.7,32.4, 30.1. HRMS (ESI): found: 225.1025, calcd. for $C_{14}H_{13}N_2O$ ([M+H]$^+$): 225.1028.

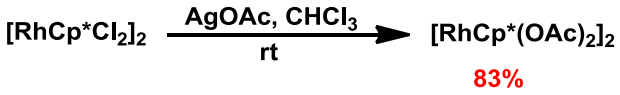


N-benzyl-N-(3,4-dimethoxyphenyl)nitrous amide (**1m**): 72% yield, yellowish brown solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30-7.23 (m, 3H), 7.18 (d, *J* = 2.4 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.91-6.84 (m, 2H), 5.22 (s, 2H), 3.88 (s, 3H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 149.7, 148.7, 135.4, 134.6, 128.9, 127.7, 127.4, 111.9, 111.2, 104.5, 56.2, 56.2, 47.8. HRMS (ESI): found: 273.1242, calcd. for $C_{15}H_{17}N_2O_3$ ([M+H]$^+$): 273.1239.



N-(4-acetylphenyl)-N-methylnitrous amide (**1n**): 84% yield, pale yellow solid. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.05 (dd, *J* = 9.0, 1.5 Hz, 2H), 7.65 (dd, *J* = 8.7, 1.5 Hz, 2H), 3.94 (s, 3H), 3.45 (s, 3H), 2.62 (s, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 197.0, 145.8, 135.4, 130.0, 118.0, 30.6, 26.7. HRMS (ESI): found: 179.0827, calcd. for $C_9H_{11}N_2O_2$ ($[M+H]^+$): 179.0821.

Synthesis of catalyst

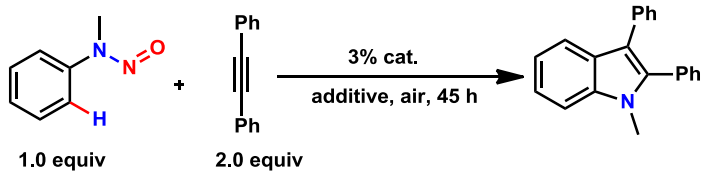


$[Cp^*RhCl_2]_2$ (750 mg, 1.0 equiv) and AgOAc (810 mg, 4.0 equiv) were weighed into an oven dried Schlenk tube. The reaction vessel was capped and vacuum/backfilled with argon three times. To this vessel, 20 mL $CHCl_3$ was added. The reaction was stirred at rt for two hours. The reaction mixture was filtered through a plug of celite and wished with n-hexane. The filtrate was concentrated by rotary evaporation and the residue yellow solid was collected as the desired catalyst (in case there is residual solvents, drying under high vacuum pump overnight maybe necessary).

Condition screening:

Initial screening quickly identified $[RhCp^*(CH_3CN)_3][SbF_6]_2$ was a good catalyst and the reaction required additives in order to achieve decent conversions. Table S1 summarized comprehensive condition tuning for substrate **1a** and 1,2-diphenylacetylene.

Table S1. Condition Screening for Rh(III)-Catalyzed Nitroso-Directed C-H Activation Indole Synthesis [a]



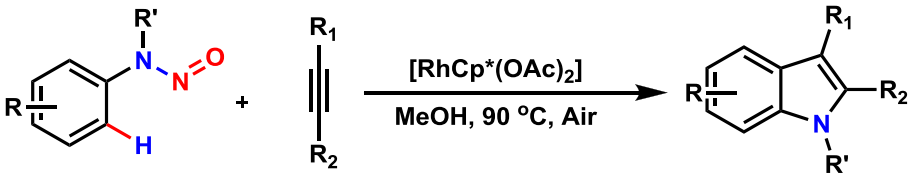
entry	temperature (^oC)	solvent (3 mL)	catalyst (3% equiv)	additive (2 equiv)	GC-MS yield (%)
1	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	NaOAc	49
2	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc	38
3	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	CsOAc	38
4	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	LiOAc	48
5	100	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc	55
6	80	MeOH	$[Ru\ (p\text{-}cymene)Cl_2]_2$	NaOAc	0
7	80	MeOH	$[Ru\ (p\text{-}cymene)Cl_2]_2$	$Cu(OAc)_2.H_2O$	<5
8	130	toluene	$Rh(PPh_3)_3Cl$	-	0
9[b,e]	60	MeOH	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2.H_2O$ $AgSbF_6$ (30%)	44
10	80	MeOH	$[RhCp^*Cl_2]_2$	NaOAc	57
11	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	Cs_2CO_3	0
12	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	K_2CO_3	0
13	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	$NaHCO_3$	0
14	80	DCE	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	$Cu(OAc)_2.H_2O$	71
15	80	DMF	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc	0
16	80	DCE	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc	15
17	80	MeCN	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc	11
18	80	toluene	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc	3
19	80	t-AmylOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc	0
20	80	THF	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc	8
21	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc (50%)	31
22	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc (1.0)	48
23[c]	90	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	KOAc	40
24[c]	90	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	CsOAc	34
25	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	$Cu(OAc)_2.H_2O$	79
26[c]	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	$Cu(OAc)_2.H_2O$ (20%)	82
27	80	MeOH	$[RhCp^*(CH_3CN)_3][SbF_6]_2$	AgOAc	67
28[d]	90	MeOH	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2.H_2O$ (10%)	79

				$AgSbF_6$ (20%)	
29[d]	90	MeOH	$[RhCp^*Cl_2]_2$	AgOAc (30%)	85
30[d]	90	DCE	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2.H_2O$ (10%)	72
31[d]	90	MeOH	$[RhCp^*Cl_2]_2$	$Cu(OPiv)_2$ (10%)	53
32[d]	90	MeOH	$[RhCp^*Cl_2]_2$	AgOAc (30%)	86
				NaOAc (1.0)	
33[d,e]	90	MeOH	$[RhCp^*Cl_2]_2$	AgOAc (30%)	82
34[d]	90	MeOH	$[RhCp^*Cl_2]_2$	$CuCl_2$ (10%)	0
35[d,e]	60	MeOH	$[RhCp^*Cl_2]_2$	AgOAc (30%)	94
36[e,f]	60	MeOH	$[RhCp^*Cl_2]_2$	AgOAc (30%)	90
37[d,e]	60	MeOH	$[RhCp^*Cl_2]_2$	NaOAc	41
38[g,e]	60	MeOH	$[RhCp^*Cl_2]_2$	AgOAc (30%)	87
39[d,e]	60	MeOH	$[RhCp^*Cl_2]_2$ (1%)	AgOAc (10%)	60
40[d,e]	60	MeOH	$[RhCp^*Cl_2]_2$ (2%)	AgOAc (20%)	50
41[e,f]	60	MeOH	$[RhCp^*(OAc)_2]$	-	53
42[e,f]	60	MeOH	$[RhCp^*(OAc)_2]$	AgOAc (10%)	73
***43*[e,f]**	***90***	***MeOH***	***[RhCp*(OAc)$_2$] (8%)***	**-**	***90***
44	80	MeOH	$[RhCp^*Cl_2]_2$	-	<5
45[e,f]	80	MeOH	$[RhCp^*(OAc)_2]$	AgOAc (5%)	88
46[e,f]	90	MeOH	$[RhCp^*(OAc)_2]$	-	66
47[e,f]	75	MeOH	$[RhCp^*(OAc)_2]$	-	76

[a] 0.3 mmol scale. [b] 23 h. [c] 4 days. [d] Under O_2. [e] Isolated yield. [f] Under Ar. [g] In a glove box

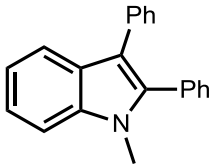
Note: for entry 26-47, only 1.3 equiv aryne and 5 mol % cat. was used, reaction was stopped when most starting material disappeared. For entry 46, 1.1 equiv aryne was used.

General Procedure for the Nitroso Directed Indole Synthesis via Rh(III)-Catalyzed C-H Activation

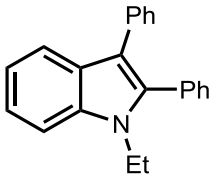


[Cp*Rh(OAc)$_2$] (0.024 mmol, 8.0 mg, 8 mol %) and N-nitroso aniline substrate **1** (0.3 mmol, 1.0 equiv) were weighed into an oven dried sealed tube. A solution of alkyne (0.45 mmol, 1.3 equiv) in methanol (3.0 mL) was added using a syringe. The vessel was sealed with a TFE cap and the reaction was stirred at 90 °C. The progress of the annulation was monitored by TLC. Upon complete consumption of **1**, the reaction was cooled to room temperature. Volatile solvent and reagents were removed by rotary evaporation and the residue was purified by silica gel flash chromatography using petroleum ether/EtOAc (80:1 to 30:1) to afford product **3**.

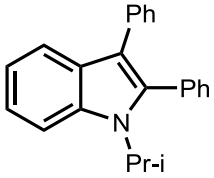
Characterization of Indole Products:



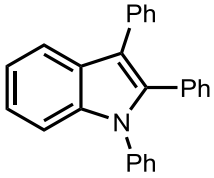
1-methyl-2,3-diphenyl-1H-indole (**3a**)[7]: 90% yield, white solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.85 (d, *J* = 8.0 Hz, 1H), 7.47-7.31 (m, 11H), 7.29-7.20 (m, 2H), 3.71 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.9, 137.5, 135.4, 132.0, 131.3, 130.0, 128.5, 128.3, 128.2, 127.1, 125.6, 122.3, 120.3, 119.7, 115.2, 109.7, 31.1. HRMS (ESI): found: 284.1439, calcd. for $C_{21}H_{18}N$ ($[M+H]^+$): 284.1439.



1-ethyl-2,3-diphenyl-1H-indole (**3b**)[8]: 90% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.84 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H),7.43-7.28 (m, 10H), 7.24-7.16 (m, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 1.32 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.4, 136.2, 135.4, 132.4, 131.2, 130.0, 128.6, 128.2, 127.4, 125.5, 122.2, 120.2, 119.9, 115.5, 109.9, 38.8, 15.5. HRMS (ESI): found: 298.1589, calcd. for $C_{22}H_{20}N$ ($[M+H]^+$): 298.1596.

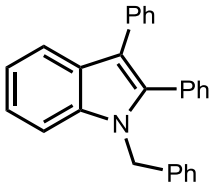


1-isopropyl-2,3-diphenyl-1H-indole (**3c**)[9]: 54% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.81 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.4 Hz, 1H),7.41-7.36 (m, 3H), 7.35-7.32 (m, 2H), 7.29-7.24 (m, 5H), 7.20-7.15 (m, 2H), 4.62-4.55 (m, 1H), 1.65 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.7, 135.4, 134.7, 132.9, 131.3, 130.1, 128.5, 128.3, 128.2, 128.1, 125.5, 121.6, 120.1, 119.8, 115.3, 112.4, 48.0, 21.7. HRMS (ESI): found: 312.1746, calcd. for $C_{23}H_{22}N$ ($[M+H]^+$): 312.1752.

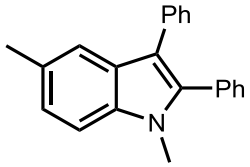


1,2,3-triphenyl-1H-indole (**3d**)[10]: 60% yield, white yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.81-7.79 (m, 1H), 7.38-7.28 (m, 8H), 7.23-7.19 (m, 5H), 7.16-7.07 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 138.3, 138.0, 137.2, 135.1, 131.7, 131.3, 130.4, 129.2, 128.4, 128.4, 128.0, 127.7,

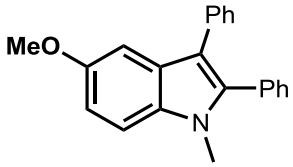
127.5, 127.3, 126.1, 122.9, 121.0, 119.7, 116.9, 110.8. HRMS (ESI): found: 346.1589, calcd. for $C_{26}H_{20}N$ ([M+H]$^+$): 346.1596.



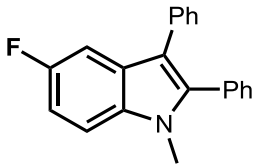
1-benzyl-2,3-diphenyl-1H-indole (**3e**)[8]: 73% yield, light yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86 (dd, *J* = 6.4, 1.6 Hz, 1H), 7.38-7.19 (m, 16H), 7.04 (d, *J* = 6.8 Hz, 2H), 5.32 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 138.2, 138.0, 137.1, 135.2, 131.9, 131.2, 130.0, 128.8, 128.5, 128.3, 127.5, 127.3, 126.3, 125.7, 122.5, 120.6, 119.9, 115.8, 110.7, 47.7. HRMS (ESI): found: 360.1755, calcd. for $C_{27}H_{22}N$ ([M+H]$^+$): 360.1752.



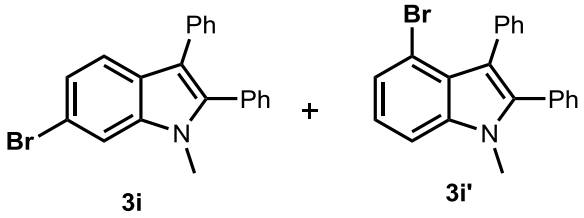
1,5-dimethyl-2,3-diphenyl-1H-indole (**3f**)[11]: 95% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.59 (s, 1H), 7.41-7.22 (m, 10H), 7.20-7.11 (m, 2H), 3.67 (s, 3H), 2.49 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 137.9, 135.9, 135.5, 132.2, 131.3, 130.1, 129.6, 128.5, 128.3, 128.1, 127.3, 125.5, 123.9, 119.3, 114.8, 109.4, 31.1, 21.7. HRMS (ESI): found: 298.1594, calcd. for $C_{22}H_{20}N$ ([M+H]$^+$): 298.1596.



5-methoxy-1-methyl-2,3-diphenyl-1H-indole (**3g**): 77% yield, white solid. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.38-7.31 (m, 3H), 7.30-7.27 (m, 7H), 7.25-7.24 (m, 1H), 7.18-7.15 (m, 1H), 6.96 (dd, *J* = 8.5, 2.5 Hz, 1H), 3.84 (s, 3H), 3.64 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 155.0, 138.6, 135.6, 133.0, 132.2, 131.3, 130.0, 128.5, 128.4, 128.1, 127.5, 125.6, 115.1, 112.6, 110.5, 101.7, 56.3, 31.2. HRMS (ESI): found: 314.1542, calcd. for $C_{22}H_{20}NO$ ([M+H]$^+$): 314.1545.

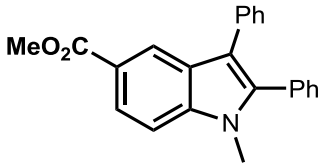


5-fluoro-1-methyl-2,3-diphenyl-1H-indole (**3h**): 50% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.43 (dd, *J* = 9.6, 2.4 Hz, 1H), 7.40-7.33 (m, 3H), 7.32-7.27 (m, 3H), 7.25-7.21 (m, 3H), 7.19-7.14 (m, 2H), 7.04 (td, *J* = 8.8, 2.4 Hz, 1H), 3.66 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.7 (J_{F1}=233.0), 139.4, 134.9, 134.1, 131.7, 131.2, 129.8, 128.6, 128.4 (J_{F4}=5.0), 128.0 (J_{F3}=5.0), 127.4 (J_{F3}=10.0), 125.8, 115.3, 110.7, 110.4(J_{F2}=11.0), 104.6 (J_{F2}=24.0). HRMS (ESI): found: 302.1340, calcd. for $C_{21}H_{17}FN$ ([M+H]$^+$): 302.1345.

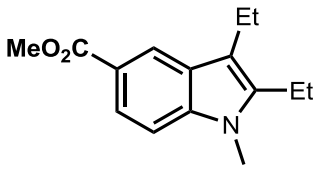


3i **3i'**

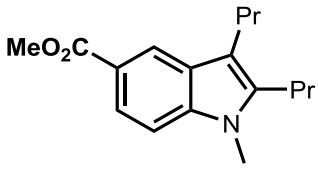
6-bromo-1-methyl-2,3-diphenyl-1H-indole (**3i**): 86% yield, as a mixture (3i/3i'=2.3), yellowish solid. ^{1}H NMR ($CDCl_3$, 400 MHz) for the major isomer: δ7.42-7.21 (m, 16 H), 7.14 (t, *J* = 8.0 Hz, 1H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) of the regiomeric mixture: δ 140.0, 138.3, 138.0, 134.8, 134.7, 132.9, 131.5, 131.3, 131.2, 131.1, 129.9, 128.6, 128.4, 128.2, 128.1, 127.0, 126.4, 126.1, 125.9, 125.4, 124.8, 123.5, 122.6, 121.0, 116.6, 115.7, 115.4, 114.5, 112.7, 108.9, 31.4, 31.2; HRMS (ESI): found: 362.0536, calcd. for $C_{21}H_{17}BrN$ ($[M+H]^+$): 362.0544.



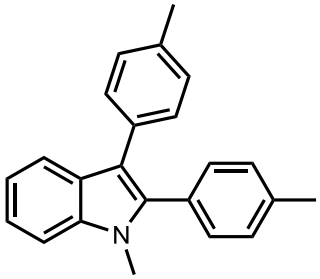
methyl 1-methyl-2,3-diphenyl-1H-indole-5-carboxylate (**3j**)[12]: 92% yield, brown solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.55 (s, 1H), 8.03 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.43-7.40 (m, 4H), 7.35-7.31 (m, 6H), 7.25-7.21 (m, 1H), 3.94 (s, 3H), 3.71 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.3, 139.8, 139.1, 134.5, 131.4, 131.2, 130.0, 128.6, 128.5, 128.2, 126.8, 126.1, 123.7, 122.8, 122.3, 116.6, 109.4, 51.9, 31.3; HRMS (ESI): found: 342.1489, calcd. for $C_{23}H_{20}NO_2$($[M+H]^+$): 342.1494.



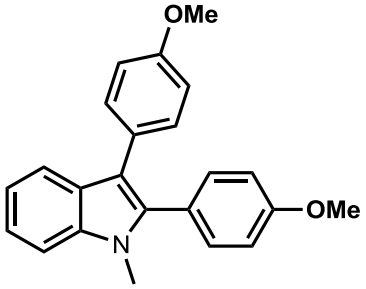
methyl 2,3-diethyl-1-methyl-1H-indole-5-carboxylate (**3k**): 51% yield, white yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.30 (d, *J* = 1.2 Hz, 1H), 7.86 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 1H), 3.94 (s, 3H), 3.69 (s, 3H), 2.81-2.74 (m, 4H), 1.27-1.21 (m, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.7, 139.5, 139.3, 127.2, 122.2, 121.2, 120.6, 114.5, 108.3, 51.9, 29.8, 17.8, 17.6, 16.5, 14.9; HRMS (ESI): found: 246.1490, calcd. for $C_{15}H_{20}NO_2$($[M+H]^+$): 246.1494.



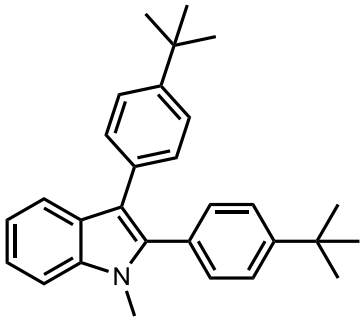
methyl 1-methyl-2,3-dipropyl-1H-indole-5-carboxylate (**3l**): 61% yield, white solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.29 (d, *J* = 1.6 Hz, 1H), 7.86 (dd, d, *J* = 8.8, 1.6 Hz, 1H), 7.22 (d, *J* = 9.2 Hz, 1H), 3.94 (s, 3H), 3.68 (s, 3H), 2.74-2.69 (m, 4H), 1.71-1.59 (m, 4H), 1.04-0.97 (m, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.7, 139.4, 138.5, 127.6, 122.2, 121.4, 120.5, 113.5, 108.3, 51.9, 29.9, 26.7, 26.7, 24.7, 23.5, 14.4, 14.2; HRMS (ESI): found: 274.1802, calcd. for $C_{17}H_{24}NO_2$($[M+H]^+$): 274.1807.



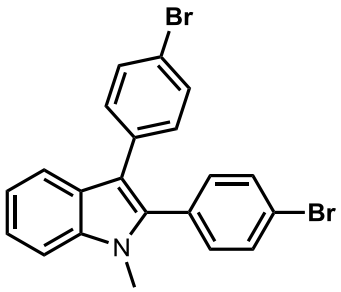
1-methyl-2,3-dip-tolyl-1H-indole (**3m**)[10]: 96% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.82 (d, *J* = 8.1 Hz, 1H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.32 (td, *J* = 6.9, 0.9 Hz, 1H), 7.27-7.19 (m, 7H) 7.12 (d, *J* = 7.8 Hz, 2H), 3.70 (s, 3H), 2.43 (s, 3H), 2.36 (s, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 137.9, 137.7, 137.4, 135.0, 132.4, 131.1, 129.8, 129.2, 129.1, 127.2, 122.1, 120.1, 119.7, 114.8, 109.6, 31.0, 21.5, 21.3; HRMS (ESI): found: 312.1749, calcd. for $C_{23}H_{22}N([M+H]^+)$: 312.1752.



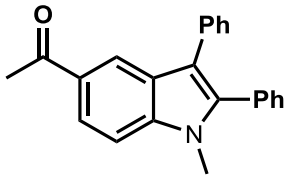
2,3-bis(4-methoxyphenyl)-1-methyl-1H-indole (**3n**)[10]: 94% yield, light yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.33-7.25 (m, 5H), 7.19 (td, *J* = 7.6, 0.8 Hz, 1H), 6.95 (td, *J* = 9.6, 2.8 Hz, 2H), 6.86 (td, *J* = 9.6, 2.8 Hz, 2H), 3.86 (s, 3H), 3.82 (s, 3H), 3.68 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.4, 157.6, 137.4, 137.3, 132.5, 131.0, 127.9, 127.3, 124.3, 122.0, 120.1, 119.6, 114.5, 114.0, 113.8, 109.6, 55.4, 55.3, 31.0; HRMS (ESI): found: 344.1642, calcd. for $C_{23}H_{22}NO_2$ ($[M+H]^+$): 344.1651.



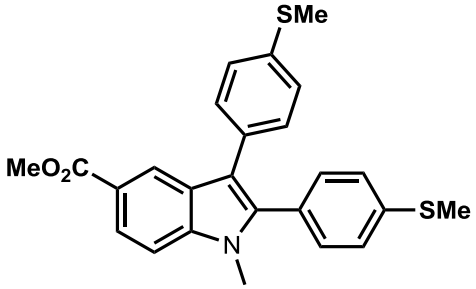
2,3-bis(4-tert-butylphenyl)-1-methyl-1H-indole (**3o**)[13]: 90% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.44-7.42 (m, 3H), 7.34-7.29 (m, 7H), 7.23-7.19 (m, 1H), 3.69 (s, 3H), 1.40 (s, 9H), 1.36 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 151.0, 148.1, 137.8, 137.4, 132.4, 130.9, 129.5, 129.1, 127.3, 125.3, 125.1, 122.0, 120.1, 119.9, 114.8, 109.6, 34.8, 34.5, 31.5, 31.1; HRMS (ESI): found: 396.2686, calcd. For $C_{29}H_{34}N$ ($[M+H]^+$): 396.2691.



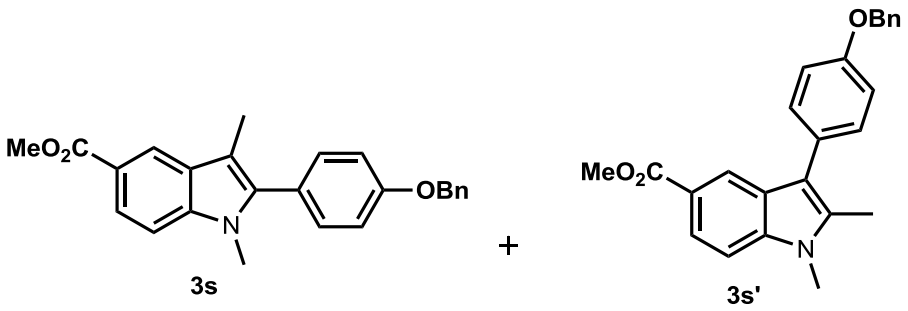
2,3-bis(4-bromophenyl)-1-methyl-1H-indole (**3p**): 88% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.76 (d, *J* = 8.0 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 3H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.27-7.17 (m, 5H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.6, 136.7, 134.0, 132.7, 132.0, 131.6, 131.5, 130.6, 126.7, 122.8, 120.7, 119.8, 119.5, 114.5, 109.9, 31.1; HRMS (ESI): found: 439.9642, calcd. for $C_{21}H_{16}Br_2N$ ($[M+H]^+$): 439.9649.



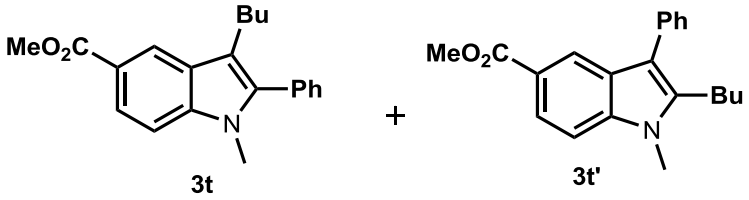
1-(1-methyl-2,3-diphenyl-1H-indol-5-yl)ethanone (**3q**): 97% yield, yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.42 (d, *J* = 1.2 Hz, 1H), 7.97 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.39 -7.38 (m, 3H), 7.38–7.30 (m, 6H), 7.25-7.19 (m, 1H), 3.69 (s, 3H), 2.65 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.4, 139.8, 139.2, 134.4, 131.2, 131.1, 130.3, 129.9, 128.6, 128.5, 126.7, 126.1, 122.6, 121.9, 116.9, 109.6, 31.3, 26.7; HRMS (ESI): found: 326.1539, calcd. for $C_{23}H_{20}NO$ ($[M+H]^+$): 326.1545.



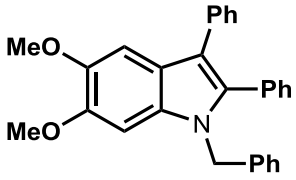
methyl 1-methyl-2,3-bis(4-(methylthio)phenyl)-1H-indole-5-carboxylate (**3r**): 87% yield, yellowish solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.47 (s, 1H), 7.99 (dd, *J* = 8.8, 1.2 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.27 -7.19 (m, 8H), 3.92 (s, 3H), 3.68 (s, 3H), 2.51 (s, 3H), 2.49 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.3, 139.9, 139.4, 138.5, 135.9, 131.4, 131.3, 130.3, 127.6, 126.8, 126.7, 126.0, 123.7, 122.6, 122.3, 116.0, 109.4, 52.0, 31.3, 16.0, 15.3; HRMS (ESI): found: 434.1246, calcd. for $C_{25}H_{24}NO_2S_2$ ($[M+H]^+$): 434.1248.



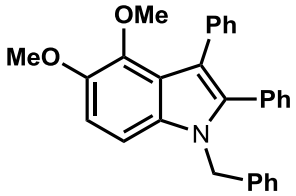
methyl 2-(4-(benzyloxy)phenyl)-1,3-dimethyl-1H-indole-5-carboxylate (**3s**): as an inseparable mixture (3s/3s'=10:1), 71% yield, yellowish solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.37 (s, 1H), 7.96 (d, *J* = 8.8 Hz, 1H), 7.49 (d, *J* = 7.6 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.38 (d, *J* = 7.2 Hz, 1H), 7.33-7.30 (m, 3H), 7.12 (d, *J* = 8.4 Hz, 2H), 5.14 (s, 2H), 3.96 (s, 3H), 3.62 (s, 3H), 2.30 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.5, 158.9, 139.6, 138.9, 136.9, 131.9, 131.3, 131.2, 128.8, 128.2, 128.2, 127.7, 124.1, 123.1, 121.8, 121.0, 117.9, 114.9, 109.9, 108.9, 52.4, 51.9, 31.2, 30.6, 9.4; HRMS (ESI): found: 386.1753, calcd. for $C_{25}H_{24}NO_3$ ($[M+H]^+$): 386.1756.



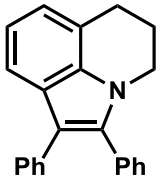
methyl 3-butyl-1-methyl-2-phenyl-1H-indole-5-carboxylate (**3t**): this isomer can be separated and mainly got **3t**, others are the mixture. From ^{1}H NMR, **3t**/**3t'**=5:1, overall yield: 86%, yellowish solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.41 (s, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.52-7.43 (m, 3H), 7.39 (d, *J* = 7.2 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 1H), 3.96 (s, 3H), 3.59 (s, 3H), 2.72 (d, *J* = 8.0 Hz, 2H), 1.66-1.57 (s, 2H), 1.35-1.27 (s, 2H), 0.84 (d, *J* = 7.6 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.5, 139.7, 139.0, 131.8, 136.9, 130.7, 128.6, 128.3, 127.5, 123.1, 122.3, 121.0, 115.6, 109.0, 51.9, 33.7, 31.1, 24.3, 22.8, 14.0; HRMS (ESI): found: 322.1796, calcd. for $C_{21}H_{24}NO_2$ ($[M+H]^+$): 322.1807.



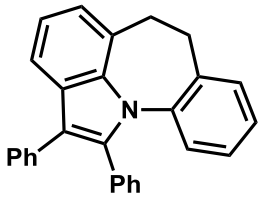
5,6-dimethoxy-1-methyl-2,3-diphenyl-1H-indole (**3u**): 53% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.33-7.18 (m, 14H), 7.00 (d, *J* = 7.2 Hz, 2H), 6.69 (s, 1H), 5.23 (s, 2H), 3.90 (s, 3H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 147.4, 145.9, 138.2, 136.6, 135.6, 132.2, 131.6, 131.2, 129.9, 128.8, 128.5, 128.4, 128.0, 127.3, 126.3, 125.6, 120.3, 115.6, 101.6, 94.2, 56.6, 56.5, 47.9; HRMS (ESI): found: 420.1958, calcd. for $C_{29}H_{26}NO_2$ ($[M+H]^+$): 420.1964.



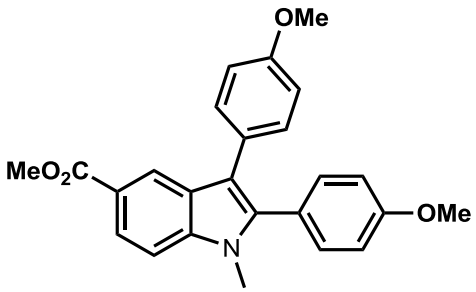
4,5-dimethoxy-1-methyl-2,3-diphenyl-1H-indole (**3u'**): 27% yield, yellowish solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.35 (d, *J* = 6.8 Hz, 2H), 7.30-7.13 (m, 11H), 7.03 (d, *J* = 6.8 Hz, 2H), 6.92 (s, 2H), 5.24 (s, 2H), 3.89 (s, 3H), 3.37 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.4, 143.1, 139.2, 138.3, 135.5, 134.4, 131.8, 131.6, 131.2, 128.8, 128.3, 128.1, 127.3, 127.1, 126.3, 125.6, 121.7, 115.2, 111.5, 105.9, 61.2, 58.4, 48.1; HRMS (ESI): found: 420.1968, calcd. for $C_{29}H_{26}NO_2$ ($[M+H]^+$): 420.1964.



1,2-diphenyl-5,6-dihydro-4H-pyrrolo[*3,2,1-ij*]quinoline (**3v**)[14]: 65% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.62 (d, *J* = 8.1 Hz, 1H), 7.35-7.24 (m, 9H), 7.18 -7.12 (m, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 6.99 (d, *J* = 7.2 Hz, 1H), 4.08 (t, *J* = 5.7 Hz, 2H), 3.05 (t, *J* = 6.0 Hz, 2H), 2.23 (t, *J* = 6.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 136.1, 135.7, 134.5, 131.9, 130.9, 129.8, 128.5, 128.3, 128.0, 125.5, 125.1, 122.2, 120.4, 119.3, 117.2, 114.6, 43.3, 25.2, 23.1; HRMS (ESI): found: 310.1589, calcd. for $C_{23}H_{20}N$ ($[M+H]^+$): 310.1596.



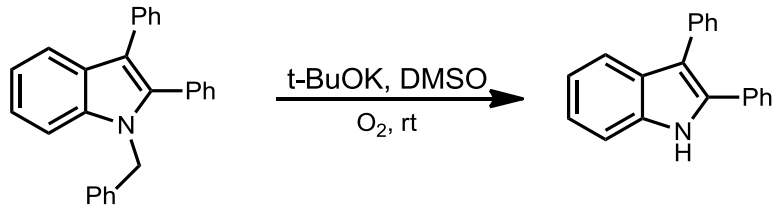
2α,8-dihydro-1,2-diphenyl-7H-Dibenz[*cd,h*]azulene (**3w**): 89% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.53-7.50 (m, 1H), 7.37-7.26 (m, 6H), 7.19-7.00 (m, 8H), 6.84-6.80 (m, 1H), 6.56-6.53 (m, 1H), 3.42-3.28 (m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 139.7, 137.4, 137.3, 137.1, 134.9, 132.5, 131.0, 130.5, 130.0, 129.3, 128.4, 128.3, 127.9, 127.2, 127.0, 126.4, 125.9, 125.0, 124.4, 121.0, 120.5, 117.6, 34.4, 33.6; HRMS (ESI): found: 372.1753, calcd. for $C_{28}H_{22}N$ ($[M+H]^+$): 372.1752.



