

Selective Synthesis of Indazoles and Indoles via Triazene–alkyne Cyclization Switched by Different Metals

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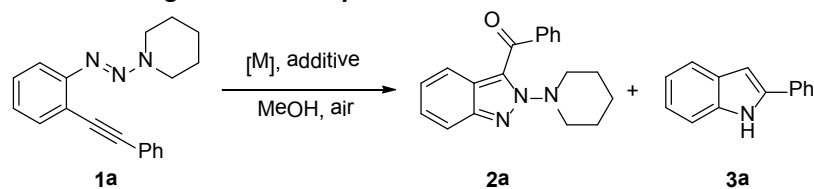
General Methods and Materials

General Information. Dichloro(η^5 -pentamethylcyclopentadienyl)rhodium(III) dimer (99%) was purchased from Sinocompound Technology Co., Ltd. Cupric acetate and silver acetate was purchased from Sinopharm Chemical Reagent Co., Ltd and used directly. All other reagents were purchased and used without further purification unless specified otherwise. Solvents for chromatography were technical grade. All compounds that were purified by flash chromatography used silica gel (200-300 mesh) with the indicated solvent system according to standard techniques. Analytical thin layer chromatography (TLC) was performed on pre-coated 0.25 mm thick silica gel 60-F254 plates (*Whatman PE SILG/UV*) and visualized using UV light (254 nm). ^1H NMR and ^{13}C NMR data were recorded on 400 MHz nuclear resonance spectrometers. Chemical shifts (δ) in ppm are reported as quoted relative to the residual signals of chloroform (^1H 7.268 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 with a quadrupole time-of-flight (QqTOF) mass spectrometer yielded ion mass/charge (m/z) ratios in atomic mass units. IR spectra were measured as dry films (KBr) and are reported in terms of frequency (cm^{-1}) and intensity of absorption.

Conditions Screening

Initial screening quickly identified $[\text{Cp}^*\text{RhCl}_2]_2$ was not necessary and this reaction required equivalent metal oxidants in order to achieve decent conversions. Table S1 summarized in-depth condition tuning for substrate **1a**.

Table S1. Conditions Screening for Selective Synthesis of Isoindazoles and Indoles from the Same Triazene Substrate^a



Entry	Catalyst (0.01 eq.)	Oxidant (2.0 eq.)	additive (0.01 eq.)	solvent	Temp.	Yield, %	
						2a	3a
1	$[\text{RhCp}^*\text{Cl}_2]_2$	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	-	MeOH	90	44	-
2	$[\text{RhCp}^*\text{Cl}_2]_2$	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	AgOAc	MeOH	90	-	-
3	$[\text{RhCp}^*\text{Cl}_2]_2$	-	AgOAc	MeOH	90	-	-
4	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	AgOAc	MeOH	90	-	-
5	-	-	-	MeOH	90	-	-
6	$\text{Pd}(\text{OAc})_2$	-	KOAc	MeOH	90	<5	-
7	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	-	MeOH	90	-	-
8	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O} (0.2)$	-	MeOH	90	-	-
9	-	AgOAc	-	MeOH	90	-	80
10	-	$\text{Ni}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	-	MeOH	90	-	-
11	-	CuBr_2	-	MeOH	90	-	-
12	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O} (0.5)$	-	MeOH	90	35	-
13	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O} (0.1)$	-	MeOH	90	<5	-
14	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O} (0.1)$	NaOAc(2.0)	MeOH	90	<5	-
15	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O} (0.1)$	CsOAc	MeOH	90	10	-
16	-	AgOAc(0.1)	-	MeOH	90	-	<5
17	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	-	MeOH	90	-	-
18	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	-	MeOH	90	-	-
19	-	$\text{Cu}(\text{OTf})_2$	-	MeOH	90	-	-
20	-	CuCl_2	-	MeOH	90	-	-
21	-	CuO	-	MeOH	90	-	-
22	-	CuCN	-	MeOH	90	-	-
23	-	$\text{Fe}(\text{OAc})_2$	-	MeOH	90	-	-
24	-	$\text{Mn}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$	-	MeOH	90	-	-
25	-	AgOOCPh	-	MeOH	90	-	-
26	-	$\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$	-	MeOH	90	-	-
27	-	$\text{Ni}(\text{OAc})_2$	-	MeOH	90	-	-
28	-	$\text{Zn}(\text{OAc})_2$	-	MeOH	90	-	-
29	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O} (1.2)$	-	MeOH	90	70	-
30	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O} (1.5)$	-	MeOH	90	70	-
31	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O} (3.0)$	-	MeOH	90	68	-
32	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	-	MeOH	90	94	-
33	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O} (1.2)$	-	MeOH	50	67	-
34	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	-	MeCN	90	20	-
35	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	-	MeCN	65	10	-
36	-	$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	-	MeCN	85	20	-

37	-	Cu(OAc) ₂ ·H ₂ O	-	MeOH	60	40	-
38	-	Cu(OAc) ₂ ·H ₂ O	-	MeOH	r.t.	<5	-
39	-	AgNO ₃	-	MeOH	90	-	-
40	-	Ag ₂ CO ₃	-	MeOH	90	-	-
41	-	AgOAc	-	MeOH	90	-	80
42	-	AgOAc(1.0)	-	MeOH	90	-	50
43	-	AgOAc(1.2)	-	MeOH	90	-	46
44	-	AgOAc(0.5)	-	MeOH	90	-	30
45	-	AgOAc(2.5)	-	MeOH	90	-	36

^a. isolated yield; entry 1-13, Ar; entries 14-17, O₂; entries 18-45, air.

Cartesian coordinates, thermal correction to Gibbs free energy (TCG), and electronic energies in MeOH (au).

React

C	1.59228800	-3.55162300	0.14497600
C	1.30423700	-2.17306500	0.02904200
C	2.39124600	-1.26752700	-0.12571300
C	3.69773400	-1.77302200	-0.20940900
C	3.95744600	-3.13526700	-0.08780500
C	2.89737500	-4.03094100	0.09708300
H	0.76072500	-4.24093500	0.26021200
H	4.50552700	-1.06236900	-0.35962600
H	4.98067300	-3.49809300	-0.14008400
H	3.08588600	-5.09731900	0.18764000
N	2.27325800	0.13227200	-0.27431000
N	1.36254400	0.65289700	0.43463300
C	0.46135000	2.62032900	1.34783200
C	2.03065800	2.77420000	-0.60666000
C	-0.29771000	3.85586600	0.85750800
H	1.19885700	2.91883200	2.11366500
H	-0.20415000	1.87962500	1.79777700
C	1.29398000	4.03087900	-1.08673600
H	2.93626000	3.04348400	-0.03558400
H	2.35245300	2.15433400	-1.44472800
C	0.63223500	4.79085000	0.07128000
H	-0.73223400	4.37178100	1.72277900
H	-1.13151400	3.53783700	0.21656900
H	2.00796300	4.67360700	-1.61685200
H	0.52646400	3.73544400	-1.81517900
H	0.07509300	5.65570300	-0.30978900
H	1.40853300	5.18541000	0.74441700
N	1.15333700	1.95822500	0.23975700
C	-0.06285500	-1.77039200	0.00808100
C	-1.25715800	-1.53500900	-0.03826400
C	-2.64315700	-1.20725800	-0.09510900
C	-3.62425200	-2.13872500	0.30604400
C	-3.06167500	0.05825100	-0.55957300
C	-4.97783400	-1.81050000	0.24608000
H	-3.31137100	-3.11555000	0.66342900
C	-4.41738400	0.37693800	-0.61937500
H	-2.31168300	0.77764800	-0.87533200
C	-5.38136600	-0.55346100	-0.21641400
H	-5.72099400	-2.53932300	0.55990000
H	-4.72375100	1.35475000	-0.98306700
H	-6.43765200	-0.30175500	-0.26390700

TCG = 0.290028 au

E = -899.534085 au

Inter1-Cu

C	4.14272000	0.43831600	0.08971200
C	2.73637100	0.32875500	0.32680300
C	2.09005800	-0.92713900	0.00394400
C	2.86059600	-1.97428300	-0.54241500
C	4.22048100	-1.80391800	-0.77085600
C	4.87784400	-0.59761900	-0.45440000
H	4.60754200	1.38409800	0.35064800

H	2.38053600	-2.91942400	-0.77168100
H	4.79074200	-2.62828100	-1.19408200
H	5.94446800	-0.49294400	-0.63022300
N	0.74497100	-1.03857000	0.31835600
N	0.14087700	-2.01333100	-0.25024900
C	-1.83275500	-3.29030300	-0.51042200
C	-1.78374100	-1.44227100	1.19262100
C	-3.19743100	-2.80707500	-1.02072600
H	-1.97397900	-4.09124800	0.23273600
H	-1.20218600	-3.67610300	-1.31456400
C	-3.15645900	-0.95709300	0.70513200
H	-1.89963000	-2.12509600	2.04861100
H	-1.13551300	-0.62156100	1.50025100
C	-3.98233100	-2.10133100	0.09628100
H	-3.75601700	-3.66875300	-1.40727100
H	-3.04124300	-2.11661500	-1.86057900
H	-3.68460200	-0.50574200	1.55378000
H	-3.00925500	-0.16240200	-0.03753800
H	-4.93297700	-1.71773300	-0.29378300
H	-4.23407700	-2.83096100	0.88099700
N	-1.10342000	-2.19319500	0.12311900
C	2.07488500	1.47208500	0.80337000
C	0.73845900	1.69507900	1.18159000
C	-0.22854200	2.36729800	0.24986600
C	-1.46096600	2.80067700	0.75746700
C	0.05740200	2.54929300	-1.11143200
C	-2.39711500	3.40384500	-0.08503200
H	-1.66072400	2.66107900	1.81612500
C	-0.87942300	3.14869700	-1.95569000
H	1.01735900	2.22916800	-1.51062300
C	-2.10945400	3.57761600	-1.44373600
H	-3.34819500	3.74511400	0.31719900
H	-0.64945900	3.28716300	-3.00934600
H	-2.83663300	4.05076600	-2.09934300
O	0.44040800	1.45392300	2.37720500

TCG = 0.333609 au

E = -1324.102917 au

Inter2-Cu

C	-0.22805000	3.79695600	-0.56786400
C	-0.31501100	2.36446900	-0.52400300
C	0.93010100	1.63190100	-0.58288000
C	2.14772600	2.31359600	-0.64388500
C	2.18418000	3.70971000	-0.68316600
C	0.98896800	4.44951600	-0.65086200
H	-1.15603500	4.35918300	-0.51897100
H	3.07933600	1.75005000	-0.66301300
H	3.14379200	4.21478900	-0.74086400
H	1.01805600	5.53553100	-0.68157200
N	0.97196700	0.20650700	-0.52545100
N	0.00895500	-0.34204700	-1.17017900
C	-1.16167600	-2.14703300	-2.09168100
C	0.55846700	-2.63202000	-0.32868200
C	-2.12005200	-3.16255200	-1.46372600
H	-0.59889400	-2.61769800	-2.91340000
H	-1.69376800	-1.28150300	-2.48896700
C	-0.39208300	-3.67020800	0.28912900

H	1.29400300	-3.11559700	-0.98885200	C	-1.03815200	-4.16207000	-0.60739500
H	1.11174600	-2.12043100	0.46345600	H	-2.66044500	-3.26161200	-1.75980000
C	-1.34498600	-4.27693300	-0.74847500	H	-2.72854200	-2.90653300	-0.04422100
H	-2.75864400	-3.57265700	-2.25568800	H	0.68872500	-4.52978800	0.67900900
H	-2.77719500	-2.64519700	-0.75268700	H	-0.63930500	-3.67106700	1.46884300
H	0.21987000	-4.44603000	0.76459900	H	-1.57068800	-5.08592500	-0.35075700
H	-0.97383000	-3.18581400	1.08426500	H	-0.45398000	-4.37537500	-1.51578700
H	-2.03690600	-4.97455800	-0.26176400	N	-0.39215900	-1.38771700	-0.04304000
H	-0.77058900	-4.86035300	-1.48365400	C	1.70080500	0.68528300	-0.96795700
N	-0.19374400	-1.63608400	-1.10747300	C	2.86253500	-0.01812200	-1.12342300
C	-1.54542000	1.76036400	-0.34045800	C	3.86219000	-0.26860500	-0.08816000
C	-2.74106400	1.25760700	-0.57531500	C	4.95867900	-1.12361400	-0.33680900
C	-3.72069000	0.83428600	0.45048200	C	3.74997600	0.33589700	1.18327500
C	-4.99479400	0.37204000	0.08110600	C	5.91224100	-1.35384100	0.65345100
C	-3.38825400	0.88961000	1.81640300	H	5.05490000	-1.59647300	-1.30775900
C	-5.91216700	-0.02638700	1.05818900	C	4.70634500	0.09856900	2.16742800
H	-5.26372200	0.33105200	-0.96858400	H	2.90933000	0.98974600	1.39235400
C	-4.30600000	0.49436800	2.78695000	C	5.79262800	-0.74613100	1.90857700
H	-2.40381000	1.24532400	2.10962700	H	6.75275700	-2.01105800	0.44545200
C	-5.57428300	0.03252100	2.41214800	H	4.60417400	0.57308900	3.13988100
H	-6.89526200	-0.37977300	0.75693300	H	6.53792400	-0.92933300	2.67807100
H	-4.03247200	0.54529400	3.83783500	O	3.09654400	-0.70184800	-2.29911100
H	-6.29003600	-0.27575600	3.16988200	H	2.37358200	-0.49280900	-2.91554900
Cu	2.54097100	-0.48612900	0.40464700	Cu	-2.63312400	0.72839500	0.52922900
O	4.08750400	-1.13800000	1.29722200	O	-4.45962800	0.76291300	1.02757200
C	5.10077200	-0.43944800	0.87393300	C	-5.10291300	-0.14310700	0.35195000
O	5.00714600	0.47058200	0.03003900	O	-4.56549700	-0.90822200	-0.46914600
C	6.44141700	-0.80907900	1.49049700	C	-6.59707700	-0.21148100	0.63317400
H	6.65214900	-1.87053800	1.31745200	H	-7.06637500	0.74299800	0.36765000
H	7.24147300	-0.19911600	1.06580700	H	-7.06052900	-1.01843000	0.06152600
H	6.40193300	-0.66134400	2.57595600	H	-6.76883600	-0.36725700	1.70417200
O	-3.19784000	1.02999900	-1.87653800				
H	-2.52667400	1.36389700	-2.49366900				

E = -1400.057542 au

TCG = 0.34347 au

TCG = 0.341278 au

E = -1400.066206 au

Inter3-Cu

TS₍₂₋₃₎-Cu

C	1.91306200	3.17626400	-0.96521700	C	-1.98993200	-2.65807400	-0.38095500
C	1.22231500	1.94660200	-0.69005100	C	-1.18413300	-1.51411800	-0.20014500
C	-0.11869500	2.03221400	-0.16071900	C	0.23212500	-1.66689000	-0.15974100
C	-0.73686900	3.28556400	0.04403800	C	0.85570900	-2.93266200	-0.23556000
C	-0.04204100	4.44176900	-0.25068900	C	0.03415600	-4.03439300	-0.38517800
C	1.28725800	4.38306300	-0.75822600	C	-1.37525700	-3.89791300	-0.47019700
H	2.92674100	3.12980900	-1.35258800	H	-3.06731700	-2.57777500	-0.46075000
H	-1.74887300	3.32367300	0.43908700	H	1.93879200	-3.01547300	-0.18757800
H	-0.51094300	5.40792300	-0.08803700	H	0.47700500	-5.02448000	-0.45134200
H	1.81301200	5.30799800	-0.98011400	H	-1.98668700	-4.78485100	-0.61196300
N	-0.74515900	0.84702300	0.09559500	N	0.85641900	-0.45809000	-0.07852600
N	0.10814400	-0.15850900	0.11332100	N	-0.15057600	0.46628300	-0.06742500
C	-1.33739500	-1.69774700	-1.14251800	C	0.69052400	2.30090300	1.23055700
C	0.60802700	-2.43220700	0.21949300	C	0.89138100	2.28110700	-1.24826700
C	-2.03911300	-3.03276800	-0.88644900	C	0.76468000	3.83015200	1.24322800
H	-0.75151100	-1.73096300	-2.07904700	H	1.69239000	1.86630900	1.37005600
H	-2.08016300	-0.90337300	-1.22142500	H	0.04196800	1.92600700	2.02809700
C	-0.08250700	-3.76443200	0.52690900	C	0.96252800	3.81041800	-1.27294100
H	1.26020500	-2.53921600	-0.66385900	H	1.90484200	1.85316400	-1.21837100
H	1.22451000	-2.09441100	1.05550400	H	0.38291900	1.88804500	-2.13410400
				C	1.55143800	4.35961800	0.03498300

H	1.23297700	4.14798900	2.18247100	H	3.17052300	1.59072700	-0.80721600
H	-0.25389000	4.24266300	1.23614100	H	2.09602100	3.29748000	2.45872000
H	1.57119500	4.11565700	-2.13255500	H	2.69174200	1.75708400	1.82768700
H	-0.04479500	4.22085100	-1.43119000	H	3.74652800	3.59496400	0.54048500
H	1.54011000	5.45597800	0.02549600	H	2.17083500	4.31340600	0.20613300
H	2.60345400	4.05236200	0.11919600	N	0.62212200	1.34329600	0.09594600
N	0.11127600	1.84200500	-0.06009700	C	-0.09356700	-1.53043500	0.80559100
C	-1.42785800	-0.09575900	-0.11394200	O	-0.48706400	-2.24342200	1.72859900
C	-2.60479400	0.67875200	-0.12016000	C	1.23176900	-1.78845100	0.16174200
C	-3.96832900	0.17360200	0.05469100	C	2.23919700	-2.40168200	0.92372700
C	-5.02508600	0.78431600	-0.65347400	C	1.45873100	-1.52975600	-1.19828600
C	-4.27783200	-0.84269400	0.98089600	C	3.46464800	-2.72256800	0.34090400
C	-6.34024500	0.36095400	-0.46972500	H	2.04480300	-2.62030700	1.96941200
H	-4.80111000	1.58716900	-1.34858400	C	2.67663700	-1.87411300	-1.78749400
C	-5.59622700	-1.25827500	1.16512200	H	0.67301300	-1.08384500	-1.80134900
H	-3.48702900	-1.28587900	1.57818600	C	3.68505200	-2.46172900	-1.01684100
C	-6.63266300	-0.66523200	0.43580700	H	4.24533400	-3.18382300	0.94029700
H	-7.14028200	0.83383800	-1.03354900	H	2.83790300	-1.68788300	-2.84627800
H	-5.81631900	-2.03679100	1.89116800	H	4.63639300	-2.72249200	-1.47381300
H	-7.65915900	-0.99136600	0.58082300				
O	-2.54069800	2.02378800	-0.30373600				
Cu	2.74816900	-0.20726800	0.06392700				
O	4.63205400	0.02368600	0.21201100				
C	5.12248200	-1.18088500	0.17030000				
O	4.41853300	-2.20186500	0.05390500				
C	6.63679500	-1.27067100	0.27419900				
H	6.96446700	-2.31148900	0.23192000				
H	7.09922400	-0.70398000	-0.54211100				
H	6.97214300	-0.81524300	1.21305300				
H	-1.57753400	2.27824500	-0.29049400				

E = -974.8176963 au
 TCG = 0.299612 au

Inter1-Ag

C	-1.16599800	3.46601400	-0.07824200
C	-0.59394200	2.17623000	-0.05319600
C	0.81961300	2.04568800	-0.05829900
C	1.61034500	3.20481000	-0.10893000
C	1.02551200	4.46781900	-0.12767100
C	-0.36737300	4.60322200	-0.11161600
H	-2.24772100	3.55509700	-0.06908000
H	2.68874100	3.10370200	-0.14253100
H	1.65941600	5.34893300	-0.16746000
H	-0.82676600	5.58664500	-0.13465200
N	1.40560100	0.74366900	-0.05847600
N	2.61827100	0.73178400	0.34839600
C	4.56498900	-0.37370400	1.04975100
C	2.84748300	-1.63377000	-0.32249100
C	5.69279900	-1.11819300	0.33499600
H	4.34618800	-0.85566000	2.01469400
H	4.80984700	0.67238600	1.24459400
C	3.99727900	-2.41261600	-0.98839800
H	2.38117300	-2.24072800	0.47372800
H	2.09347000	-1.39692000	-1.07979800
C	5.23424300	-2.51911500	-0.08925900
H	6.55187300	-1.17388900	1.01294300
H	6.01207300	-0.54484900	-0.54523500
H	3.61855900	-3.40429600	-1.26158800
H	4.26553500	-1.90294000	-1.92251500
H	6.03583400	-3.03990300	-0.62419100
H	5.00374300	-3.12270800	0.80081200
N	3.32081700	-0.36941700	0.25219100
C	-1.50326600	1.05854600	-0.01261100
C	-2.51857700	0.35502300	0.03556100
C	-3.73975000	-0.39004600	0.08354800
C	-4.47043300	-0.62391400	-1.10108900
C	-4.23802300	-0.86437400	1.31578300
C	-5.67723000	-1.31860500	-1.04739200

E = -1400.131599 au
 TCG = 0.350235 au

Prod-Cu

C	-2.75983100	0.74615500	-0.39260900
C	-2.39846900	-0.54107800	0.12386100
C	-3.38460000	-1.53967000	0.31678600
C	-4.68866600	-1.22688800	-0.00844900
C	-5.04577100	0.05559700	-0.52706200
C	-4.10557900	1.04412000	-0.72625400
C	-1.00119200	-0.47565400	0.29489300
H	-3.11647600	-2.50899600	0.72475600
H	-5.46997500	-1.96844400	0.13629700
H	-6.08801600	0.25034000	-0.76691700
H	-4.37060600	2.02062900	-1.12079800
N	-1.68263500	1.55971400	-0.48434700
N	-0.65389900	0.79300000	-0.09173500
C	1.08873300	2.05990900	-1.10724700
C	0.64889300	2.19964900	1.30423900
C	2.54470100	2.48816000	-0.89822600
H	0.45301400	2.93598600	-1.31083000
H	1.00073400	1.37762500	-1.95800600
C	2.08907700	2.64086300	1.57955300
H	-0.00674800	3.07536100	1.16468000
H	0.25495400	1.61031200	2.13822700
C	2.69091000	3.35621300	0.36081300
H	2.88336200	3.03532800	-1.78716700

H	-4.09107500	-0.25128200	-2.04810300
C	-5.44542300	-1.55861600	1.35621500
H	-3.68201200	-0.67386600	2.22922300
C	-6.16487800	-1.78752000	0.17765000
H	-6.23951500	-1.49167600	-1.96037800
H	-5.82862700	-1.91716600	2.30714600
H	-7.10675900	-2.32746500	0.21459100
Ag	-0.21917100	-0.90057300	-0.12048600

E = -1045.243684 au

TCG = 0.28741 au

Inter2-Ag

C	2.26962100	-2.78973400	-0.10496800
C	1.23496400	-1.83655400	-0.04151000
C	-0.12062900	-2.26735300	0.00752900
C	-0.38002000	-3.65138900	-0.01729000
C	0.65778800	-4.57501000	-0.07618100
C	1.99375800	-4.15037800	-0.12122000
H	3.30466900	-2.45123500	-0.14315700
H	-1.41071600	-3.98593000	0.00624900
H	0.42704800	-5.63661200	-0.09434500
H	2.80248500	-4.87250100	-0.17357000
N	-1.10625300	-1.26581900	0.04937200
N	-2.27479100	-1.72553700	0.29263200
C	-4.56292000	-1.37372500	0.74814800
C	-3.13206200	0.56788000	0.01599000
C	-5.70960200	-0.88171700	-0.14090900
H	-4.70717600	-1.01566900	1.77963200
H	-4.49464100	-2.46327300	0.77459300
C	-4.29083000	1.07674300	-0.85464900
H	-3.12096000	1.08365400	0.98921800
H	-2.16588900	0.72980500	-0.46080500
C	-5.65799600	0.64401500	-0.30613600
H	-6.65953700	-1.19464900	0.30795100
H	-5.64042300	-1.36696500	-1.12376600
H	-4.22319200	2.16979700	-0.91558900
H	-4.16456700	0.68948600	-1.87467200
H	-6.45681400	0.98166500	-0.97621500
H	-5.83663400	1.12598800	0.66665700
N	-3.26971800	-0.87447900	0.26291100
C	1.49601000	-0.41876100	-0.01872900
C	1.10396000	0.76958600	0.01006200
C	0.66965900	2.11912900	0.05351700
C	0.44806500	2.75472200	1.29862100
C	0.42376200	2.82688100	-1.14741600
C	-0.00722700	4.06913800	1.33502200
H	0.63015700	2.20552700	2.21757200
C	-0.03051100	4.14125200	-1.09714800
H	0.58766200	2.33336000	-2.10083200
C	-0.24421100	4.76231100	0.14057700
H	-0.17783300	4.55625700	2.29054200
H	-0.21914700	4.68407500	-2.01866200
H	-0.59623800	5.78961500	0.17430000
Ag	3.65335400	0.27609000	-0.03530600

E = -1045.230099 au

TCG = 0.284123 au

TS₍₂₋₃₎-Ag

C	-2.79596100	2.52059100	-0.13997200
C	-1.69653500	1.65830400	-0.07704900
C	-0.39357600	2.18908000	0.03362900
C	-0.19563500	3.57383900	0.07492500
C	-1.30400500	4.42086100	0.02235800
C	-2.60050600	3.90113000	-0.09145400
H	-3.79976600	2.11102600	-0.22466000
H	0.80956600	3.97610400	0.14179900
H	-1.15456200	5.49619700	0.05823400
H	-3.45264200	4.57175000	-0.14639600
N	0.62486600	1.21648800	0.02383500
N	1.74648800	1.61024600	0.50594000
C	4.00738200	1.34517800	1.08944100
C	2.94227900	-0.28722400	-0.52907200
C	5.22974100	1.47066700	0.17461000
H	4.20079500	0.60802300	1.88200500
H	3.74032000	2.29174200	1.56346000
C	4.18269900	-0.15980100	-1.42890000
H	3.00570300	-1.18413300	0.09978400
H	2.02973500	-0.34720500	-1.12022600
C	5.44720200	0.18270800	-0.63102400
H	6.10325400	1.69985200	0.79576800
H	5.08696900	2.31952700	-0.50729800
H	4.30320600	-1.10590600	-1.96987200
H	3.99890900	0.61839900	-2.18148900
H	6.29959800	0.29780500	-1.30955500
H	5.69488500	-0.64459700	0.05026800
N	2.81713500	0.89279300	0.34526400
C	-1.71856100	0.20350300	-0.07677900
C	-0.64234000	-0.51149100	-0.03100100
C	0.06018800	-1.75194800	0.09978900
C	0.48171800	-2.20071100	1.37117200
C	0.30191600	-2.55685600	-1.03558200
C	1.12460600	-3.43006600	1.50003600
H	0.29095500	-1.58265300	2.24385700
C	0.93565500	-3.79026900	-0.89605800
H	-0.02136900	-2.20938500	-2.01282700
C	1.35053300	-4.22535700	0.36887300
H	1.44074800	-3.77544500	2.48023600
H	1.10661900	-4.41294600	-1.76952500
H	1.84477000	-5.18718000	0.47447700
Ag	-3.53506200	-0.95511700	-0.07363700

E = -1045.215552 au

TCG = 0.289402 au

Inter3-Ag

C	0.46557800	-1.82624400	-0.38012100
C	-0.91009200	-1.96444500	-0.08697700
C	-1.46814400	-3.24372200	-0.06639600
C	-0.66557200	-4.34726100	-0.37586600
C	0.67660200	-4.17756300	-0.73897400
C	1.26259600	-2.90523200	-0.75813500
C	-0.56267200	0.28031200	-0.25616400
C	-1.52182300	-0.64212500	0.02051000
H	-2.52373600	-3.37193100	0.15750700

H	-1.09417200	-5.34498800	-0.36337200	C	2.41443200	-1.96049100	-0.64550200
H	1.27635900	-5.03944000	-1.01501800	C	2.55226300	-0.01413300	0.77819400
H	2.29222100	-2.79303700	-1.07592900	C	3.80724000	-2.06082900	-0.64386300
N	0.71004300	-0.41436800	-0.43919200	H	1.82807900	-2.66435200	-1.23126100
C	-0.61502800	1.75688600	-0.28364100	C	3.94435800	-0.10983200	0.77164100
C	-0.27469300	2.48285800	-1.43853300	H	2.06250200	0.75976600	1.36213600
C	-1.06233000	2.45520300	0.85165400	C	4.58041700	-1.13443600	0.06209800
C	-0.38554400	3.87398500	-1.45690100	H	4.28896600	-2.85762400	-1.20543300
H	0.05856900	1.95627200	-2.32847700	H	4.53471300	0.60746500	1.33694600
C	-1.17132200	3.84815400	0.83131000	H	5.66459100	-1.21150700	0.06282200
H	-1.31176100	1.90217200	1.75345000	Ag	-0.02732700	2.26884000	-0.15024300
C	-0.83300300	4.56019400	-0.32266900	H	-0.09994200	-2.92561900	0.25790100
H	-0.13157300	4.42254200	-2.35983100				
H	-1.51483700	4.37528000	1.71727400				
H	-0.91888800	5.64311700	-0.33993500				
N	1.77782600	0.29423400	-0.68223600				
C	3.36511100	-1.13159200	0.61597200				
C	4.05256300	0.72293700	-0.94812200				
C	4.14011100	-0.42077400	1.74291500				
H	3.99518900	-1.88358200	0.12690200				
H	2.47891600	-1.62194600	1.00912000				
C	4.83150700	1.41769600	0.17462800				
H	4.70922700	0.06060500	-1.52628300				
H	3.58376300	1.43083700	-1.63268900				
C	5.31989100	0.40293900	1.21506400				
H	4.47757500	-1.19911100	2.43758300				
H	3.44611900	0.22483900	2.29655100				
H	5.67103800	1.95752000	-0.27794100				
H	4.18343300	2.16707700	0.64756500				
H	5.81543100	0.91803400	2.04500800				
H	6.06936600	-0.26357800	0.76482600				
N	2.96431100	-0.13416000	-0.41229100				
Ag	-3.54446600	-0.18327400	0.39707200				

E = -1045.229566 au

TCG = 0.293336 au

Inter4-Ag

C	-1.81153800	-1.68292600	0.07956200
C	-1.89872800	-0.25965400	0.05055100
C	-3.17553000	0.33263600	0.03508200
C	-4.30643000	-0.47679600	0.06818400
C	-4.19204800	-1.88409900	0.11279300
C	-2.94464000	-2.50438900	0.11746000
C	0.29396500	-0.83583900	0.06599500
C	-0.55465400	0.25733500	0.04463800
H	-3.27040200	1.41636300	0.00299600
H	-5.29461800	-0.02373000	0.06134100
H	-5.09162600	-2.49370300	0.14062800
H	-2.85801500	-3.58842400	0.14536400
N	-0.47122200	-2.00845200	0.05339700
C	1.76067600	-0.93237400	0.06220300

E = -740.0341223 au

TCG = 0.157598 au

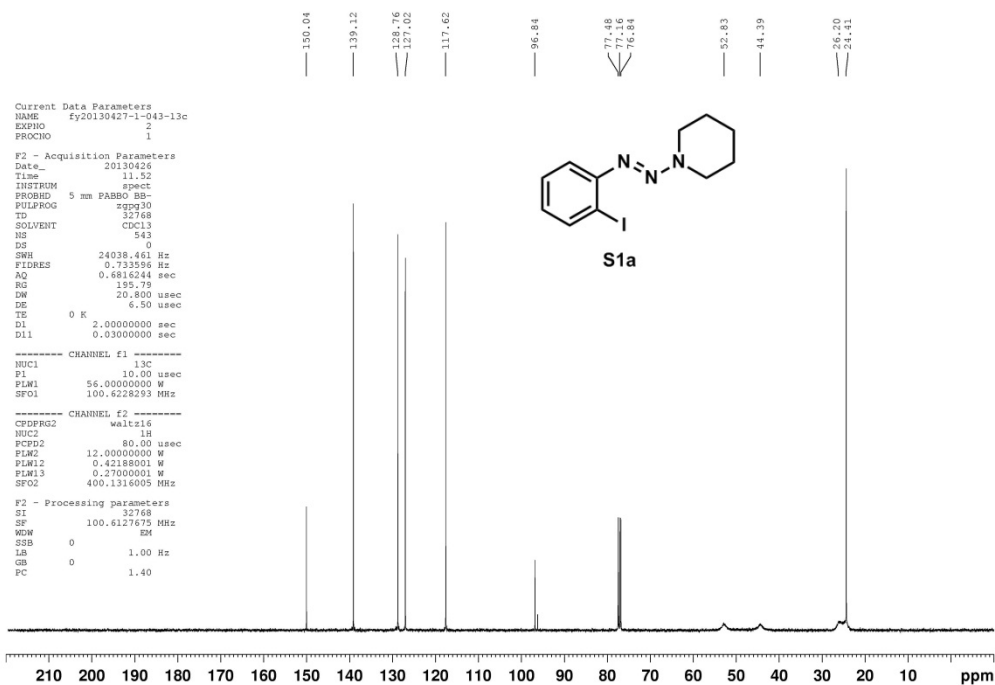
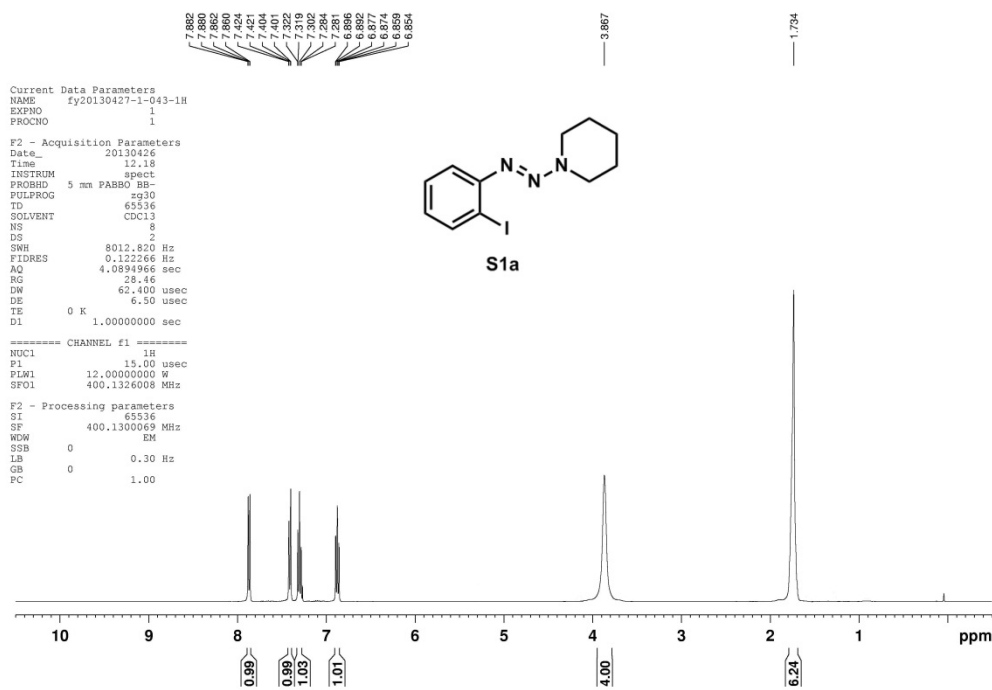
Prod-Ag