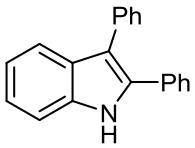
methyl 2,3-bis(4-methoxyphenyl)-1-methyl-1H-indole-5-carboxylate (**3X**): 70% yield, yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.47 (d, *J* = 1.6 Hz, 1H), 7.97 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.35

(d, *J* = 8.4 Hz, 1H), 7.21 (d, *J* = 8.8 Hz, 4H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 3.90 (s, 3H), 3.81 (s, 3H), 3.78 (s, 3H), 3.64 (s, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 168.4, 159.6, 157.9, 139.6, 138.6, 132.3, 131.0, 127.0, 126.9, 123.6, 123.4, 122.6, 122.0, 115.9, 114.1, 114.0, 109.2, 55.3, 55.3, 51.9, 31.1; HRMS (ESI): found: 402.1712, calcd. for $C_{25}H_{24}NO_4$ ($[M+H]^+$): 402.1705.

Debenzylation of the indole product[15]



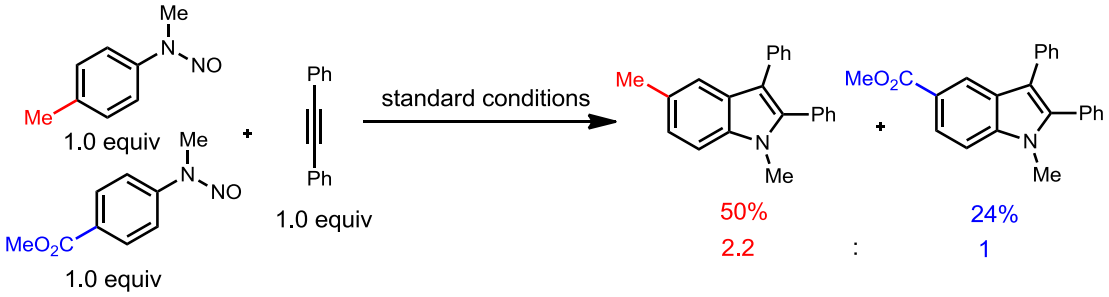
To an indole product **3e** (0.3mmol, 107.8 mg) in 10 mL DMSO, t-BuOK (1.5 mmol, 168.0 mg) was added slowly at rt under O_2. The reaction mixture was stirred at rt for 5 h. Solvent was removed by high vacuum evaporation, and the residue was purified by silica gel flash chromatography using petroleum ether/EtOAc (20:1) to afford NH indole product **4a**.

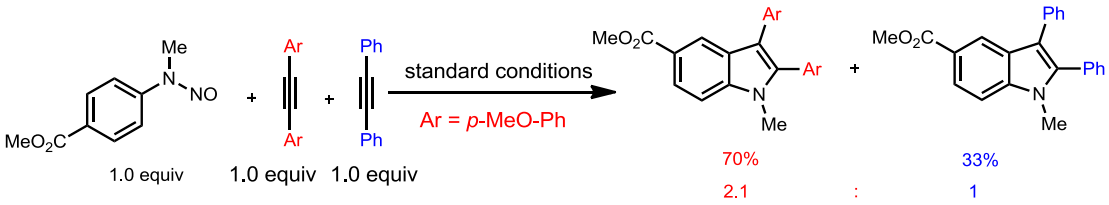


2,3-diphenyl-1H-indole (**4a**)[16]: 93% yield, white solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.27 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.50-7.27 (m, 12H), 7.18 (td, *J* = 8.0, 0.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 136.0, 135.2, 134.2, 132.8, 130.3, 128.9, 128.8, 128.7, 128.3, 127.8, 126.4, 122.8, 120.6, 119.8, 115.2, 111.0. HRMS (ESI): found: 270.1276, calcd. for $C_{20}H_{16}N$ ($[M+H]^+$): 270.1283.

Mechanistic Experiments

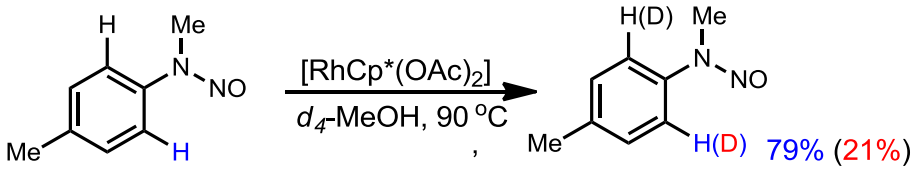
Competing experiments





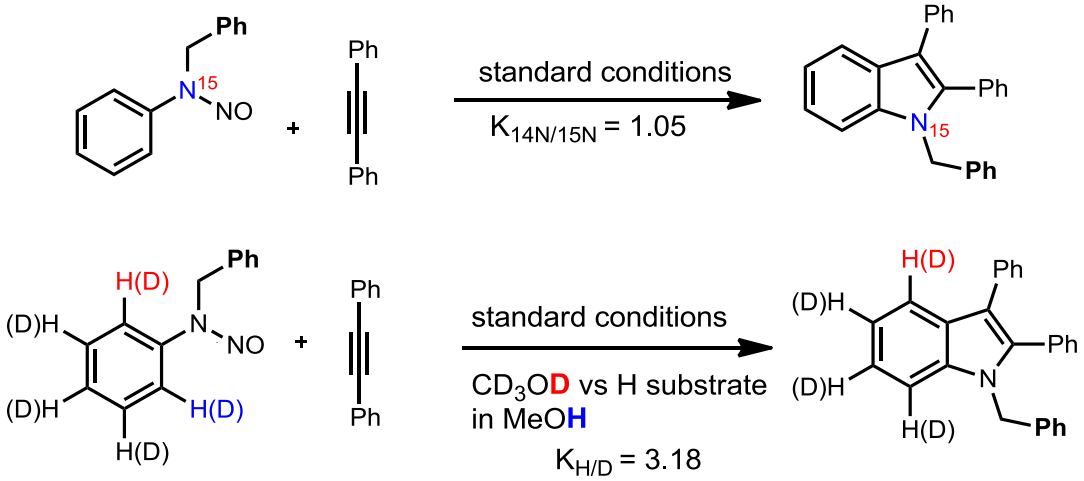
The reactions were carried out as described above for the **General Procedure for the Nitroso Directed Indole Synthesis via Rh(III)-Catalyzed C-H Activation**. The above ratio is calculated using the isolated yield (for the NMR data of this OMe-indole product, see above **3x**).

Reversibility of triazene cyclorhodation



The reactions were carried out as described above for the General Procedure for Rh(III)-Catalyzed C-H Activation/Cyclization directed by N-nitrosoamine. After 22.5 h, the residue was subjected to ^{1}H NMR analysis, the results of which are shown as above.

Deuterium kinetic isotope effect (DKIE) measurements

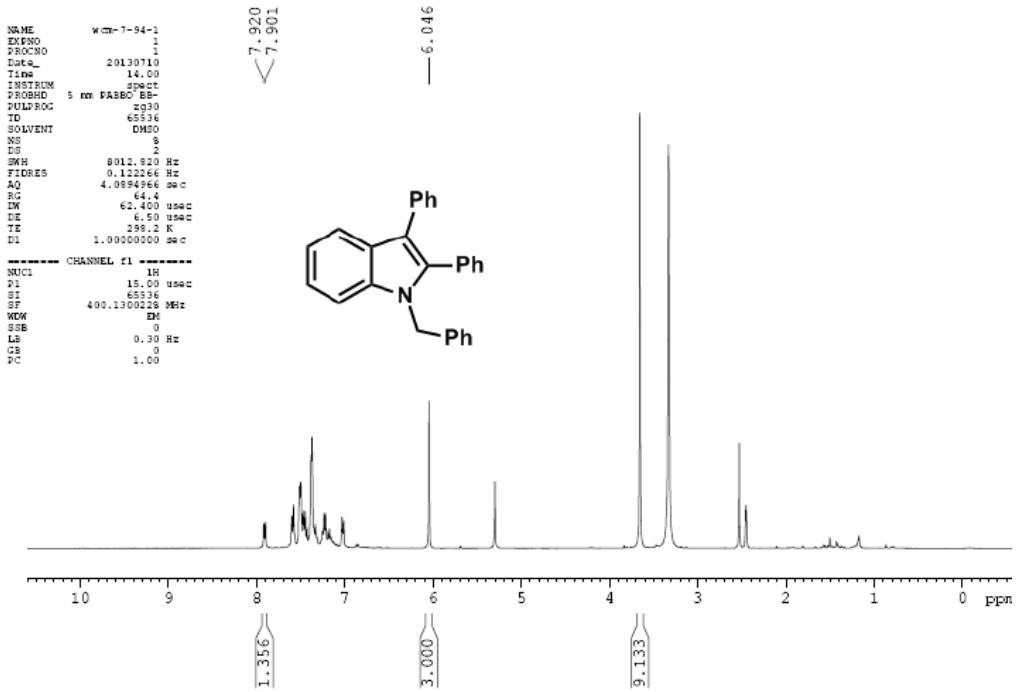


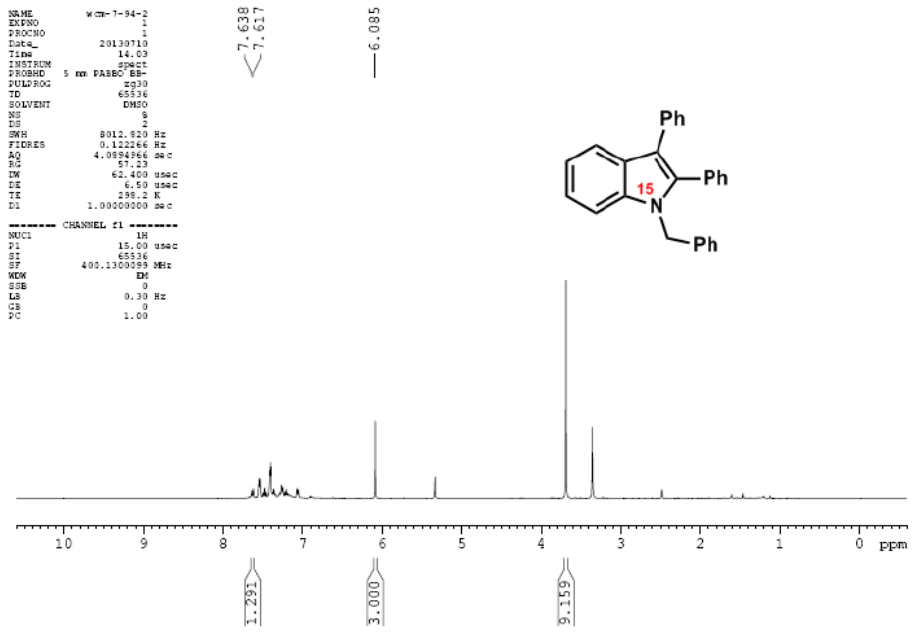
A sample experiment was carried out as the following: Nitroso aniline **1e** (31.8 mg, 0.15 mmol; or **1e'**: 32.0 mg, 0.15 mmol), [RhCp*$(OAc)_2$] (4.0 mg, 8% equiv), diphenylacetylene (35.0 mg, 0.195 mmol) were weighed into two vials containing a stir bar and fitted with a cap lined with a septa. MeOH (3 mL, for N15-amine **1e'** d_4- methanol was used) was quickly added via a syringe and the vial was capped and put into an oil bath (110 °C) to react for 2.5 h. After reaction, 1,3,5-trimethoxybenzene (25.2mg, 0.15 mmol) was added as an internal standard. Then the mixture was subjected to ^{1}HNMR.

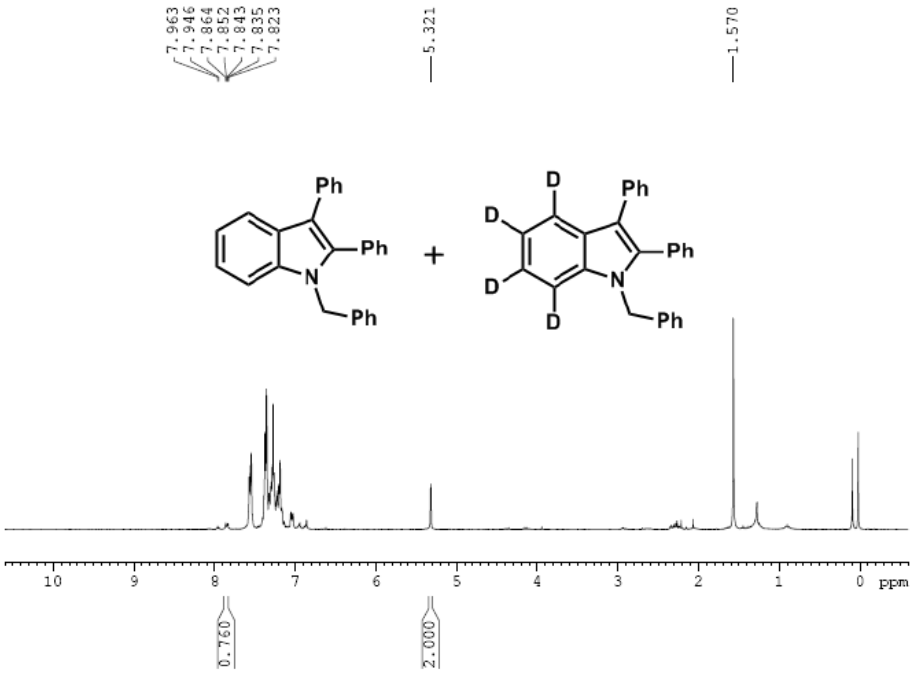
For $K_{H/D}$, the procedure is same as above. After the reaction, no internal standard was added. The H and D reactions were combined and a quick flash column was performed, mainly to remove the remaining N-nitroso aniline starting material (the residual

diphenylethyne doesn't affect the results). The mixture was subjected to ^{1}HNMR analysis.

The isotope effect $K_{14N/15N}$ was calculated as 1.05.
The isotope effect $K_{H/D}$ was calculated as 3.18.



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D
D
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Ph
N
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9
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7
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5
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References

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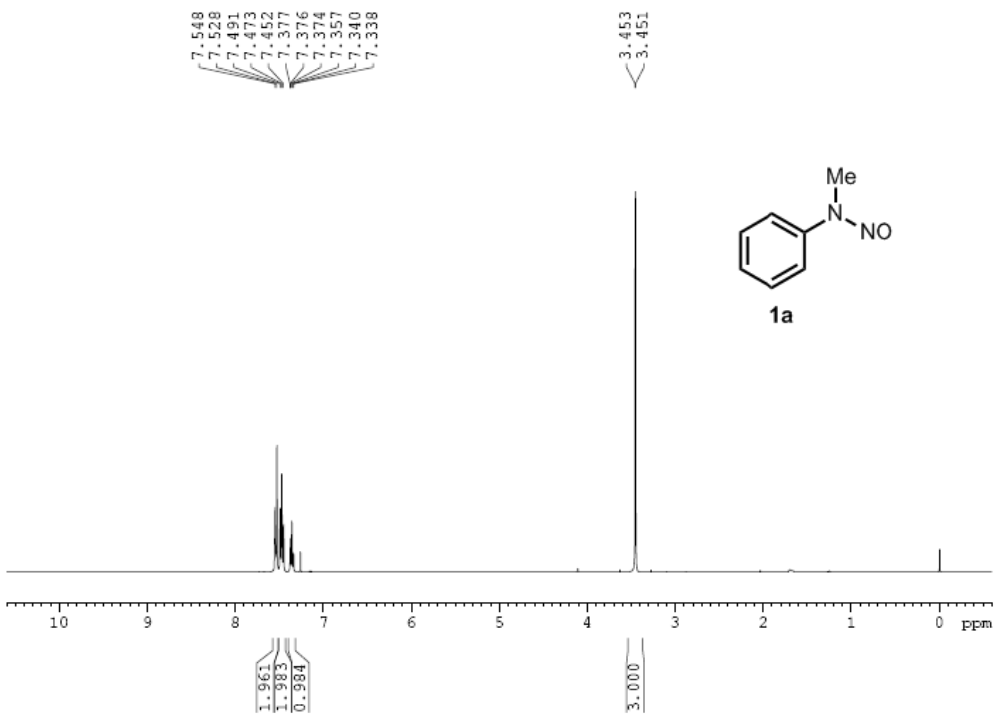
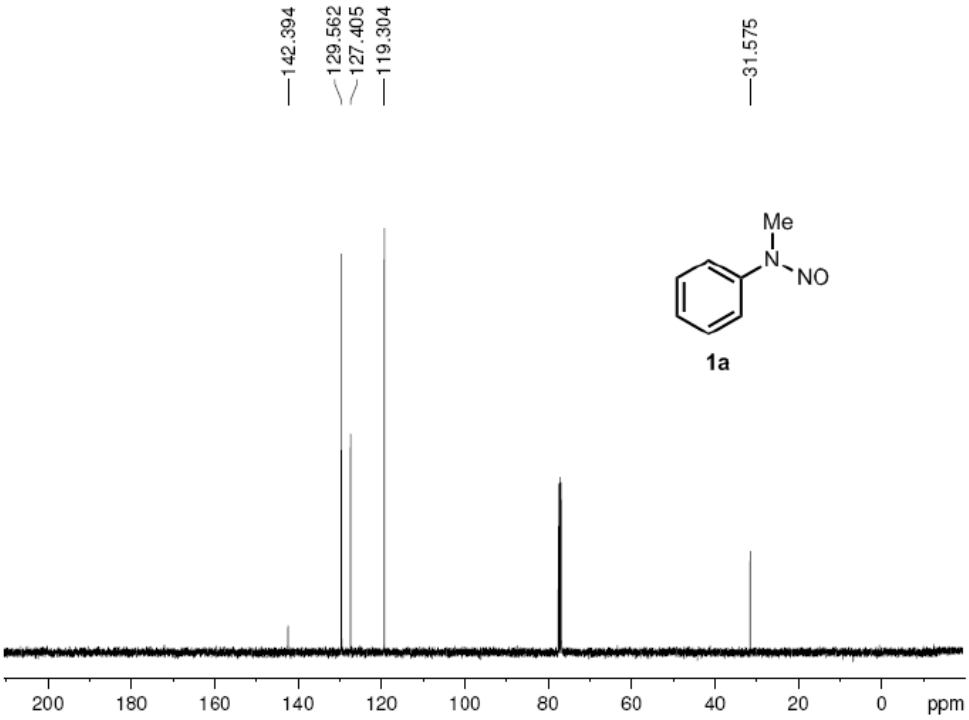
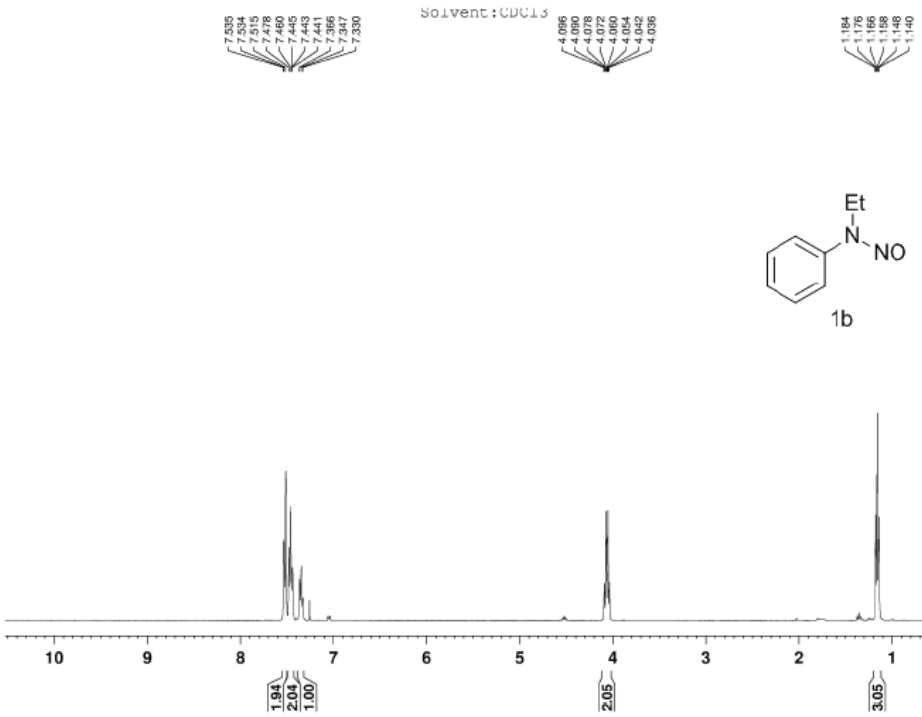
NMR Spectra Images of Nitroso Substrates and Products



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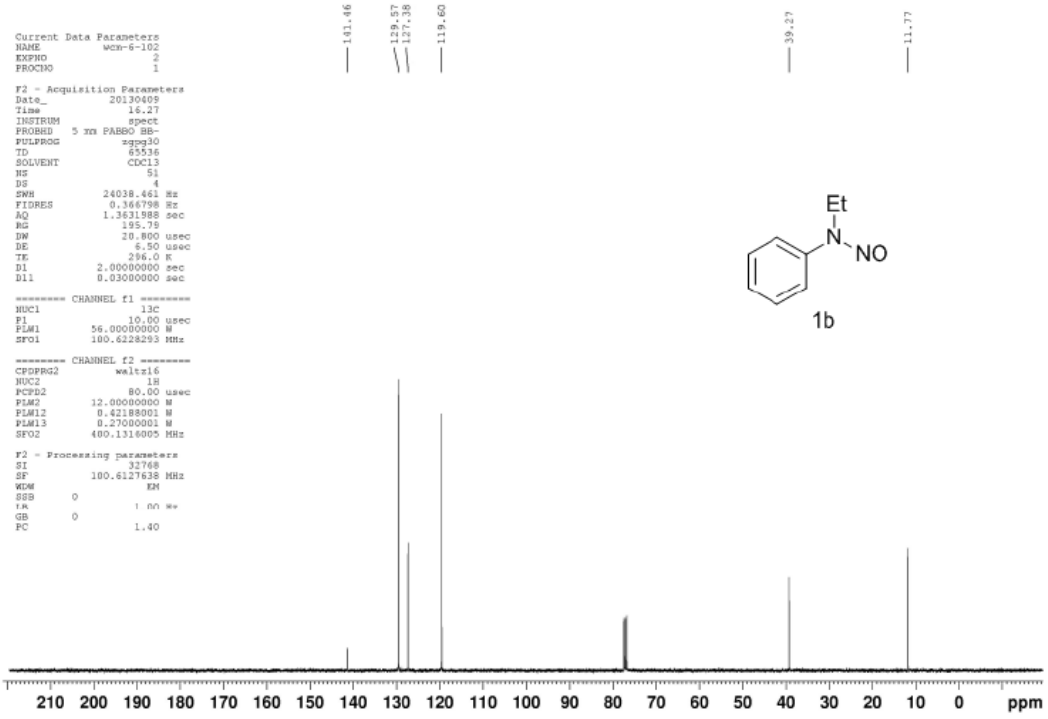
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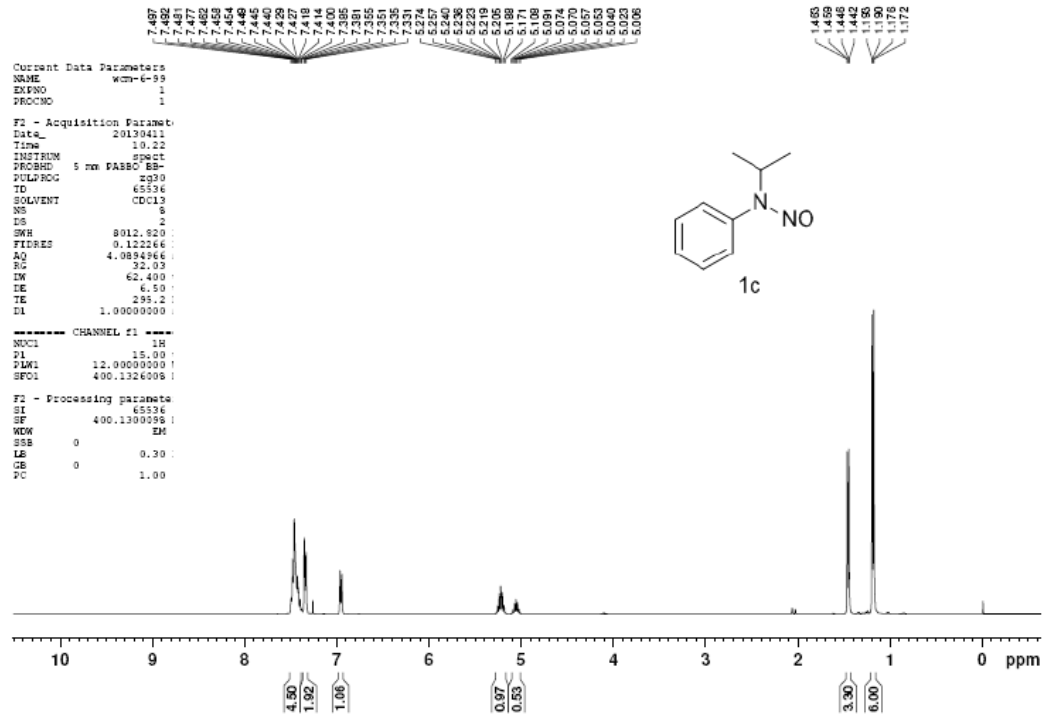
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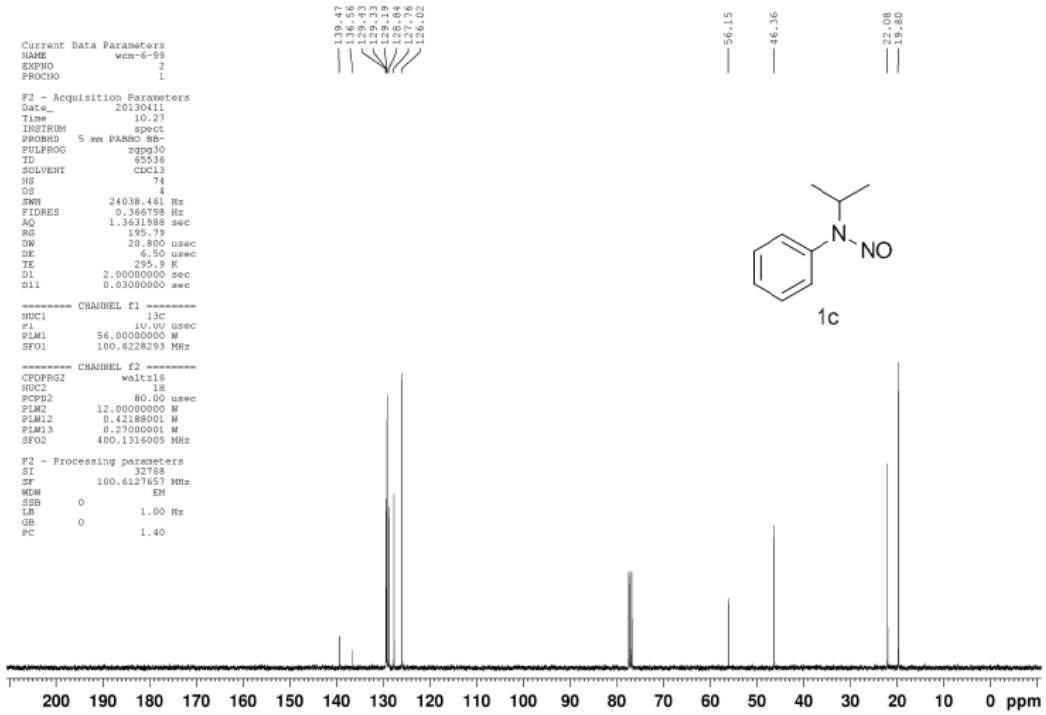
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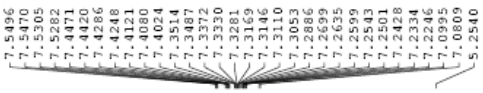
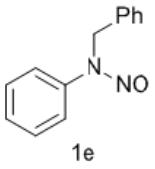
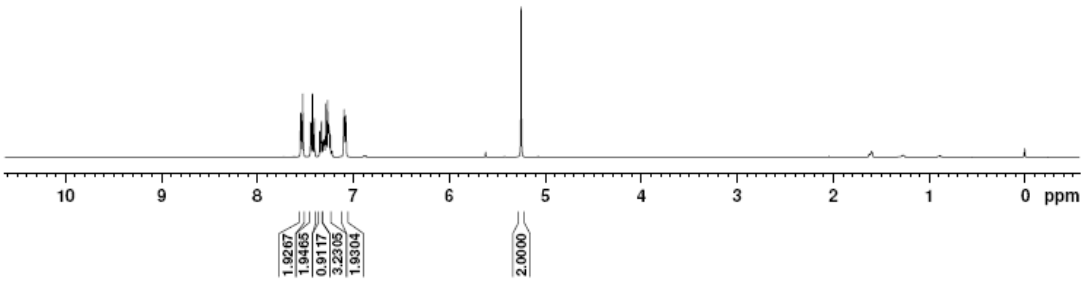
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127657 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
NO
1c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



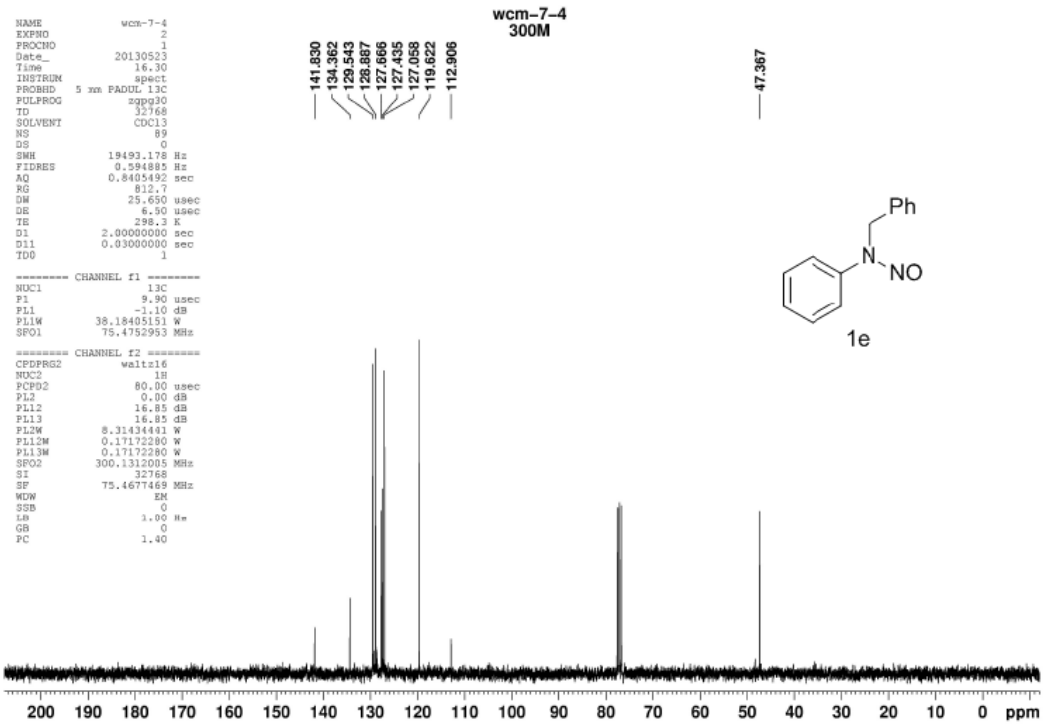


1e

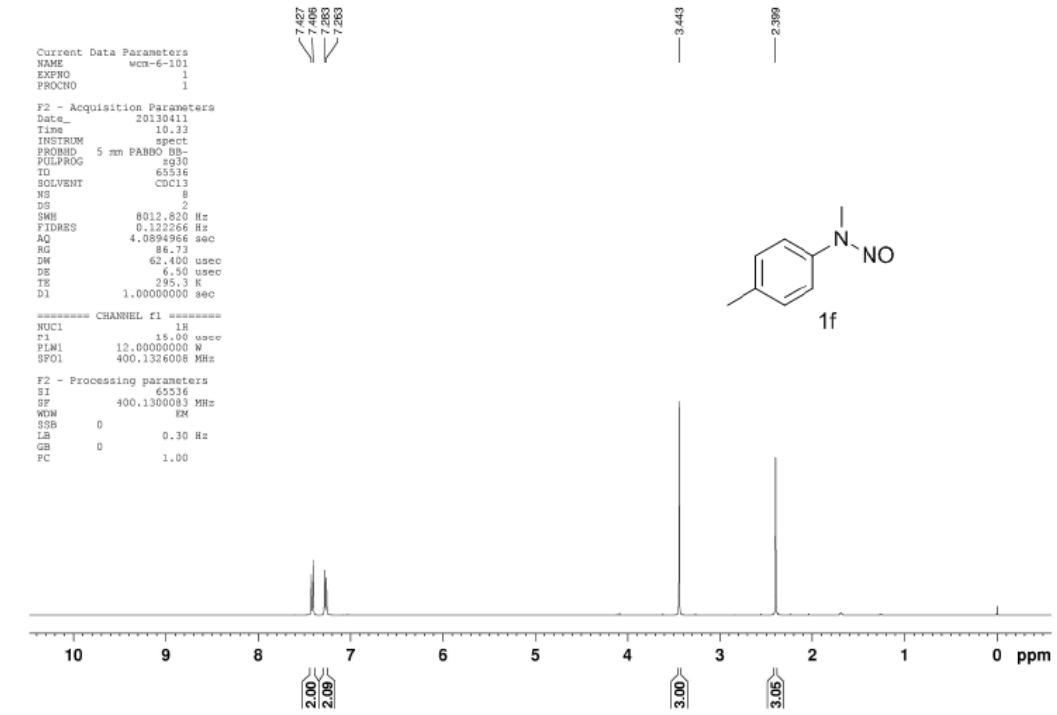


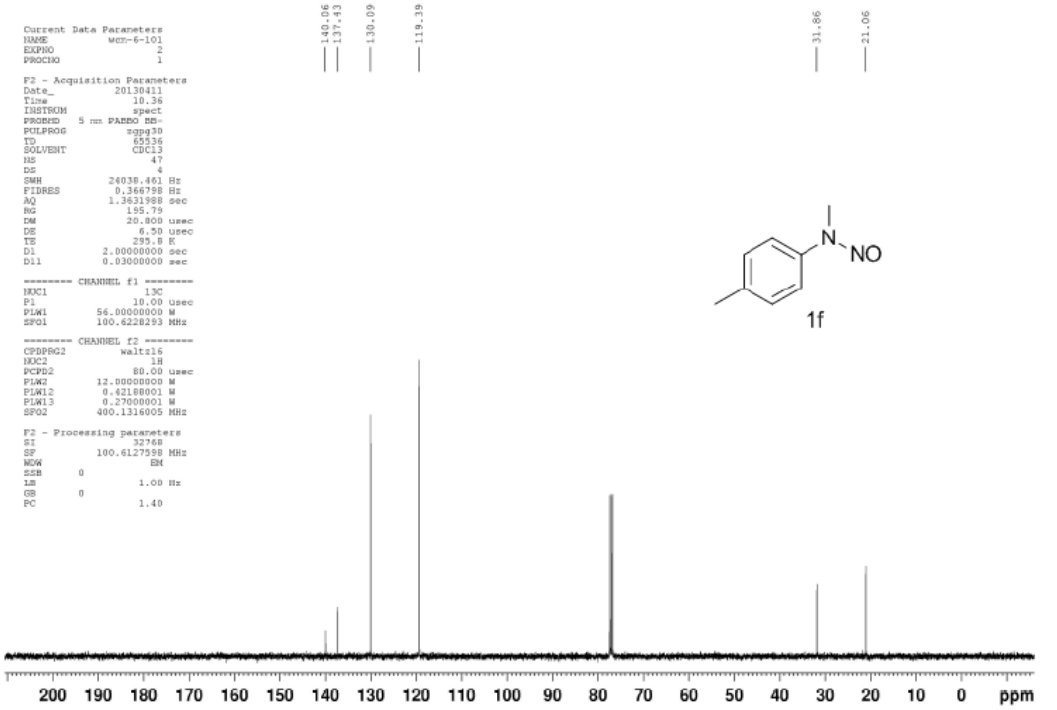
wcm–7–4
300M

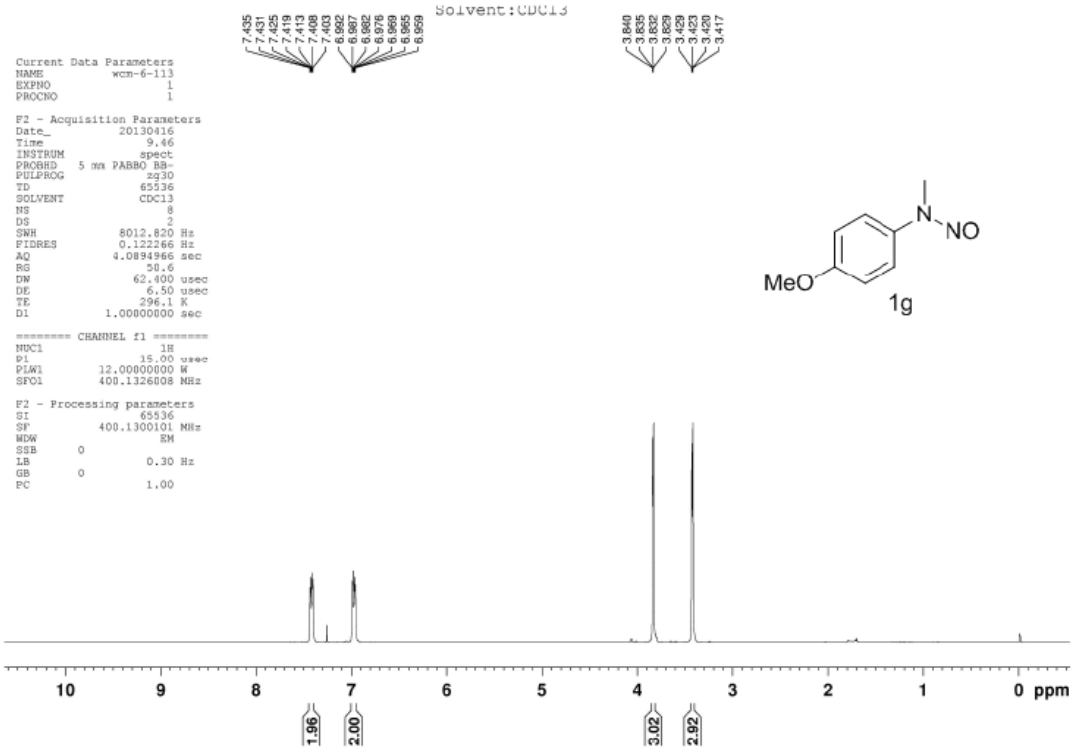
```
NAME                wcm-7-4
EXPNO                     2
PROCNO                    1
Date_              20130523
Time                  16.30
INSTRUM                spect
PROBHD   5 mm PADUL 13C
PULPROG             zgpg30
TD                     32768
SOLVENT                CDCl3
NS                        89
DS                         0
SWH               19493.178 Hz
FIDRES                0.594885 Hz
AQ                    0.8405492 sec
RG                        812.7
DW                       25.650 usec
DE                        6.50 usec
TE                      298.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.90 usec
PL1                     -1.10 dB
PL1W             38.18405151 W
SFO1              75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    16.85 dB
PL13                    16.85 dB
PL2W              8.31434441 W
PL12W             0.17172280 W
PL13W             0.17172280 W
SFO2            300.1312005 MHz
SI                     32768
SF                75.4677469 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

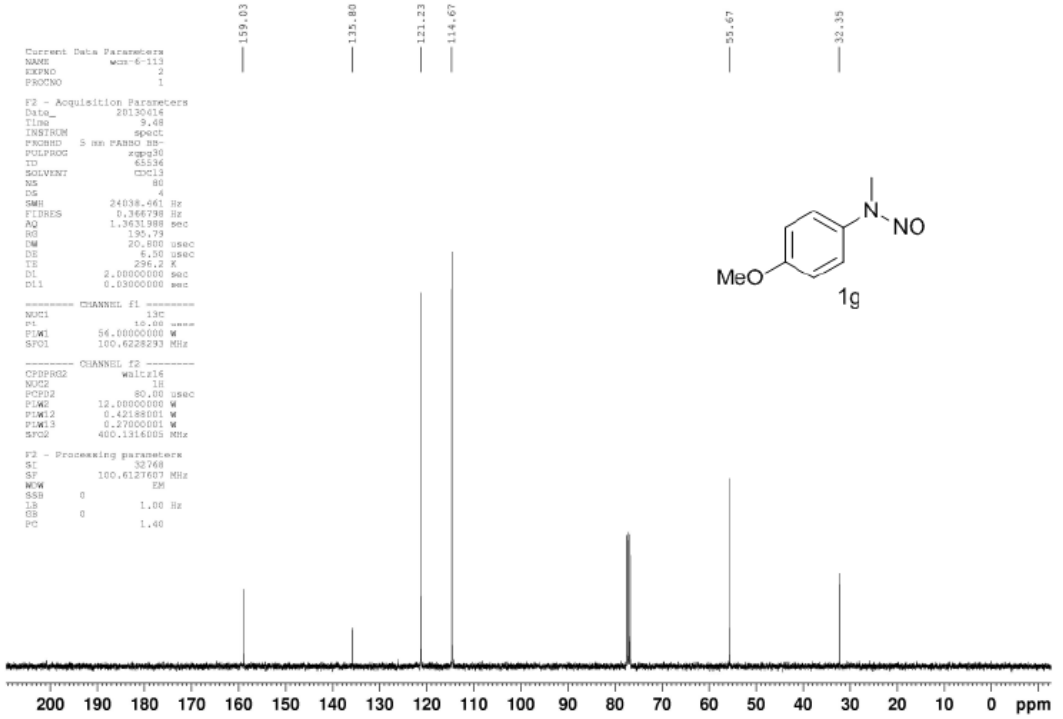


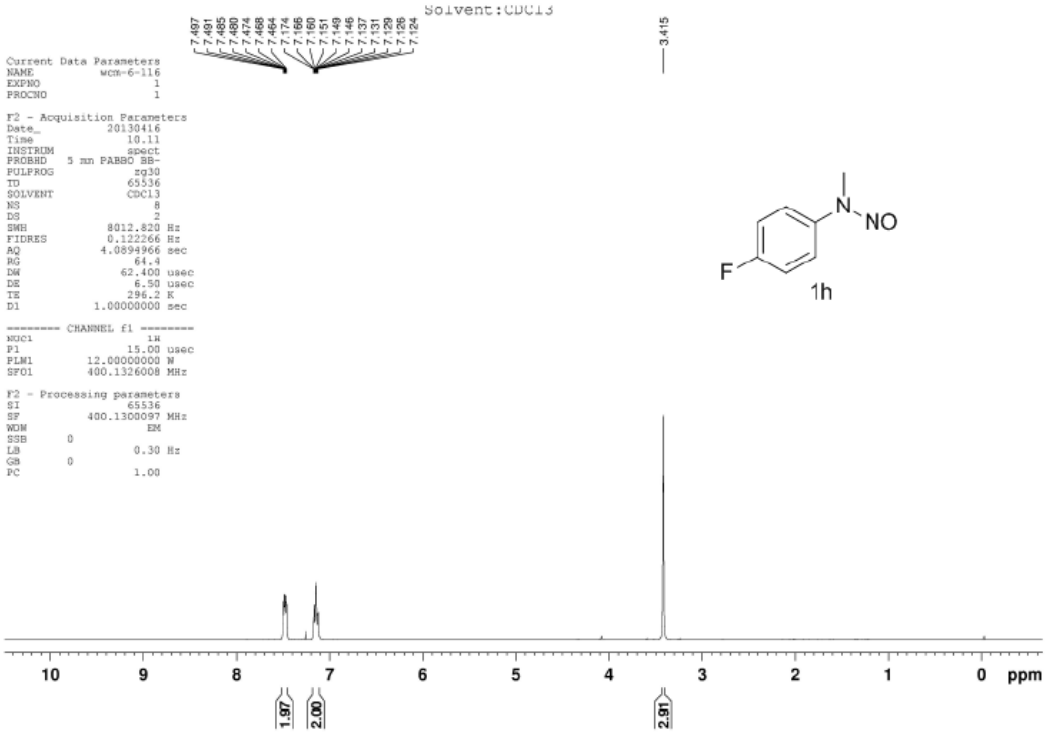
1e

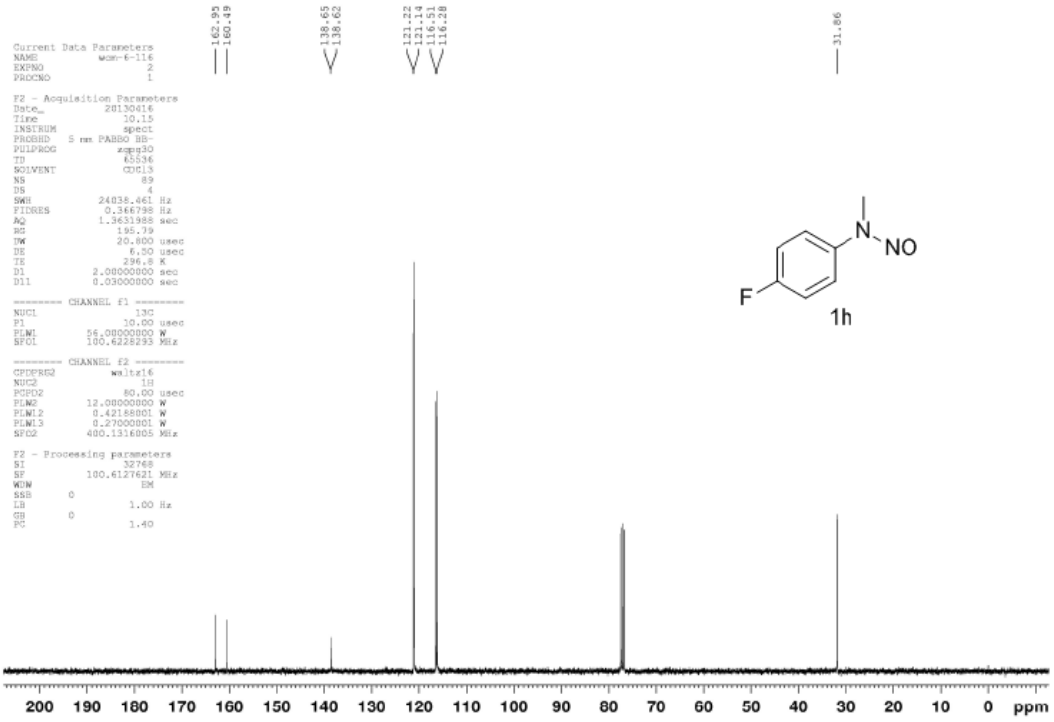

7.427
7.406
7.283
7.263
3.443
2.399
Current Data Parameters
NAME wcm-6-101
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130411
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 86.73
DW 62.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
NO
1f
10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.09
3.00
3.05

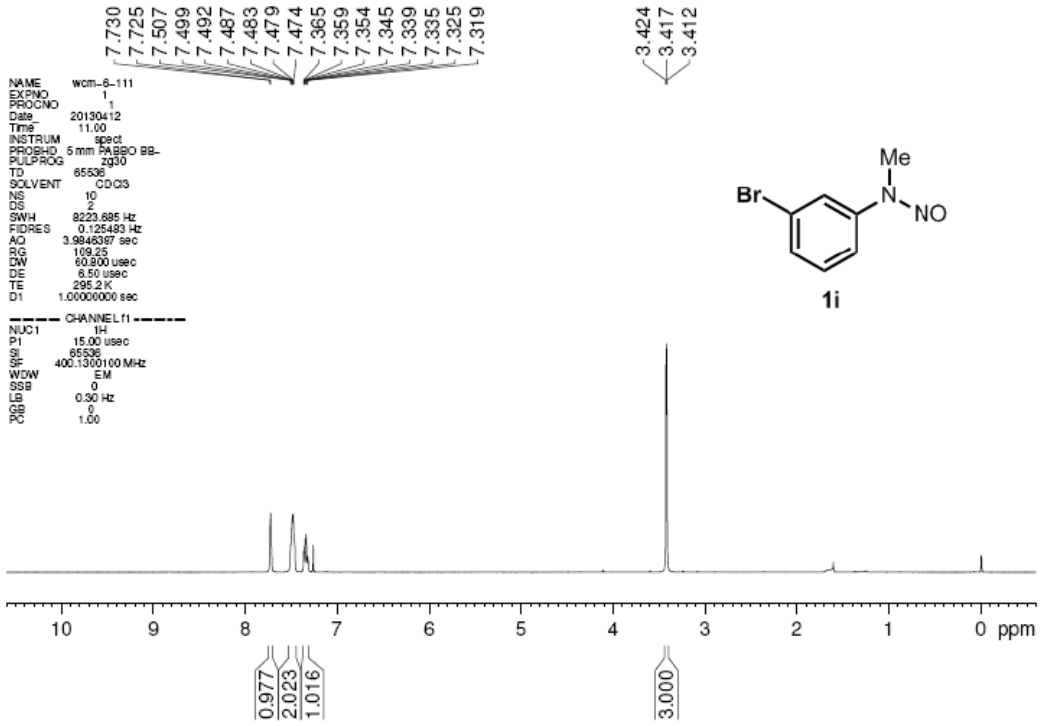

140.06
137.43
130.09
119.39
31.86
21.06
Current Data Parameters
NAME wcm-6-101
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130411
Time 10.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 47
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42180001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127598 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
NO
1f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

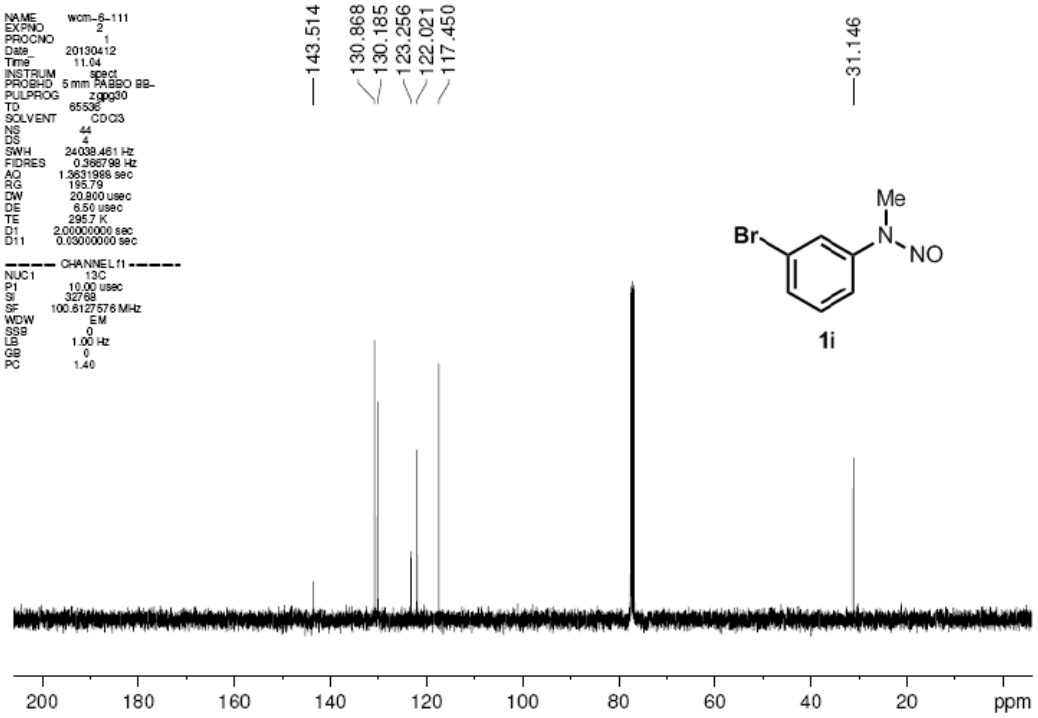

Solvent:CDCl3
7.435
7.431
7.425
7.419
7.413
7.408
7.403
6.992
6.987
6.982
6.976
6.969
6.965
6.959
3.840
3.835
3.832
3.829
3.429
3.423
3.420
3.417
Current Data Parameters
NAME wcm-6-113
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130416
Time 9.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 50.6
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
N
NO
1g
10
9
8
7
6
5
4
3
2
1
0 ppm
1.96
2.00
3.02
2.92

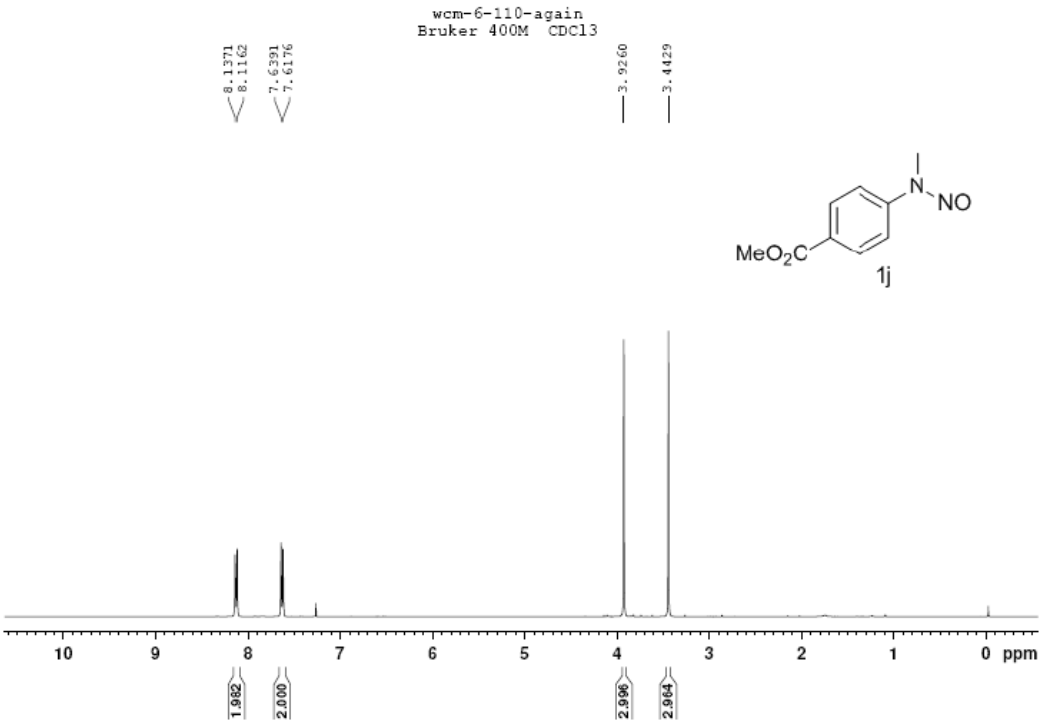

159.03
135.80
121.23
114.67
55.67
32.35
Current Data Parameters
NAME wcm-6-113
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130416
Time 9.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 80
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127607 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
MeO
N
NO
1g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

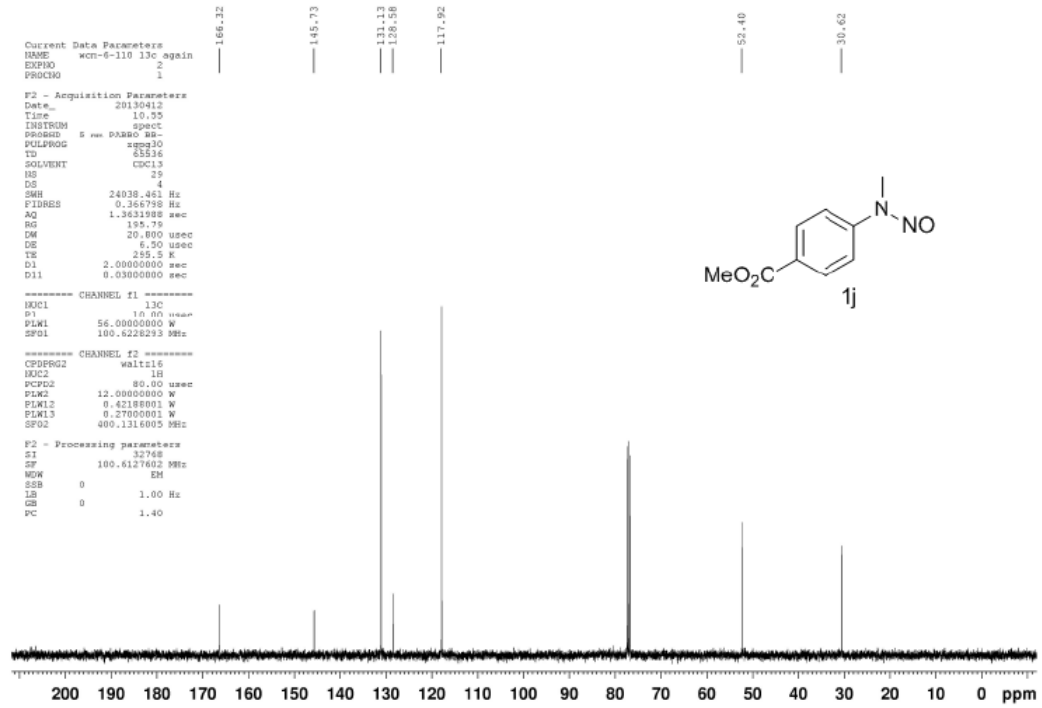

Solvent:CDCl3
7.497
7.491
7.485
7.480
7.474
7.468
7.464
7.174
7.166
7.160
7.151
7.146
7.137
7.131
7.129
7.126
7.124
3.415
Current Data Parameters
NAME wcm-6-116
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130416
Time 10.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 64.4
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
NO
F
1h
10
9
8
7
6
5
4
3
2
1
0
ppm
1.97
2.00
2.91

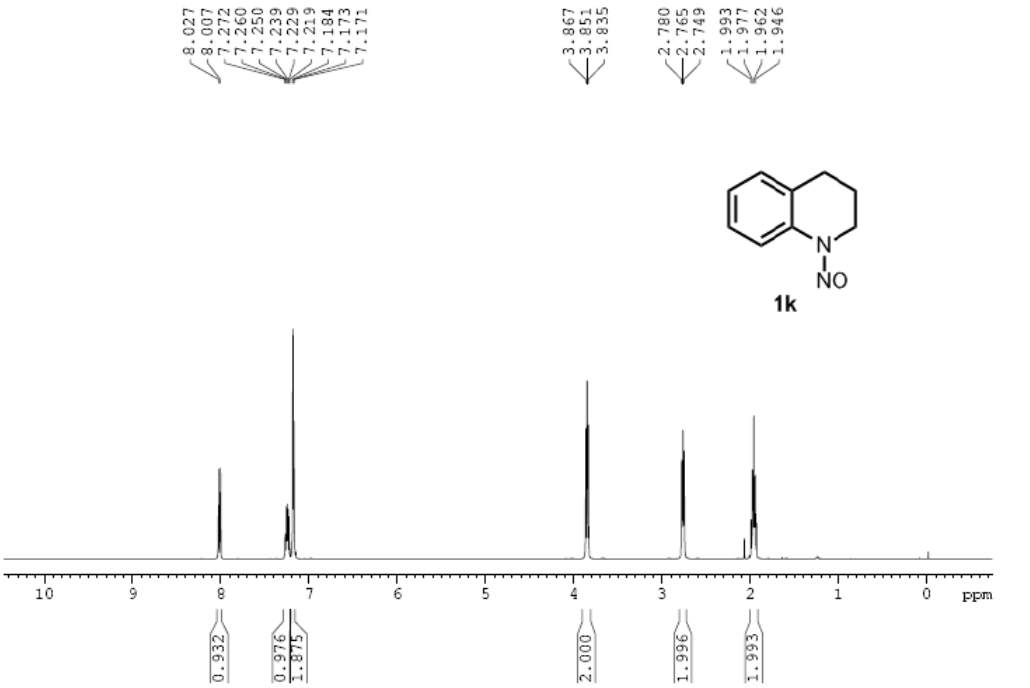

162.95
160.49
138.65
138.62
121.22
121.14
116.51
116.28
31.86
Current Data Parameters
NAME wcm-6-116
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130416
Time 10.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 89
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127621 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
NO
F
1h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

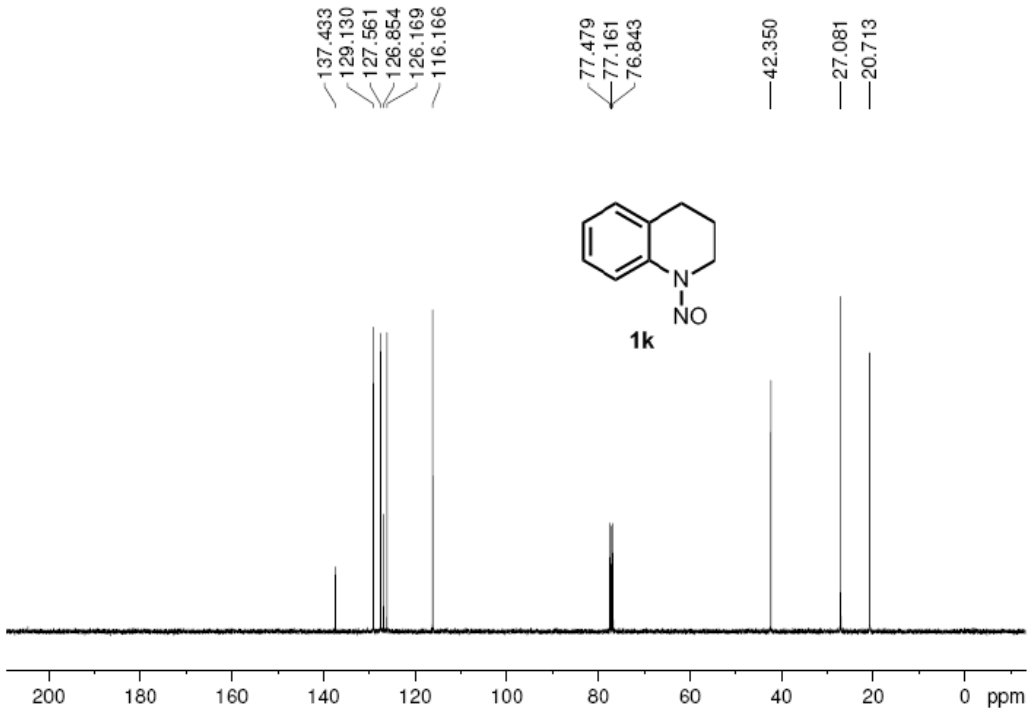

7.730
7.725
7.507
7.499
7.492
7.487
7.483
7.479
7.474
7.365
7.359
7.354
7.345
7.339
7.335
7.325
7.319
3.424
3.417
3.412
NAME wcm-6-111
EXPNO 1
PROCNO 1
Date_ 20130412
Time 11.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 109.25
DW 60.800 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
N
NO
Br
1i
10
9
8
7
6
5
4
3
2
1
0 ppm
0.977
2.023
1.016
3.000

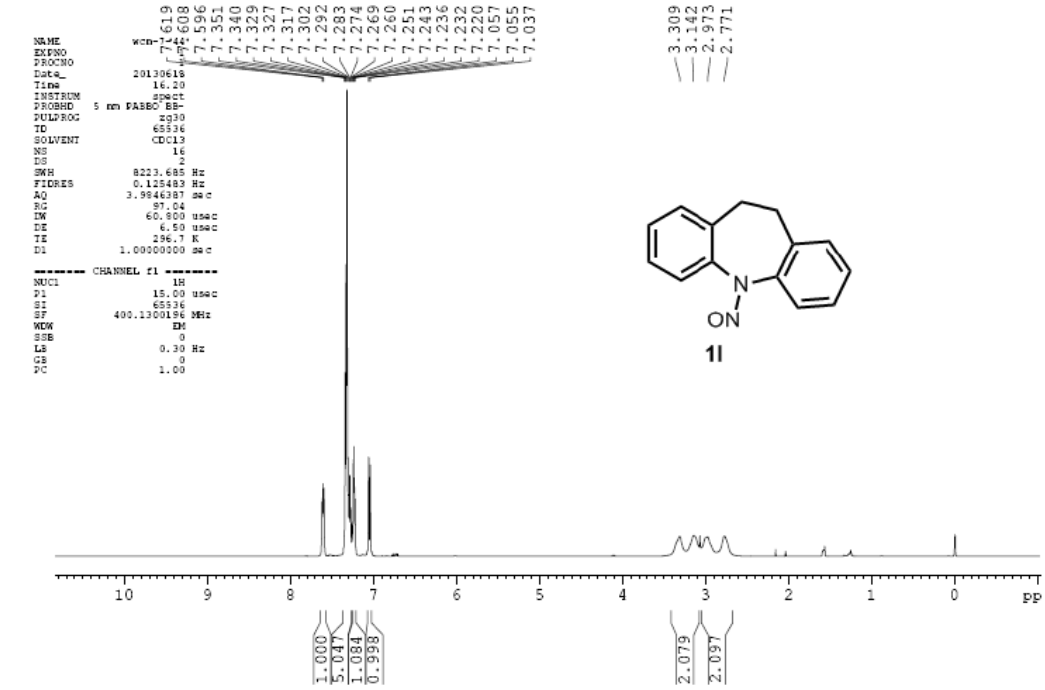

NAME wcm-6-111
EXPNO 2
PROCNO 1
Date_ 20130412
Time 11.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 44
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631986 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127576 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
143.514
130.868
130.185
123.256
122.021
117.450
31.146
Me
N
NO
Br
1i
200
180
160
140
120
100
80
60
40
20
ppm

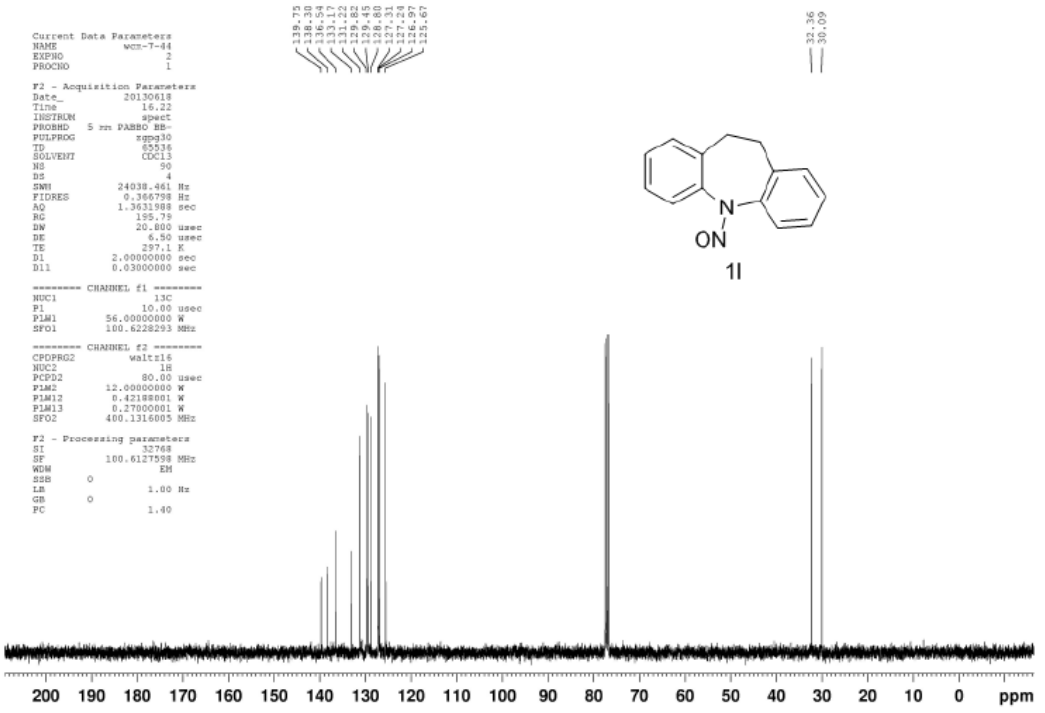

wcm-6-110-again
Bruker 400M CDCl3
8.1371
8.1162
7.6391
7.6176
3.9260
3.4429
MeO2C
N
NO
1j
10 9 8 7 6 5 4 3 2 1 0 ppm
1.982
2.000
2.996
2.964

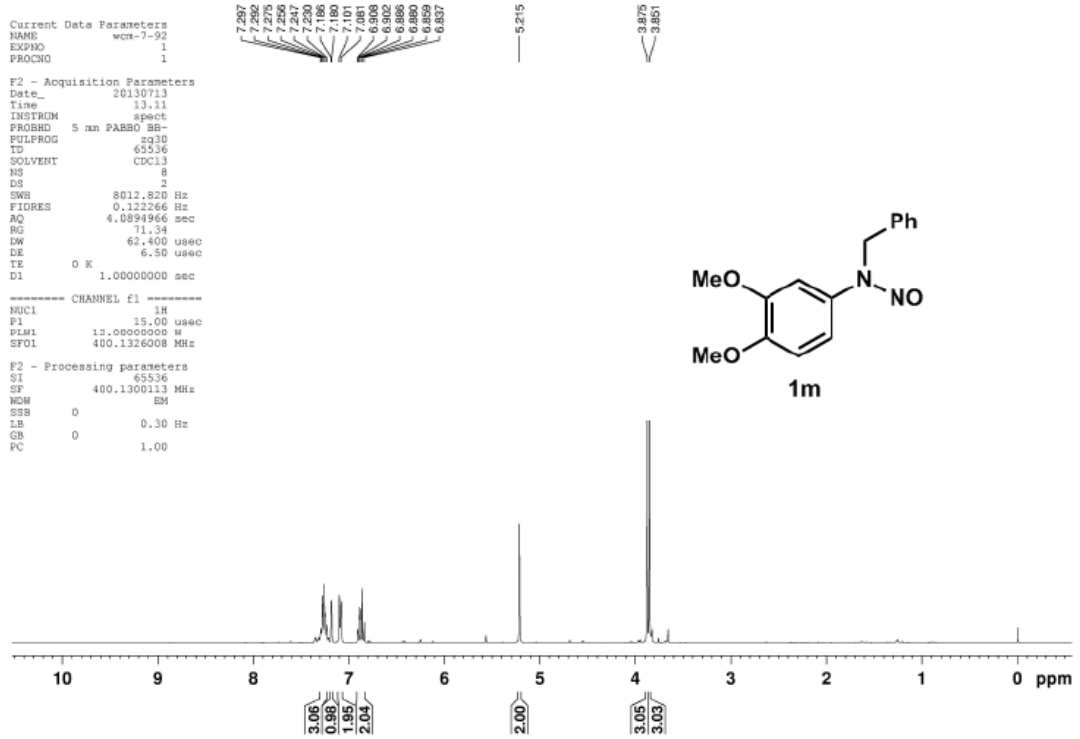

166.32
145.73
131.13
128.58
117.92
52.40
30.62
Current Data Parameters
NAME wcm-6-110 13c again
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130412
Time 10.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 29
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 255.5 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127602 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
MeO2C
N
NO
1j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

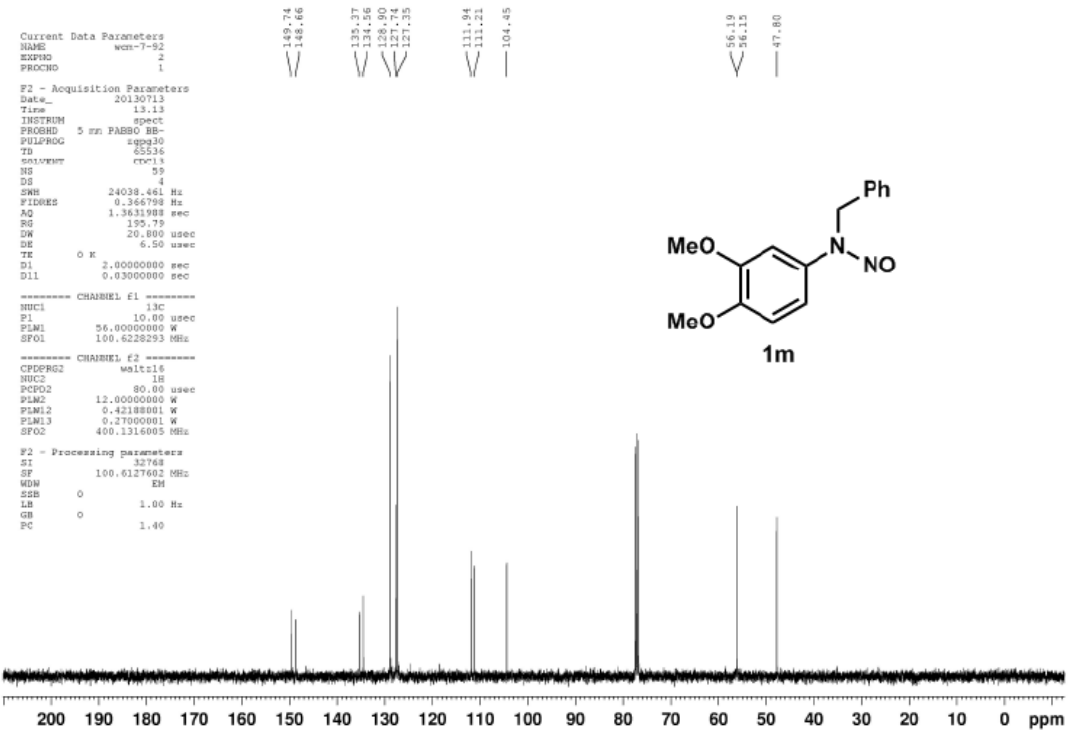