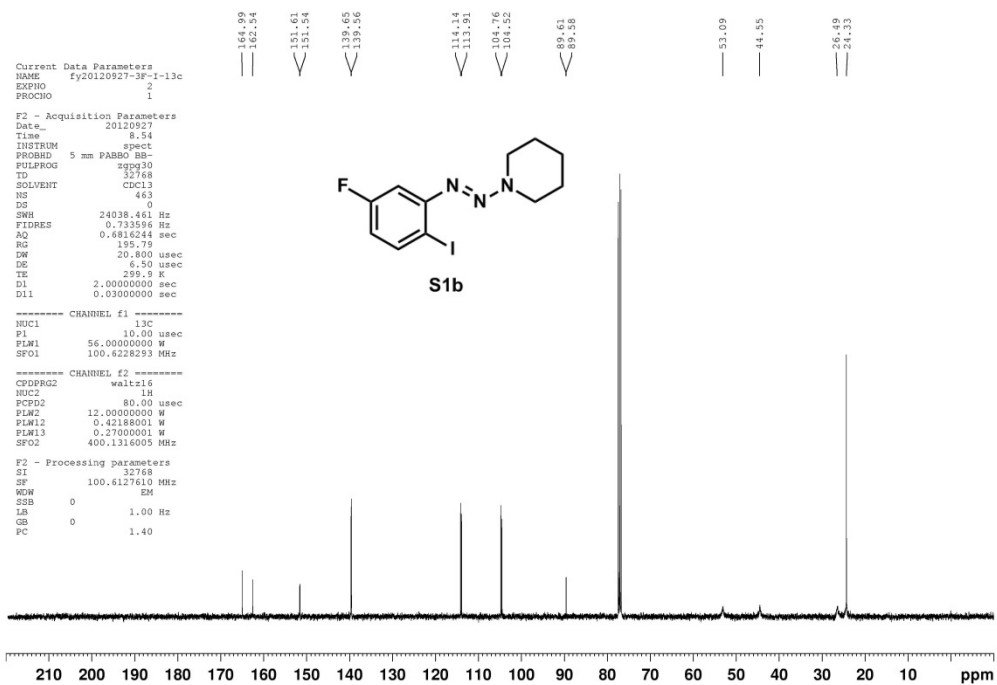
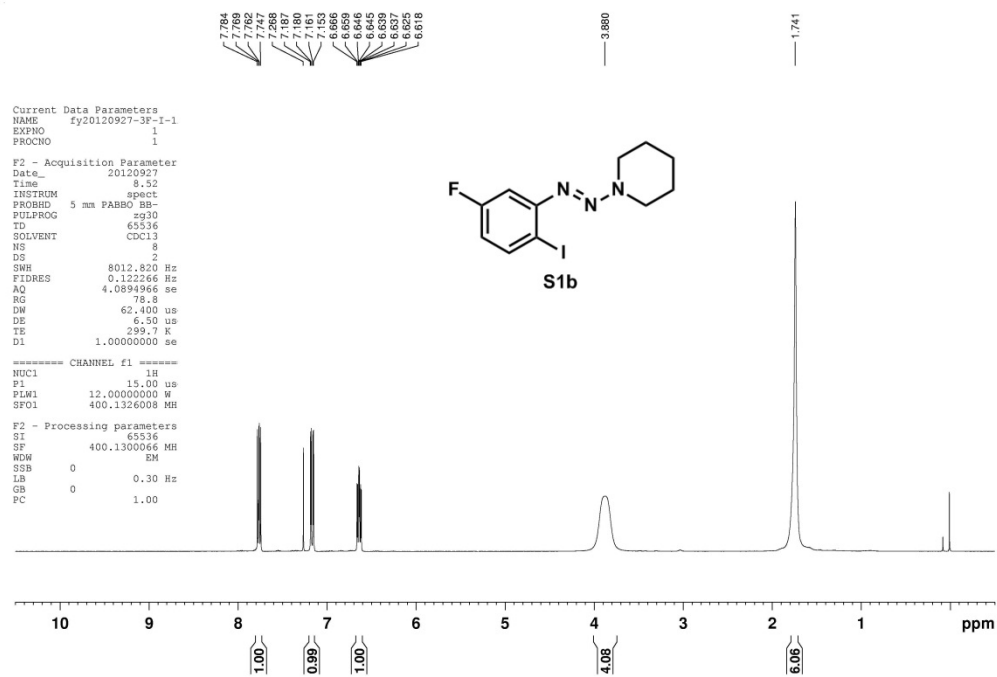
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C	-1.89583900	0.75864100	-0.14523100
C	-3.15547000	1.37615600	-0.26789400
C	-4.30268400	0.60628700	-0.11098400
C	-4.22143400	-0.77693500	0.16403600
C	-2.99074200	-1.41809800	0.28027300
C	0.28916400	0.13503300	-0.02208200
C	-0.54100100	1.21994700	-0.22568300
H	-3.22830800	2.44054400	-0.47807600
H	-5.28024600	1.07310000	-0.19977200
H	-5.13575500	-1.35212900	0.28401200
H	-2.93077200	-2.48425500	0.48595700
N	-0.50472200	-0.99417500	0.16088500
C	1.75270000	0.05281900	-0.01142300
C	2.42439400	-1.13782700	-0.34797800
C	2.52549400	1.17714700	0.33716300
C	3.81874400	-1.20268900	-0.33198200
H	1.85696600	-2.01138200	-0.65987300
C	3.91786700	1.11335100	0.34229600
H	2.02548400	2.09831900	0.62306600
C	4.57306700	-0.07799000	0.01194500
H	4.31563200	-2.13148200	-0.60099600
H	4.49400100	1.99340200	0.61699700
H	5.65863600	-0.12786100	0.02212100
H	-0.15759500	-1.88280700	0.49055000
H	-0.21527600	2.22639000	-0.45286400

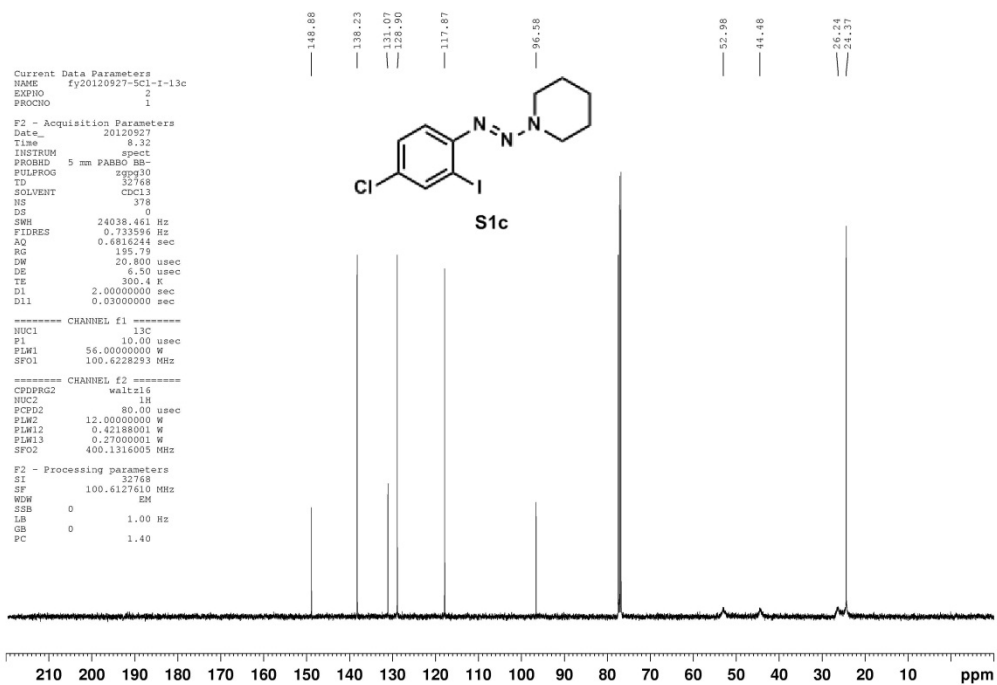
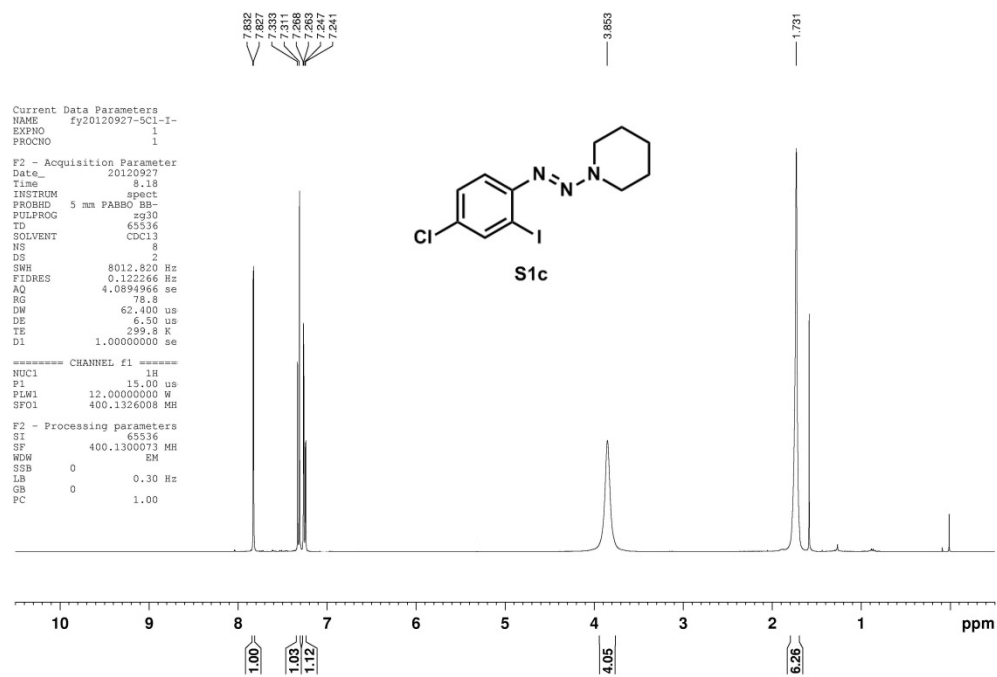
E = -594.8281719 au

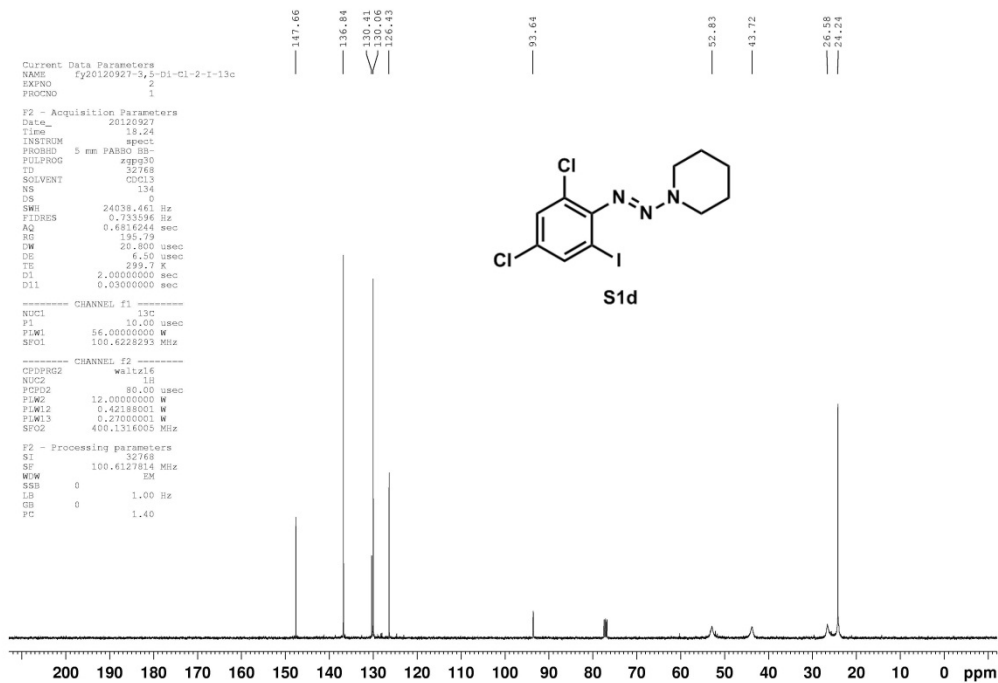
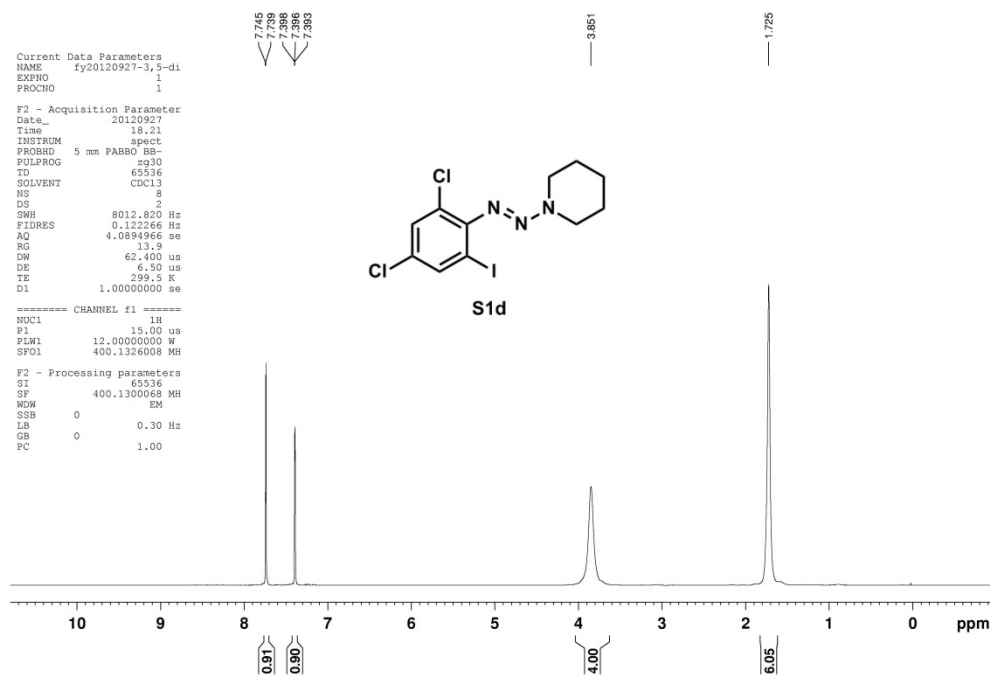
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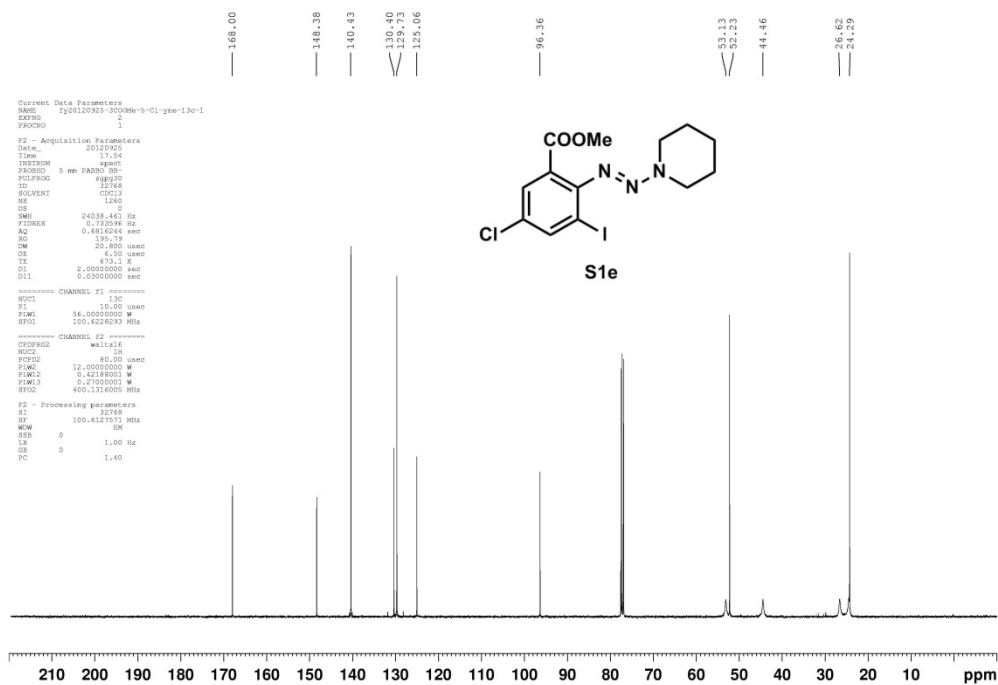
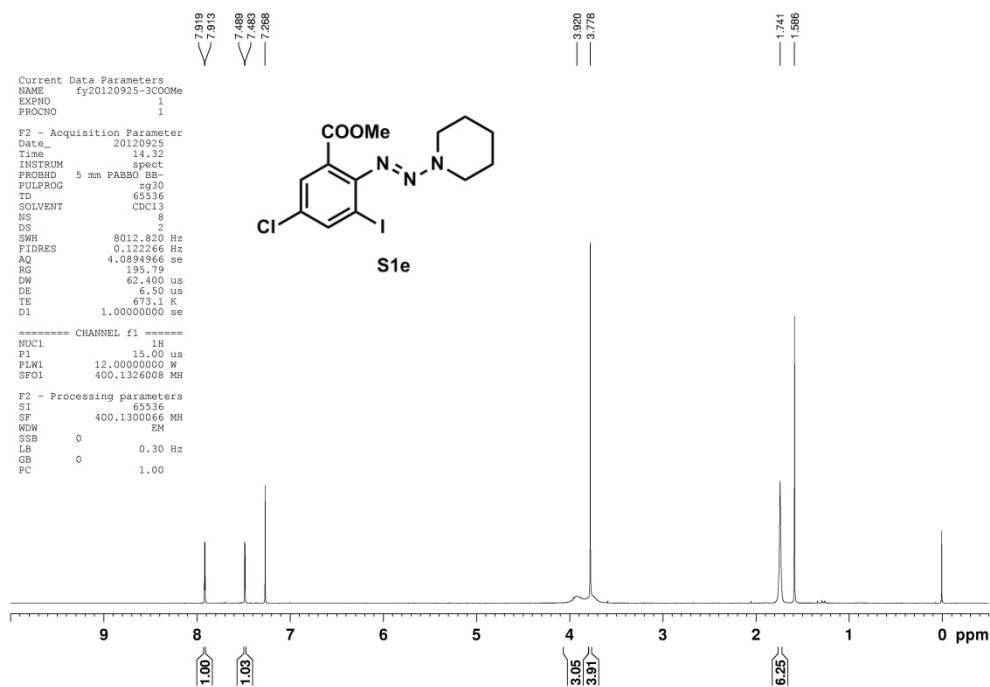
NMR Spectra Images of Triazene Substrates and Products