8.027
8.007
7.272
7.260
7.250
7.239
7.229
7.219
7.184
7.173
7.171
3.867
3.851
3.835
2.780
2.765
2.749
1.993
1.977
1.962
1.946
N
NO
1k
10
9
8
7
6
5
4
3
2
1
0
ppm
0.932
0.976
1.875
2.000
1.996
1.993

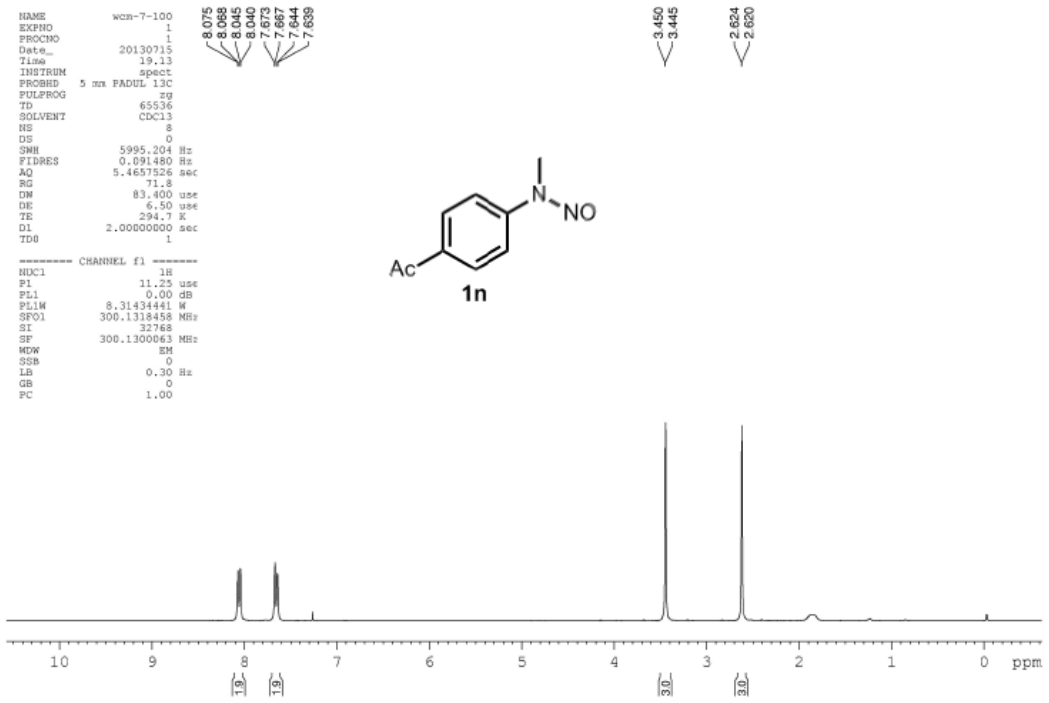

137.433
129.130
127.561
126.854
126.169
116.166
77.479
77.161
76.843
42.350
27.081
20.713
N
NO
1k
200
180
160
140
120
100
80
60
40
20
0
ppm

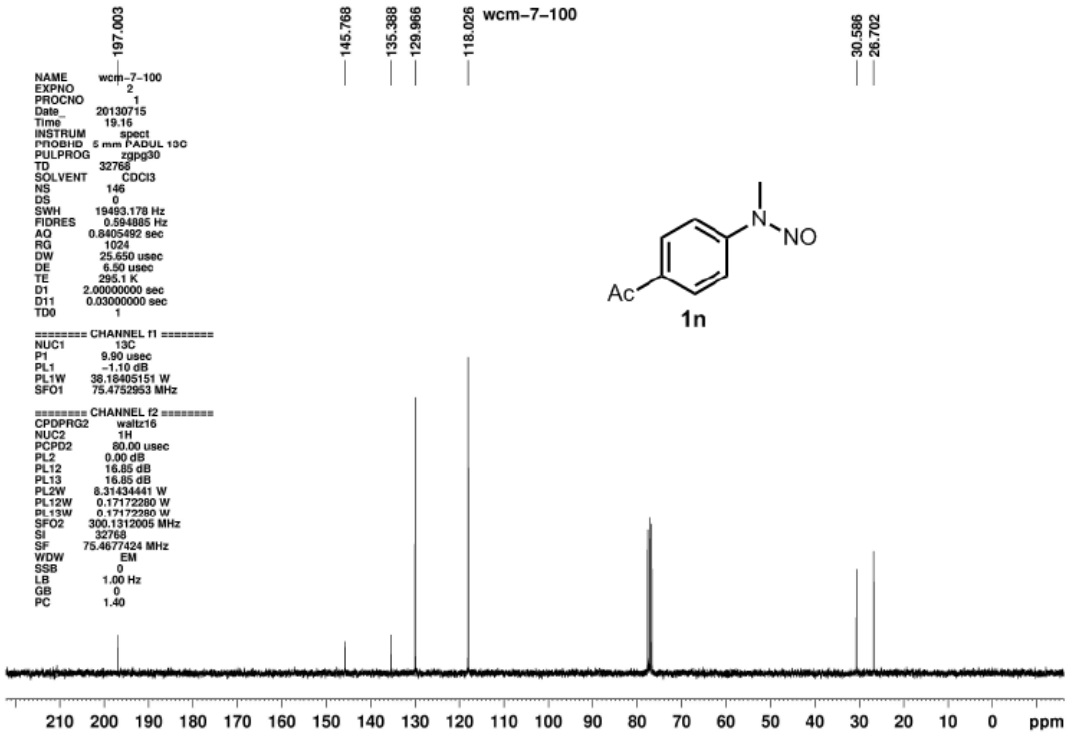

7.619
7.608
7.596
7.351
7.340
7.329
7.327
7.317
7.302
7.292
7.283
7.274
7.269
7.260
7.251
7.243
7.236
7.232
7.220
7.057
7.055
7.037
3.309
3.142
2.973
2.771
NAME wcn-T-44
EXPNO 1
PROCNO 1
Date_ 20130618
Time 16.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 97.04
DW 60.800 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
SI 65536
SF 400.1300196 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
ON
1l
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
5.047
1.084
0.998
2.079
2.097

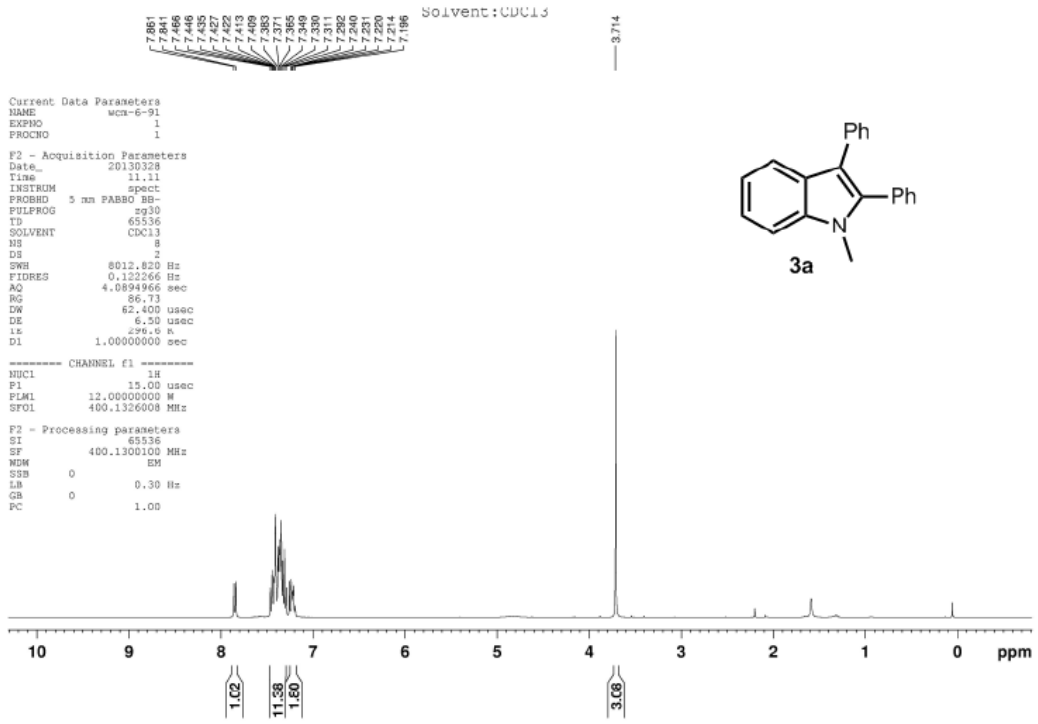

139.75
138.30
135.59
133.17
131.22
129.82
129.45
128.60
128.31
127.24
126.97
125.67
32.36
30.09
Current Data Parameters
NAME wcn-T-44
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130618
Time 16.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 90
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127598 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
ON
1l
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

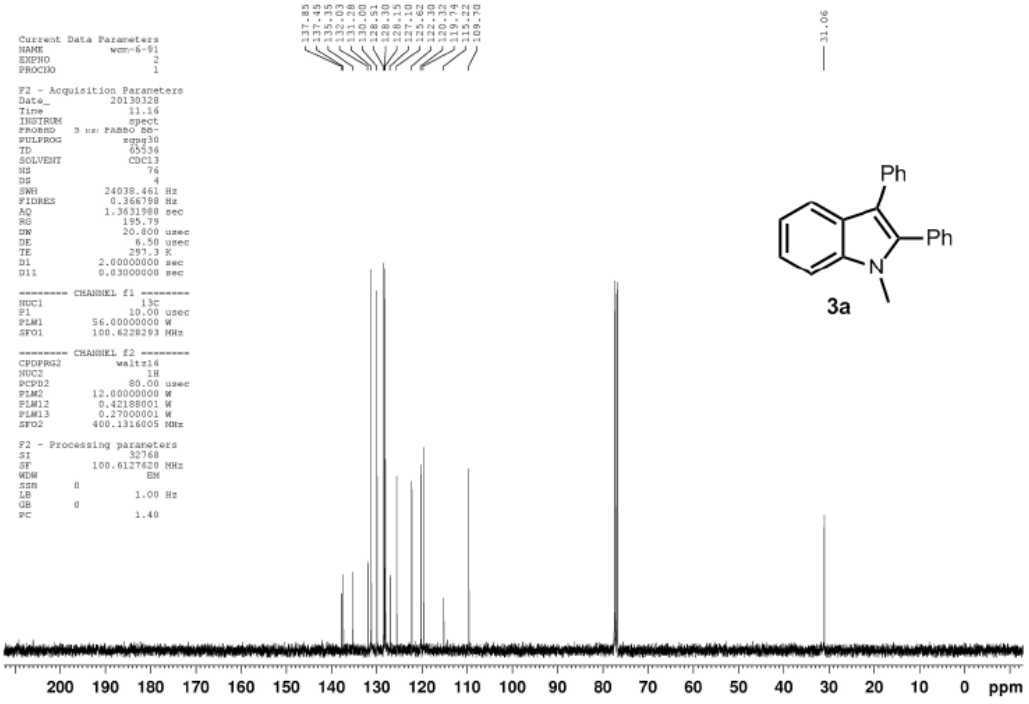

Current Data Parameters
NAME wcm-7-92
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130713
Time 13.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.34
DW 62.400 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.297
7.292
7.275
7.256
7.247
7.230
7.186
7.180
7.101
7.081
6.908
6.902
6.886
6.880
6.859
6.837
5.215
3.875
3.851
MeO
MeO
N
NO
Ph
1m
10
9
8
7
6
5
4
3
2
1
0 ppm
3.06
0.98
1.95
2.04
2.00
3.05
3.03

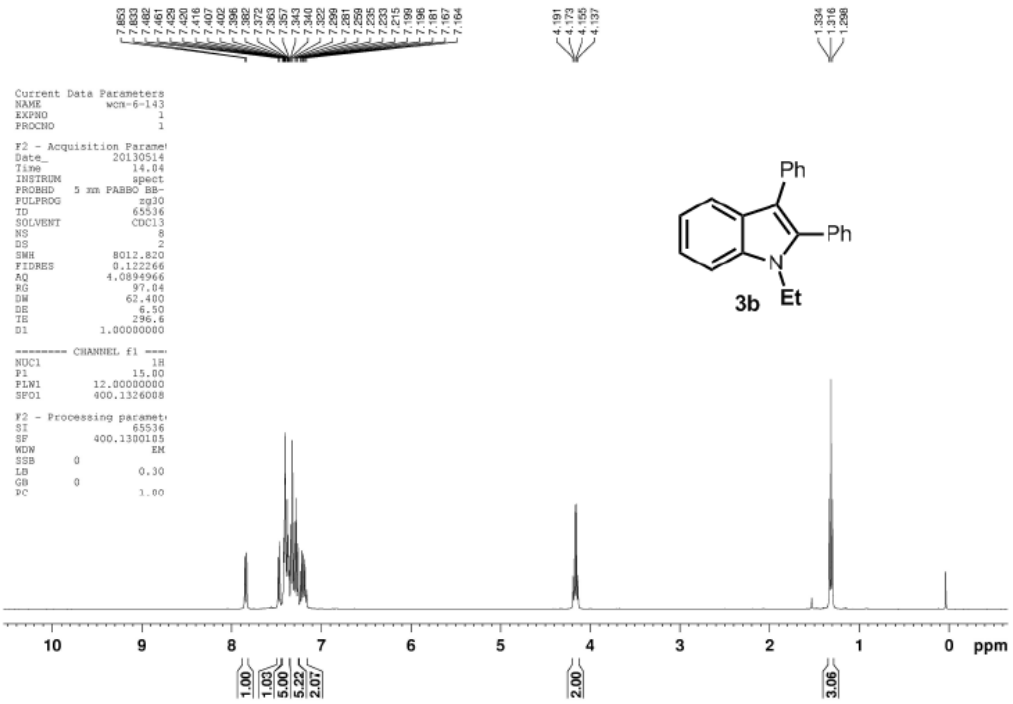

Current Data Parameters
NAME wcm-7-92
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130713
Time 13.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 59
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127602 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
149.74
148.66
135.37
134.56
128.90
127.74
127.35
111.94
111.21
104.45
56.19
56.15
47.80
MeO
MeO
N
NO
Ph
1m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

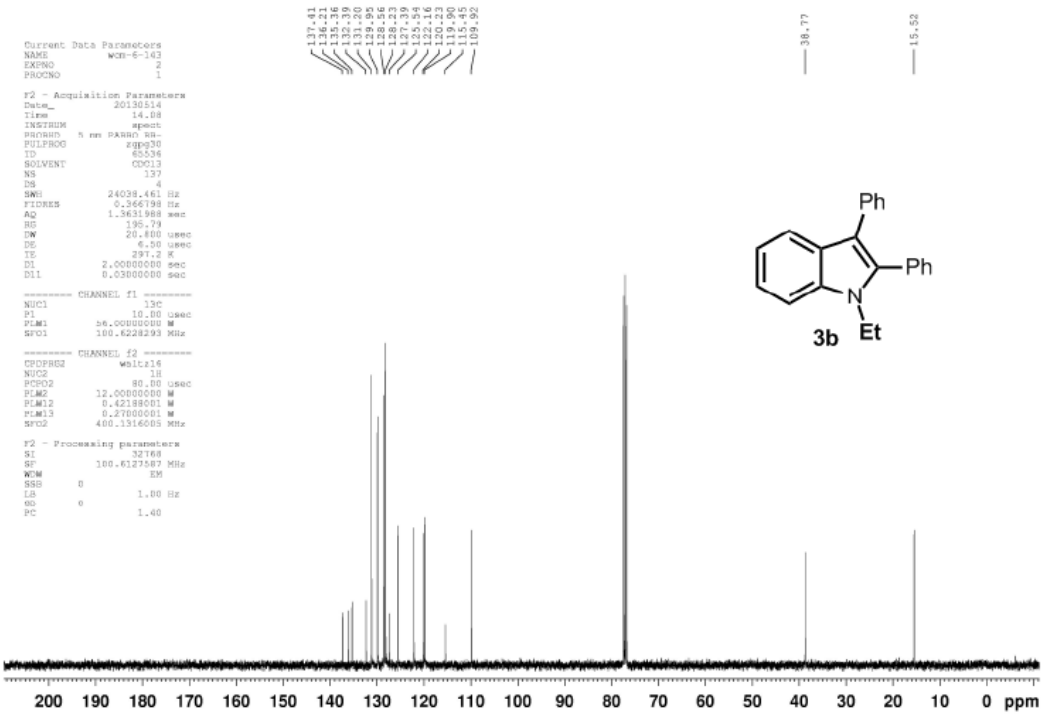

NAME wcm-7-100
EXPNO 1
PROCNO 1
Date_ 20130715
Time 19.13
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 71.8
DW 83.400 use
DE 6.50 use
TE 294.7 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.25 use
PL1 0.00 dB
PL1W 8.31434441 W
SFO1 300.1318458 MHz
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.075
8.068
8.045
8.040
7.673
7.667
7.644
7.639
3.450
3.445
2.624
2.620
N
NO
Ac
1n
10
9
8
7
6
5
4
3
2
1
0
ppm
1.9
1.9
3.0
3.0

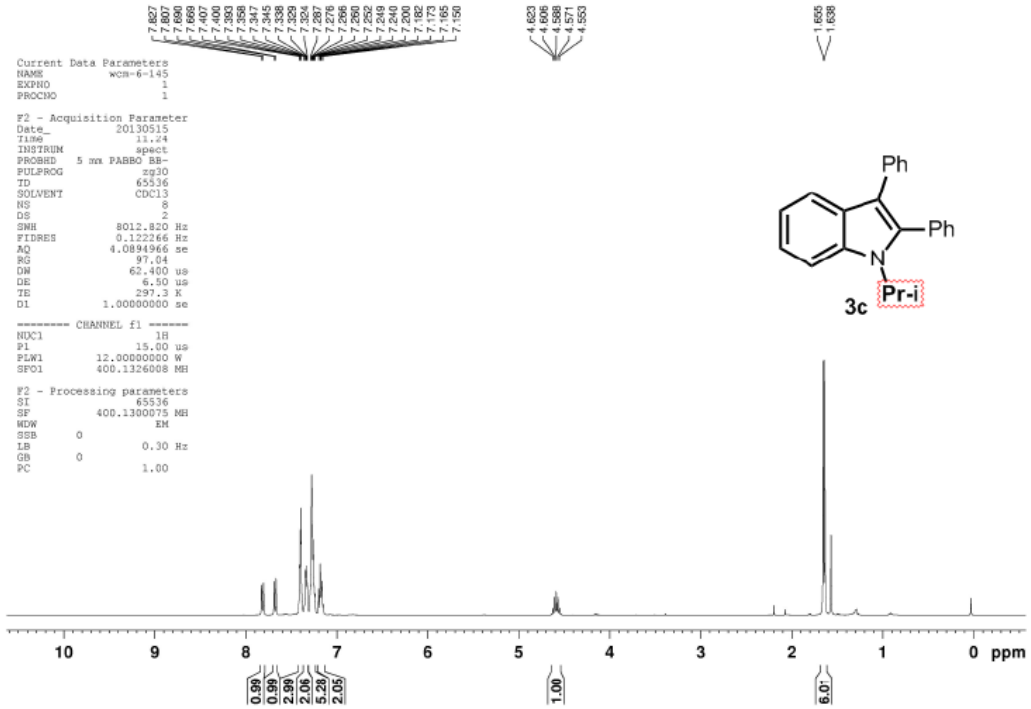

wcm-7-100
197.003
145.768
135.388
129.966
118.026
30.586
26.702
NAME wcm-7-100
EXPNO 2
PROCNO 1
Date_ 20130715
Time 19.16
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 146
DS 0
SWH 19493.178 Hz
FIDRES 0.594885 Hz
AQ 0.8405492 sec
RG 1024
DW 25.650 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.90 usec
PL1 -1.10 dB
PL1W 38.18405151 W
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 16.85 dB
PL13 16.85 dB
PL2W 8.31434441 W
PL12W 0.17172280 W
PL13W 0.17172280 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677424 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
NO
Ac
1n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

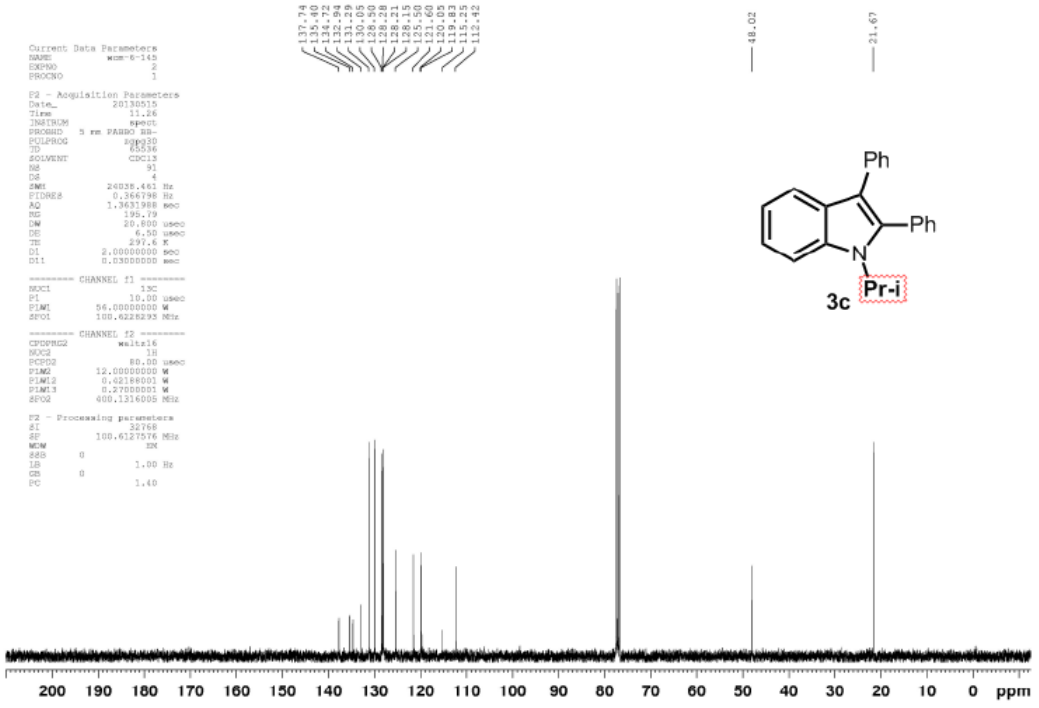

Solvent:CDCl3
7.861
7.841
7.466
7.446
7.435
7.427
7.422
7.413
7.409
7.383
7.377
7.365
7.349
7.330
7.311
7.292
7.240
7.231
7.220
7.214
7.196
3.714
Current Data Parameters
NAME wcm-6-91
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130328
Time 11.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 86.73
DW 62.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
Ph
N
3a
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
11.38
1.80
3.08

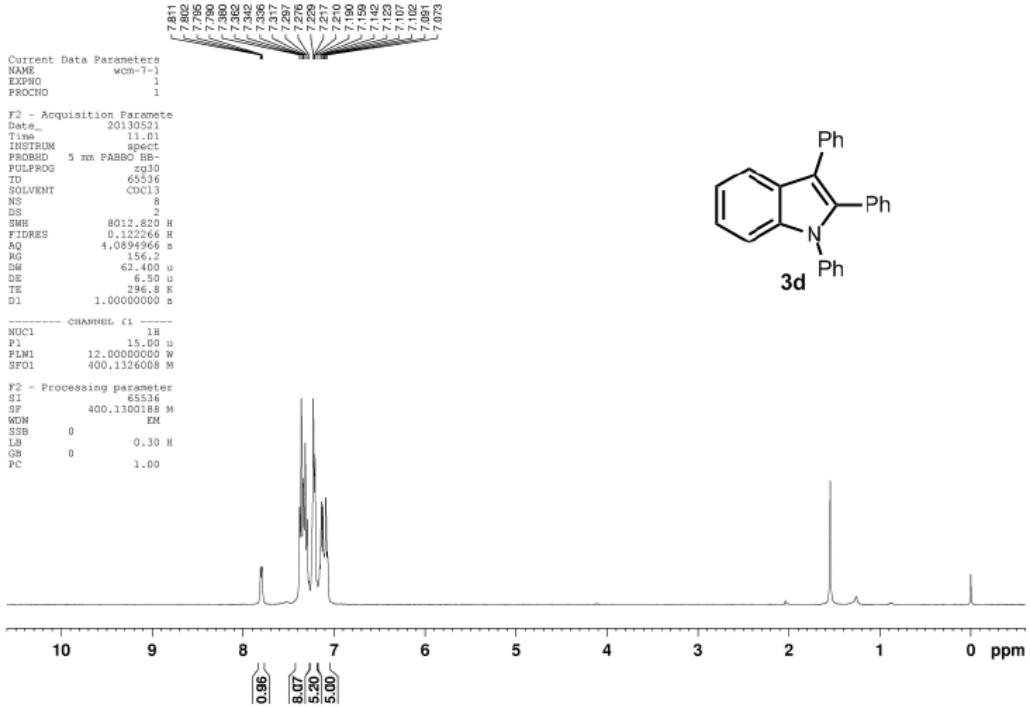

137.85
137.45
135.35
132.03
131.28
131.00
128.51
128.30
128.15
127.10
125.62
120.90
120.32
119.74
115.22
109.70
31.06
Current Data Parameters
NAME wcm-6-91
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130328
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 76
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
Ph
N
3a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

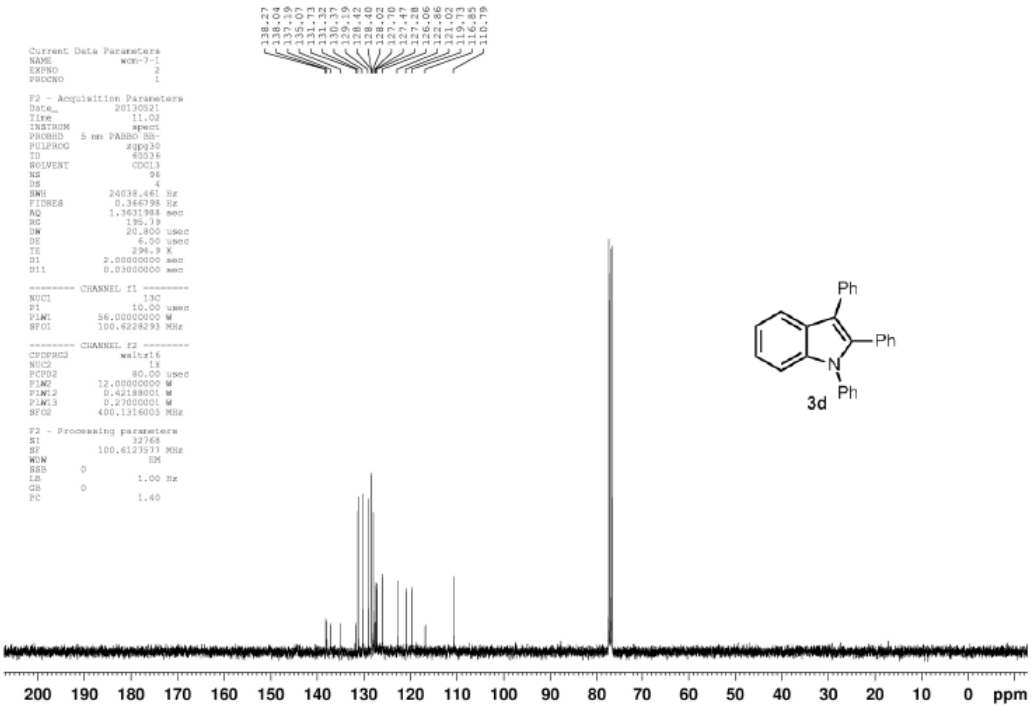

7.853
7.833
7.482
7.461
7.454
7.420
7.418
7.407
7.402
7.396
7.382
7.372
7.363
7.357
7.343
7.340
7.322
7.299
7.281
7.259
7.235
7.233
7.215
7.198
7.196
7.181
7.167
7.164
4.191
4.173
4.155
4.137
1.334
1.316
1.298
Current Data Parameters
NAME wcm-6-143
EXPNO 1
PROCNO 1
F2 - Acquisition Parame
Date_ 20130514
Time 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820
FIDRES 0.122266
AQ 4.0894966
RG 97.04
DW 62.400
DE 6.50
TE 296.6
D1 1.00000000
CHANNEL f1
NUC1 1H
P1 15.80
PLW1 12.00000000
SFO1 400.1326008
F2 - Processing parame
SI 65536
SF 400.1300105
WDN EM
SSB 0
LB 0.30
GB 0
PC 1.00
Ph
Ph
N
Et
3b
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
5.00
5.22
2.07
2.00
3.06

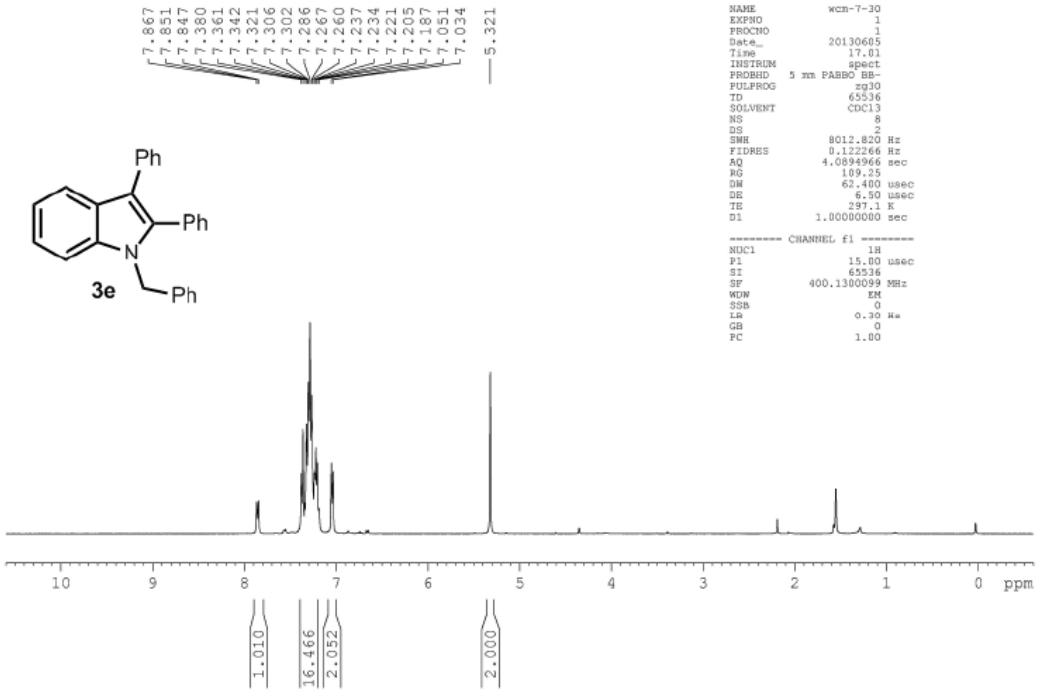

137.41
136.21
135.36
132.39
131.20
129.95
128.85
128.23
127.39
125.54
122.16
120.13
119.40
115.45
109.92
38.77
15.52
Current Data Parameters
NAME wcm-6-143
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130514
Time 14.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 137
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.79
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127587 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
Ph
N
Et
3b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

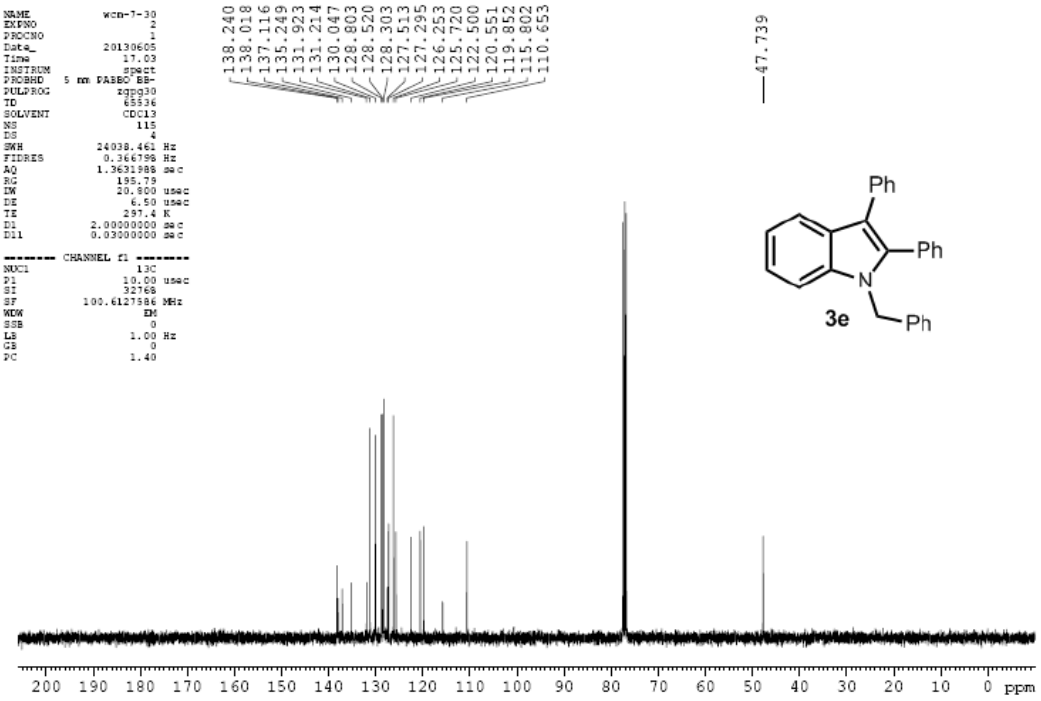

7.827
7.807
7.690
7.669
7.407
7.400
7.393
7.358
7.347
7.345
7.338
7.329
7.324
7.287
7.276
7.266
7.260
7.252
7.249
7.246
7.200
7.182
7.173
7.165
7.150
4.623
4.606
4.588
4.571
4.553
1.656
1.638
Current Data Parameters
NAME wcm-6-145
EXPNO 1
PROCNO 1
F2 - Acquisition Parameter
Date_ 20130515
Time 11.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 se
RG 97.04
DW 62.400 us
DE 6.50 us
TE 297.3 K
D1 1.00000000 se
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 us
PLW1 12.00000000 W
SFO1 400.1326008 MH
F2 - Processing parameters
SI 65536
SF 400.1300075 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
Ph
N
Pr-i
3c
10
9
8
7
6
5
4
3
2
1
0 ppm
0.99
0.99
2.99
2.06
5.28
2.05
1.00
6.01

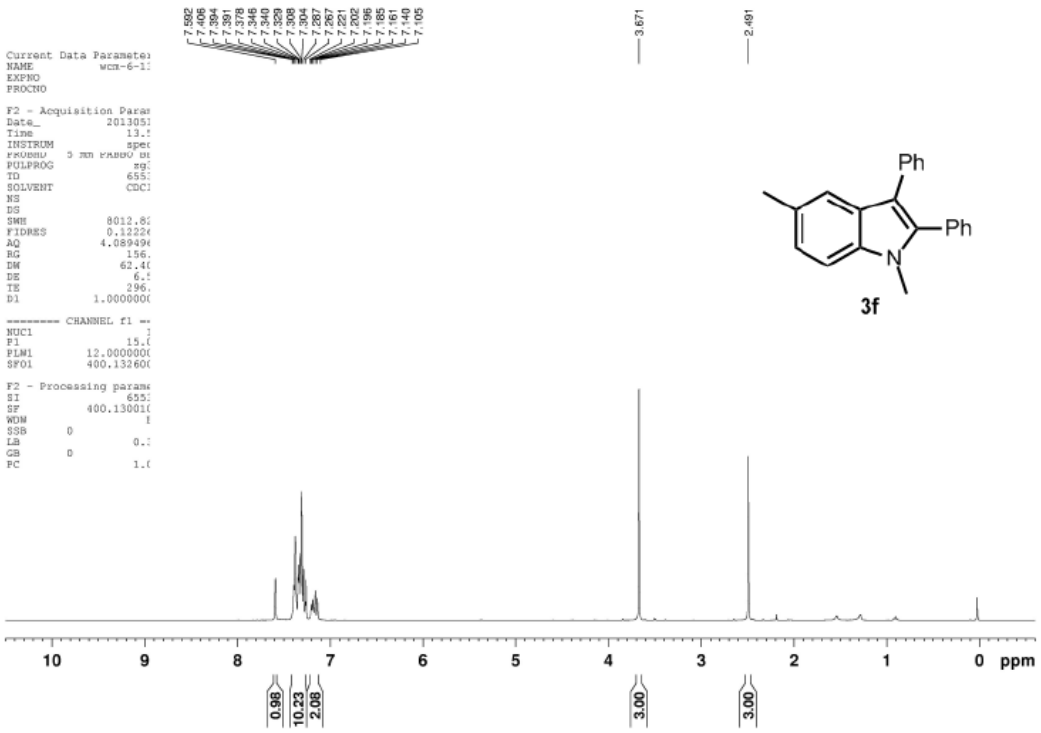

137.74
135.40
134.72
132.94
131.29
130.65
128.69
128.29
128.21
128.15
125.50
121.60
120.05
119.83
115.25
112.42
48.02
21.67
Current Data Parameters
NAME wcm-6-145
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130515
Time 11.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 91
DS 4
SWH 26038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 199.79
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.02188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127576 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
Ph
N
Pr-i
3c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

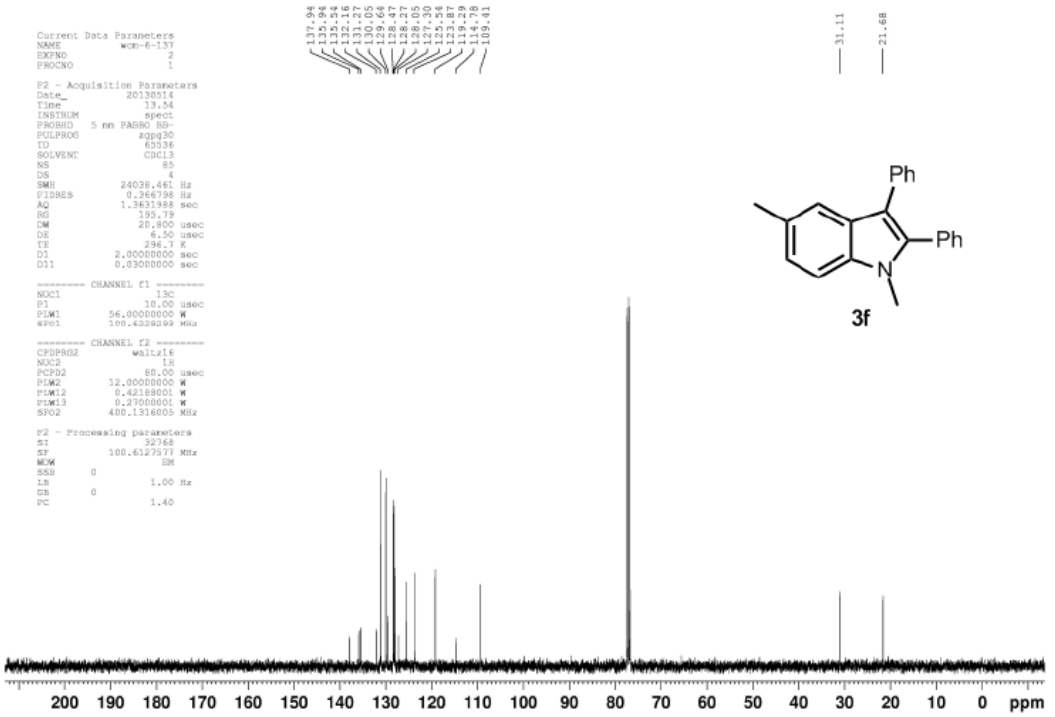

7.811
7.802
7.795
7.790
7.380
7.362
7.342
7.336
7.317
7.297
7.276
7.229
7.217
7.210
7.190
7.159
7.142
7.123
7.107
7.102
7.091
7.073
Current Data Parameters
NAME wcm-7-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130521
Time 11.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 156.2
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300188 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
Ph
N
Ph
3d
10
9
8
7
6
5
4
3
2
1
0 ppm
0.96
8.07
5.20
5.00

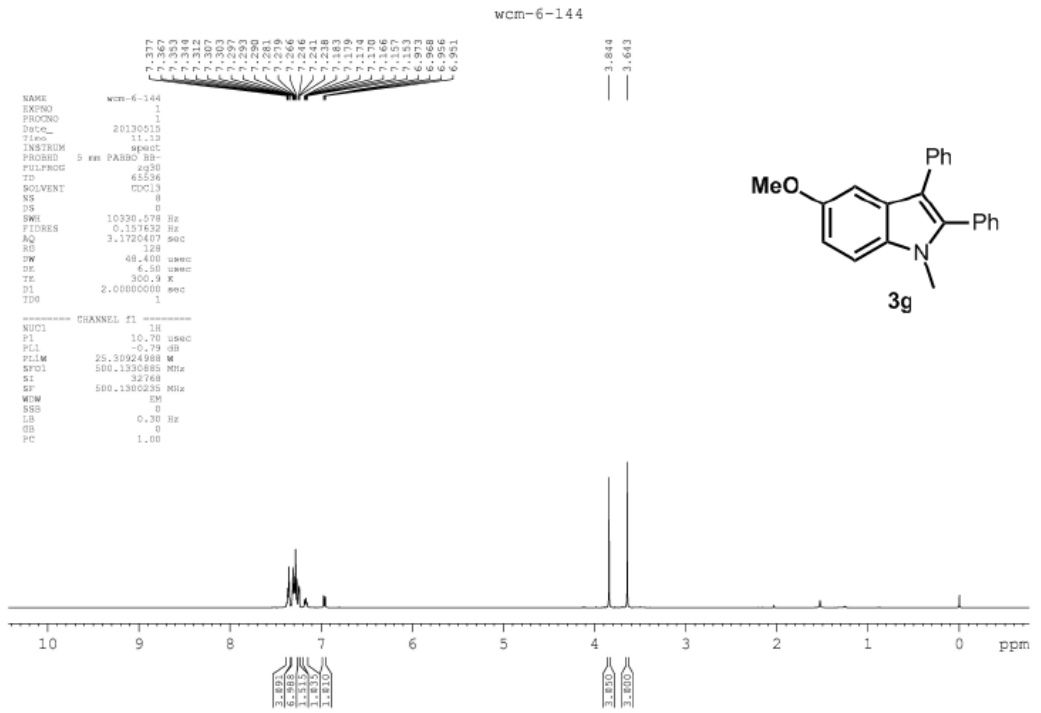

138.27
138.04
135.19
135.07
131.73
131.32
130.37
129.19
128.42
128.40
128.02
123.70
122.47
122.28
121.06
122.86
121.02
119.73
116.85
110.19
Current Data Parameters
NAME wcm-7-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130521
Time 11.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 96
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 199.19
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127533 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
Ph
N
Ph
3d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

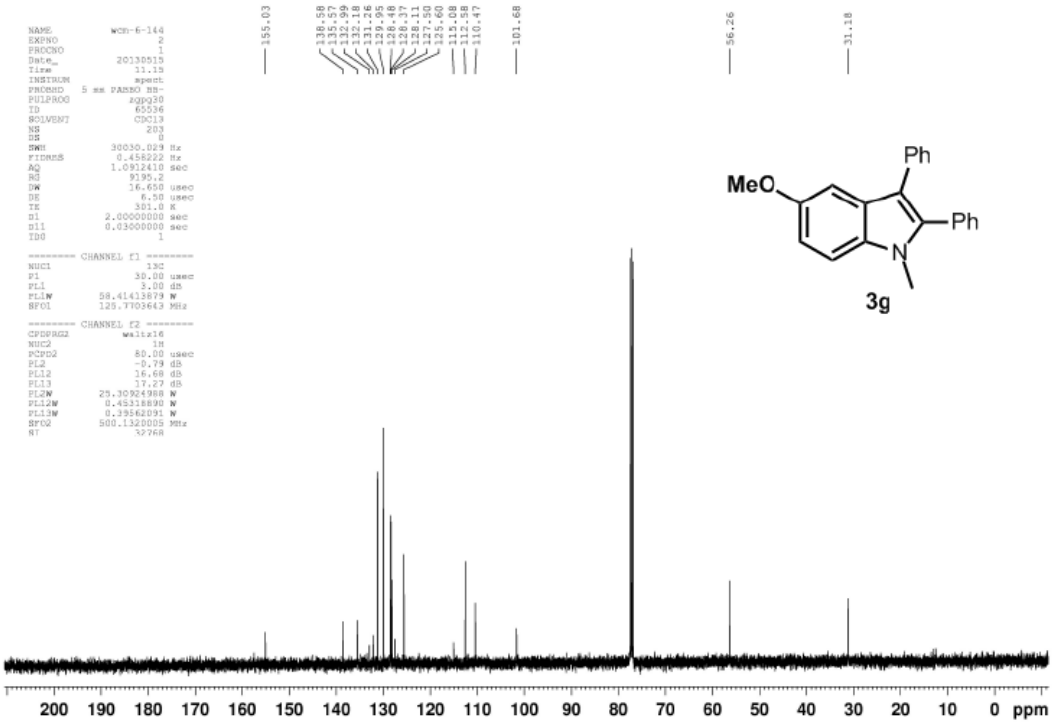

7.867
7.851
7.847
7.380
7.361
7.342
7.321
7.306
7.302
7.286
7.267
7.260
7.237
7.234
7.221
7.205
7.187
7.051
7.034
5.321
Ph
Ph
N
Ph
3e
NAME wcm-7-30
EXPNO 1
PROCNO 1
Date_ 20130605
Time 17.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 109.25
DW 62.400 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
1.010
16.466
2.052
2.000

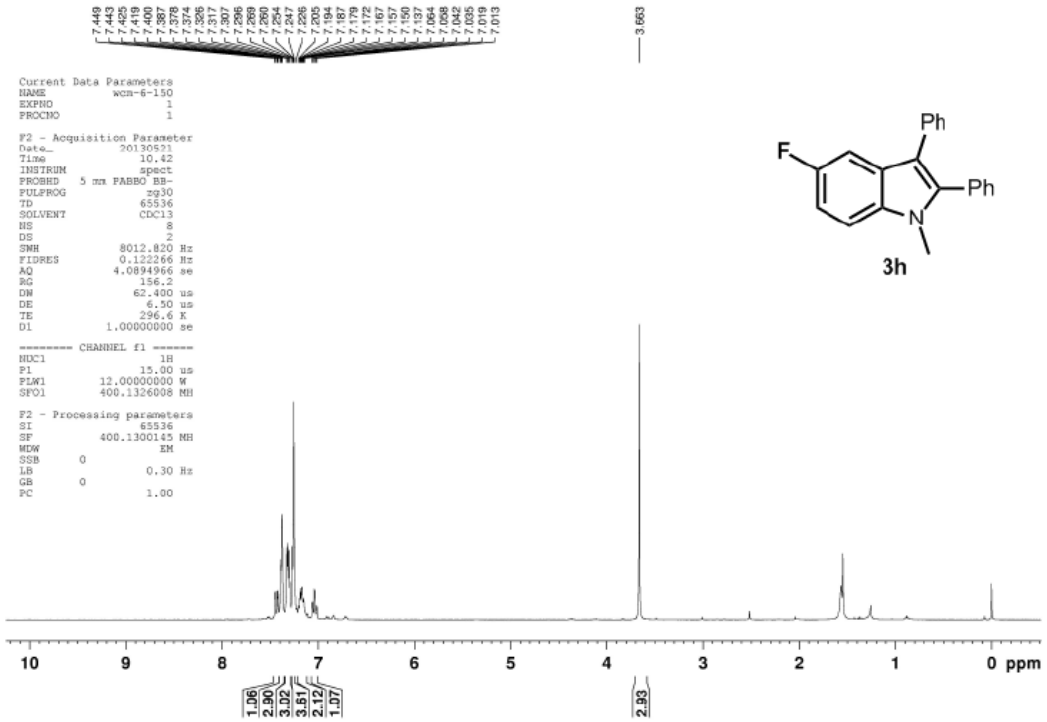

NAME wcm-7-30
EXPNO 2
PROCNO 1
Date_ 20130605
Time 17.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 115
DS 4
SWH 24038.461 Hz
FIDRES 0.366796 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127586 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
138.240
138.018
137.116
135.249
131.923
131.214
130.047
128.803
128.520
128.303
127.513
127.295
126.253
125.720
122.500
120.551
119.852
115.802
110.653
47.739
Ph
Ph
N
Ph
3e
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

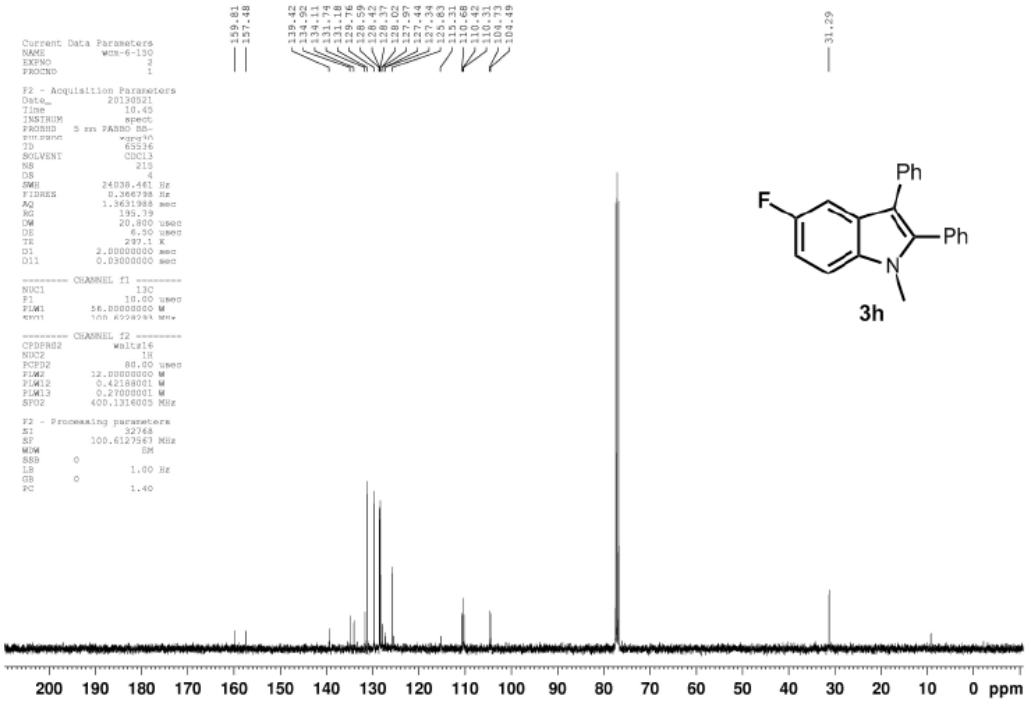

7.592
7.406
7.394
7.391
7.378
7.346
7.340
7.329
7.308
7.304
7.287
7.267
7.221
7.202
7.196
7.185
7.161
7.140
7.105
3.671
2.491
Ph
Ph
N
3f
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
10.23
2.08
3.00
3.00

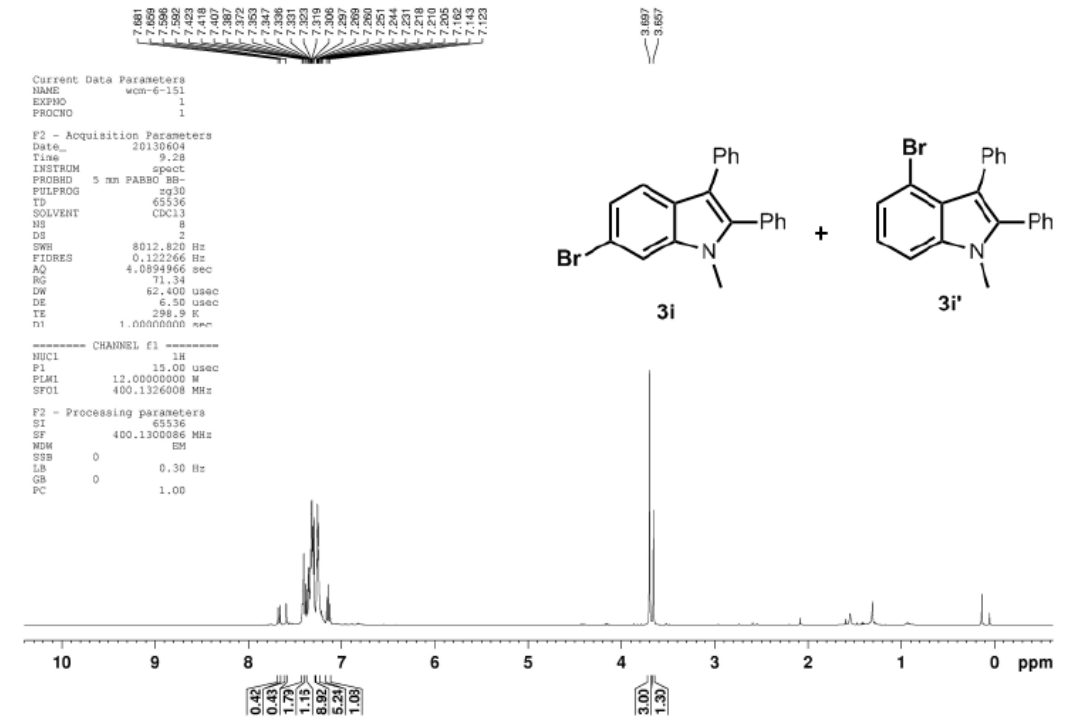

137.94
135.94
135.16
132.18
131.27
130.05
129.64
128.47
128.27
128.05
127.30
125.54
123.87
119.29
114.78
109.41
31.11
21.68
Ph
Ph
N
3f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

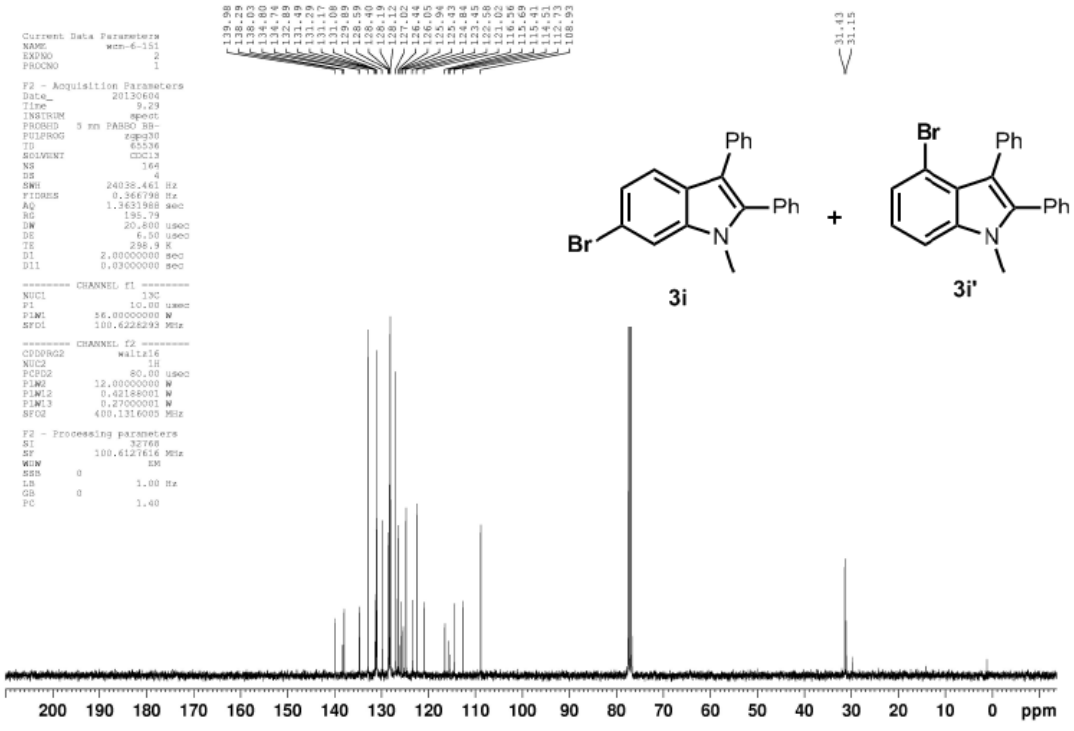

wcm-6-144
7.377
7.367
7.353
7.344
7.312
7.307
7.303
7.297
7.293
7.290
7.281
7.279
7.266
7.246
7.241
7.238
7.183
7.179
7.174
7.170
7.166
7.157
7.153
6.973
6.968
6.956
6.951
3.844
3.643
NAME wcm-6-144
EXPNO 1
PROCNO 1
Date_ 20130515
Time 11.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 300.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 -0.79 dB
PL1W 25.30924988 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300235 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
Ph
Ph
N
3g
10
9
8
7
6
5
4
3
2
1
0
ppm
3.89
6.98
6.51
1.83
1.81
3.85
3.80

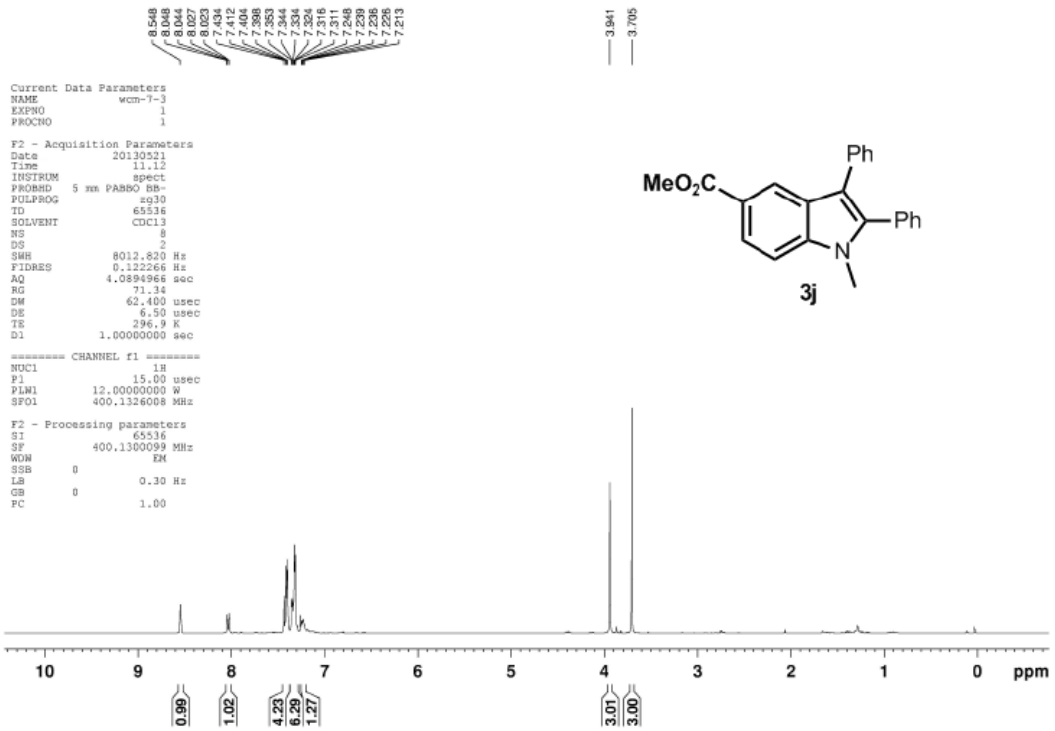

155.03
138.58
135.57
132.99
131.18
129.95
128.48
128.37
128.11
127.50
125.60
115.08
112.58
110.47
101.68
56.26
31.18
NAME wcm-6-144
EXPNO 2
PROCNO 1
Date_ 20130515
Time 11.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 203
DS 2
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 9195.2
DW 16.650 usec
DE 6.50 usec
TE 301.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 30.00 usec
PL1 3.00 dB
PL1W 58.41413879 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -0.79 dB
PL12 16.68 dB
PL13 17.27 dB
PL2W 25.30924988 W
PL12W 0.45318890 W
PL13W 0.39562091 W
SFO2 500.1320005 MHz
SI 32768
MeO
Ph
Ph
N
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

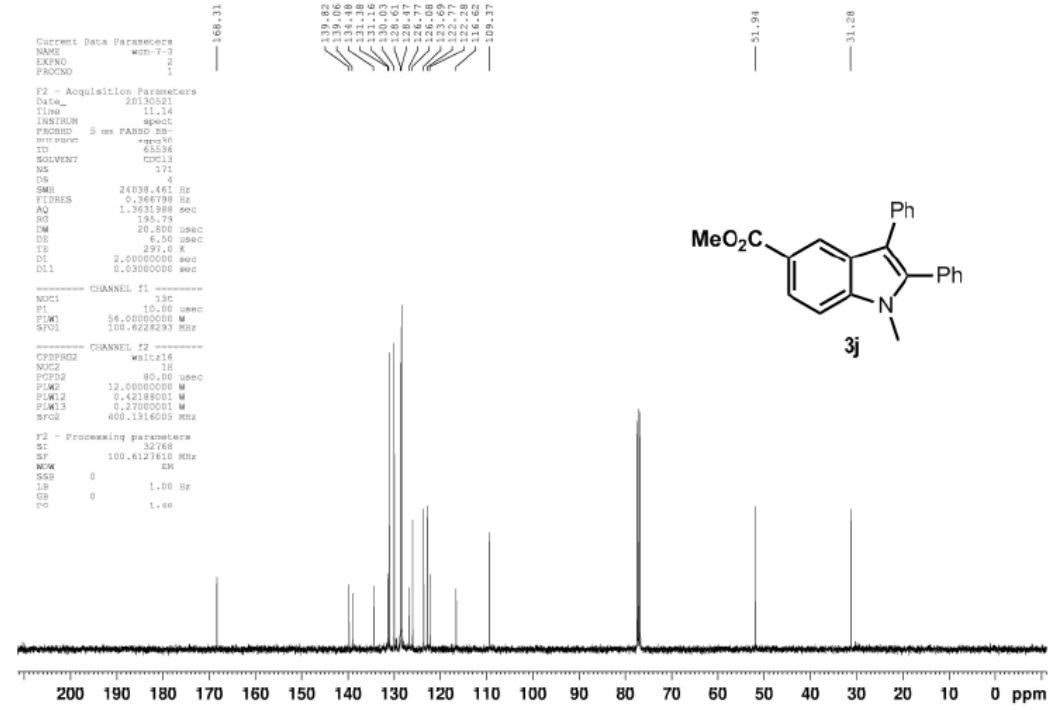

7.449
7.443
7.425
7.419
7.400
7.387
7.378
7.374
7.326
7.317
7.307