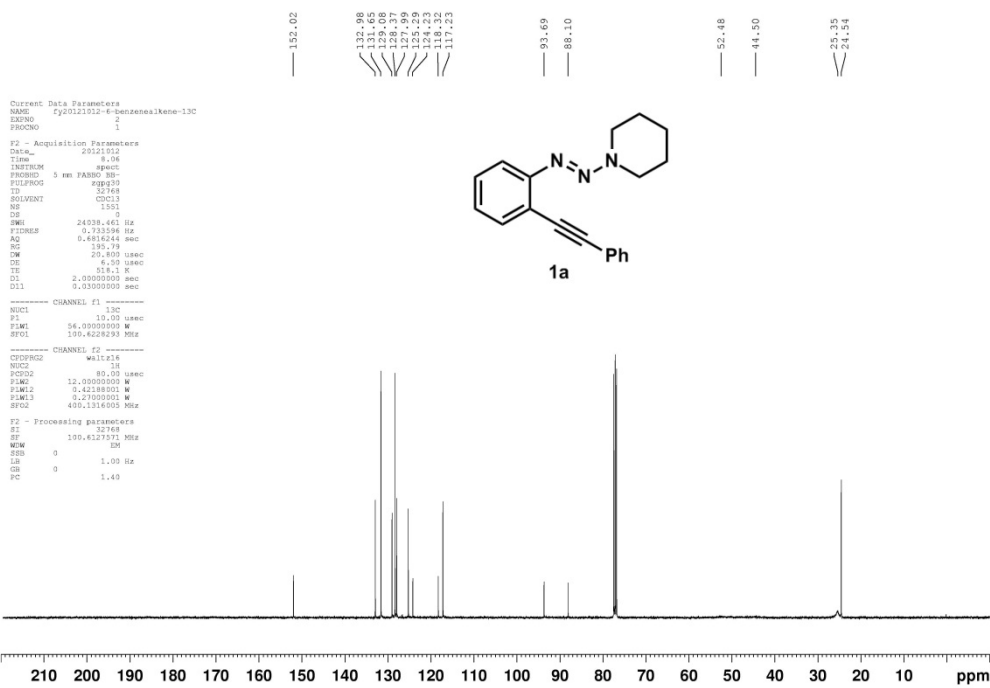
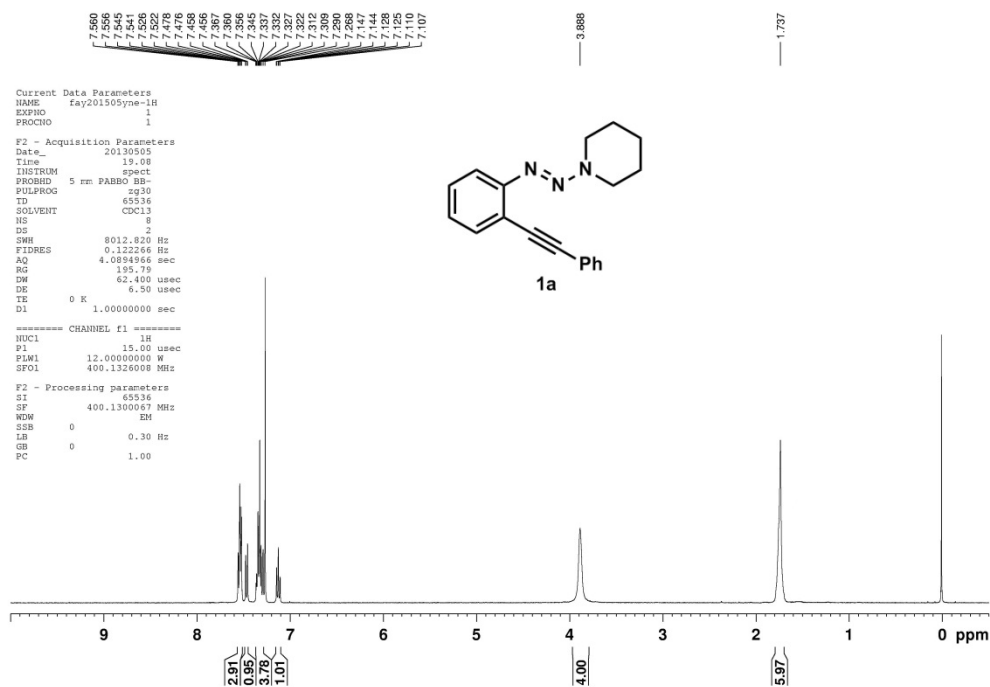


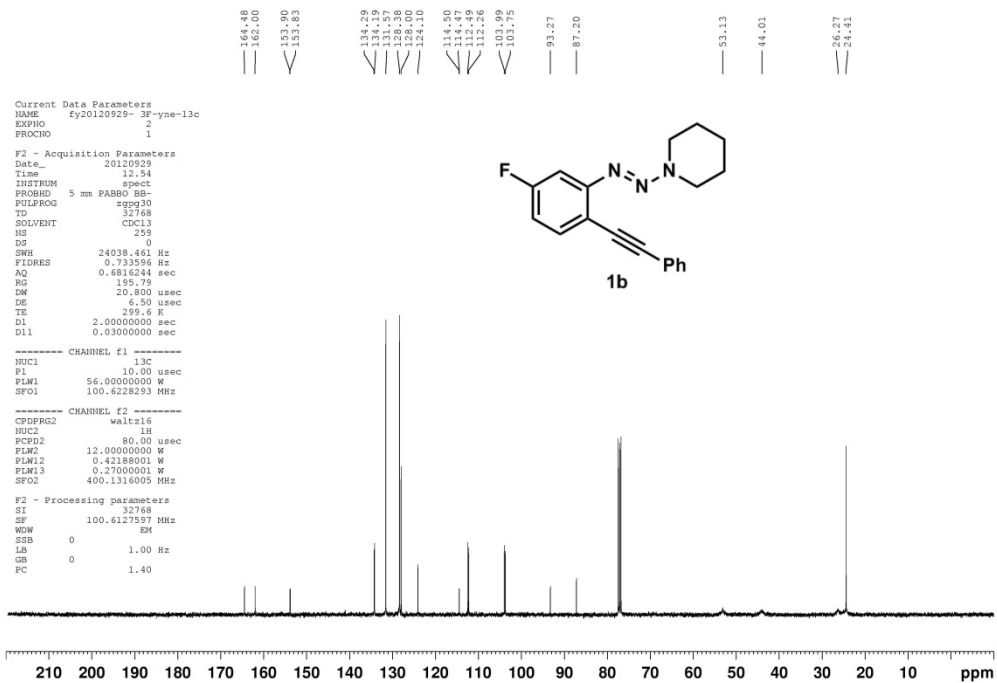
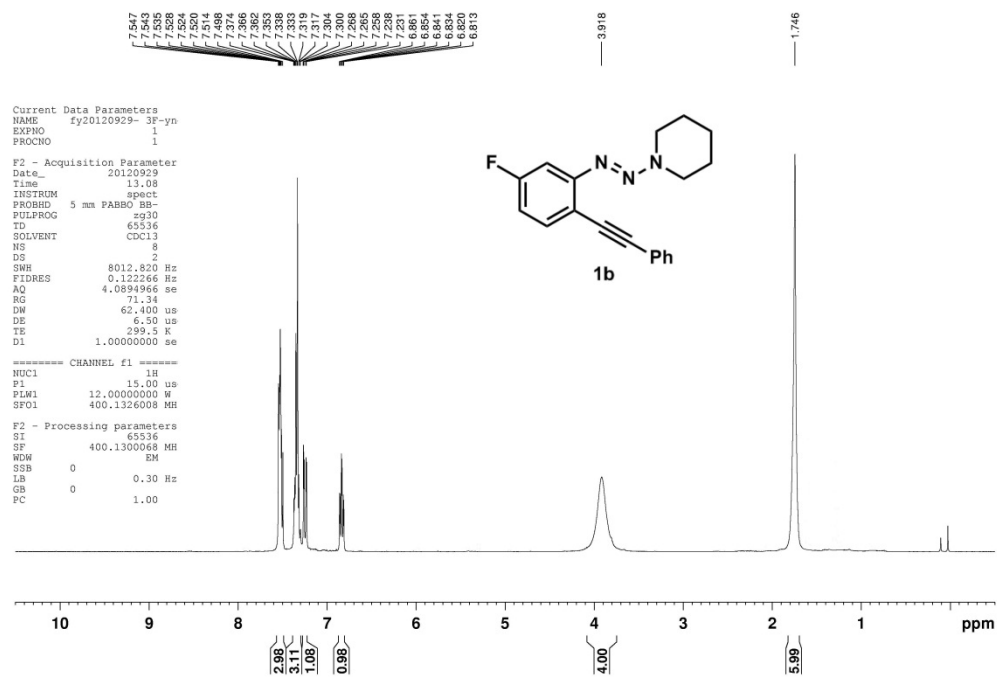


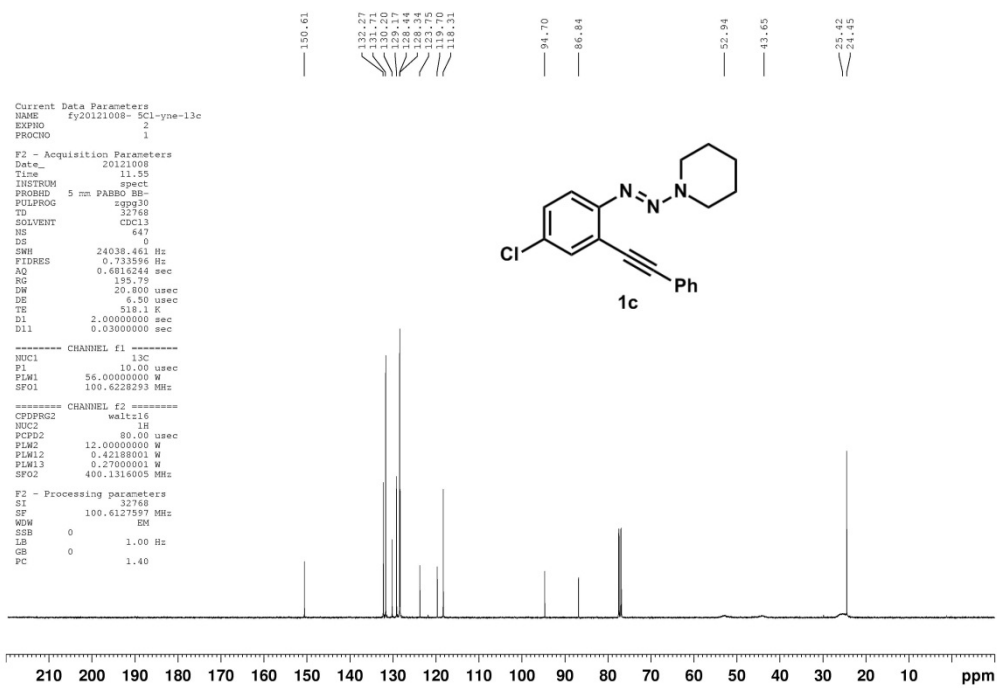
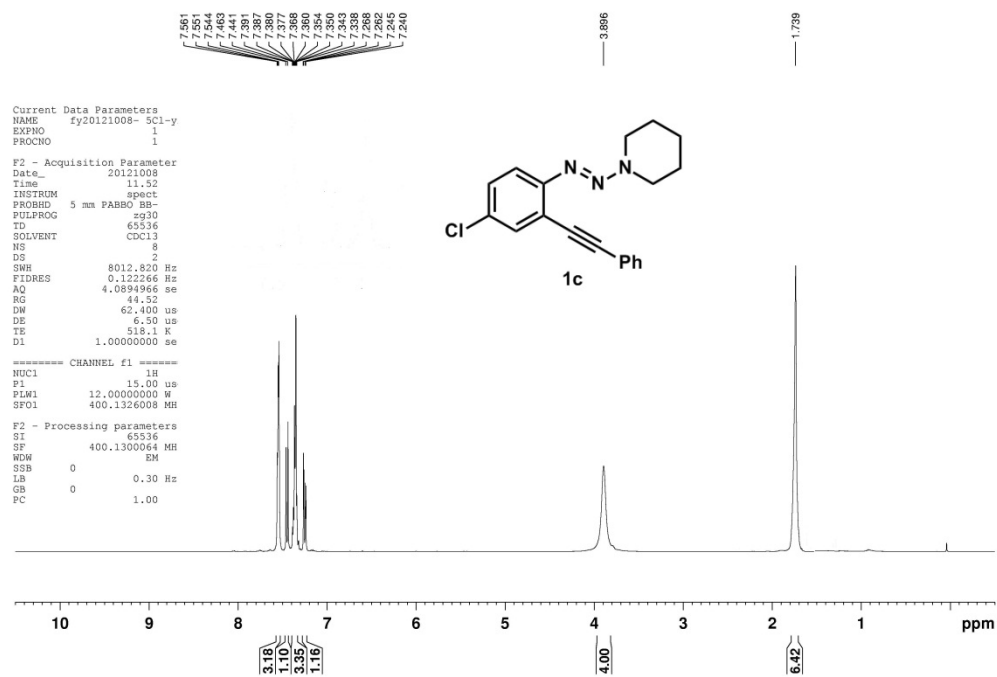


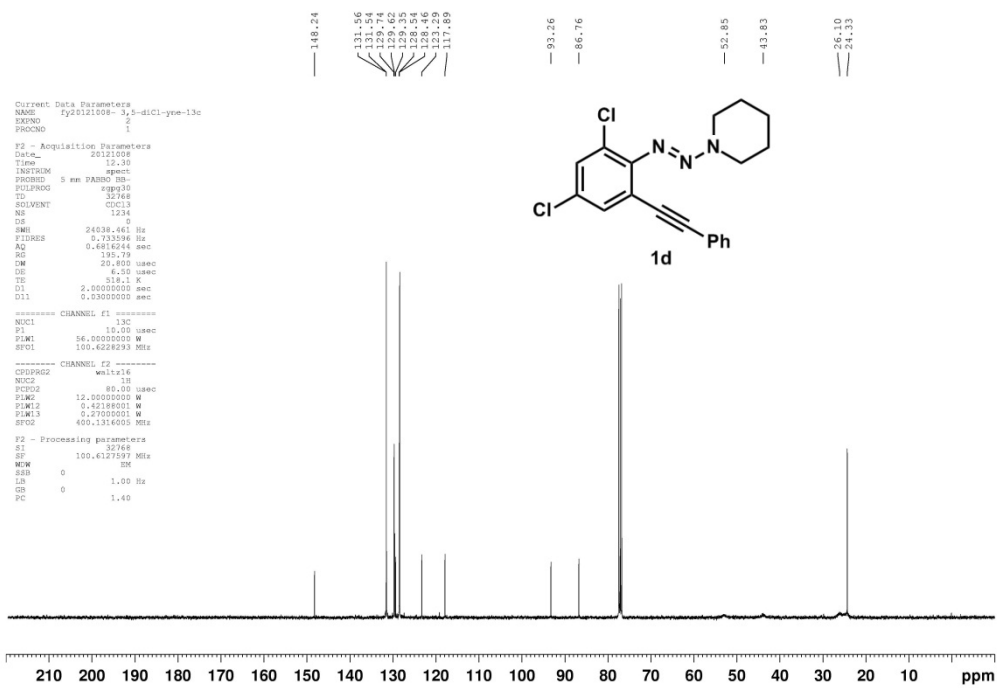
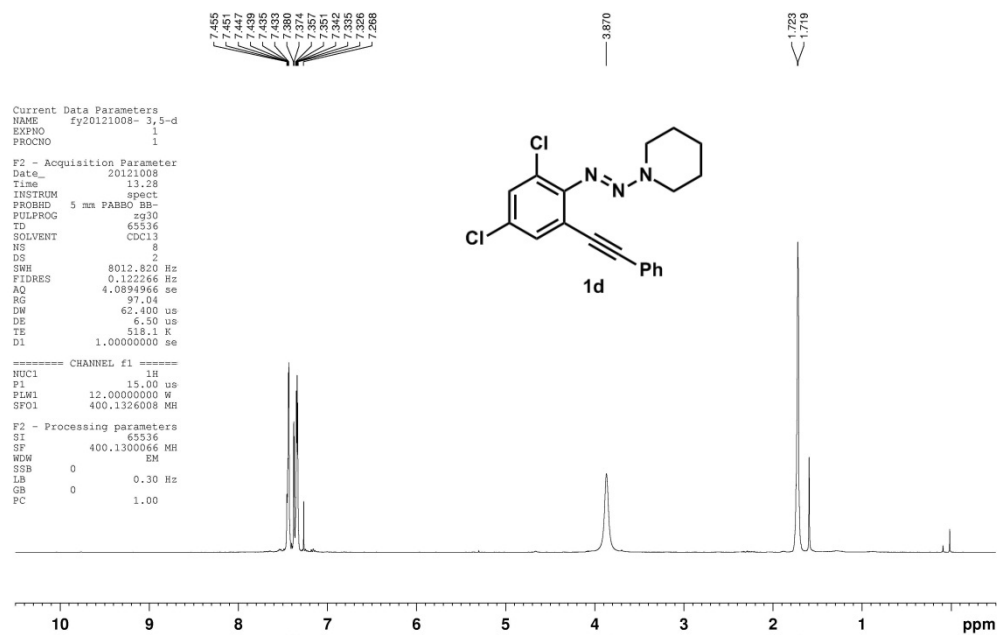


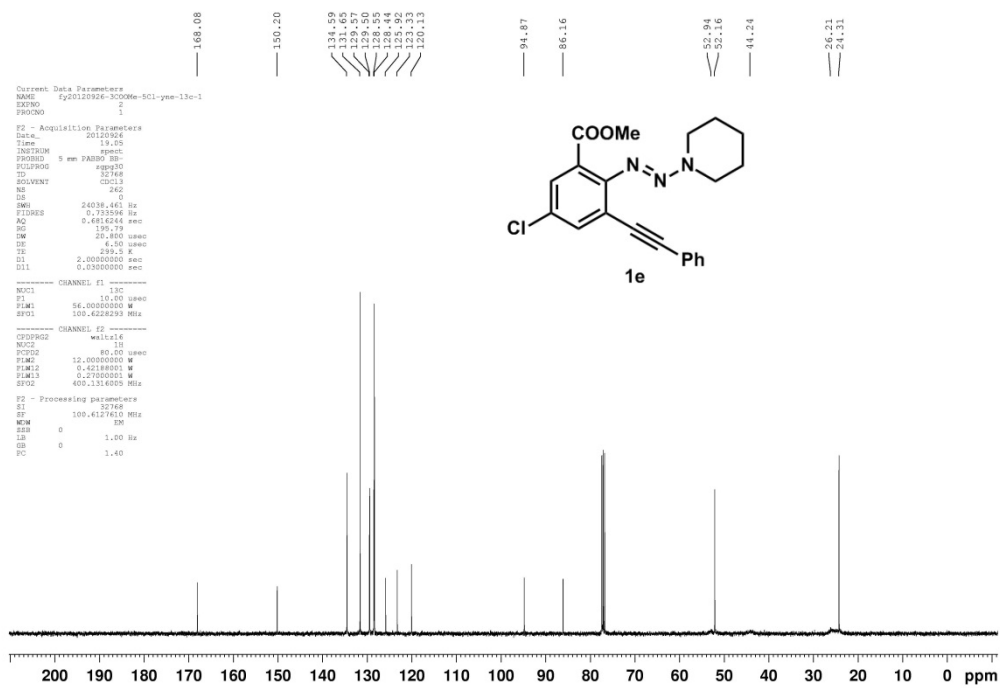
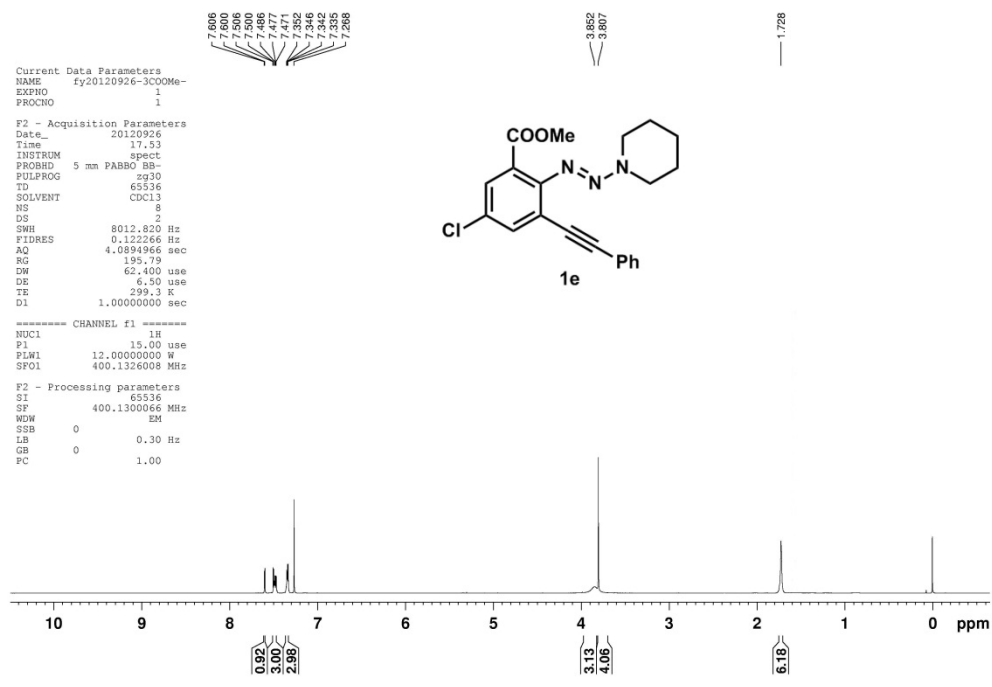


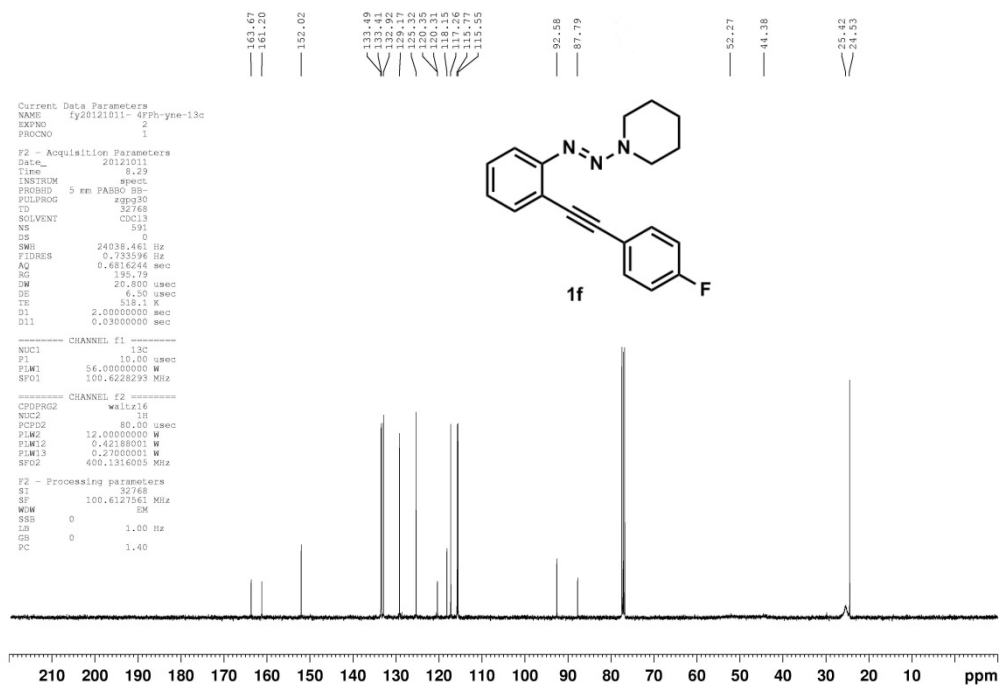
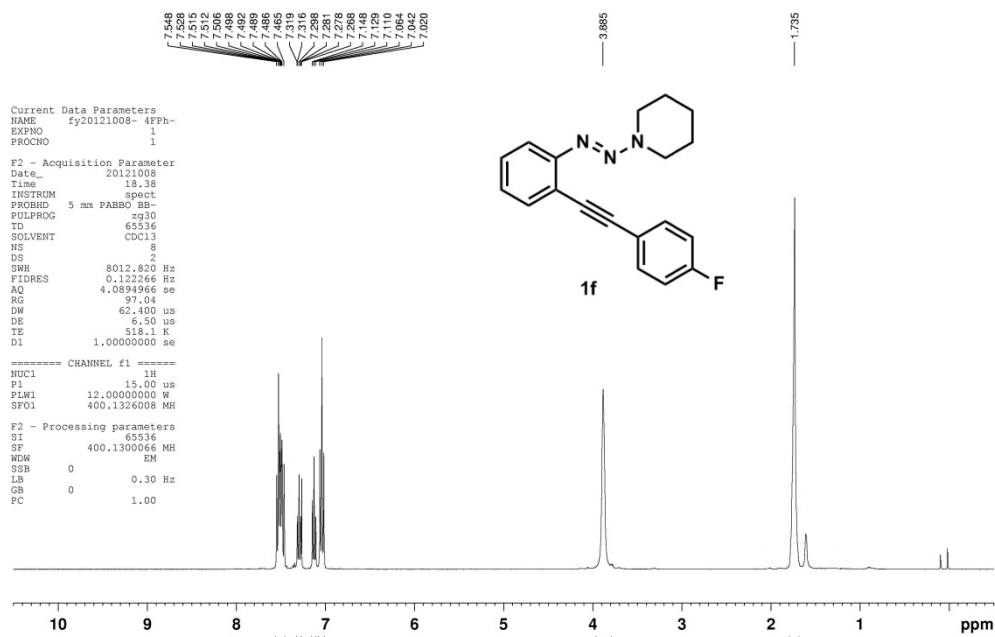


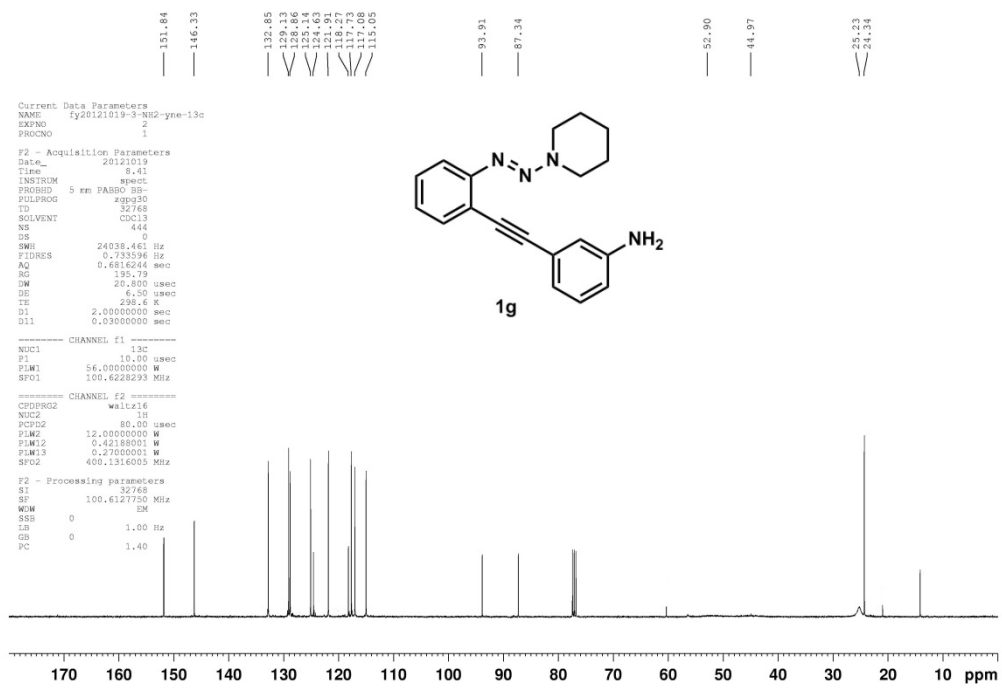
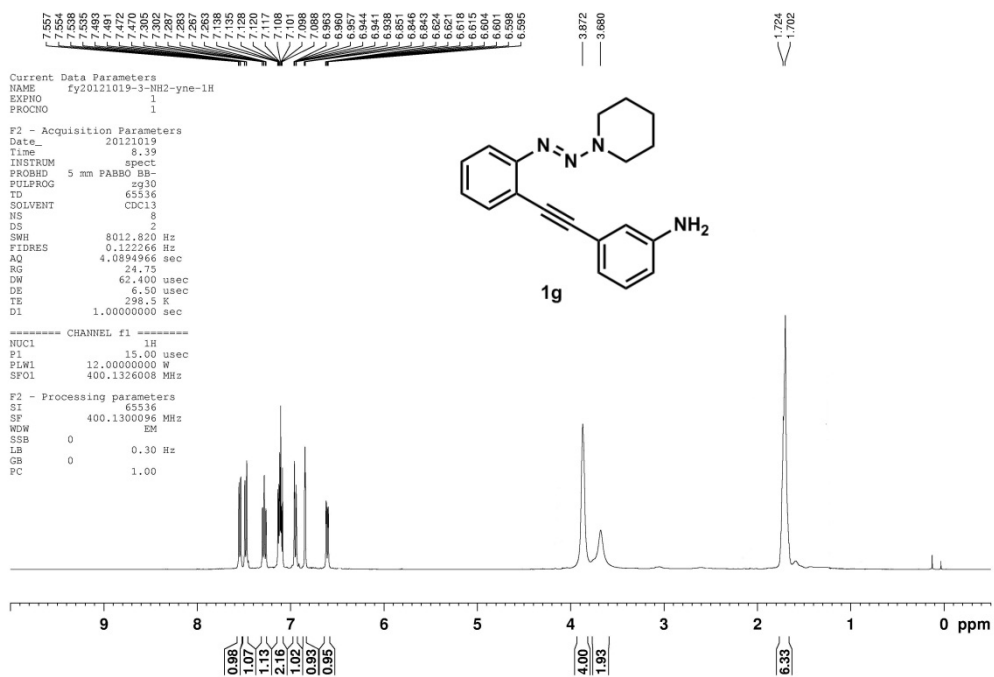


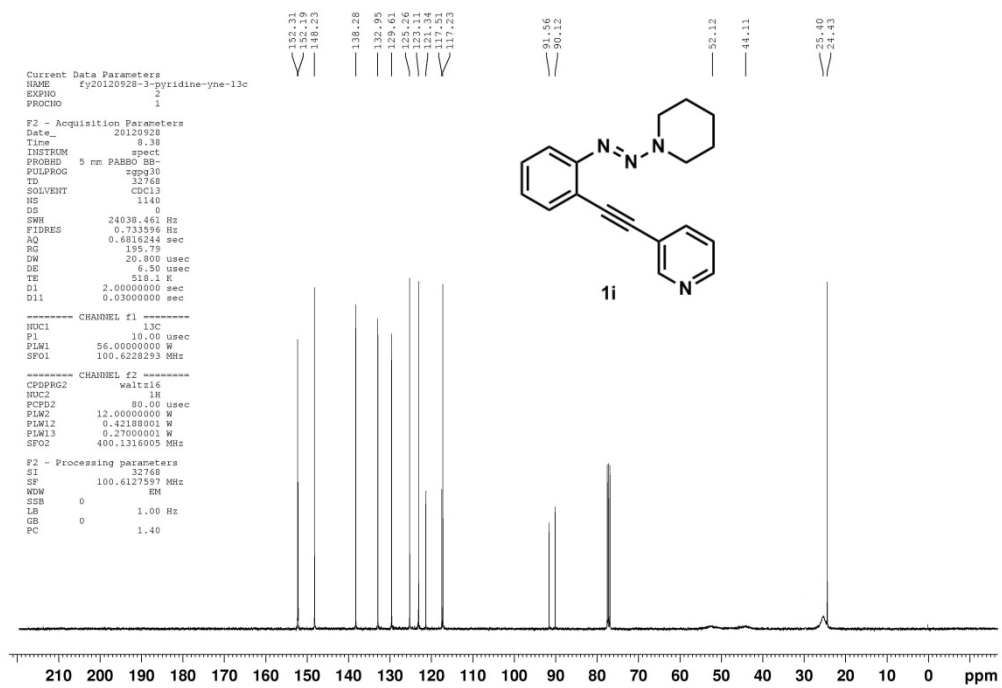
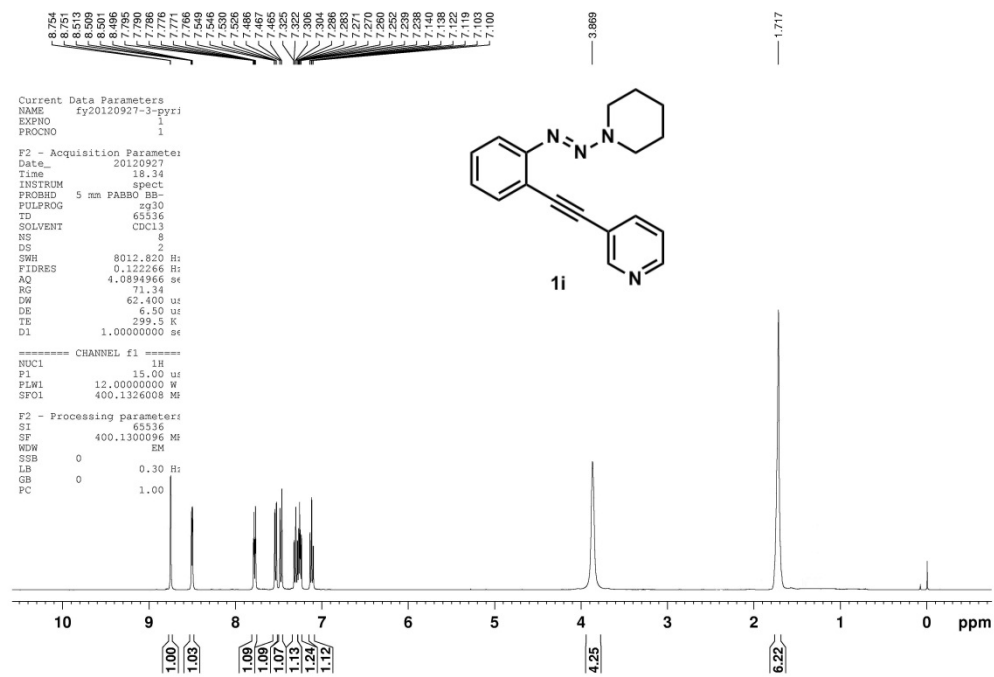


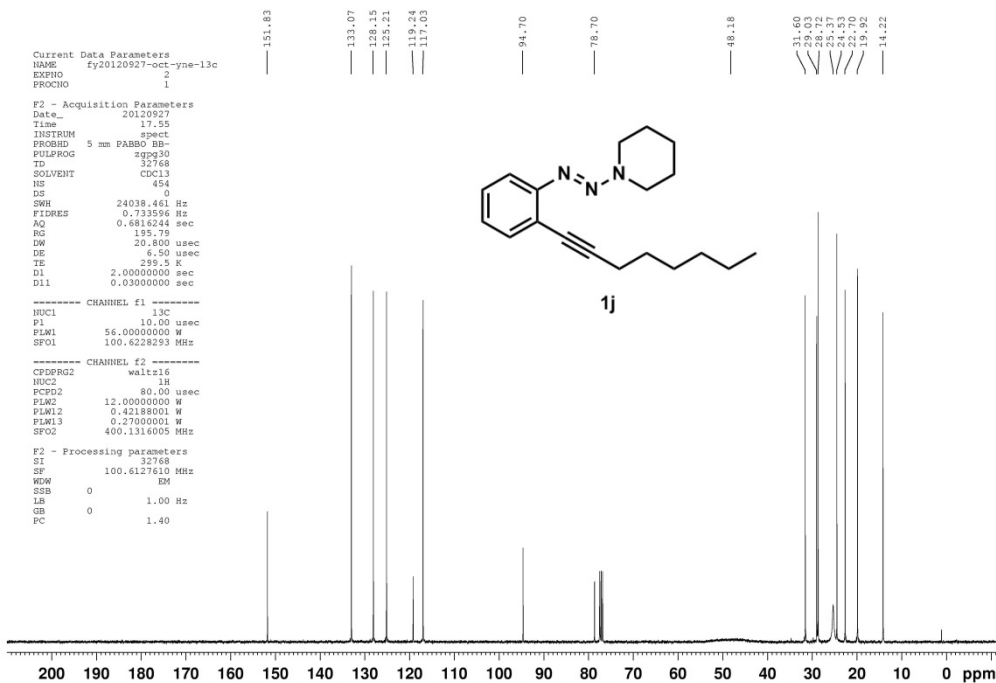
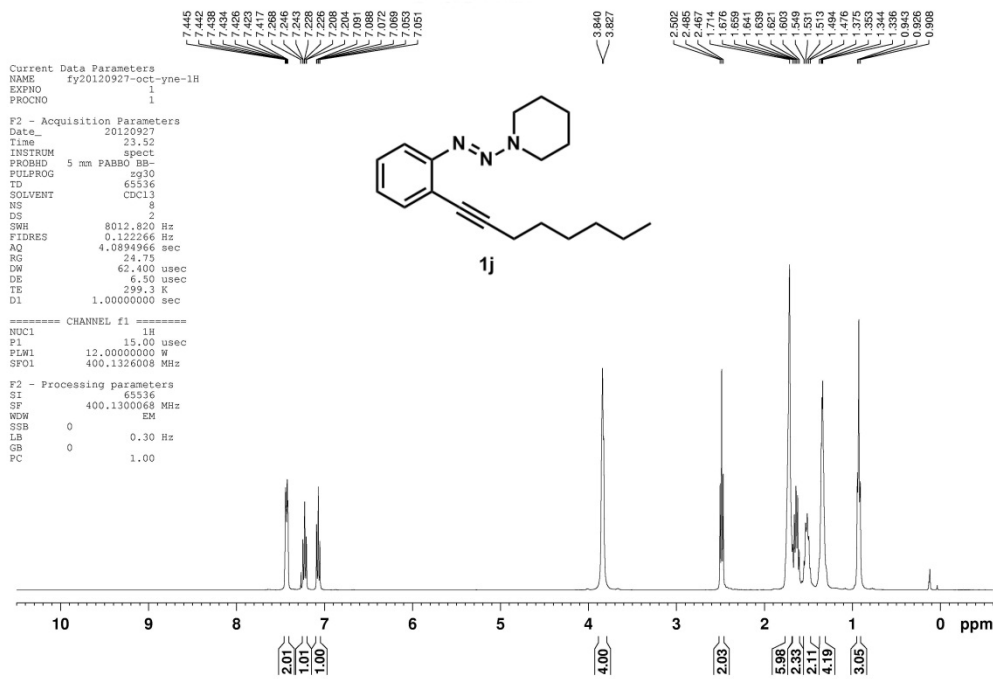


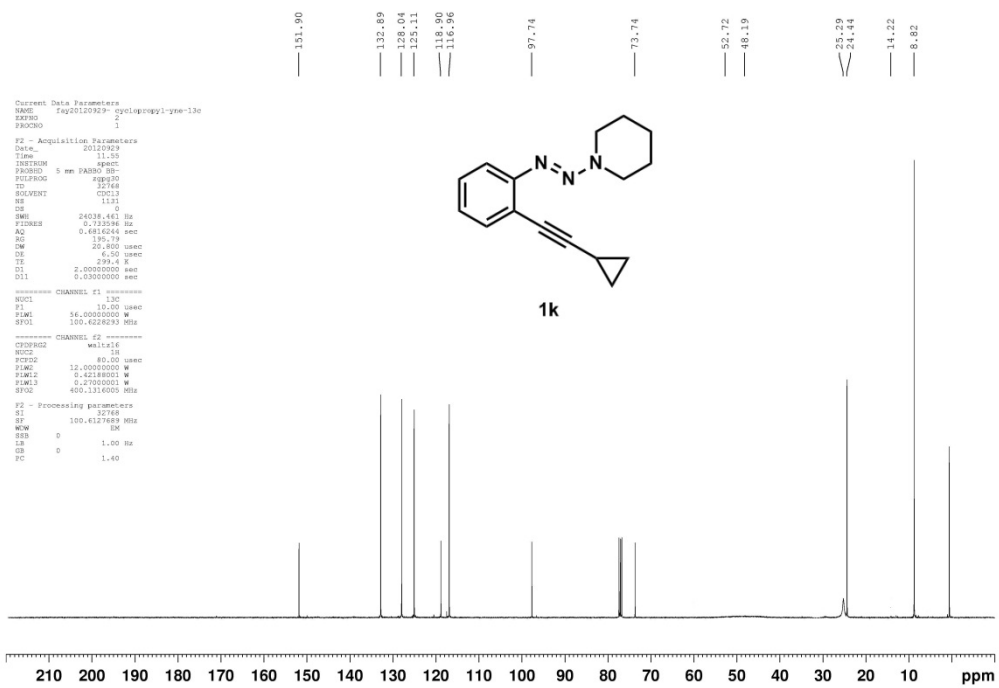
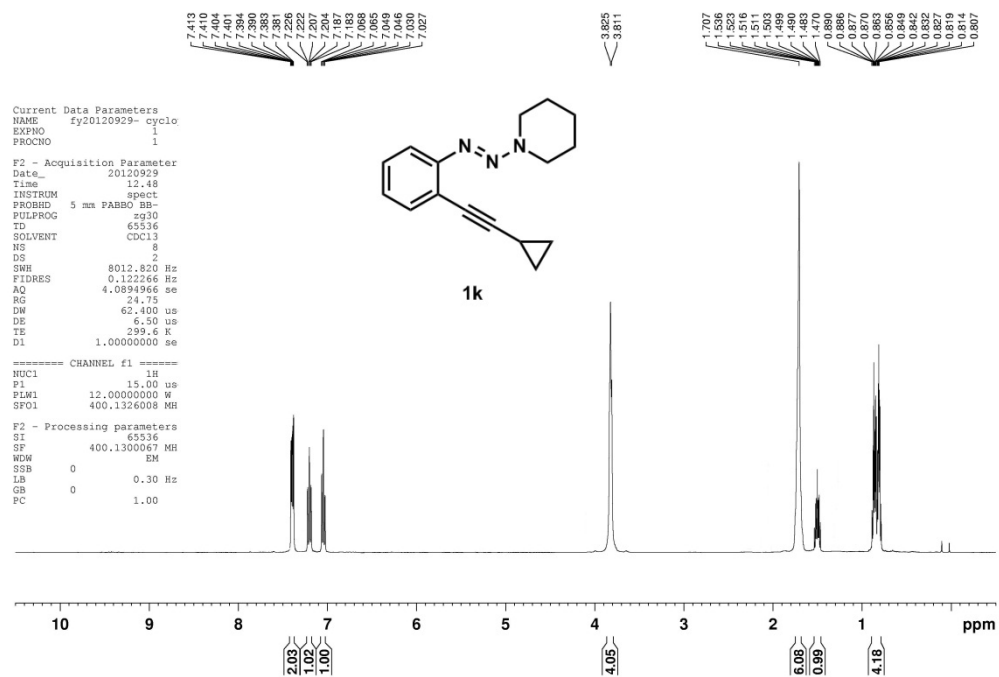


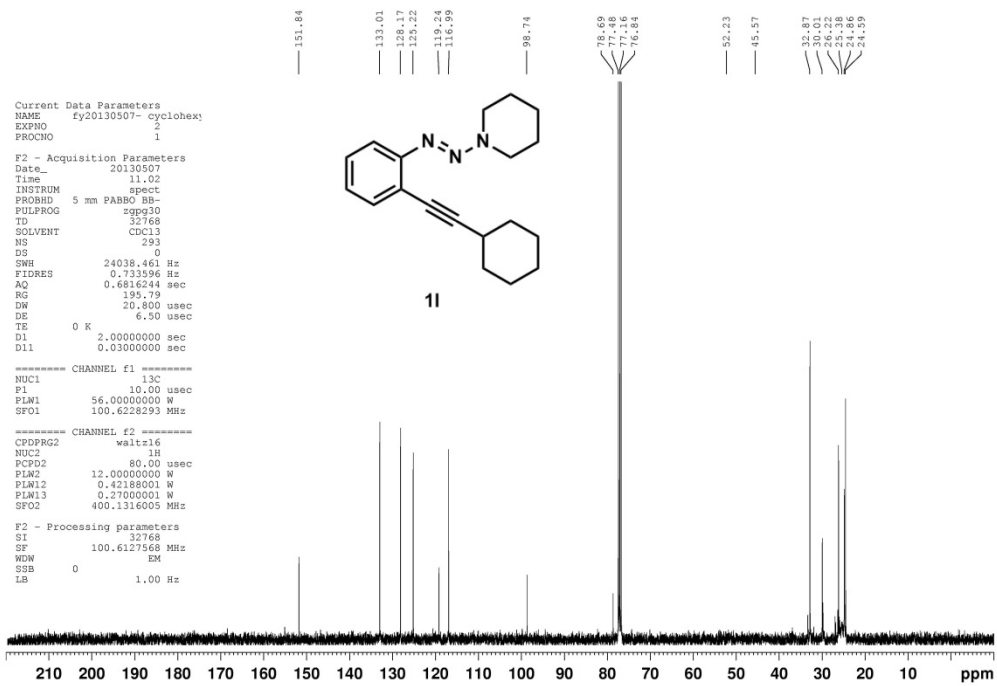
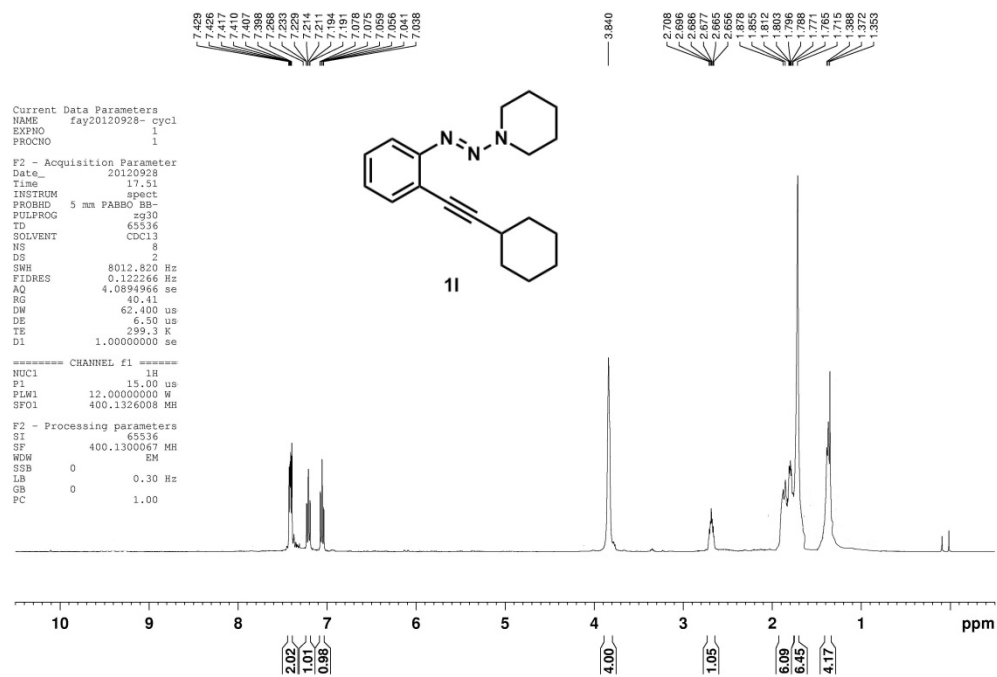


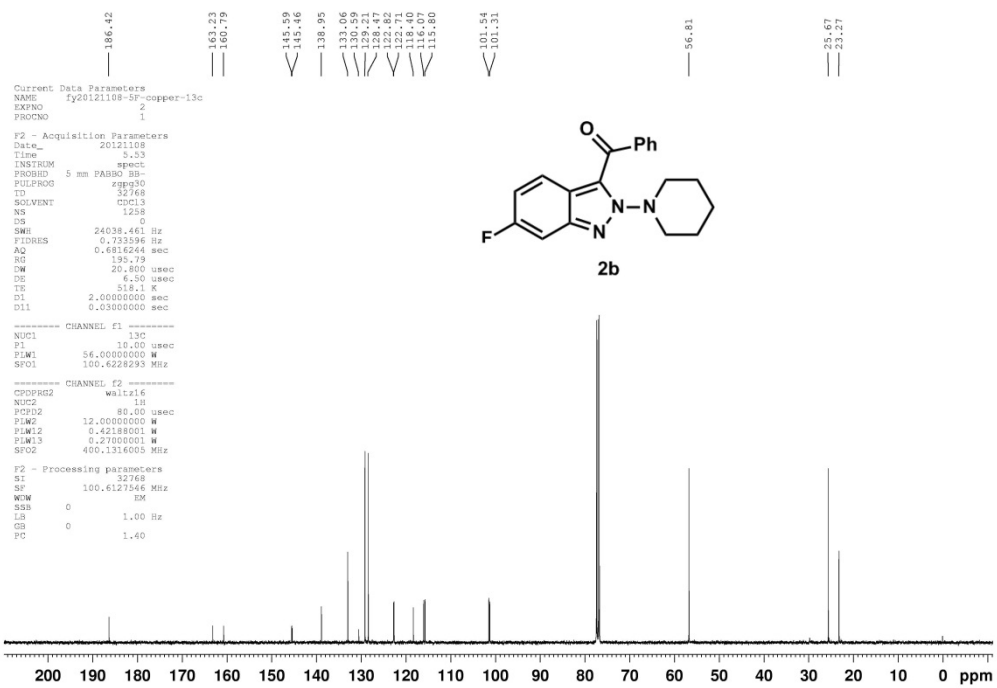
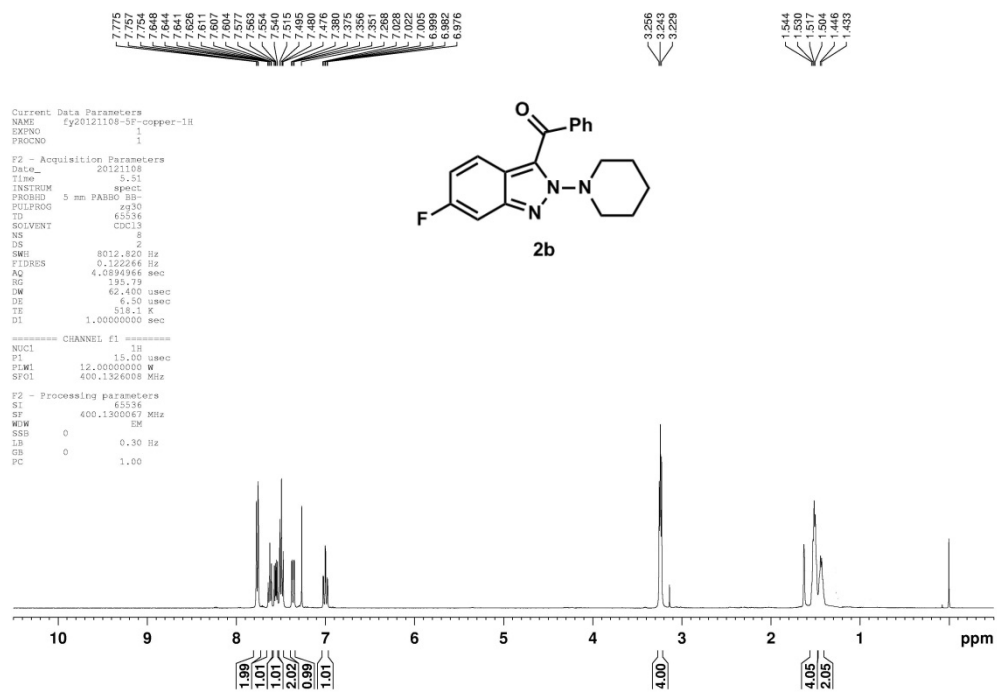


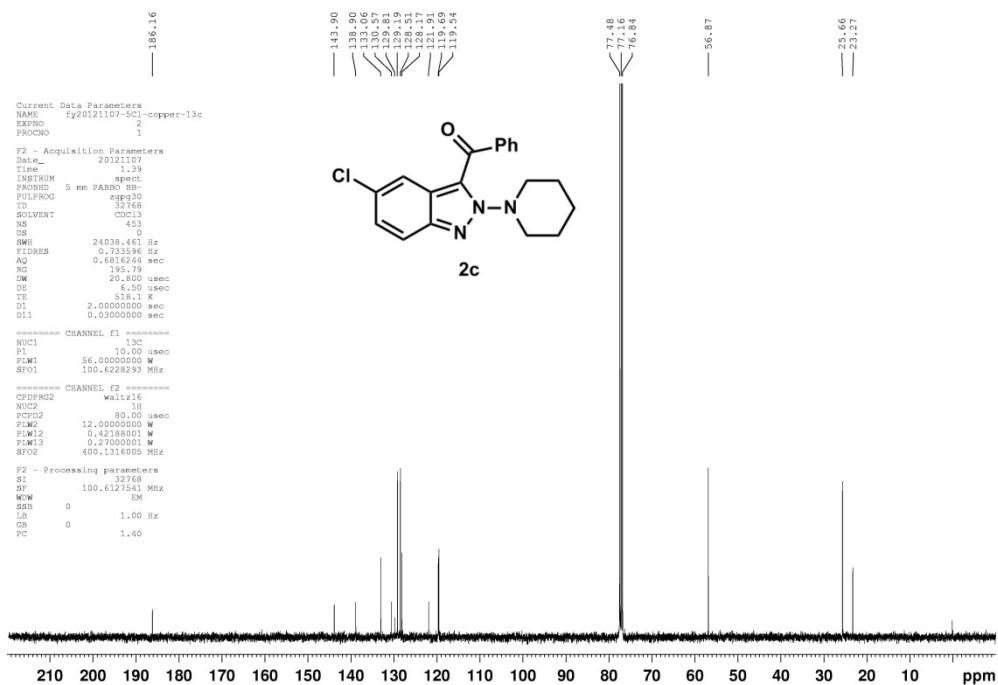
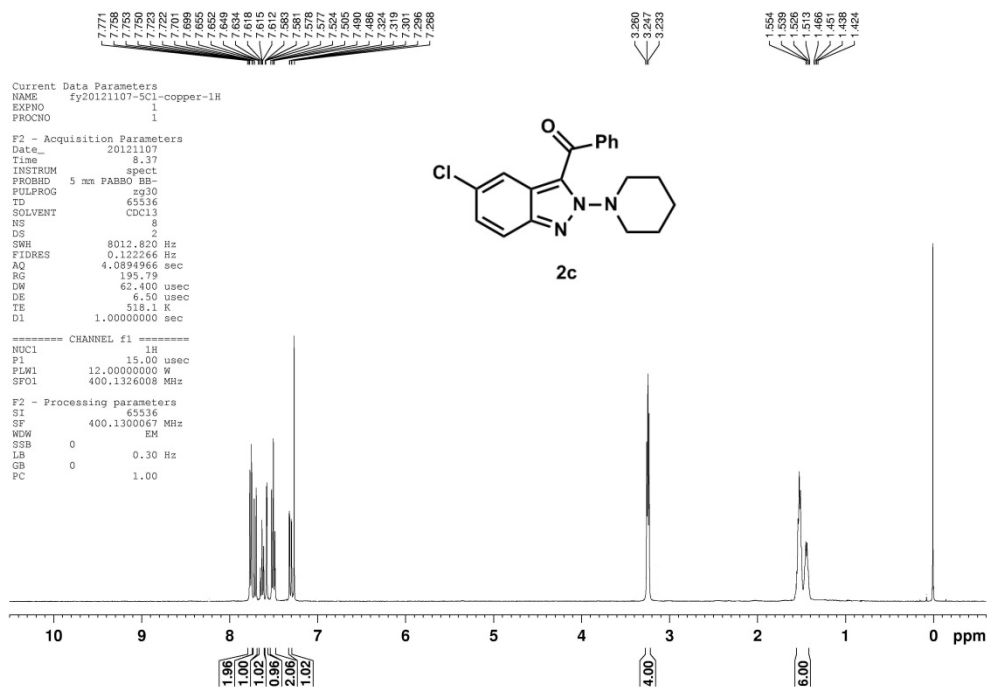


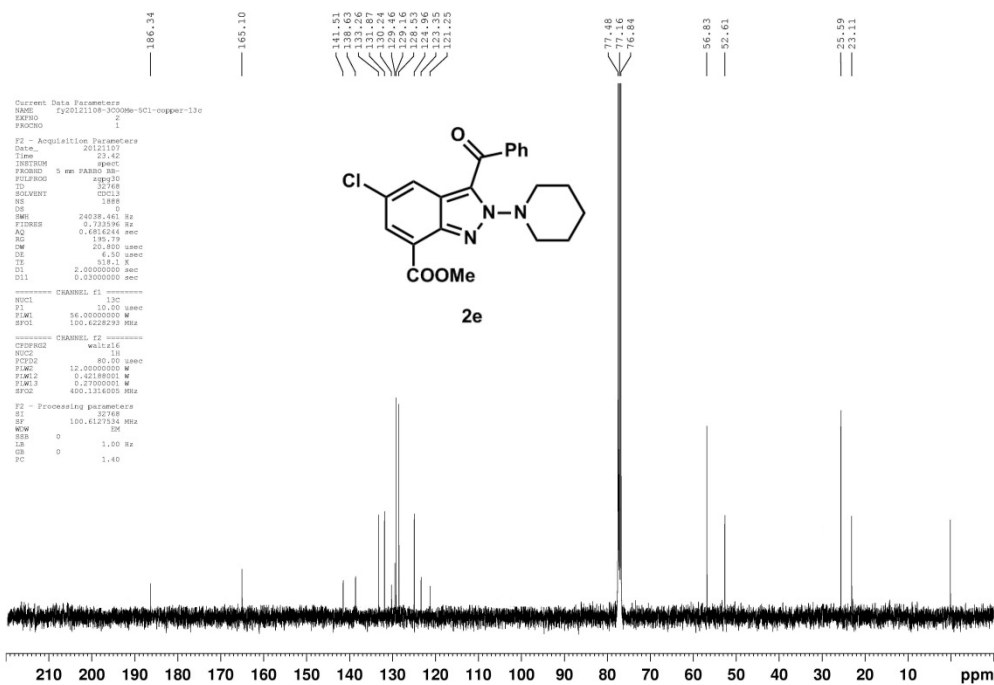
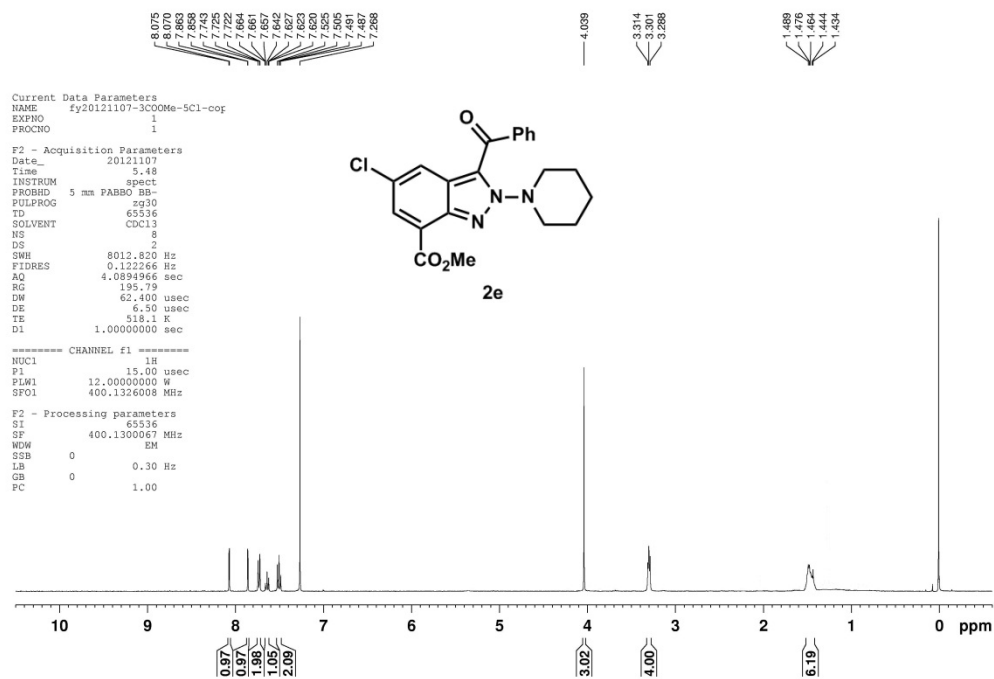


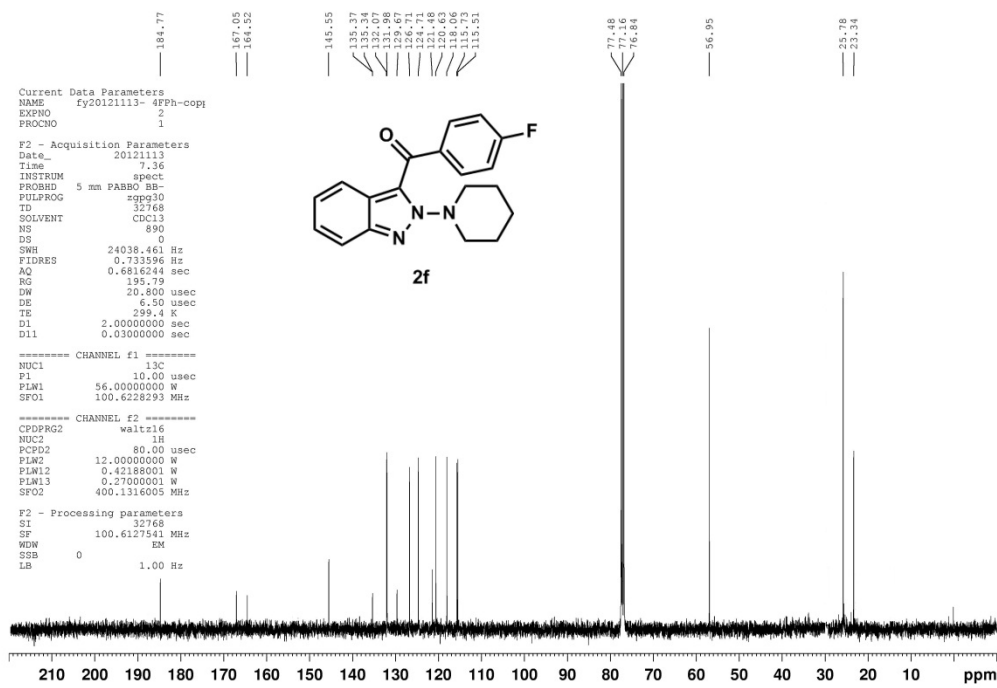
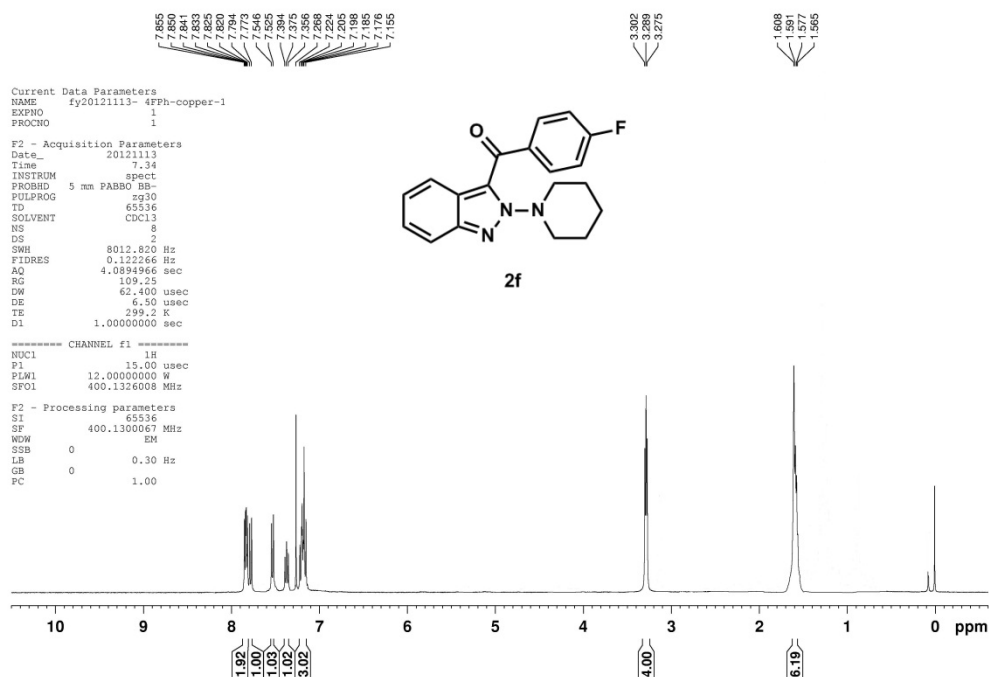


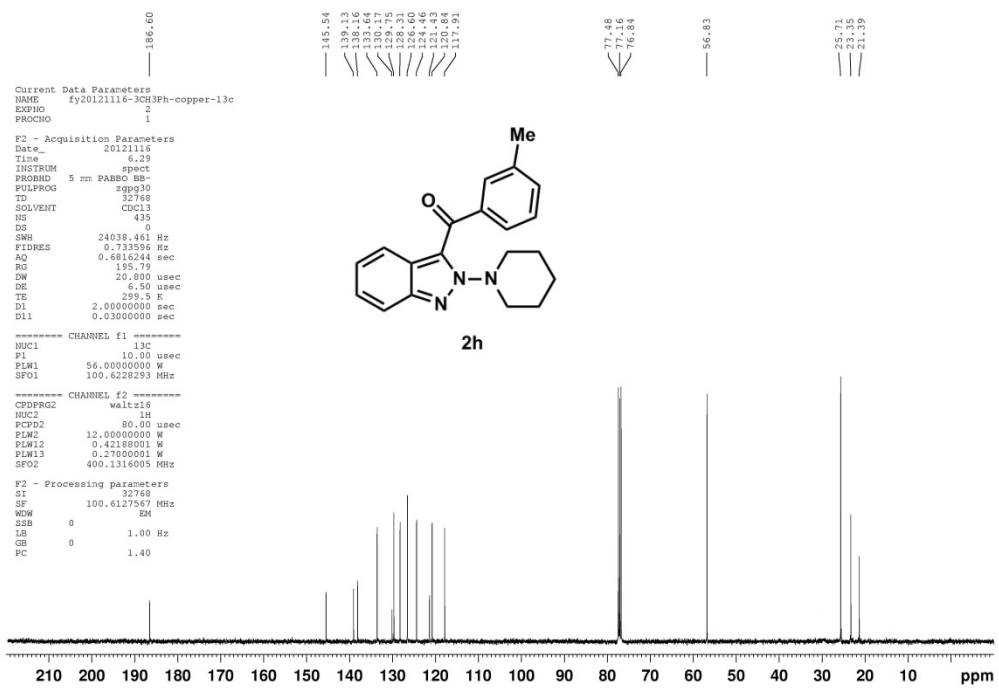
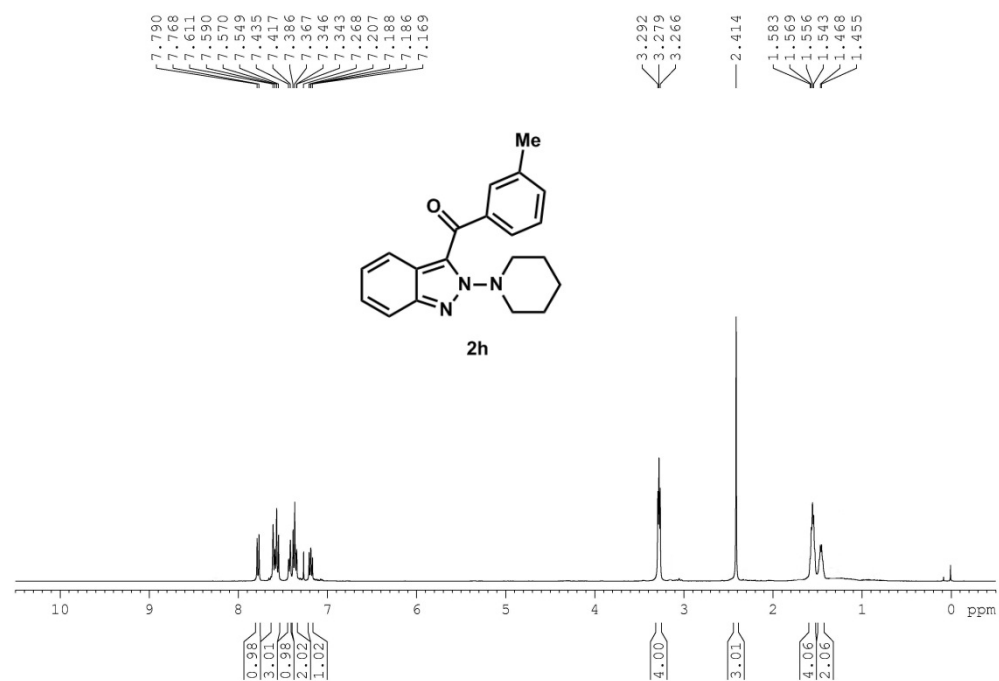












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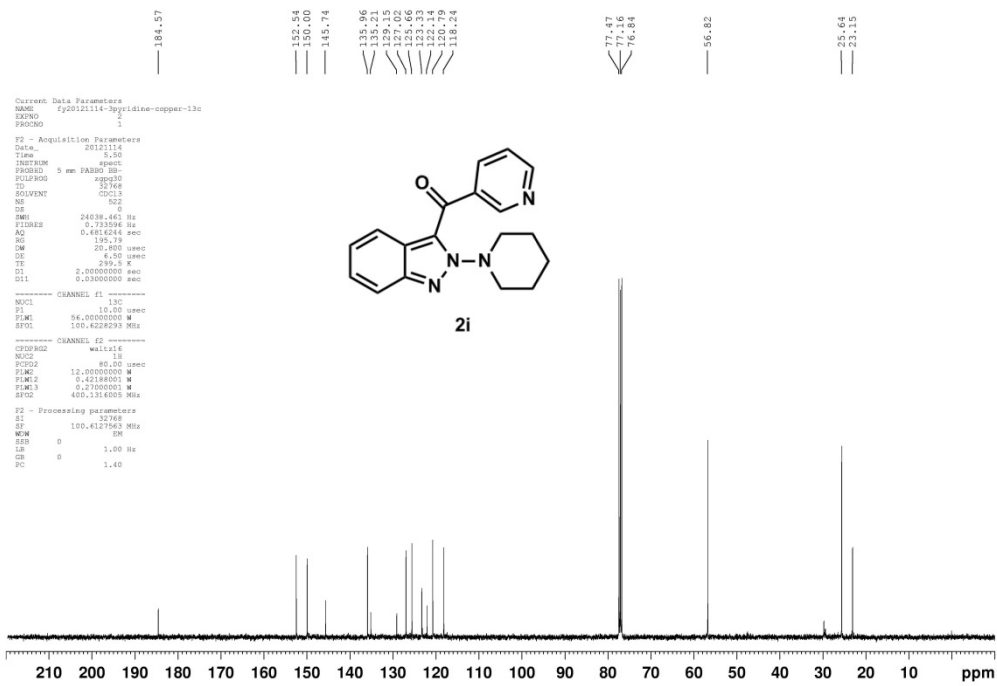
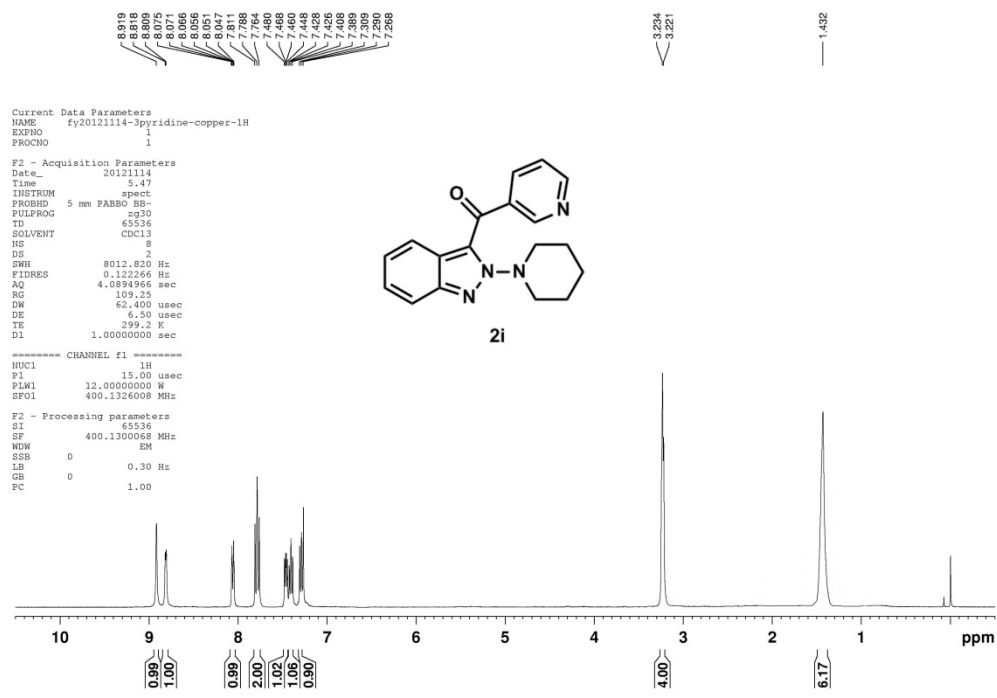
Current Data Parameters
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EXPNO    2
PROCNO   1

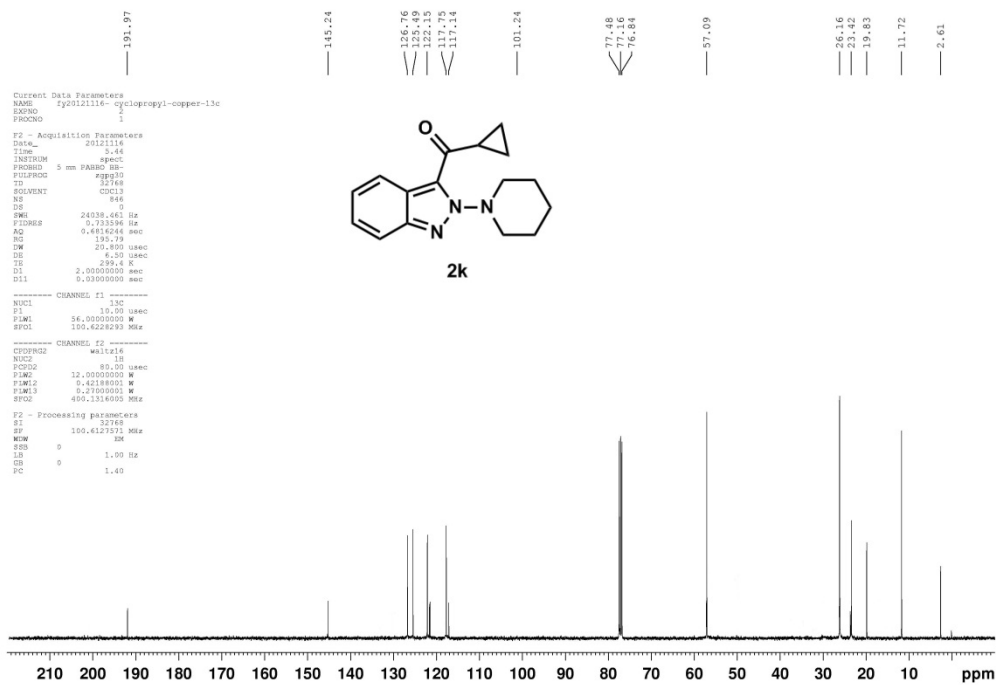
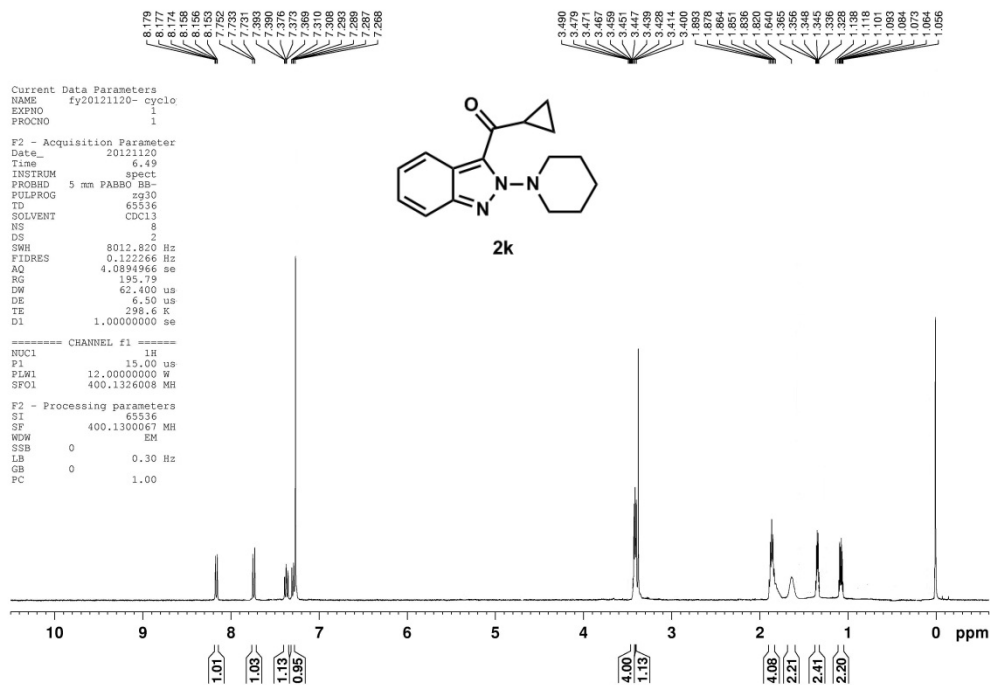
F2 - Acquisition Parameters
Date_    20121116
Time     6.29
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        435
DS        0
SWH       24038.461 Hz
FIDRES    0.733596 Hz
AQ        0.4816244 sec
RG        195.79
DW        20.800 usec
DE        6.50 usec
TE        299.5 K
D1        2.00000000 sec
D11       0.03000000 sec

===== CHANNEL f1 =====
NUC1      13C
P1        10.00 usec
PLM1     56.00000000 W
SFO1     100.6228293 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2     80.00 usec
PLM2     12.00000000 W
PLM12    0.42188001 W
PLM13    0.27000031 W
SFO2     400.1316095 MHz

F2 - Processing parameters
SI        32768
SF        100.6127967 MHz
WDW       EM
SSB       0
GB        0
PC        1.40
    
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6.882
7.784
7.686
7.673
7.656
7.647
7.473
7.458
7.429
7.427
7.409
7.386
7.367
7.354
7.338
7.323
7.320
7.317
7.298
7.226
7.211
7.191
7.188
7.154
7.132
7.117
7.115
6.848
6.843

0.014