7.296
7.269
7.260
7.254
7.247
7.226
7.205
7.194
7.187
7.179
7.172
7.167
7.157
7.150
7.137
7.064
7.058
7.042
7.035
7.019
7.013
3.663
Current Data Parameters
NAME wcm-6-150
EXPNO 1
PROCNO 1
F2 - Acquisition Parameter
Date_ 20130521
Time 10.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 se
RG 156.2
DW 62.400 us
DE 6.50 us
TE 296.6 K
D1 1.00000000 se
======== CHANNEL f1 =======
NUC1 1H
P1 15.00 us
PLW1 12.00000000 W
SFO1 400.1326008 MH
F2 - Processing parameters
SI 65536
SF 400.1300145 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
F
Ph
N
3h
10 9 8 7 6 5 4 3 2 1 0 ppm
1.06
2.90
3.02
3.51
2.12
1.07
2.93

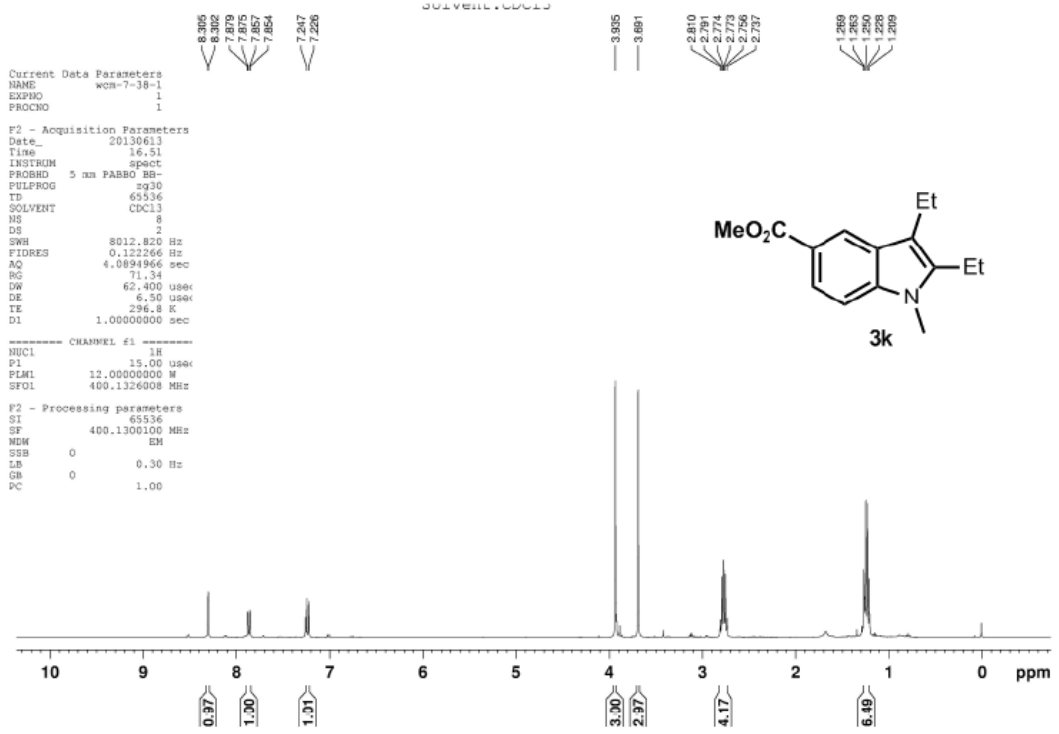

159.81
157.48
139.42
134.92
134.11
131.74
131.18
128.76
128.59
128.42
128.37
128.02
127.87
127.44
127.34
125.83
115.21
110.68
110.42
110.31
104.73
104.49
31.29
Current Data Parameters
NAME wcm-6-150
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130521
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG wgpg90
TD 65536
SOLVENT CDCl3
NS 213
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228283 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127563 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
F
Ph
N
3h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

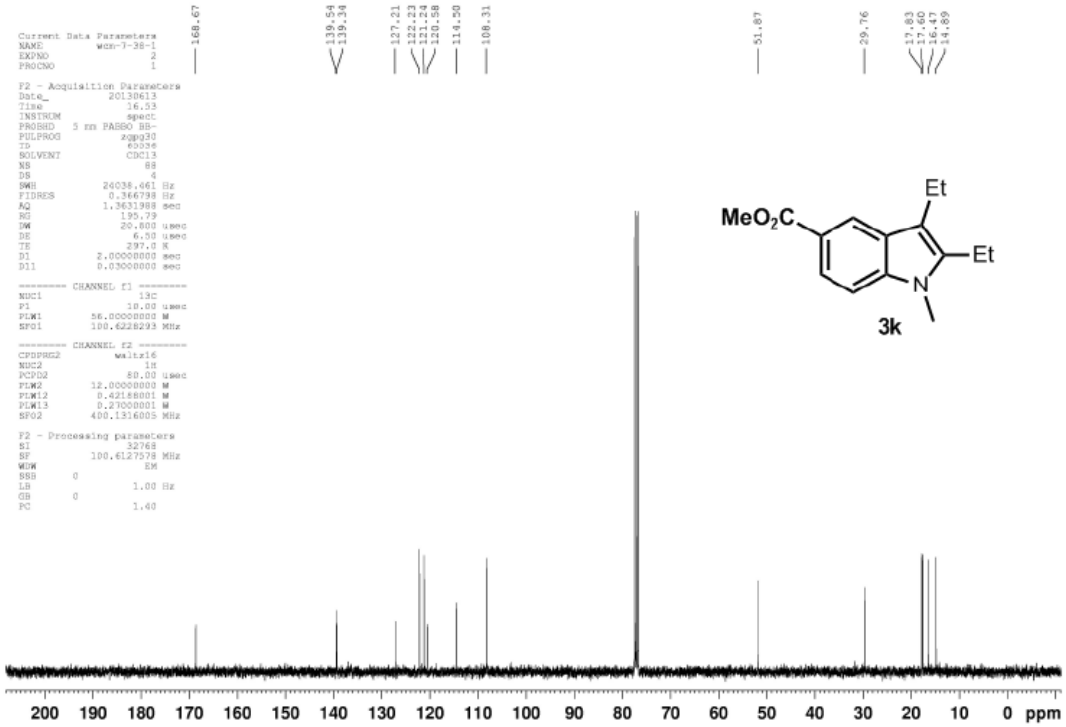

7.681
7.658
7.598
7.592
7.423
7.418
7.407
7.387
7.372
7.353
7.347
7.336
7.331
7.323
7.319
7.306
7.297
7.269
7.260
7.251
7.244
7.231
7.218
7.210
7.205
7.162
7.143
7.123
3.697
3.657
Current Data Parameters
NAME wcm-6-151
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130604
Time 9.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.34
DW 62.400 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
Br
Ph
N
3i
+
Br
Ph
Ph
N
3i'
10
9
8
7
6
5
4
3
2
1
0
ppm
0.42
0.43
1.79
1.15
8.92
5.24
1.08
3.00
1.30

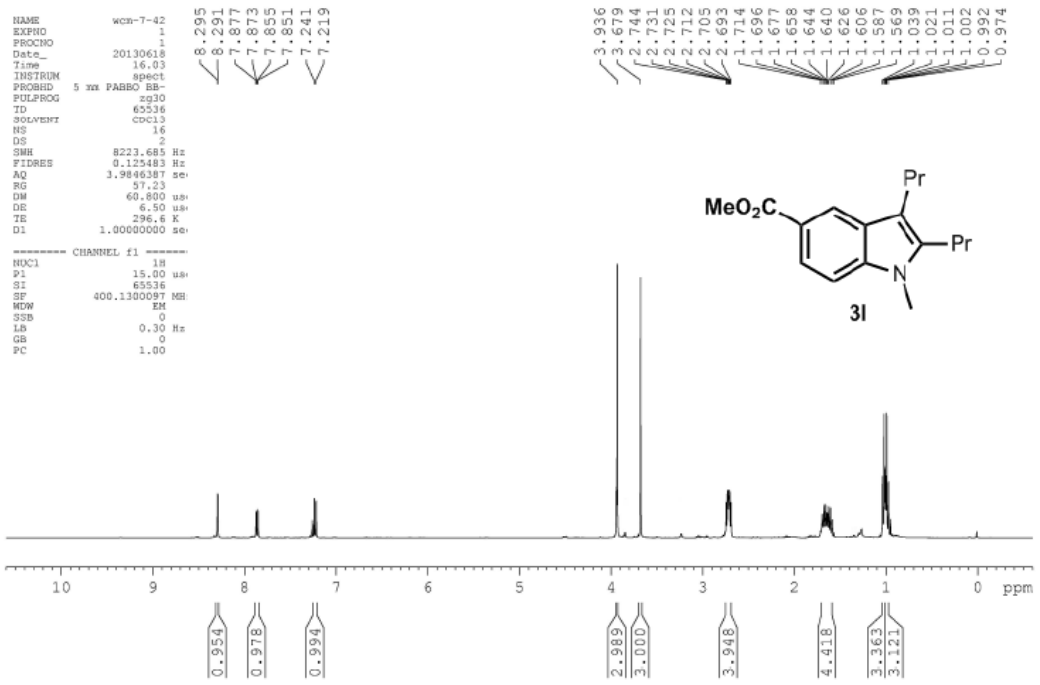

139.98
138.29
138.03
136.80
134.74
132.89
131.49
131.29
131.17
131.08
129.89
128.59
128.40
128.19
128.12
127.94
126.05
125.96
125.43
124.84
123.55
123.08
121.02
116.56
115.69
115.41
114.51
114.33
108.93
31.43
31.15
Current Data Parameters
NAME wcm-6-151
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130604
Time 9.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 164
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127616 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
Br
Ph
N
3i
+
Br
Ph
Ph
N
3i'
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

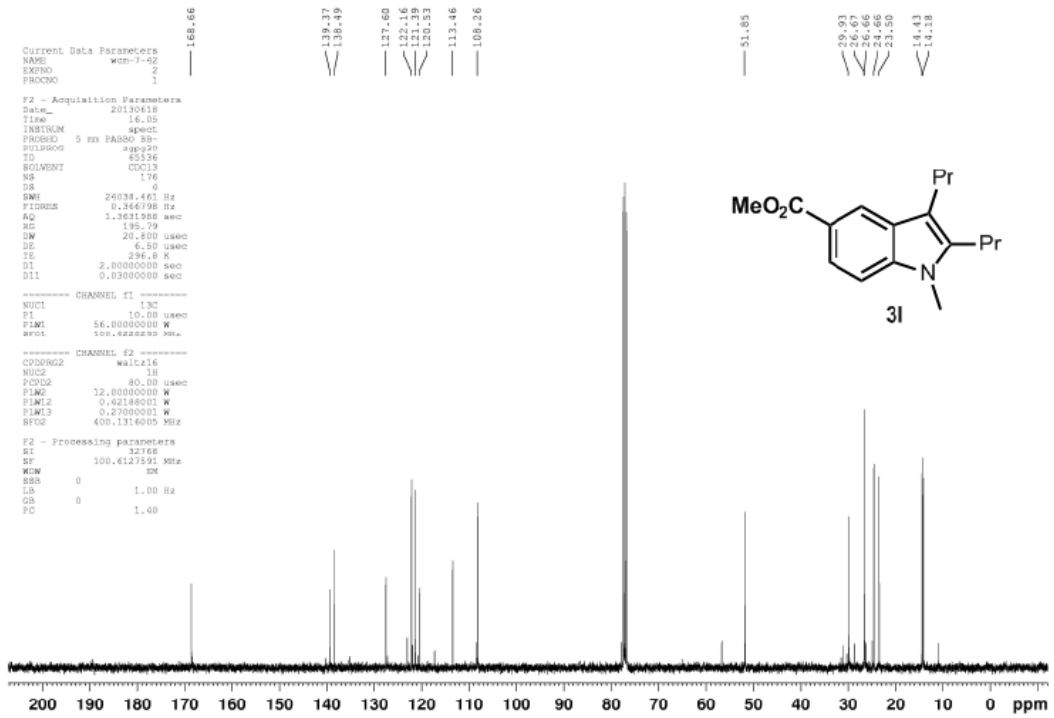

8.548
8.048
8.044
8.027
8.023
7.434
7.412
7.404
7.398
7.353
7.344
7.334
7.324
7.316
7.311
7.248
7.239
7.236
7.226
7.213
3.941
3.705
Current Data Parameters
NAME wcm-7-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20130521
Time 11.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.34
DW 62.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
MeO2C
Ph
N
3j
10 9 8 7 6 5 4 3 2 1 0 ppm
0.99 1.02 4.23 6.29 1.27 3.01 3.00

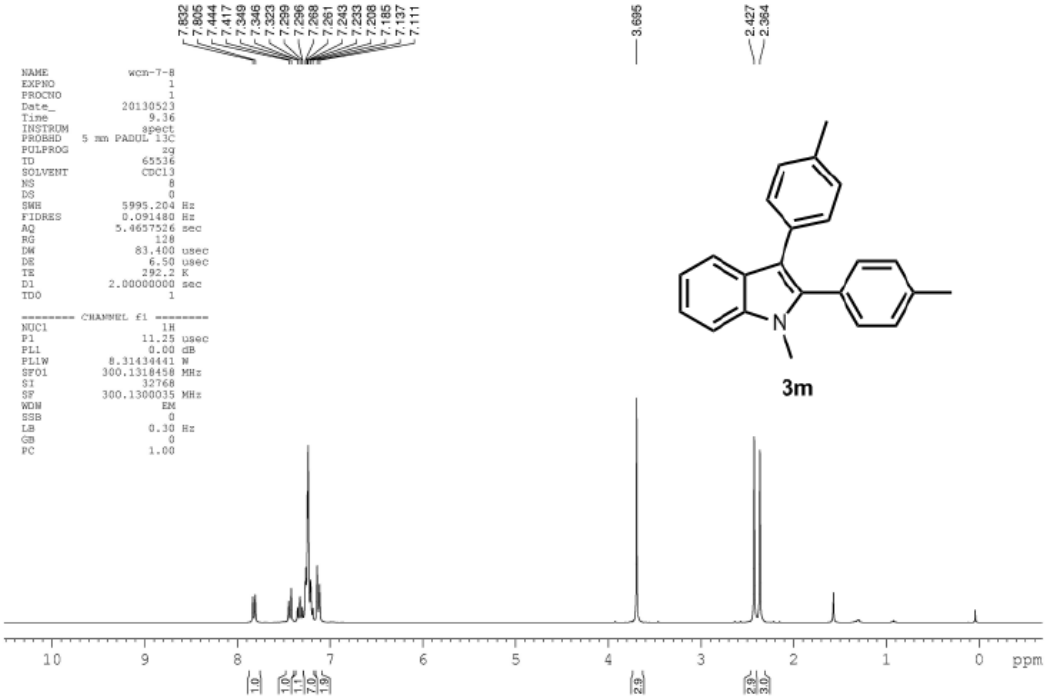

168.31
139.82
139.66
137.40
131.38
131.16
130.03
128.61
128.47
126.77
126.08
123.69
122.77
122.28
112.62
109.37
51.94
31.28
Current Data Parameters
NAME wcm-7-3
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130521
Time 11.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 171
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
MeO2C
Ph
N
3j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

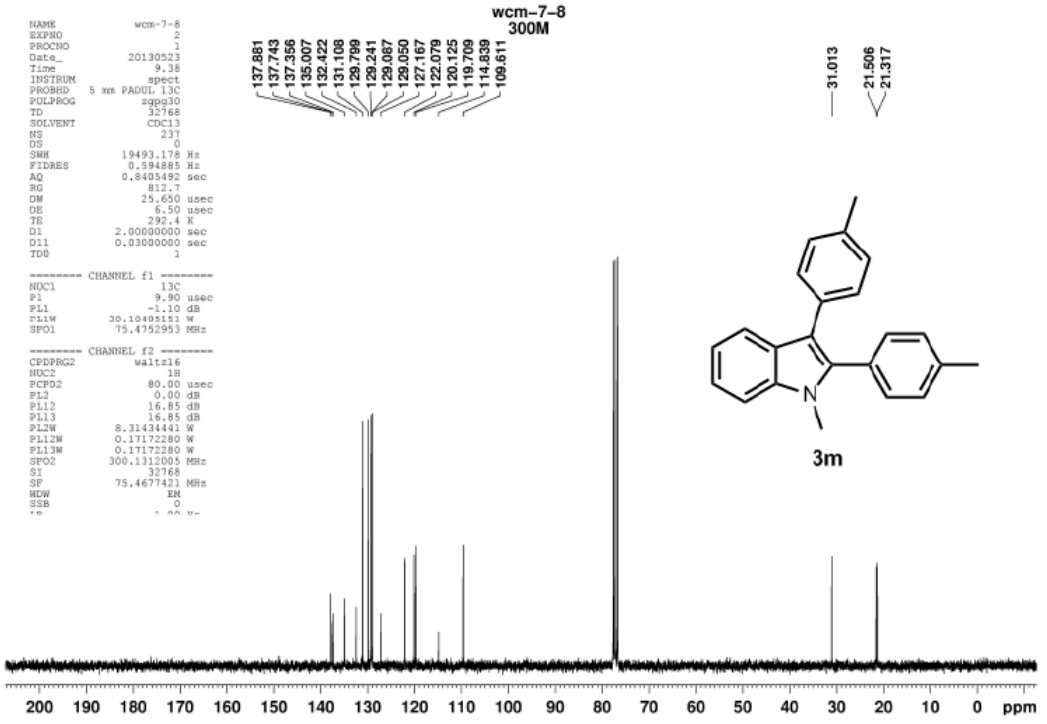

8.305
8.302
7.879
7.875
7.857
7.854
7.247
7.226
3.935
3.691
2.810
2.791
2.774
2.773
2.756
2.737
1.269
1.263
1.250
1.228
1.209
Current Data Parameters
NAME wcm-7-38-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130613
Time 16.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.34
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO2C
Et
Et
N
3k
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
1.00
1.01
3.00
2.97
4.17
6.49

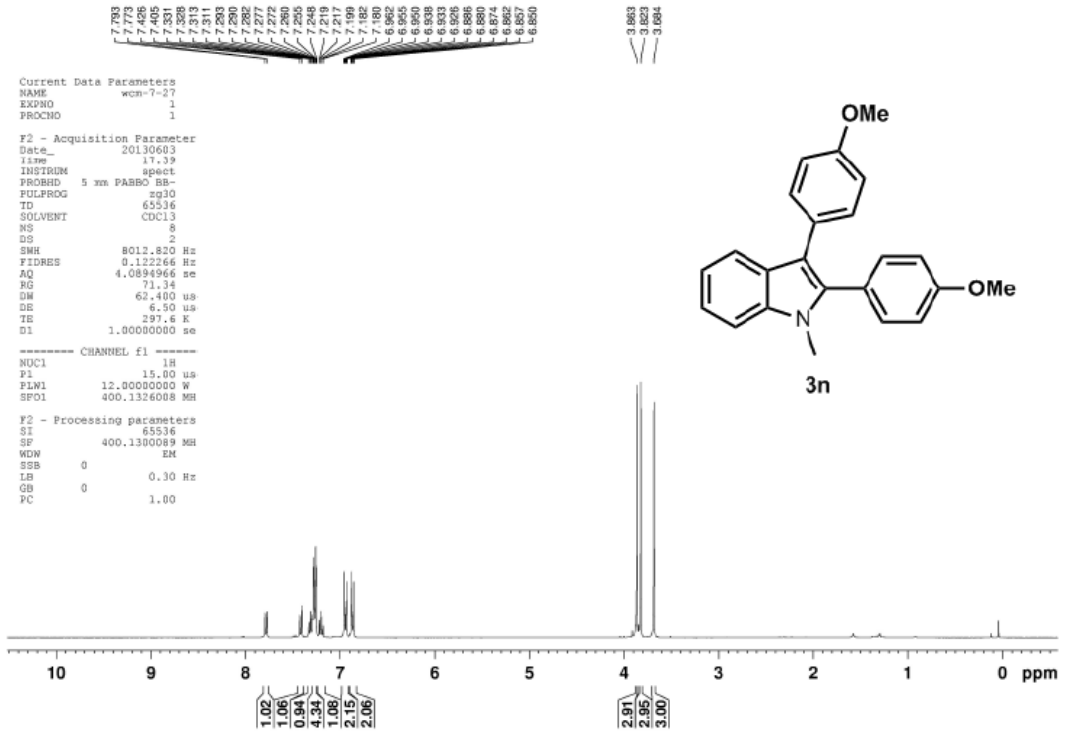

168.67
139.54
139.34
127.21
122.23
121.28
120.58
114.50
108.31
51.87
29.76
17.83
17.60
16.47
14.89
Current Data Parameters
NAME wcm-7-38-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130613
Time 16.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 88
DS 4
SWH 26038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127578 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
MeO2C
Et
Et
N
3k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

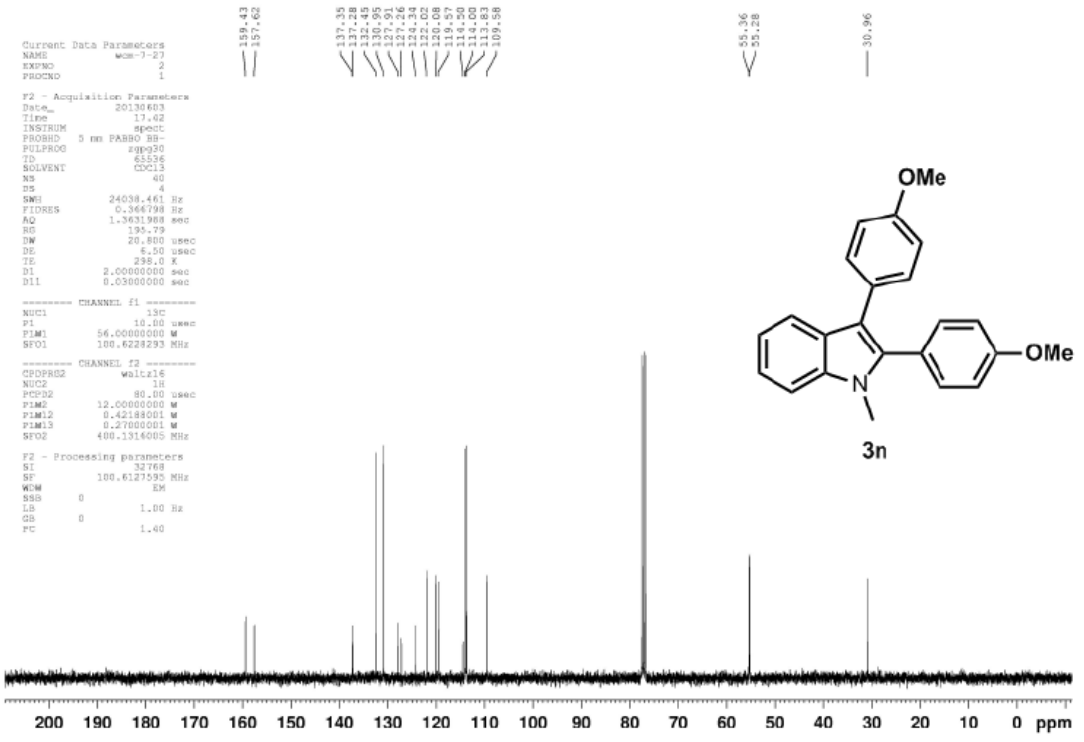

MeO2C
Pr
Pr
N
3l
ppm

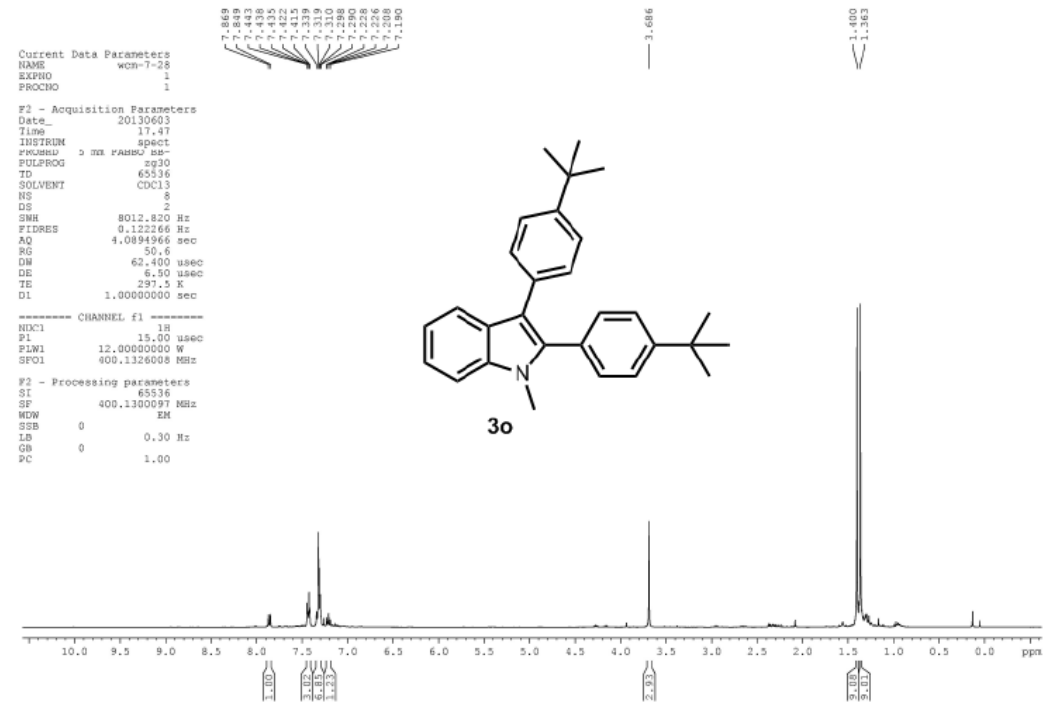

MeO2C
Pr
Pr
N
3l
ppm

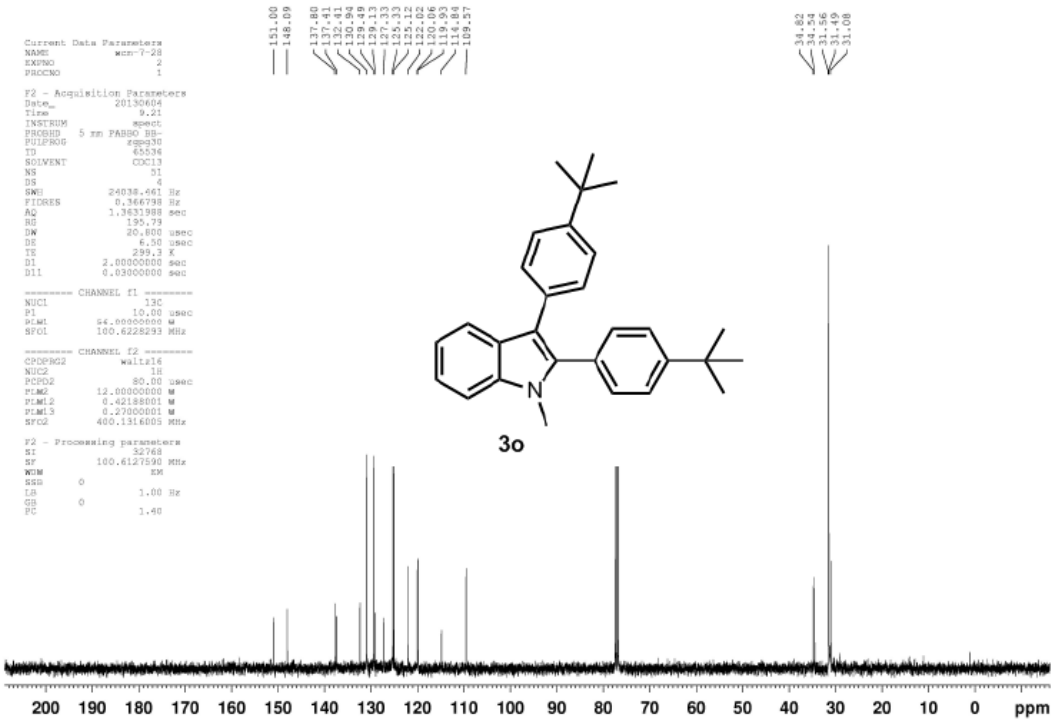

7.832
7.805
7.444
7.417
7.349
7.346
7.323
7.299
7.296
7.288
7.261
7.243
7.233
7.208
7.185
7.137
7.111
3.695
2.427
2.364
NAME wcm-7-8
EXPNO 1
PROCNO 1
Date_ 20130523
Time 9.36
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 128
DW 83.400 usec
DE 6.50 usec
TE 292.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.25 usec
PL1 0.00 dB
PL1W 8.31434441 W
SFO1 300.1318458 MHz
SI 32768
SF 300.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
3m
10 9 8 7 6 5 4 3 2 1 0 ppm
1.0 1.0 1.1 1.9 1.9 2.9 2.8 3.0

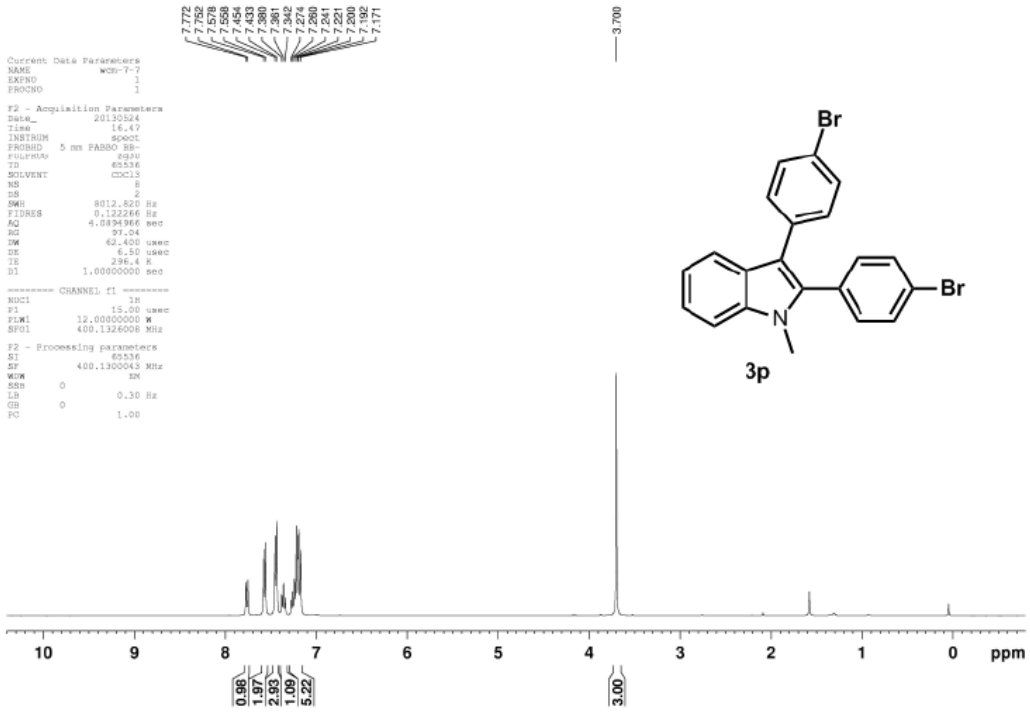

wcm-7-8
300M
137.881
137.743
137.356
135.007
132.422
131.108
129.799
129.241
129.067
129.050
127.167
122.079
120.125
119.709
114.839
109.611
31.013
21.506
21.317
NAME wcm-7-8
EXPNO 2
PROCNO 1
Date_ 20130523
Time 9.38
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 237
DS 0
SWH 19493.178 Hz
FIDRES 0.594885 Hz
AQ 0.8405492 sec
RG 812.7
DW 25.650 usec
DE 6.50 usec
TE 292.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.90 usec
PL1 -1.10 dB
PL1W 30.10405151 W
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 16.85 dB
PL13 16.85 dB
PL2W 8.31434441 W
PL12W 0.17172280 W
PL13W 0.17172280 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677421 MHz
WDW EM
SSB 0
3m
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

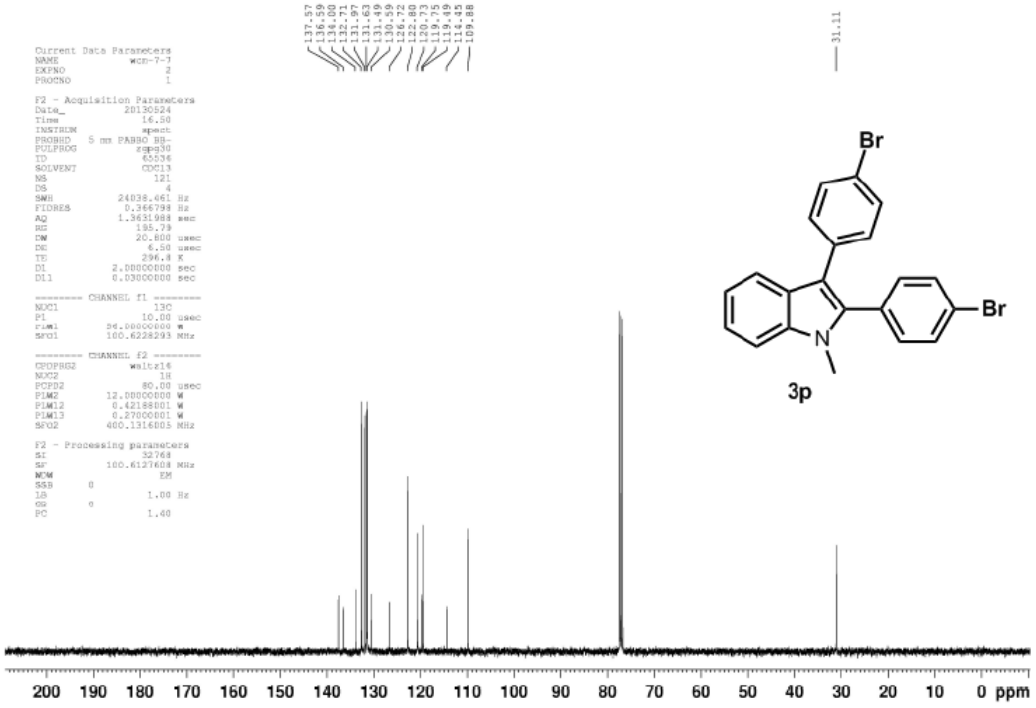

7.793
7.773
7.426
7.405
7.331
7.328
7.313
7.311
7.291
7.290
7.282
7.277
7.272
7.260
7.255
7.248
7.219
7.217
7.199
7.182
7.180
6.962
6.955
6.950
6.938
6.933
6.926
6.886
6.880
6.874
6.862
6.857
6.850
3.863
3.823
3.684
Current Data Parameters
NAME wcm-7-27
EXPNO 1
PROCNO 1
F2 - Acquisition Parameter
Date_ 20130603
Time 17.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 se
RG 71.34
DW 62.400 us
DE 6.50 us
TE 297.6 K
D1 1.00000000 se
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 us
PLW1 12.00000000 W
SFO1 400.1326008 MH
F2 - Processing parameters
SI 65536
SF 400.1300089 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
OMe
N
3n
10
9
8
7
6
5
4
3
2
1
0 ppm
1.02
1.06
0.94
4.34
1.08
2.15
2.06
2.91
2.95
3.00

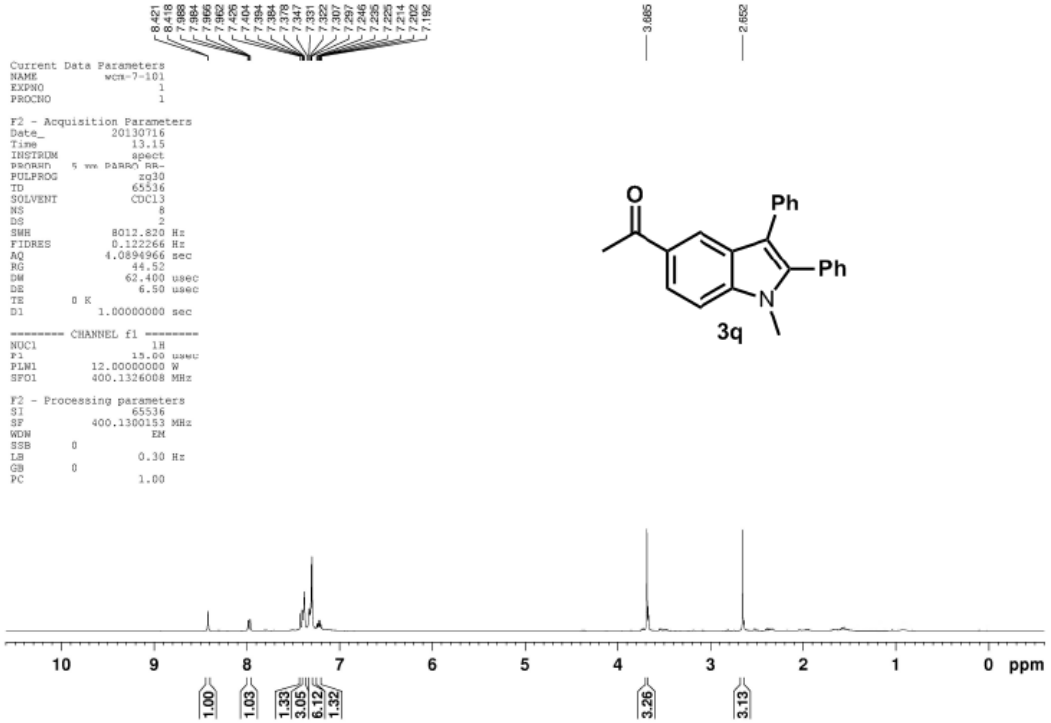

159.43
157.62
137.35
137.28
132.45
130.95
127.91
127.26
124.34
122.00
120.08
119.57
114.50
114.00
113.83
109.58
55.36
55.28
30.96
Current Data Parameters
NAME wcm-7-27
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130603
Time 17.62
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 40
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631968 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127595 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OMe
OMe
N
3n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

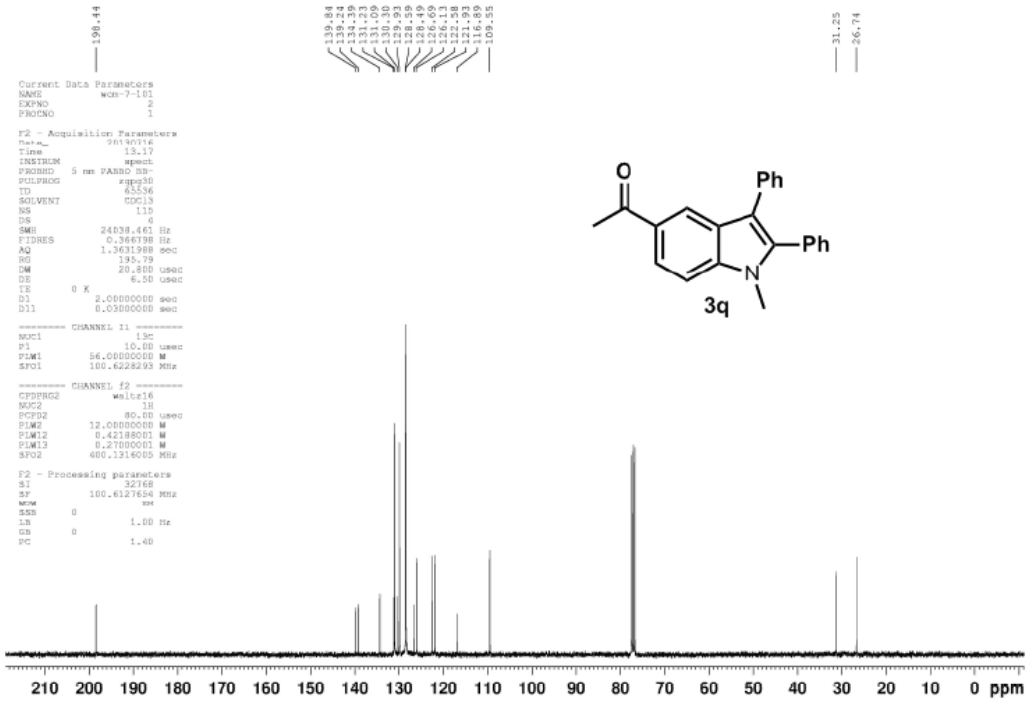

Current Data Parameters
NAME wcm-7-28
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130603
Time 17.47
INSTRUM spect
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 50.6
DW 62.400 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.869
7.849
7.443
7.438
7.435
7.422
7.415
7.339
7.319
7.310
7.298
7.290
7.228
7.226
7.208
7.190
3.686
1.400
1.363
3o
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
3.02
6.85
2.83
2.93
9.08
9.01

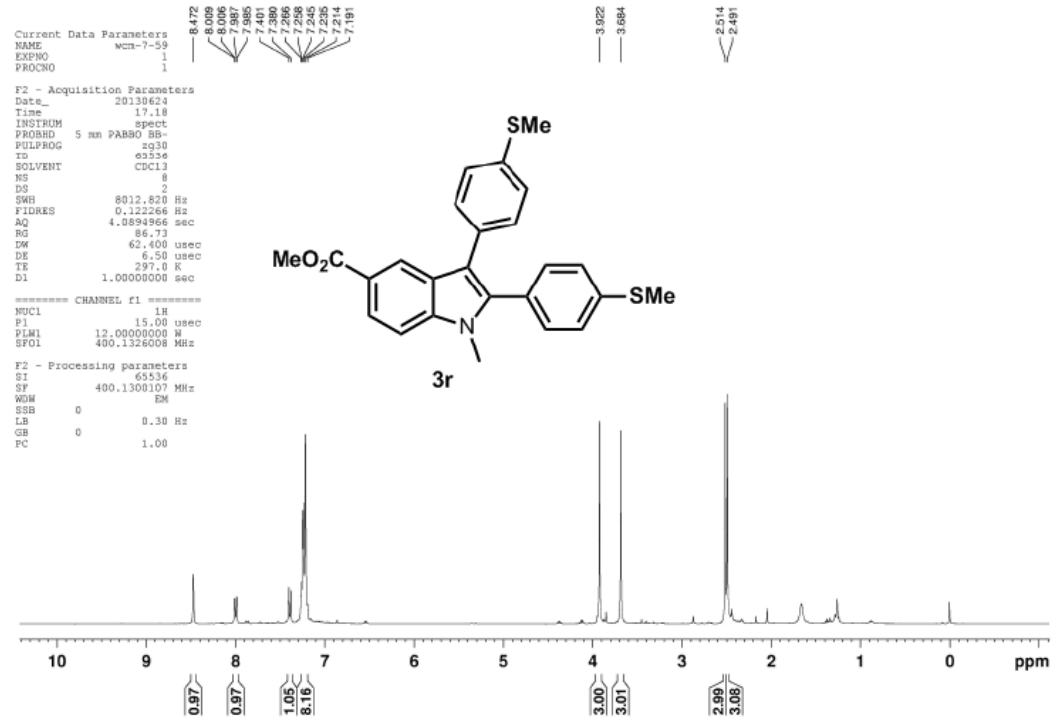

Current Data Parameters
NAME wcm-7-28
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130604
Time 9.21
INSTRUM spect
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 51
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TS 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W
SFO1 100.6228293 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316003 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
151.00
148.09
137.80
137.41
132.41
130.94
129.49
129.13
126.33
125.12
122.02
120.06
119.93
114.84
103.57
34.82
34.54
31.56
31.49
31.08
3o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

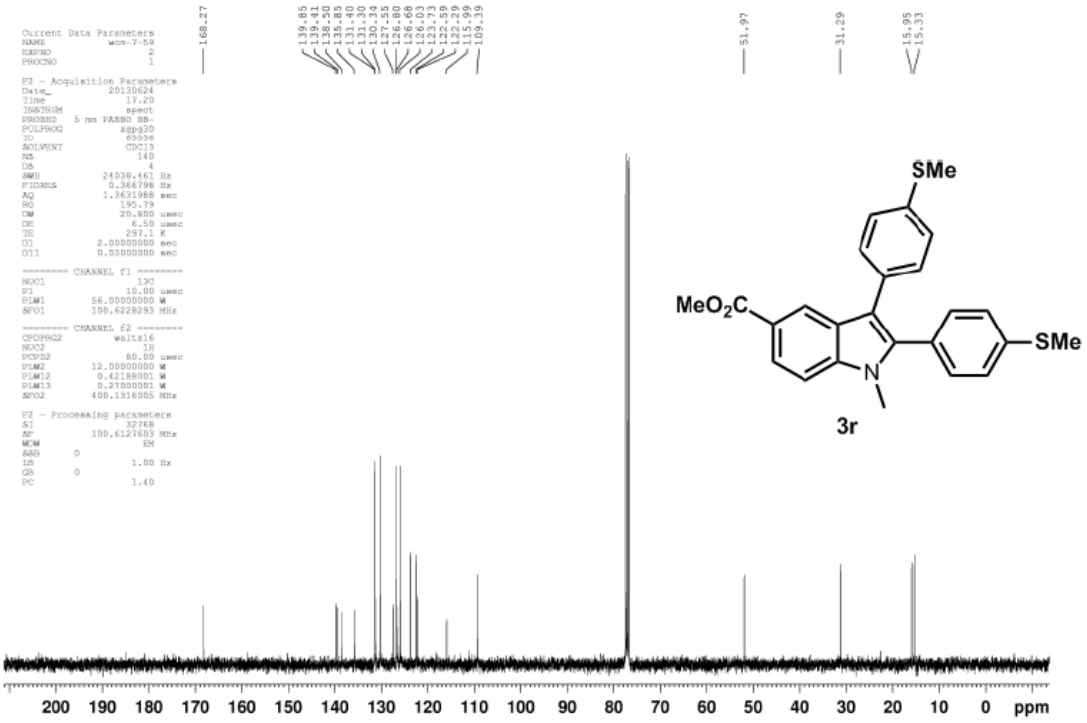

7.772
7.752
7.578
7.558
7.454
7.433
7.380
7.361
7.342
7.274
7.260
7.241
7.221
7.200
7.192
7.171
3.700
Br
Br
N
3p
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.97
2.93
1.09
5.22
3.00

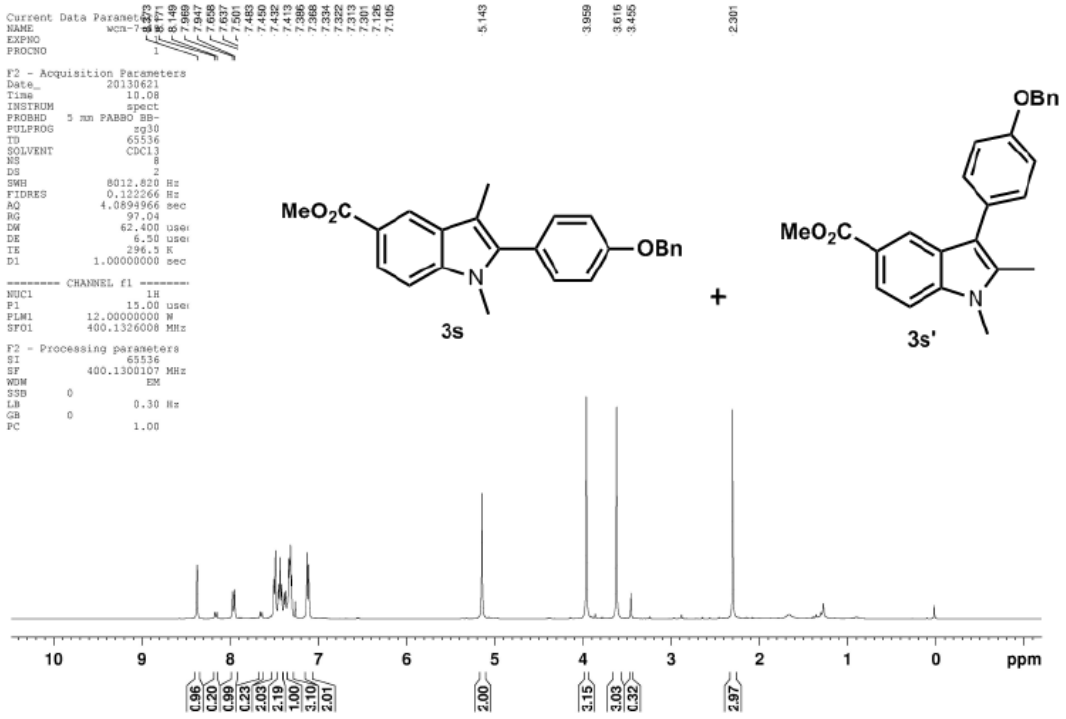

137.57
136.59
134.00
132.71
131.97
131.63
131.49
130.59
126.72
125.80
120.73
119.75
119.49
114.45
109.88
31.11
Br
Br
N
3p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

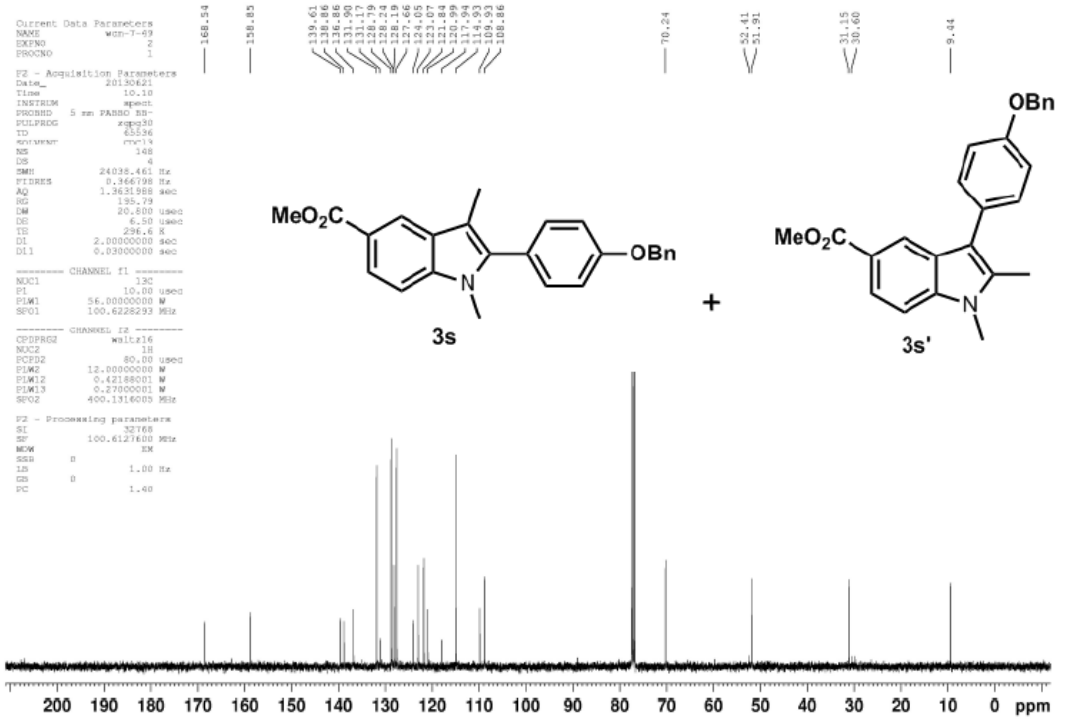

8.421
8.418
7.988
7.984
7.966
7.962
7.426
7.404
7.384
7.378
7.347
7.331
7.322
7.307
7.297
7.246
7.235
7.225
7.214
7.202
7.192
3.685
2.652
O
Ph
Ph
N
3q
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.03
1.33
3.05
6.12
1.32
3.26
3.13

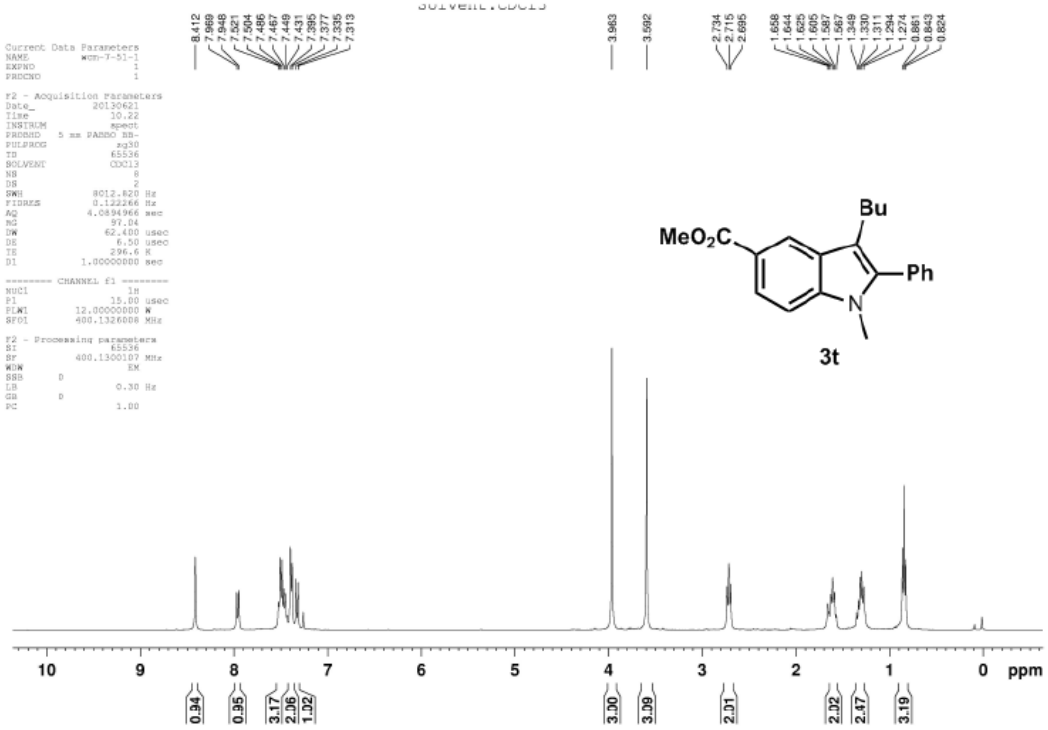

190.44
139.84
139.24
134.39
131.23
131.09
131.00
129.93
128.59
128.49
126.69
126.13
125.18
121.93
116.89
109.55
31.25
26.74
O
Ph
Ph
N
3q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

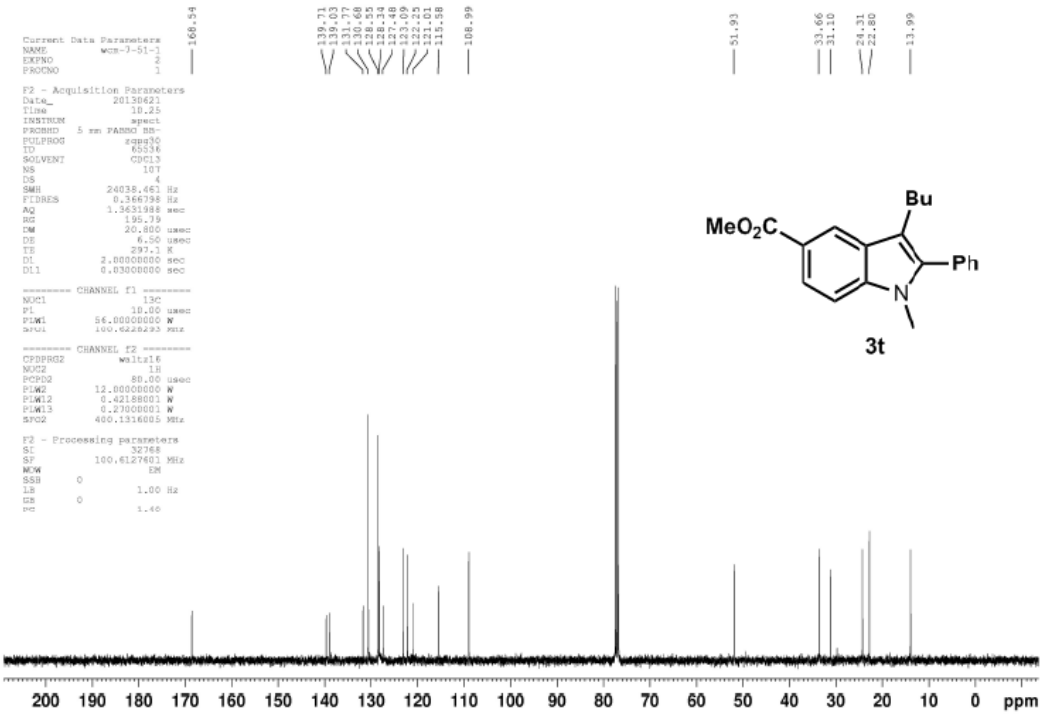

SMe
MeO2C
SMe
N
3r
10
9
8
7
6
5
4
3
2
1
0
ppm

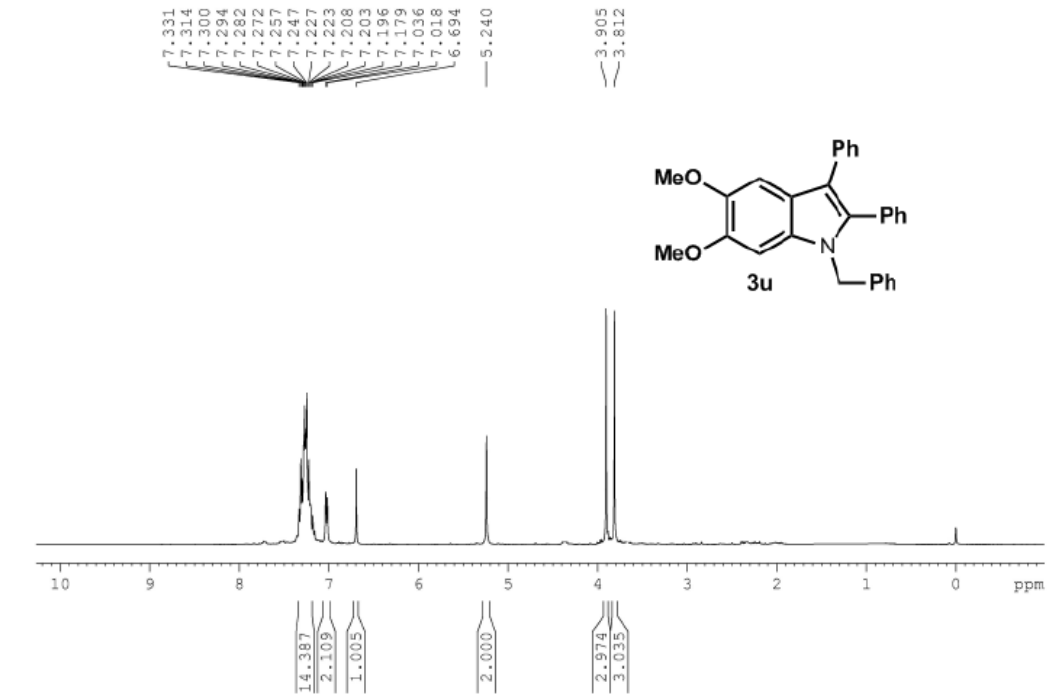

SMe
MeO2C
SMe
N
3r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

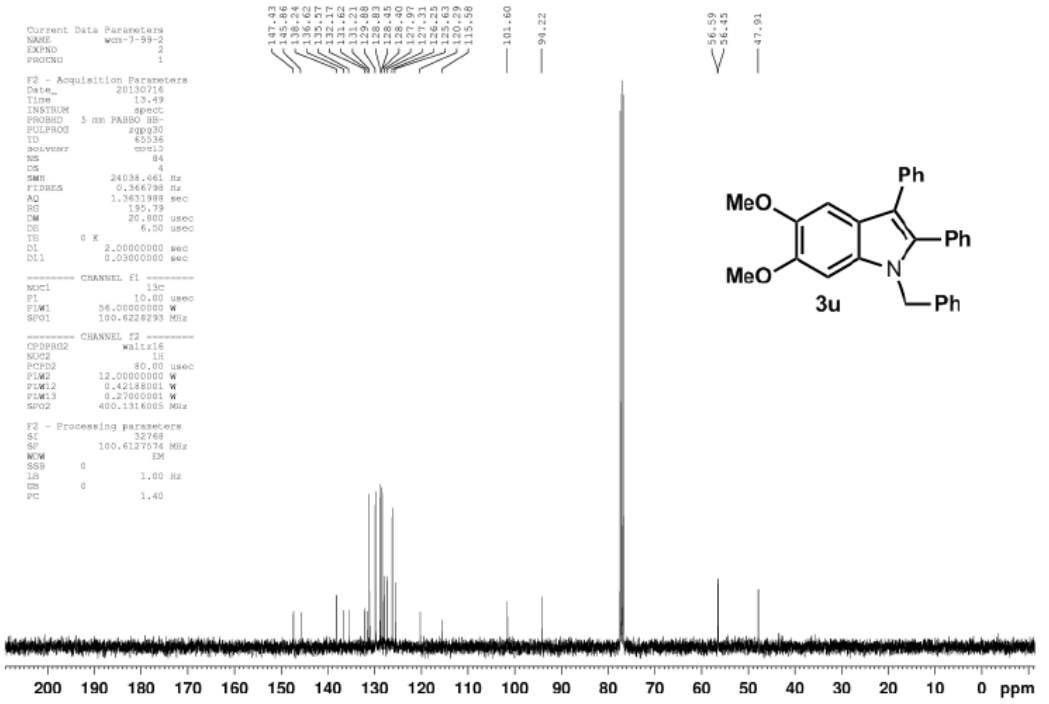

MeO2C
OBn
3s
+
MeO2C
OBn
3s'
ppm

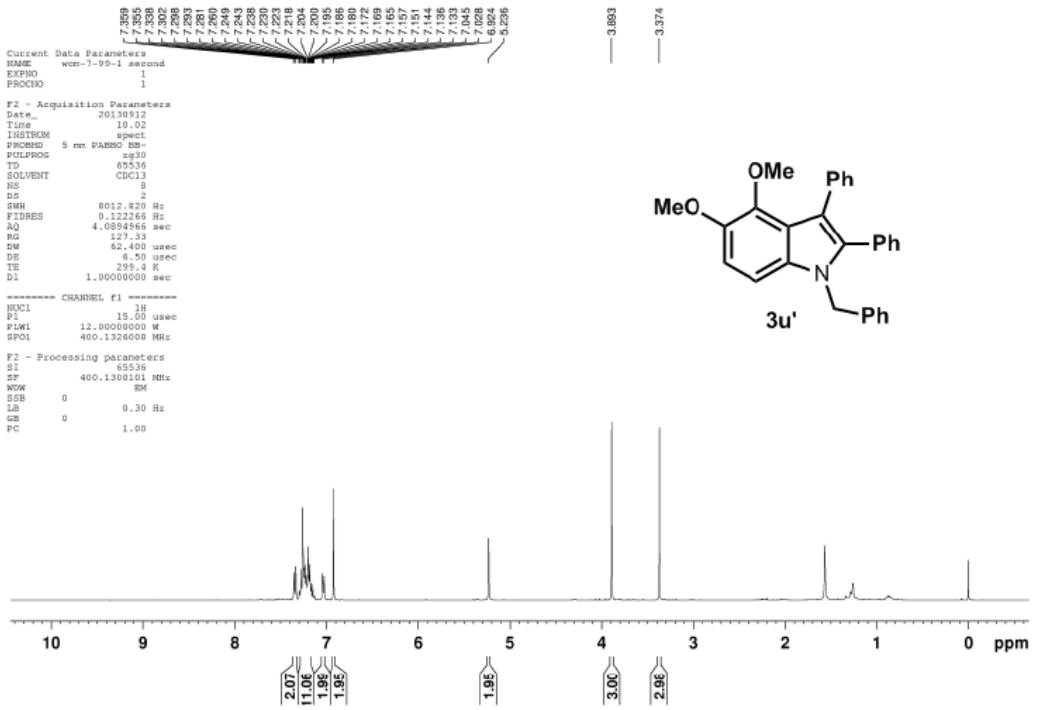

MeO2C
OBn
3s
+
MeO2C
OBn
3s'
ppm

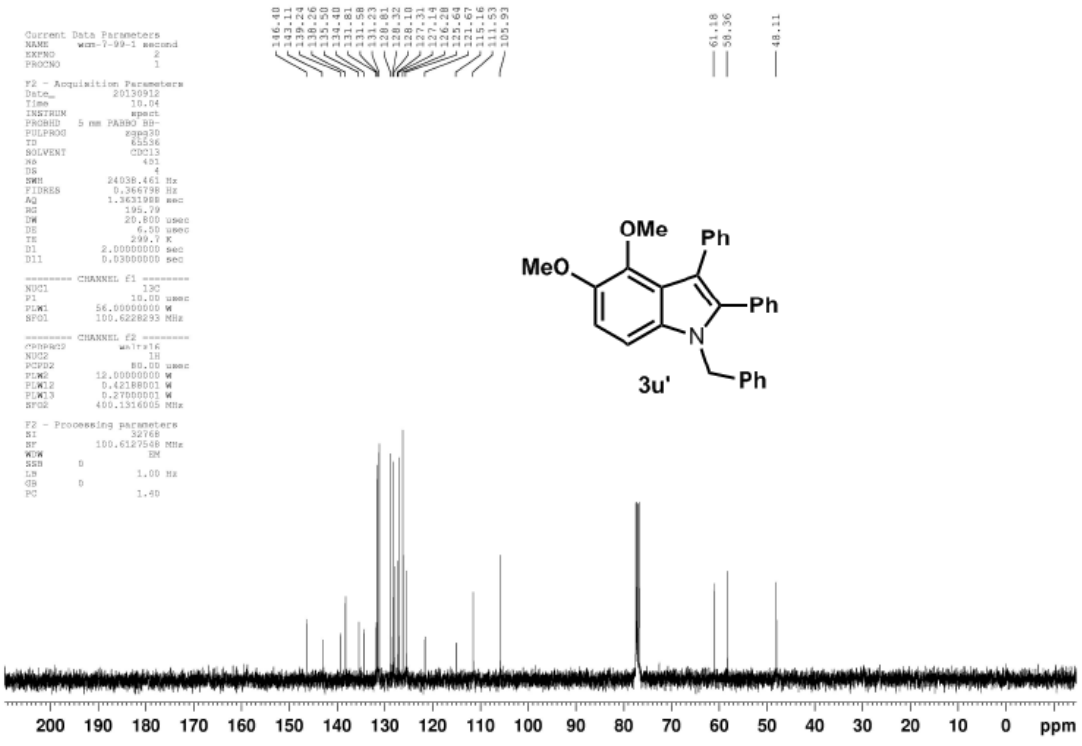

Bu
MeO2C
Ph
N
3t
ppm

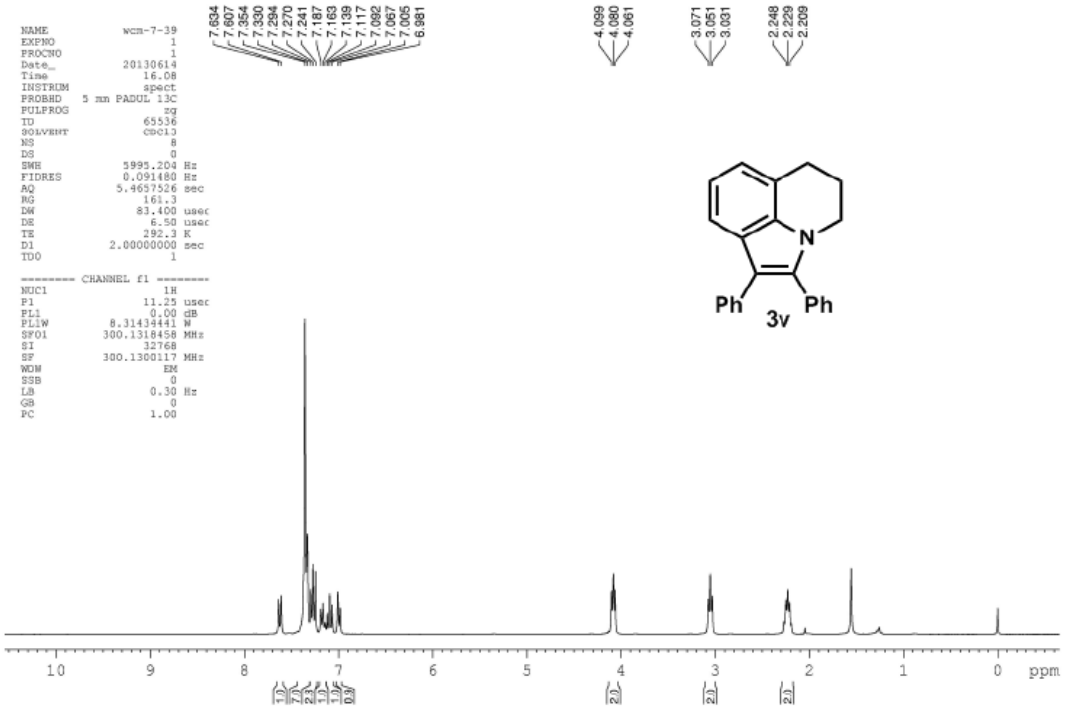

Bu
MeO2C
Ph
N
3t
ppm

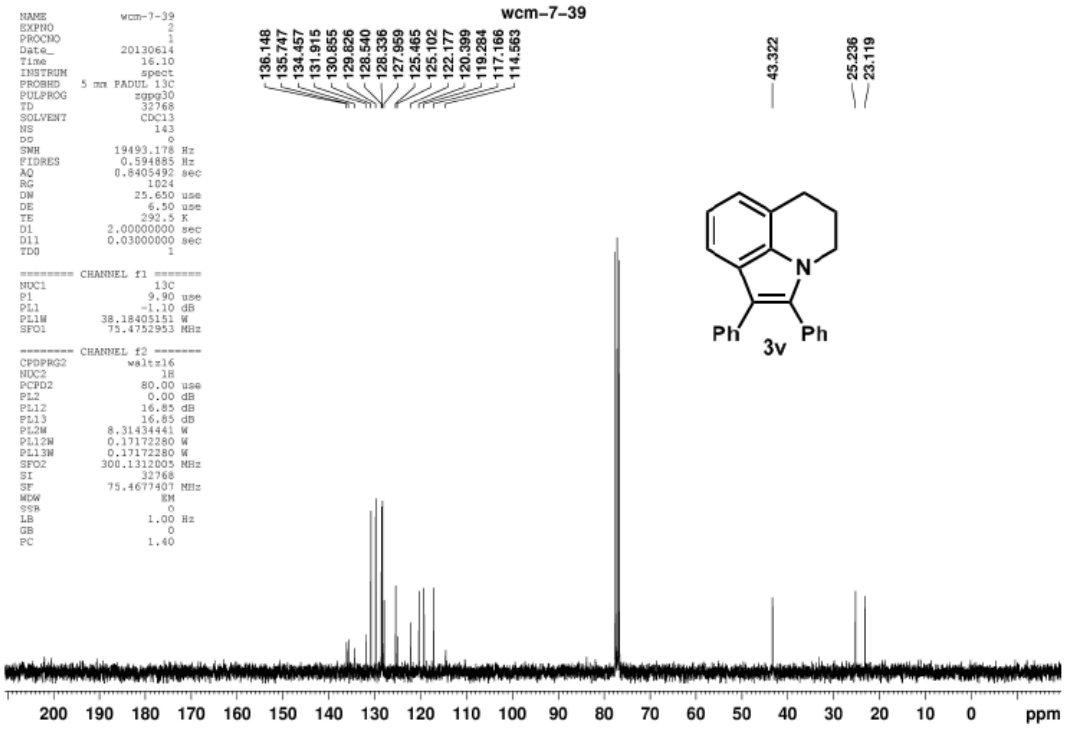

7.331
7.314
7.300
7.294
7.282
7.272
7.257
7.247
7.227
7.223
7.208
7.203
7.196
7.179
7.036
7.018
6.694
5.240
3.905
3.812
MeO
MeO
Ph
Ph
Ph
N
3u
10
9
8
7
6
5
4
3
2
1
0
ppm
14.387
2.109
1.005
2.000
2.974
3.035

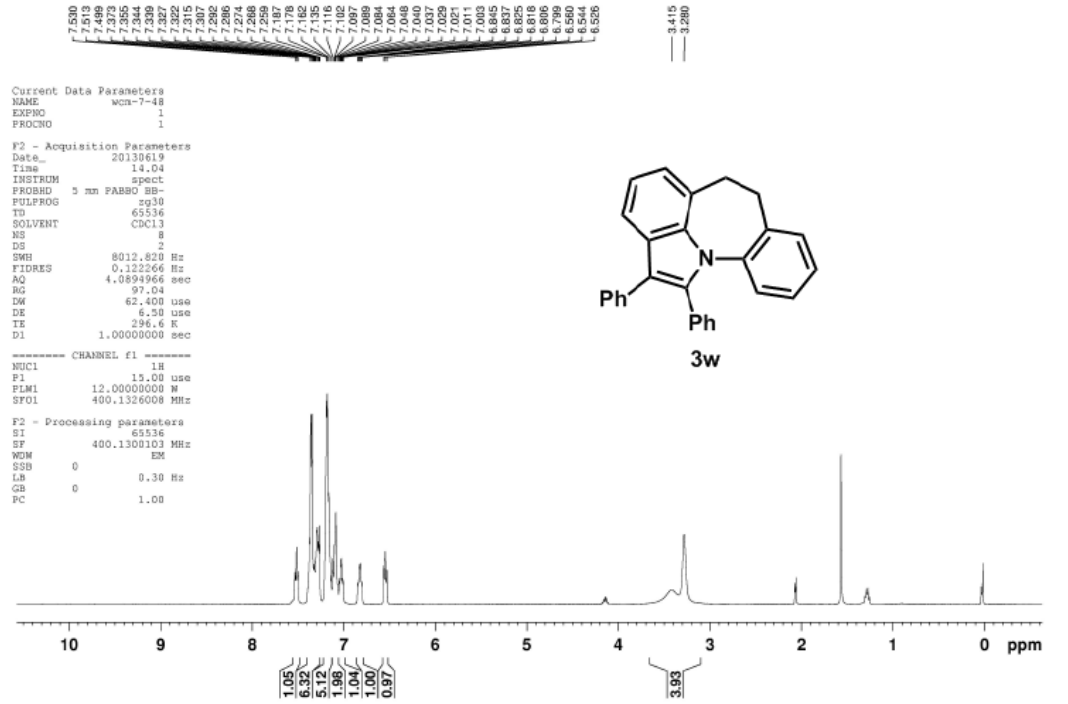

147.43
145.86
138.24
136.60
135.57
132.17
131.62
131.21
129.88
128.83
128.45
128.40
127.97
127.31
126.75
125.63
120.29
115.58
101.60
94.22
56.59
56.45
47.91
Current Data Parameters
NAME wcs-3-99-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130716
Time 13.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT cmtl3
NS 84
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13c
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127574 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
MeO
MeO
Ph
Ph
Ph
N
3u
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

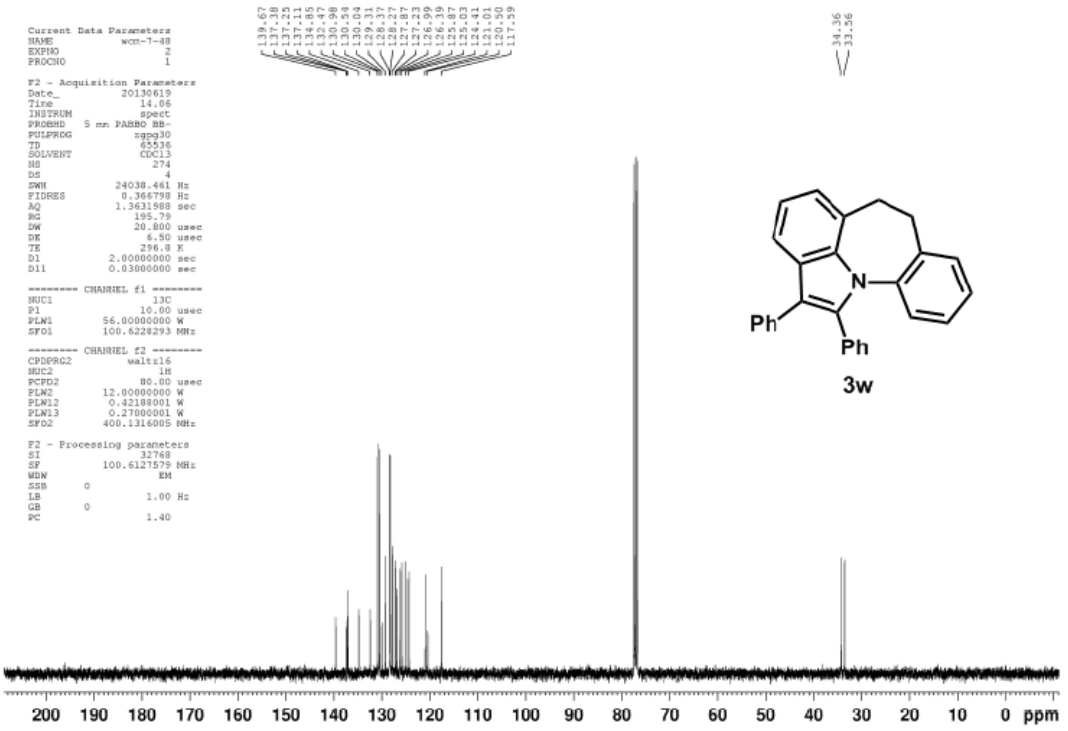

7.359
7.355
7.335
7.302
7.298
7.293
7.281
7.260
7.249
7.243
7.238
7.230
7.223
7.218
7.204
7.200
7.195
7.186
7.180
7.172
7.169
7.165
7.157
7.151
7.144
7.136
7.133
7.045
7.028
6.924
5.236
3.893
3.374
Current Data Parameters
NAME wcm-7-99-1 second
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130912
Time 10.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 127.33
DW 62.400 usec
DE 6.50 usec
TE 299.4 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
Ph
MeO
Ph
N
Ph
3u'
10
9
8
7
6
5
4
3
2
1
0
ppm
2.07
11.06
1.96
1.95
1.95
3.00
2.96

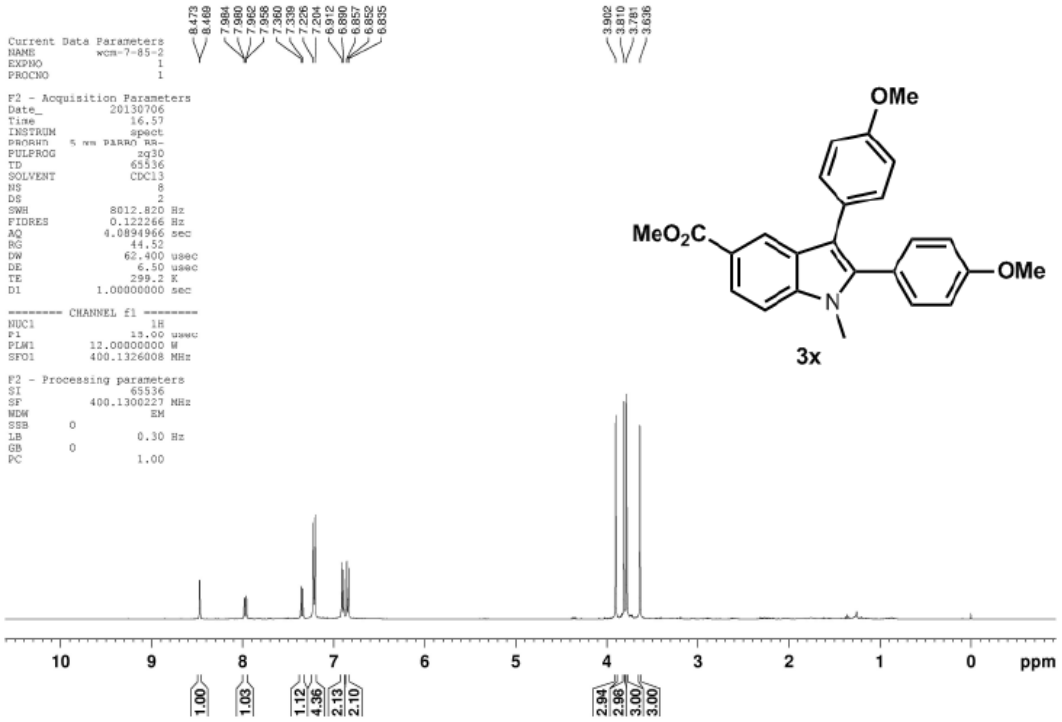

146.40
143.11
139.24
136.26
134.40
133.40
131.81
131.58
131.23
129.81
128.32
128.10
127.31
127.14
126.28
125.64
121.67
115.16
111.53
105.93
61.18
58.36
48.11
Current Data Parameters
NAME wcm-7-99-1 second
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130912
Time 10.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 401
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127568 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OMe
Ph
MeO
Ph
N
Ph
3u'
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

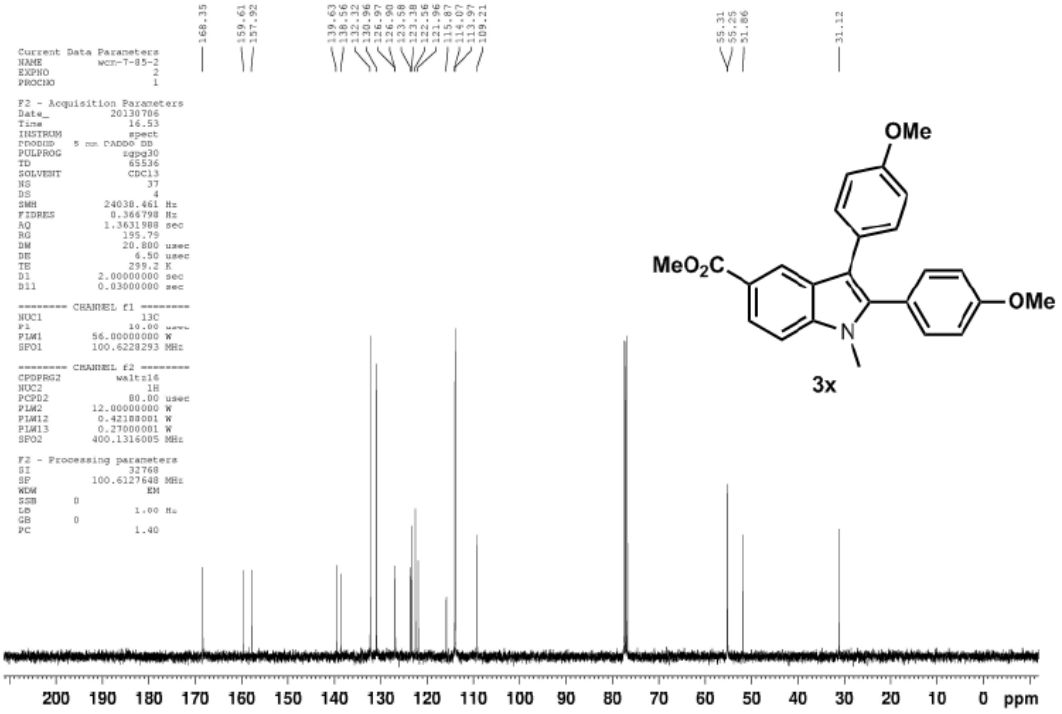

7.634
7.607
7.354
7.330
7.294
7.270
7.241
7.187
7.163
7.139
7.117
7.092
7.067
7.005
6.981
4.099
4.080
4.061
3.071
3.051
3.031
2.248
2.229
2.209
NAME wcm-7-39
EXPNO 1
PROCNO 1
Date_ 20130614
Time 16.08
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 161.3
DW 83.400 usec
DE 6.50 usec
TE 292.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.25 usec
PL1 0.00 dB
PL1W 8.31434441 W
SFO1 300.1318458 MHz
SI 32768
SF 300.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
Ph
3v
10
9
8
7
6
5
4
3
2
1
0
ppm
1.0
1.0
2.3
1.0
1.0
0.9
2.0
2.0
2.0

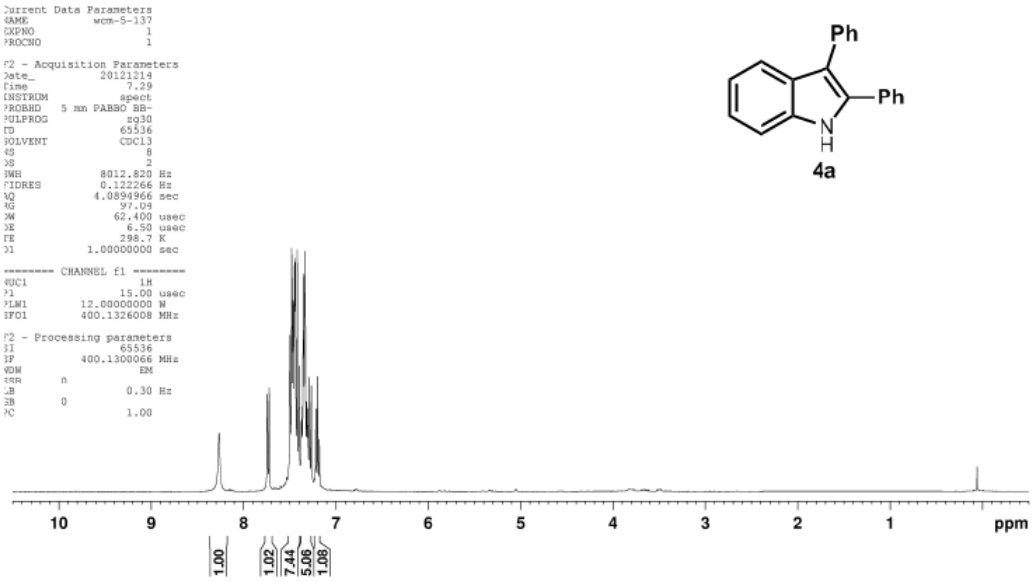

wcm-7-39
136.148
135.747
134.457
131.915
130.855
129.826
128.540
128.336
127.959
125.465
125.102
122.177
120.399
119.284
117.166
114.563
43.322
25.236
23.119
NAME wcm-7-39
EXPNO 2
PROCNO 1
Date_ 20130614
Time 16.10
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 143
DS 0
SWH 19493.178 Hz
FIDRES 0.594885 Hz
AQ 0.8405492 sec
RG 1024
DW 25.650 use
DE 6.50 use
TE 292.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.90 use
PL1 -1.10 dB
PL1W 38.18405151 W
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 0.00 dB
PL12 16.85 dB
PL13 16.85 dB
PL2W 8.31434441 W
PL12W 0.17172280 W
PL13W 0.17172280 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677407 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph
Ph
3v
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

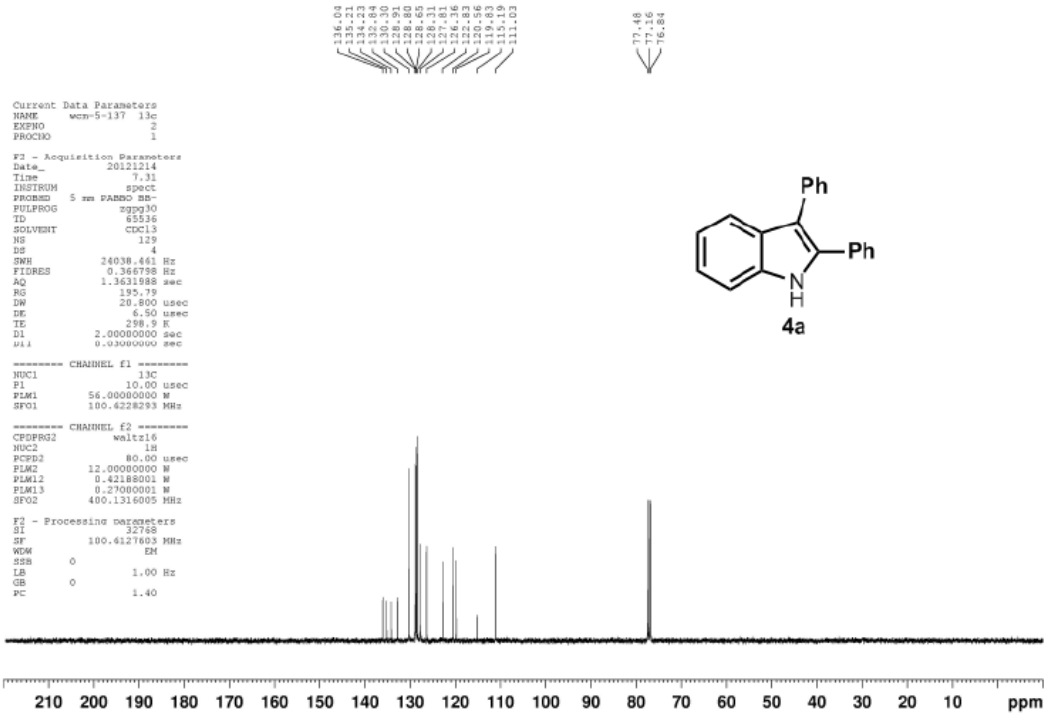

7.530
7.513
7.499
7.373
7.365
7.344
7.339
7.327
7.322
7.315
7.307
7.292
7.286
7.274
7.268
7.259
7.197
7.178
7.162
7.135
7.116
7.102
7.097
7.089
7.084
7.048
7.040
7.037
7.029
7.021
7.011
7.003
6.845
6.837
6.825
6.818
6.806
6.799
6.580
6.544
6.526
3.415
3.280
Current Data Parameters
NAME wcm-7-48
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130619
Time 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 97.04
DW 62.400 use
DE 6.50 use
TE 296.6 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 use
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
Ph
Ph
3w
10
9
8
7
6
5
4
3
2
1
0 ppm
1.05
6.32
5.12
1.98
1.04
1.00
0.97
3.93


139.67
137.39
137.25
137.11
134.85
132.47
130.98
130.58
130.04
129.31
128.37
128.27
127.87
127.23
126.99
126.39
125.87
125.03
124.41
123.00
120.50
117.59
34.36
33.56
Current Data Parameters
NAME wcm-7-48
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130619
Time 14.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 274
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127579 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
Ph
Ph
3w
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


8.473
8.469
7.984
7.980
7.962
7.958
7.360
7.359
7.226
7.204
6.912
6.890
6.857
6.852
6.835
3.902
3.810
3.781
3.636
OMe
MeO2C
OMe
N
3x
Current Data Parameters
NAME wcm-7-85-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130706
Time 16.57
INSTRUM spect
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 44.52
DW 62.400 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
PL1 13.90 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300227 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.03 1.12 4.36 2.13 2.10 2.94 2.96 3.00 3.00


168.35
159.61
157.92
139.63
138.56
132.32
130.96
126.97
126.68
123.58
123.38
122.56
121.96
115.87
114.57
111.97
109.21
55.31
55.25
51.86
31.12
OMe
MeO2C
OMe
N
3x
Current Data Parameters
NAME wcm-7-85-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130706
Time 16.53
INSTRUM spect
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 37
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
PL1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127648 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Current Data Parameters
NAME wcm-5-137
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121214
Time 7.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 97.09
DW 62.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.00000000 W
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 65536
SF 400.1300066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
Ph
N
H
4a
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
7.44
5.06
1.08


Current Data Parameters
NAME wcm-5-137 13c
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121214
Time 7.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 129
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 195.79
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 56.00000000 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.42188001 W
PLW13 0.27000001 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127603 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
136.04
135.21
134.23
132.84
130.30
128.91
128.80
128.65
128.31
127.81
126.36
122.83
120.56
119.85
115.19
111.03
77.48
77.16
76.84
Ph
Ph
N
H
4a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm