Electronic Supplementary Information

Cascade double isocyanide insertion and C-N coupling of 2-iodo-2'-isocyano-1,1'-biphenyls

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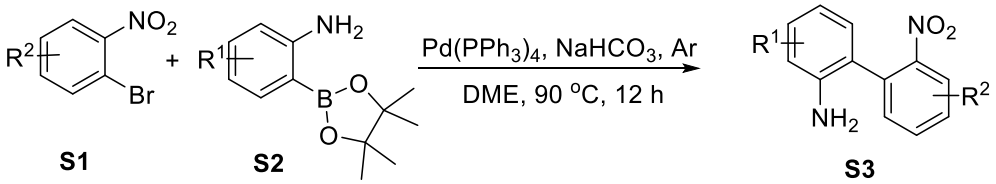
1. General Information

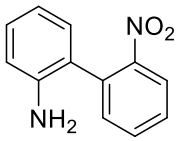
All the solvents and reagents were purchased from commercial suppliers. ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz or/and 500 MHz Bruker FT-NMR spectrometers. All chemical shifts were given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, *J*, are reported in Hertz (Hz). High Resolution Mass (MS) analysis was obtained using on a LC/MSD TOF spectrometer system with Electrospray Ionization (ESI). Melting points were measured on a Mel-Temp apparatus and are uncorrected. IR was recorded on a Bruker Tensor 27 FT-IR spectrometer. Reactions were monitored by thin-layer chromatography (TLC) carried out on commercial silica gel plates (GF254) under UV light. Flash chromatography was performed on silica gel 60 (200–300 mesh).

2. Synthesis and Characterization of the Starting Materials

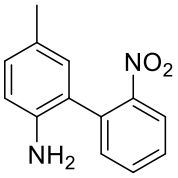
2.1 Preparation of 2'-nitro-[1,1'-biphenyl]-2-amines



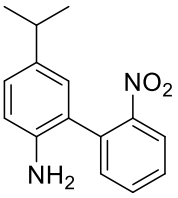
S1 **S2** **S3**



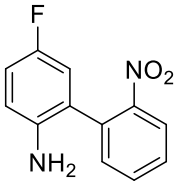
5.2 mmol, 85%
S3a



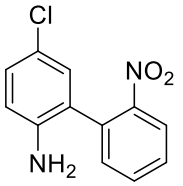
5.1 mmol, 64%
S3b



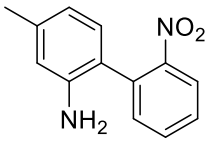
4.4 mmol, 74%
S3c



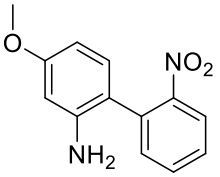
5.9 mmol, 90%
S3d



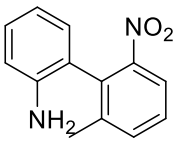
6.2 mmol, 86%
S3e



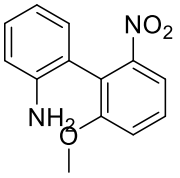
2.5 mmol, 51%
S3f



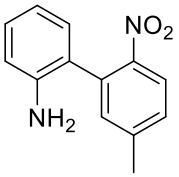
6.9 mmol, 86%
S3g



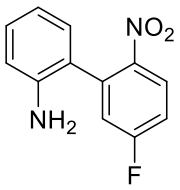
5.0 mmol, 83%
S3j



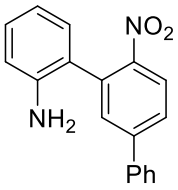
4.6 mmol, 92%
S3k



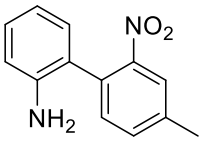
3.9 mmol, 65%
S3l



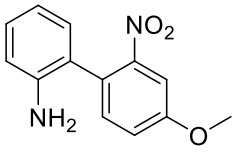
4.5 mmol, 90%
S3m



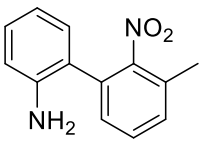
7.8 mmol, 85%
S3n



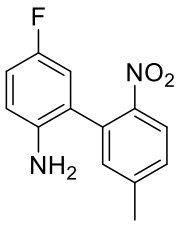
5.4 mmol, 90%
S3o



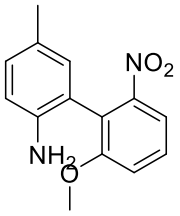
5.0 mmol, 83%
S3p



5.3 mmol, 88%
S3r



5.0 mmol, 83%
S3s

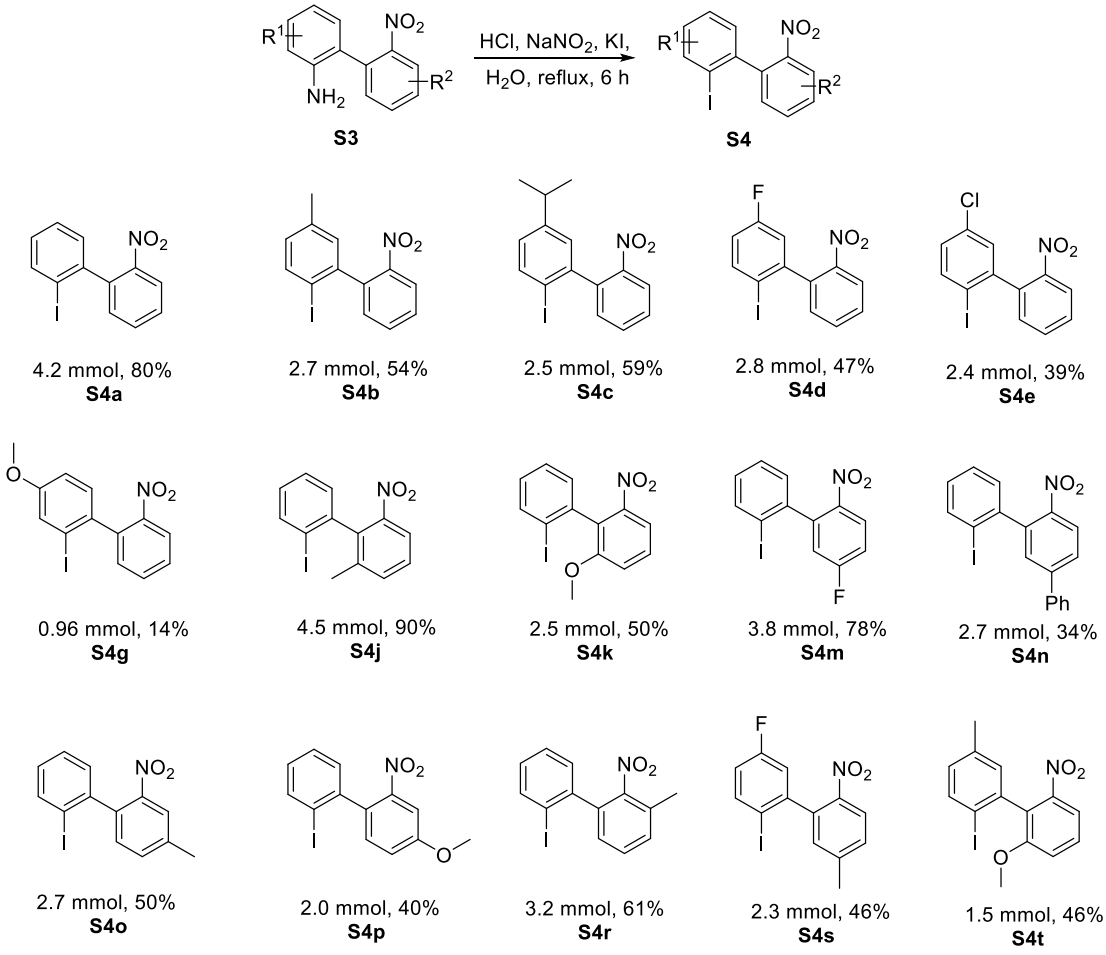


3.3 mmol, 56%
S3t

The above 2'-nitro-[1,1'-biphenyl]-2-amines were prepared by following a reported procedure.[1] In a 250 mL Schlenk flask, 1-bromo-2-nitrobenzene (1.0 equiv,

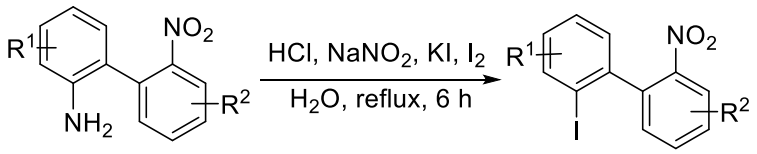
2.0-6.0 mmol) and 2-aminophenylboronic acid pinocal esters (1.2 equiv) were charged under the protection of argon. Then, dimenthoxyethane (80 mL) and $NaHCO_3$ aqueous solution (5.0 equiv, 1.0 mol/L) were added to the above flask and was degassed for 30 minutes. $Pd(PPh_3)_4$ (5 mol %) was added, then the mixture was heated to 90 °C and stirred for 12 hours (monitored by TLC). After completion of the reaction, it was cooled to room temperature. The reaction mixture was extracted with ethyl acetate (50 mL×3) and the combined organic phase was dired over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/30 to 1/10) to afford the desired 2'-nitro-[1,1'-biphenyl]-2-amines.

2.2 Iodination of 2'-nitro-[1,1'-biphenyl]-2-amines

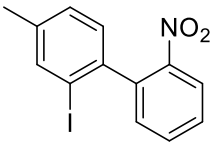


The above 2'-nitro-[1,1'-biphenyl]-2-amines were prepared by following a reported procedure.[2] A mixture of 2'-nitro-[1,1'-biphenyl]-2-amines (1.0 equiv, 1.0-5.0 mmol), water (72 mL), and conc. hydrochloric acid (12 mL) was warmed at 60-70 °C

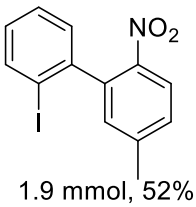
until a clear solution was obtained. Then the mixture was diazotized at 5 °C with sodium nitrite (1.6 equiv) in water (12 mL). After stirring for 30 minutes, a solution of potassium iodine (3.0 equiv) in the minimum amount of water was rapidly added and the mixture was cautiously warmed up to its boiling point and refluxed for 6 hours. After completion of the reaction (monitored by TLC), it was cooled to room temperature. The mixture was quenched by adding saturated aqueous sodium thiosulfate solution and pH was regulated with saturated sodium hydroxide aqueous solution to 8-10. After extraction with ethyl acetate (30 mL×3) and the combined organic phase was dired over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/30) to afford the desired product**.**



S3 **S4**



1.3 mmol, 53%
S4f

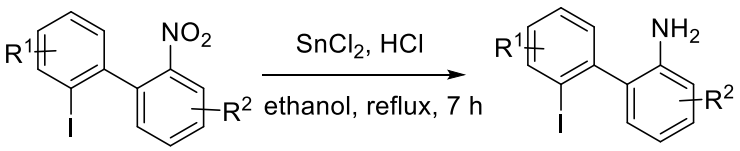


1.9 mmol, 52%
S4l

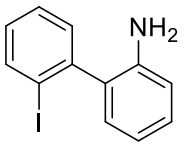
The above 2'-nitro-[1,1'-biphenyl]-2-amines were prepared by following a reported procedure.[3] A mixture of 2'-nitro-[1,1'-biphenyl]-2-amines (1.0 equiv, 1.0-5.0 mol), water (30 mL), and conc. hydrochloric acid (5 mL) was warmed at 60-70 °C until a clear solution was obtained. Then the mixture was diazotized at 5 °C with sodium nitrite (1.2 equiv) in water (5 mL). After stirring for 30 minutes, the resulting solution was poured into a solution of potassium iodine (2.0 equiv) and iodine (0.3 equiv) and the mixture was cautiously warmed up to its boiling point. After completion of the reaction (monitored by TLC), it was cooled to room temperature. The mixture was quenched by adding saturated aqueous sodium thiosulfate solution and pH was regulated with saturated sodium hydroxide aqueous solution to 8-10. The solution was extracted with ethyl acetate (10 mL×3) and the combined organic phase was dired over Na_2SO_4 and concentrated under reduced pressure. The residue was

purified by flash chromatography (ethyl acetate/petroleum ether = 1/30) to afford the desired product.

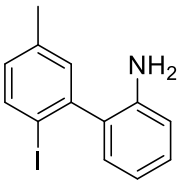
2.3 Preparation of 2'-iodo-[1,1'-biphenyl]-2-amines



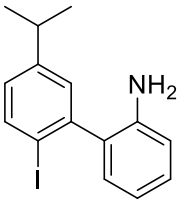
S4 **S5**



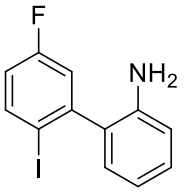
1.2 mmol, 30%
S5a



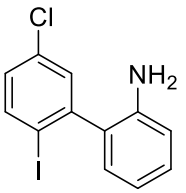
1.0 mmol, 40%
S5b



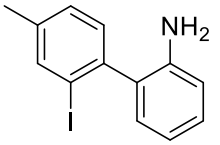
2.0 mmol, 87%
S5c



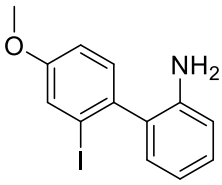
2.3 mmol, 84%
S5d



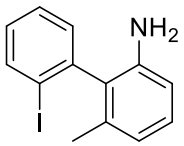
1.8 mmol, 74%
S5e



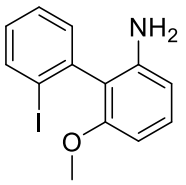
1.1 mmol, 85%
S5f



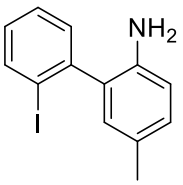
0.57 mmol, 57%
S5g



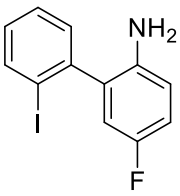
4.1 mmol, 91%
S5j



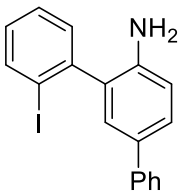
1.1 mmol, 44%
S5k



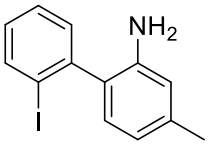
1.2 mmol, 64%
S5l



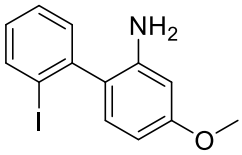
1.9 mmol, 50%
S5m



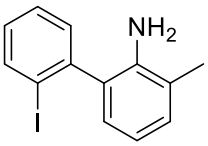
1.9 mmol, 71%
S5n



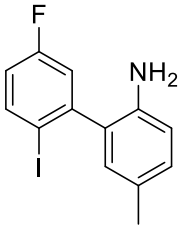
2.4 mmol, 90%
S5o



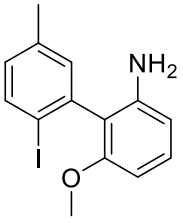
1.7 mmol, 84%
S5p



1.5 mmol, 49%
S5r



2.0 mmol, 89%
S5s

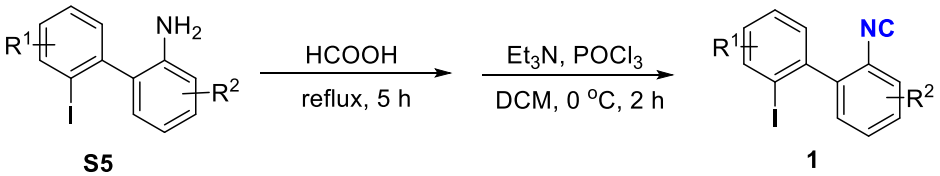


1.3 mmol,85%
S5t

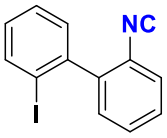
The above 2'-nitro-[1,1'-biphenyl]-2-amines were prepared by following a

reported procedure.[4] A mixture of 2-iodo-2'-nitro-1,1'-biphenyl (1.0 equiv, 1.0-4.0 mmol), anhydrous tin (II) chloride (4.0 equiv), and concentrated hydrochloric acid (4.0 equiv) in absolute ethanol (15 mL) were refluxed for 7 hours. After completion of the reaction (monitored by TLC), it was cooled to room temperature and pH was regulated with saturated sodium hydroxide aqueous solution to 8-10. The mixture was filtered through diatomaceous earth. The filtrate was extracted with ethyl acetate (30 mL×3) and the combined organic phase was dired over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/10) to afford the desired product.

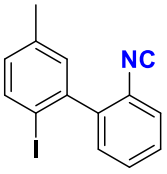
2.4 Preparation of substituted 2-iodo-2'-isocyano-1,1'-biphenyl



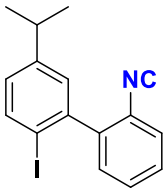
S5 **1**



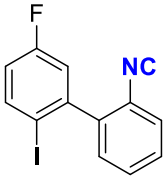
0.8 mmol, 67%
1a



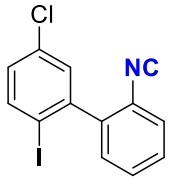
0.6 mmol, 61%
1b



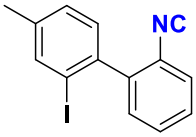
1.1 mmol, 57%
1c



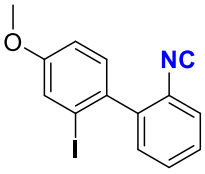
1.3 mmol, 69%
1d



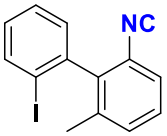
0.6 mmol, 34%
1e



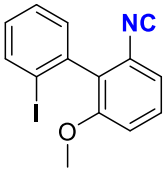
0.5 mmol, 50%
1f



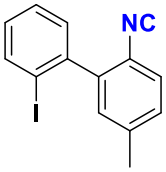
0.3 mmol, 59%
1g



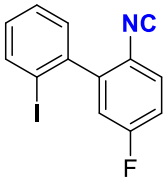
1.7 mmol, 42%
1j



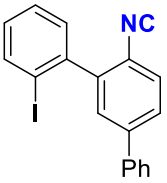
0.6 mmol, 54%
1k



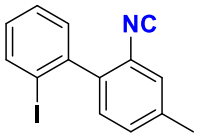
0.7 mmol, 58%
1l



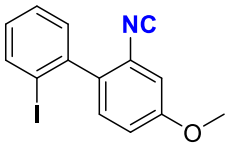
1.45 mmol, 76%
1m



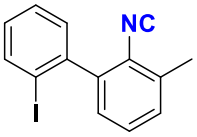
0.7 mmol, 37%
1n



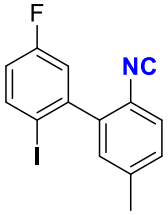
1.3 mmol, 56%
1o



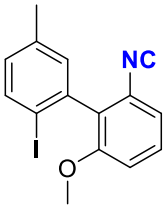
1.1 mmol, 68%
1p



1.1 mmol, 76%
1r



1.3 mmol, 64%
1s



0.6 mmol, 53%
1t

The above substituted 2-iodo-2'-isocyano-1,1'-biphenyl were prepared by following a reported procedure with minor changes.[5] A mixture of

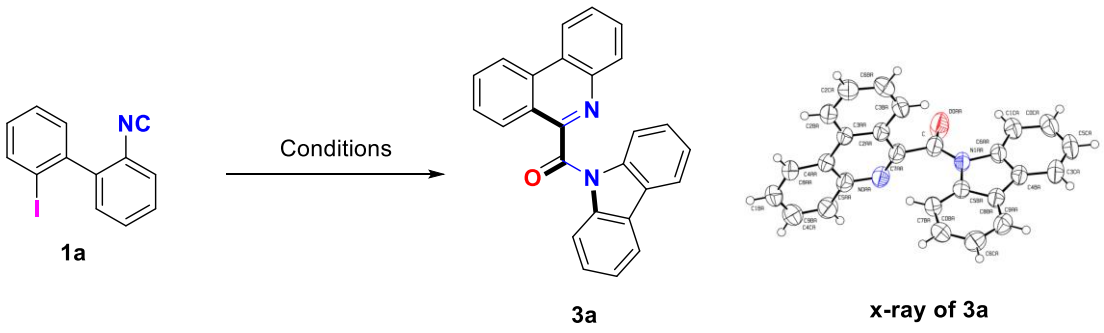
2'-iodo-[1,1'-biphenyl]-2-amine (1.0 equiv, 0.3-2.0 mmol) and formic acid (15 mL) was refluxed for 5 hours. After completion of the reaction (monitored by TLC), the mixture was concentrated under reduced pressure to afford crude product as a yellow oil for next step without further purification.

The crude product was dissolved in dichloromethane (20 mL) and NEt_3 (3.0 equiv) and cooled to 0 °C by ice bath. To the above mixture was added phosphory chloride (1.1 equiv) dropwise. After stirring for an hour, the reaction temperature was warmed to room temperature and the mixture was stirred for another hour. When the reaction was completed, the resulting mixture was cooled to 0 °C and aqueous saturated solution of sodium carbonate (10 mL) was added dropwise to quench the reaction. After vigorous stirring for an hour, the mixture was extracted with ethyl acetate (10 mL×3) and the combined organic phase was dired over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/50) to afford the desired product.

3. Optimization of Reaction Condition and General Procedures

3.1 Optimization of Reaction Condition for the Synthesis of 3a

Table S1. Optimization of the Reaction Conditions [a]



Entry	[Pd]	[Cu]	Base	Solvent	Yield (%) [b]
1[c]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	48
2	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	67
3	$Pd(acac)_2$	CuI	K_2CO_3	DMSO	56
4	$Pd(CF_3COO)_2$	CuI	K_2CO_3	DMSO	65

5	$PdCl_2(CH_3CN)_2$	CuI	K_2CO_3	DMSO	44
6	$Pd(OAc)_2$	CuCl	K_2CO_3	DMSO	50
7	$Pd(OAc)_2$	CuBr	K_2CO_3	DMSO	62
8	$Pd(OAc)_2$	$Cu(acac)_2$	K_2CO_3	DMSO	62
9	$Pd(OAc)_2$	Cu_2O	K_2CO_3	DMSO	52
10 [d]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	46
11 [e]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	18
12 [f]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	60
13 [g]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	45
14	$Pd(OAc)_2$	CuI	K_2CO_3	acetone	19
15	$Pd(OAc)_2$	CuI	K_2CO_3	DCM	4
16	$Pd(OAc)_2$	CuI	K_2CO_3	EtOH	11
17	$Pd(OAc)_2$	CuI	Na_2CO_3	DMSO	48
18	$Pd(OAc)_2$	CuI	Cs_2CO_3	DMSO	48
19	$Pd(OAc)_2$	CuI	DBU	DMSO	56
20	$Pd(OAc)_2$	CuI	DIPEA	DMSO	5
21 [h]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	59
22 [i]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	65
23 [j]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	80
24 [k]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	70
25 [l, o]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	72
26 [m, o]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	90
27 [n, o]	$Pd(OAc)_2$	CuI	K_2CO_3	DMSO	84

[a] Reaction conditions: an aqueous solution of base (0.12 mmol) in water (0.15 mL) was added to a mixture of **1a** (0.1 mmol), [Pd] (10 mol%), [Cu] (20 mol%) in solvent (1.5 mL) via syringe bump within 15 minutes and stirred for 30 minutes, at 23 °C, in Ar. [b] The yields were determined by ^1H NMR using CH_2Br_2 as internal standard. [c] PPh_3 (0.01 mmol) was used. [d] At 40 °C. [e] At 60 °C. [f] 0.5 equiv base was used. [g] 2.0 equiv base was used. [h] $Pd(OAc)_2$ (5 mol%), CuI (20 mol%) were used. [i] $Pd(OAc)_2$ (2 mol%), CuI (20 mol%) were used. [j] $Pd(OAc)_2$ (10 mol%), CuI (15 mol%) were used. [k] $Pd(OAc)_2$ (10 mol%), CuI (10 mol%) were used. [l] $Pd(OAc)_2$ (10 mol%), CuI (20 mol%) were used. [m] $Pd(OAc)_2$ (2 mol%), CuI (20 mol%) were used. [n] $Pd(OAc)_2$ (2 mol%), CuI (15 mol%) were used. [o]CuI was added to the mixture after addition of

aqueous solution of K_2CO_3 when the substrate was consumed completely.

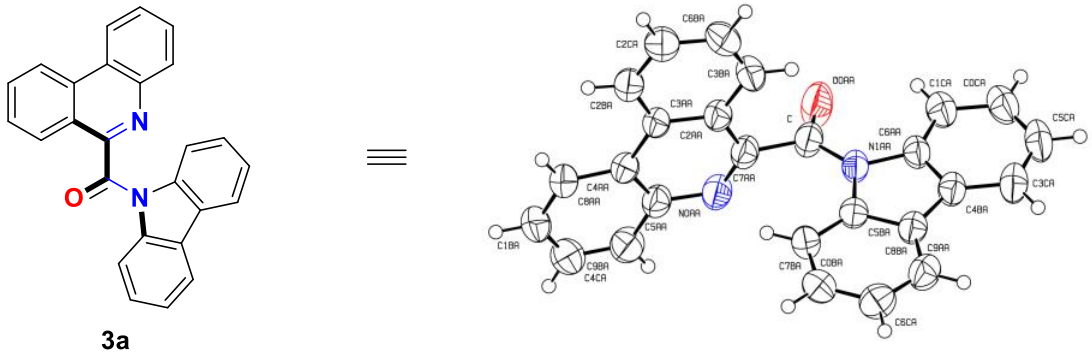
3.2 Procedures for the Synthesis of 2a

To a solution of **1a** (1.0 equiv, 0.1 mmol) in anhydrous DMSO (1.5 mL) was added $Pd(OAc)_2$ (2 mol%). The tube was then evacuated and backfilled with argon for 3 times and stirred at 23 ^oC for 15 minutes. Then an aqueous solution of K_2CO_3 (1.2 equiv) in H_2O (0.15 mL) was added to the mixture via syringe bump with a duration time of 15 minutes and stirred for 30 minutes. After completion of the reaction (monitored by TLC), the mixture was washed with saturated aqueous NH_4Cl solution. The solution was extracted with ethyl acetate (10 mL×3) and the combined organic phase was dired over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/50-1/30) to afford the desired product **2a**.

3.3 General Procedures for the Synthesis of 3

To a 10 mL oven-dried Schlenk tube was added **1** (1.0 equiv, 0.1 mmol), $Pd(OAc)_2$ (2 mol%) and anhydrous DMSO (1.5 mL). The tube was then evacuated and backfilled with argon for 3 times and stirred at 23 ^oC. Then an aqueous solution of K_2CO_3 (1.2 equiv) in H_2O (0.15 mL) was added to the mixture via syringe bump with a duration time of 15 minutes and stirred for 30 minutes to 4 hours. After complete consumption of **1** (monitored by TLC), CuI (20 mol%) was added to the mixture and stirred for 30 minutes. The mixture was washed with saturated aqueous NH_4Cl solution. The solution was extracted with ethyl acetate (10 mL×3) and the combined organic phase was dired over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/50-1/30) to afford the desired product **3**.

4. X-ray Crystallography of 3a



3a

Crystallographic data for compound **3a** (CCDC-1582339) has been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained, free of charge, on application to CCDC (Email:deposit@ccdc.cam.ac.uk).

Bond precision: C-C = 0.0033 A Wavelength=1.54184

Cell: a=8.9209(3) b=9.1610(3) c=12.7949(4)
alpha=101.938(2) beta=106.434(3) gamma=107.197(3)
Temperature: 293 K

	Calculated	Reported
Volume	908.67(6)	908.67(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H16 N2 O	C26 H16 N2 O
Sum formula	C26 H16 N2 O	C26 H16 N2 O
Mr	372.41	372.41
Dx,g cm-3	1.361	1.361
Z	2	2
Mu (mm-1)	0.660	0.660
F000	388.0	388.0
F000'	389.10	
h,k,lmax	10,10,15	10,10,15
Nref	3225	3191
Tmin,Tmax	0.789,0.876	0.678,1.000
Tmin'	0.719	

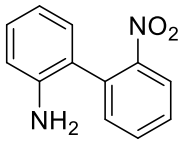
Correction method= # Reported T Limits: Tmin=0.678 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 66.780

R(reflections)= 0.0457(2767) wR2(reflections)= 0.1563(3191)

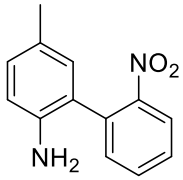
S = 1.214 Npar= 262

5. Characterization Data



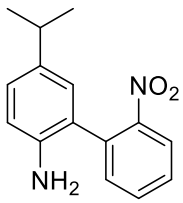
2'-Nitro-[1,1'-biphenyl]-2-amine (S3a)

Yellow oil (1112.8 mg, 85% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.96 (d, *J* = 13.5 Hz, 1H), 7.67-7.64 (m, 1H), 7.54-7.50 (m, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.21-7.18 (m, 1H), 6.99 (d, *J* = 7.5 Hz, 1H), 6.84-6.80 (m, 1H), 6.77 (d, *J* = 12.0 Hz, 1H), 3.16 (br, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 150.16, 144.02, 134.06, 133.20, 133.10, 129.83, 129.58, 128.98, 124.66, 123.70, 119.2, 116.20; HRMS (ESI) calcd for $C_{12}H_{11}N_2O_2^+$ $[M+H]^+$ 215.0815, found 215.0819.



5-Methyl-2'-nitro-[1,1'-biphenyl]-2-amine (S3b)

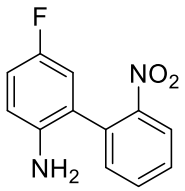
Yellow solid (1162.8 mg, 64% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (dd, *J* = 0.8 Hz, *J* = 8.0 Hz, 1H), 7.66-7.62 (m, 1H), 7.53-7.49 (m, 1H), 7.44 (dd, *J* = 0.8 Hz, *J* = 8.4 Hz, 1H), 7.01 (dd, *J* = 1.6 Hz, *J* = 8.0 Hz, 1H), 6.80 (d, *J* = 1.2 Hz, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 2.98 (br, 2H), 2.25 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 149.76, 141.15, 133.89, 132.78, 132.76, 130.06, 129.57, 128.48, 128.11, 124.22, 123.52, 116.05, 20.34; HRMS (ESI) calcd for $C_{13}H_{13}N_2O_2^+$ $[M+H]^+$ 229.0972, found 229.0962.



5-Isopropyl-2'-nitro-[1,1'-biphenyl]-2-amine (S3c)

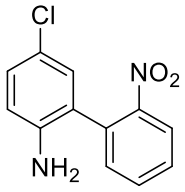
Yellow oil (1126.4 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95-7.93 (m, 1H),

7.66-7.62 (m, 1H), 7.52-7.47 (m, 2H), 7.07 (dd, *J* = 1.6 Hz, *J* = 8.4 Hz, 1H), 6.85 (d, *J* = 1.6 Hz, 1H), 6.72 (d, *J* = 8.4 Hz, 1H), 3.20 (br, 2H), 2.87-2.77 (m, 1H), 1.21 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): 149.96, 141.50, 139.47, 134.15, 132.84, 132.76, 128.52, 127.45, 127.21, 124.27, 123.36, 116.08, 33.18, 24.17; HRMS (ESI) calcd for $C_{15}H_{17}N_2O_2^+$ $[M+H]^+$ 257.1285, found 257.1282.



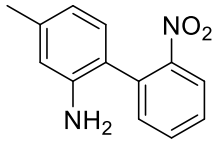
5-Fluoro-2'-nitro-[1,1'-biphenyl]-2-amine (S3d)

Yellow solid (1368.8 mg, 90% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.70-7.67 (m, 1H), 7.57-7.54 (m, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 6.94-6.90 (m, 1H), 6.75 (dd, *J* = 2.5 Hz, *J* = 8.0 Hz, 1H), 6.75 (dd, *J* = 5.0 Hz, *J* = 9..0 Hz, 1H), 3.33 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 156.31 (d, *J* = 236.3 Hz), 149.55, 139.94, 133.25, 132.77, 132.66, 129.20, 124.65, 124.60, 116.98 (d, *J* = 7.6 Hz), 116.18 (d, *J* = 22.1 Hz), 115.95 (d, *J* = 23.3 Hz); ^{19}F NMR (470 MHz, $CDCl_3$): -126.33 (s, 1F); HRMS (ESI) calcd for $C_{12}H_{10}FN_2O_2^+$ $[M+H]^+$ 233.0721, found 233.0712.



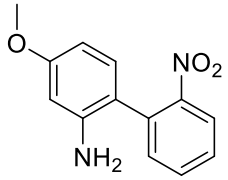
5-chloro-2'-nitro-[1,1'-biphenyl]-2-amine (S3e)

Yellow oil (1513.9 mg, 86% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 2.4 Hz, 1H), 7.63 (dd, *J* = 2.0 Hz, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 1H), 7.23-7.19 (m, 1H), 6.96 (dd, *J* = 1.6 Hz, *J* = 7.6 Hz, 1H), 6.84-6.80 (m, 1H), 6.76 (d, *J* = 7.2 Hz, 1H), 3.28 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 150.30, 143.96, 134.71, 134.26, 133.37, 132.47, 130.14, 129.51, 124.87, 122.49, 119.32, 116.33; HRMS (ESI) calcd for $C_{12}H_{10}ClN_2O_2^+$ $[M+H]^+$ 249.0425, found 249.0431.



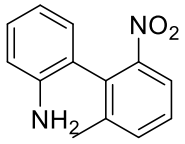
4-Methyl-2'-nitro-[1,1'-biphenyl]-2-amine (S3f)

Yellow oil (570.0 mg, 51% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (dd, *J* = 0.8 Hz, *J* = 8.0 Hz, 1H), 7.65-7.61 (m, 1H), 7.52-7.48 (m, 1H), 7.48-7.44 (m, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 6.64 (d, *J* = 8.0 Hz, 1H), 6.60 (s, 1H), 3.27 (br, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 150.32, 143.82, 139.84, 134.08, 133.22, 133.07, 129.47, 128.77, 124.58, 120.92, 120.18, 116.90, 21.62; HRMS (ESI) calcd for $C_{13}H_{13}N_2O_2^+$ $[M+H]^+$ 229.0972, found 229.0965.



4-Methoxy-2'-nitro-[1,1'-biphenyl]-2-amine (S3g)

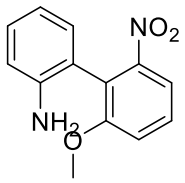
Yellow oil (1683.6 mg, 86% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (d, *J* = 7.5 Hz, 1H), 7.64-7.61 (m, 1H), 7.51-7.47 (m, 1H), 7.45 (dd, *J* = 0.5 Hz, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 8.5 Hz, 1H), 7.39 (dd, *J* = 2.5 Hz, *J* = 8.5 Hz, 1H), 6.32 (d, *J* = 2.0 Hz, 1H), 3.79 (s, 3H), 3.55 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.93, 150.24, 145.01, 133.49, 133.18, 132.74, 130.33, 128.46, 124.30, 116.18, 104.69, 101.49, 55.24; HRMS (ESI) calcd for $C_{13}H_{13}N_2O_3^+$ $[M+H]^+$ 245.0921, found 245.0914.



2'-Methyl-6'-nitro-[1,1'-biphenyl]-2-amine (S3j)

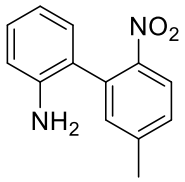
Yellow oil (1140.0 mg, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.42-7.38 (m, 1H), 7.22-7.18 (m, 1H), 6.86-6.84 (m, 1H), 6.81-6.77 (m, 2H), 3.25 (br, 2H), 2.16 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 151.40, 144.38, 141.08, 134.25, 132.57, 129.74, 129.08, 128.63, 122.06, 121.50, 119.15, 115.98, 20.23; HRMS (ESI) calcd for $C_{13}H_{13}N_2O_2^+$ $[M+H]^+$ 229.0972, found

229.0962.



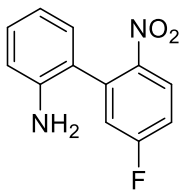
2'-Methoxy-6'-nitro-[1,1'-biphenyl]-2-amine (S3k)

Yellow solid (1122.4 mg, 92% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50-7.44 (m, 2H), 7.21-7.18 (m, 2H), 6.92 (d, *J* = 7.2 Hz, 1H), 6.81-6.78 (m, 2H), 3.81 (s, 3H), 3.20 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 158.15, 151.61, 144.60, 129.64, 129.45, 122.19, 118.82, 118.67, 115.78, 115.65, 114.77, 56.64; HRMS (ESI) calcd for $C_{13}H_{13}N_2O_3^+$ $[M+H]^+$ 245.0921, found 245.0921.



5'-Methyl-2'-nitro-[1,1'-biphenyl]-2-amine (S3l)

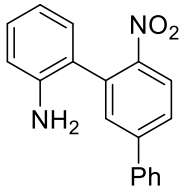
Yellow oil (809.2 mg, 65% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.89 (d, *J* = 8.5 Hz, 1H), 7.29 (d, *J* = 8.5 Hz, 1H), 7.23 (s, 3H), 7.19-7.16 (m, 1H), 6.96 (dd, *J* = 1.5 Hz, *J* = 7.5 Hz, 1H), 6.81-6.79 (m, 1H), 6.75 (d, *J* = 8.0 Hz, 1H), 3.50 (br, 2H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 147.40, 144.21, 143.72, 133.88, 133.30, 129.33, 129.22, 129.16, 124.60, 123.93, 118.81, 115.81, 21.40; HRMS (ESI) calcd for $C_{13}H_{13}N_2O_2^+$ $[M+H]^+$ 229.0972, found 229.0973.



5'-Fluoro-2'-nitro-[1,1'-biphenyl]-2-amine (S3m)

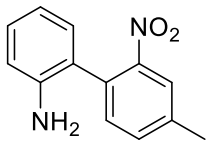
Yellow oil (1044.0 mg, 90% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05-8.02 (m, 1H), 7.23-7.15 (m, 3H), 6.98 (dd, *J* = 1.2 Hz, *J* = 7.6 Hz, 1H), 6.85-6.81 (m, 1H), 6.77 (d, *J*

= 8.0 Hz, 1H), 3.36 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 164.34 (d, *J* = 256.3 Hz), 145.78, 143.40, 137.05 (d, *J* = 8.8 Hz), 129.85, 128.91, 127.15 (d, *J* = 10.0 Hz), 122.52, 119.63 (d, *J* = 23.8 Hz), 118.97, 116.03, 115.60 (d, *J* = 22.9 Hz); ^{19}F NMR (470 MHz, $CDCl_3$): -103.95 (s, 1F);HRMS (ESI) calcd for $C_{12}H_{10}FN_2O_2^+$ $[M+H]^+$ 233.0721, found 233.0717.



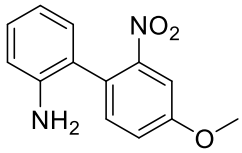
6'-Nitro-[1,1':3',1''-terphenyl]-2-amine (S3n)

Yellow oil (2262.0 mg, 85% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.08 (d, *J* = 8.5 Hz, 1H), 7.73 (dd, *J* = 1.5 Hz, *J* = 8.5 Hz, 1H), 7.68 (d, *J* = 1.5 Hz, 1H), 7.64 (d, *J* = 7.5 Hz, 2H), 7.50-7.47 (m, 2H), 7.45-7.42 (m, 1H), 7.24-7.21 (m, 1H), 7.06-7.05 (m, 1H), 6.87-6.84 (m, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 3.54 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 148.42, 146.12, 143.77, 138.55, 134.51, 131.38, 129.58, 129.30, 129.22, 128.93, 127.42, 127.04, 125.22, 123.72, 118.95, 115.94; HRMS (ESI) calcd for $C_{18}H_{15}N_2O_2^+$ $[M+H]^+$ 291.1128, found 291.1124.



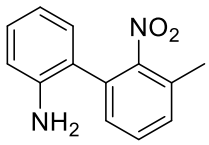
4'-Methyl-2'-nitro-[1,1'-biphenyl]-2-amine (S3o)

Yellow oil (1231.2 mg, 90% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 0.4 Hz, 1H), 7.46 (dd, *J* = 0.8 Hz, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.21-7.16 (m, 1H), 6.98-6.96 (m, 1H), 6.82-6.78 (m, 1H), 6.76 (d, *J* = 8.0 Hz, 1H), 3.35 (br, 2H), 2.48 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 149.90, 144.13, 139.54, 134.00, 132.82, 131.02, 129.67, 129.63, 124.97, 123.73, 119.12, 116.08, 21.28; HRMS (ESI) calcd for $C_{13}H_{13}N_2O_2^+$ $[M+H]^+$ 229.0972, found 229.0966.



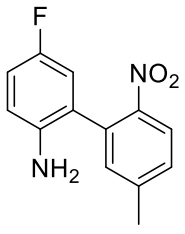
5'-Methoxy-2'-nitro-[1,1'-biphenyl]-2-amine (S3p)

Yellow oil (1220.0 mg, 83% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.48 (s, 1H), 7.35 (d, *J* = 8.5 Hz, 1H), 7.20-7.17 (m, 2H), 6.97 (d, *J* = 7.5 Hz, 1H), 6.81-6.78 (m, 1H), 6.76 (d, *J* = 8.0 Hz, 1H), 3.91 (s, 3H), 3.54 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.52, 150.30, 144.11, 133.64, 129.64, 129.33, 125.72, 123.34, 119.45, 118.86, 115.79, 109.31, 56.01; HRMS (ESI) calcd for $C_{13}H_{13}N_2O_3^+$ $[M+H]^+$ 245.0921, found 245.0918.



3'-Methyl-2'-nitro-[1,1'-biphenyl]-2-amine (S3r)

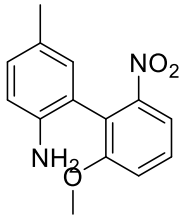
Yellow oil (1208.4 mg, 88% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46-7.42 (m, 1H), 7.32 (dd, *J* = 0.4 Hz, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.20-7.15 (m, 1H), 6.99 (dd, *J* = 1.2 Hz, *J* = 7.6 Hz, 1H), 6.79-6.74 (m, 2H), 3.44 (br, 2H), 2.39 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 152.12, 144.42, 131.96, 131.03, 130.59, 130.43, 130.12, 129.63, 122.11, 118.88, 116.2017.83; HRMS (ESI) calcd for $C_{13}H_{13}N_2O_2^+$ $[M+H]^+$ 229.0972, found 229.0969.



5-Fluoro-5'-methyl-2'-nitro-[1,1'-biphenyl]-2-amine (S3s)

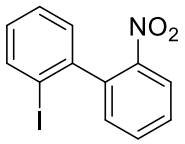
Yellow oil (1230.0 mg, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 8.4 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.21 (s, 1H), 6.93-6.88 (m, 1H), 6.75-6.68 (m, 2H), 3.44 (br, 2H), 2.47 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 156.31 (d, *J* = 236.3 Hz), 147.14, 144.60, 139.92, 133.02 (d, *J* = 30.0 Hz), 129.69, 125.19 (d, *J* = 7.6 Hz),

124.81, 116.83 (d, *J* = 8.8 Hz), 115.91 (d, *J* = 7.9 Hz), 115.73 (d, *J* = 9.0 Hz), 21.45; ^{19}F NMR (470 MHz, $CDCl_3$): -126.43 (s, 1F); HRMS (ESI) calcd for $C_{13}H_{12}FN_2O_2^+$ $[M+H]^+$ 247.0877, found 247.0867.



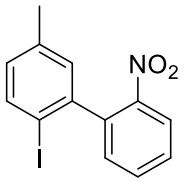
2'-Methoxy-5-methyl-6'-nitro-[1,1'-biphenyl]-2-amine (S3t)

Yellow oil (851.0 mg, 56% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48-7.42 (m, 2H), 7.18 (dd, *J* = 1.6 Hz, *J* = 7.6 Hz, 1H), 7.01-6.99 (m, 1H), 6.72-6.69 (m, 2H), 3.82 (s, 3H), 3.43 (br, 2H), 2.23 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 158.24, 151.76, 124.28, 130.25, 130.01, 129.42, 128.00, 122.54, 119.08, 116.10, 115.72, 114.78, 56.76, 24.94, 20.49; HRMS (ESI) calcd for $C_{14}H_{15}N_2O_3^+$ $[M+H]^+$ 259.1077, found 259.1072.



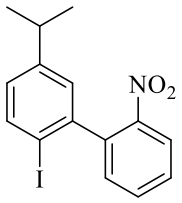
2-Iodo-2'-nitro-1,1'-biphenyl (S4a)

Yellow solid (1352.0 mg, 80% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.11 (d, *J* = 8.0 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.70-7.67 (m, 1H), 7.60-7.57 (m, 1H), 7.43-7.39 (m, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 9.0 Hz, 1H), 7.10-7.07 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 148.46, 143.70, 139.45, 139.30, 133.29, 133.76, 129.76, 139.39, 129.19, 128.46, 124.78, 98.41; HRMS (ESI) calcd for $C_{12}H_9INO_2^+$ $[M+H]^+$ 325.9672, found 325.9673.



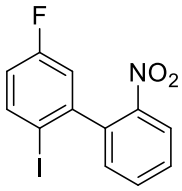
2-Iodo-5-methyl-2'-nitro-1,1'-biphenyl (S4b)

Yellow solid (915.3 mg, 54% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 4.0 Hz, 1H), 7.69-7.65 (m, 1H), 7.58-7.54 (m, 1H), 7.31-7.29 (m, 1H), 7.03 (d, *J* = 1.2 Hz, 1H), 6.92-6.90 (m, 1H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 148.13, 143.08, 139.15, 138.66, 138.18, 132.86, 132.44, 130.45, 129.65, 128.90, 124.37, 93.94, 20.92; HRMS (ESI) calcd for $C_{13}H_{11}INO_2^+$ $[M+H]^+$ 339.9829, found 339.9828.



2-Iodo-5-isopropyl-2'-nitro-1,1'-biphenyl (S4c)

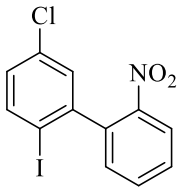
Yellow oil (917.5 mg, 59% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.08 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.68-7.66 (m, 1H), 7.58-7.55 (m, 1H), 7.32 (d, *J* = 7.5 Hz, 1H), 7.07 (s, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 2.92-2.84 (m, 1H), 1.25-1.23 (m, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): 149.49, 148.52, 143.35, 139.58, 139.06, 133.14, 132.84, 129.22, 128.11, 127.58, 124.65, 94.60, 33.98, 24.07, 24.06; HRMS (ESI) calcd for $C_{15}H_{15}INO_2^+$ $[M+H]^+$ 368.0142, found 368.0163.



5-Fluoro-2-iodo-2'-nitro-1,1'-biphenyl (S4d)

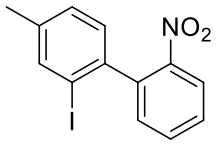
Yellow solid (960.4 mg, 47% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, *J* = 8.4 Hz, 1H), 7.84 (dd, *J* = 5.6 Hz, *J* = 8.8 Hz, 1H), 7.73-7.69 (m, 1H), 7.63-7.59 (m, 1H), 7.28 (d, *J* = 7.8 Hz, 1H), 6.98 (dd, *J* = 2.8 Hz, *J* = 8.8 Hz, 1H), 6.89-6.84 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 162.73 (d, *J* = 247.5 Hz), 147.76, 145.26 (d, *J* = 7.5 Hz), 140.15 (d, *J* = 7.5Hz), 138.10 (d, *J* = 1.3 Hz), 133.25, 132.08, 129.48, 124.64, 116.77 (d, *J* = 51.5 Hz), 116.60 (d, *J* = 53.1 Hz), 91.14 (d, *J* = 3.8 Hz); ^{19}F NMR (470 MHz, $CDCl_3$): -113.87 (s, 1F); HRMS (ESI) calcd for $C_{12}H_8FINO_2^+$ $[M+H]^+$ 343.9578,

found 343.9592.



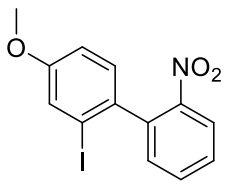
5-chloro-2-iodo-2'-nitro-1,1'-biphenyl (S4e)

Yellow solid (853.9 mg, 39% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 2.4 Hz, 1H), 7.90 (dd, *J* = 0.8 Hz, *J* = 8.0 Hz, 1H), 7.64 (dd, *J* = 2.0 Hz, *J* = 8.0 Hz, 1H), 7.42-7.38 (m, 1H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.17 (dd, *J* = 1.6 Hz, *J* = 7.6 Hz, 1H), 7.11-7.07 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 148.68, 142.55, 139.39, 137.81, 135.24, 133.87, 133.45, 130.09, 129.17, 128.59, 122.02, 98.31; HRMS (ESI) calcd for $C_{12}H_8ClINO_2^+$ $[M+H]^+$ 359.9283, found 359.9279.



2-Iodo-4-methyl-2'-nitro-1,1'-biphenyl (S4f)

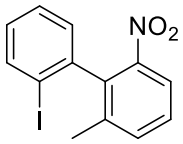
Yellow solid (440.7 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08-8.06 (m, 1H), 7.76 (s, 1H), 7.66-7.64 (m, 1H), 7.58-7.56(m, 1H), 7.31-7.29 (m, 1H), 7.22-7.20 (m, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 148.67, 140.62, 139.95, 139.76, 139.31, 133.15, 132.95, 129.30, 129.22, 128.83, 124.68, 98.25; HRMS (ESI) calcd for $C_{13}H_{11}INO_2^+$ $[M+H]^+$ 339.9829, found 339.9859.



2-Iodo-4-methoxy-2'-nitro-1,1'-biphenyl (S4g)

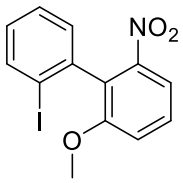
Yellow oil (340.8 mg, 14% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.06 (d, *J* = 0.5 Hz, 1H), 7.67-7.64 (m, 1H), 7.57-7.53 (m, 1H), 7.45 (d, *J* = 2.5 Hz, 1H), 7.31 (dd, *J* = 1.0

Hz, *J* = 8.0 Hz, 1H), 7.11 (d, *J* = 8.5 Hz, 1H), 6.95 (dd, *J* = 2.5 Hz, *J* = 8.0 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.49, 148.72, 138.77, 135.47, 132.99, 132.77, 129.31, 128.94, 124.40, 124.32, 114.32, 98.22, 55.64; HRMS (ESI) calcd for $C_{13}H_{11}INO_3^+$ $[M+H]^+$ 355.9778, found 355.9775.



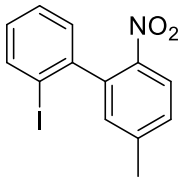
2'-Iodo-2-methyl-6-nitro-1,1'-biphenyl (S4j)

Pale yellow solid (1525.5 mg, 90% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.94 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.47-7.44 (m, 1H), 7.43-7.40 (m, 1H), 7.13 (d, *J* = 7.5 Hz, 1H), 7.10-7.07 (m, 1H), 2.06 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 149.25, 142.23, 139.63, 139.43, 138.10, 134.95, 129.67, 129.19, 128.90, 128.74, 122.09, 99.35, 20.68; HRMS (ESI) calcd for $C_{13}H_{11}INO_2^+$ $[M+H]^+$ 339.9829, found 339.9871.



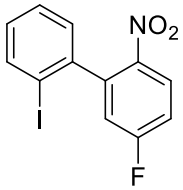
2'-Iodo-2-methoxy-6-nitro-1,1'-biphenyl (S4k)

Pale yellow solid (887.5 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93-7.91 (m, 1H), 7.61-7.59 (m, 1H), 7.54-7.50 (m, 1H), 7.41-7.37 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 1H), 7.14-7.12 (m, 1H), 7.09-7.05 (m, 1H), 3.81 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 157.69, 149.56, 139.11, 138.78, 129.65, 129.48, 129.31, 128.03, 127.88, 115.85, 115.38, 99.77, 56.60; HRMS (ESI) calcd for $C_{13}H_{11}INO_3^+$ $[M+H]^+$ 355.9778, found 355.9767.



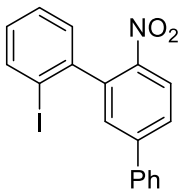
2'-Iodo-5-methyl-2-nitro-1,1'-biphenyl (S4l)

Yellow solid (644.1 mg, 52% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.90 (dd, *J* = 0.8 Hz, *J* = 8.0 Hz, 1H), 7.42-7.38 (m, 1H), 7.36 (dd, *J* = 1.6 Hz, *J* = 8.4 Hz, 1H), 7.21-7.19 (m, 1H), 7.10-7.05 (m, 2H), 2.47 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 145.82, 144.38, 143.86, 139.27, 138.90, 132.91, 129.64, 129.30, 128.82, 128.14, 124.71, 98.15, 21.50; HRMS (ESI) calcd for $C_{13}H_{11}INO_2^+$ $[M+H]^+$ 339.9829, found 339.9821.



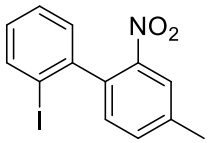
5-Fluoro-2'-iodo-2-nitro-1,1'-biphenyl (S4m)

Pale yellow oil (1303.4 mg, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (dd, *J* = 5.2 Hz, *J* = 9.2 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.44-7.40 (m, 1H), 7.28-7.23 (m, 1H), 7.20 (dd, *J* = 1.2 Hz, *J* = 7.6 Hz, 1H), 7.13-7.09 (m, 1H), 7.01 (dd, *J* = 2.4 Hz, *J* = 8.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 164.34 (d, *J* = 256.3 Hz), 144.20, 142.43, 142.13 (d, *J* = 10.0 Hz), 139.03, 129.75, 128.53, 128.23, 127.38 (d, *J* = 10.0 Hz), 119.43 (d, *J* = 22.5 Hz), 116.05 (d, *J* = 22.5 Hz), 97.38; ^{19}F NMR (470 MHz, $CDCl_3$): -103.39 (s, 1F); HRMS (ESI) calcd for $C_{12}H_8FINO_2^+$ $[M+H]^+$ 343.9578, found 343.9546.



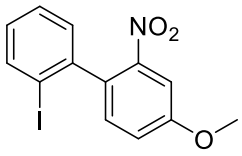
2-Iodo-6'-nitro-1,1':3',1''-terphenyl (S4n)

Yellow oil (1082.7 mg, 34% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (d, *J* = 8.4 Hz, 1H), 7.95-7.93 (m, 1H), 7.77 (dd, *J* = 2.0 Hz, *J* = 8.4 Hz, 1H), 7.65-7.64 (m, 2H), 7.51-7.40 (m, 5H), 7.26 (dd, *J* = 2.0 Hz, *J* = 7.6 Hz, 1H), 7.12-7.08 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 146.69, 146.00, 143.56, 139.70, 138.97, 138.41, 130.99, 129.41, 129.13, 128.93, 128.81, 128.14, 127.37, 127.30, 125.20, 98.12; HRMS (ESI) calcd for $C_{18}H_{13}INO_2^+$ $[M+H]^+$ 401.9985, found 401.9995.



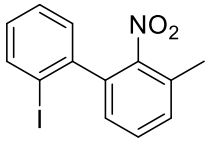
2'-Iodo-4-methyl-2-nitro-1,1'-biphenyl (S4o)

Yellow oil (915.3 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92-7.90 (m, 2H), 7.49 (dd, *J* = 0.8 Hz, *J* = 8.0 Hz, 1H), 7.41-7.37 (m, 1H), 7.21-7.17 (m, 2H), 7.09-7.05 (m, 1H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 148.17, 143.73, 139.98, 139.20, 136.65, 134.07, 132.46, 129.61, 129.30, 128.43, 125.08, 98.80, 21.40; HRMS (ESI) calcd for $C_{13}H_{11}INO_2^+$ $[M+H]^+$ 339.9829, found 339.9837.



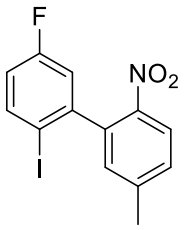
2'-Iodo-5-methoxy-2-nitro-1,1'-biphenyl (S4p)

Pale yellow oil (710.0 mg, 40% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.91 (d, *J* = 7.5 Hz, 1H), 7.61 (s, 1H), 7.40-7.37 (m, 1H), 7.20 (s, 3H), 7.08-7.05 (m, 1H), 3.94 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.76, 148.67, 143.36, 138.96, 133.26, 131.63, 129.32, 129.28, 128.19, 119.52, 109.17, 99.15, 56.03; HRMS (ESI) calcd for $C_{13}H_{11}INO_3^+$ $[M+H]^+$ 355.9778, found 355.9756.



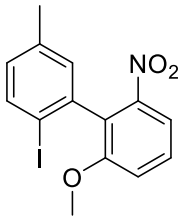
2'-Iodo-3-methyl-2-nitro-1,1'-biphenyl (S4r)

Yellow oil (1084.8 mg, 61% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.0 Hz, 1H), 7.45-7.42 (m, 1H), 7.36-7.34 (m, 2H), 7.25-7.23 (m, 1H), 7.15 (d, *J* = 7.5 Hz, 1H), 7.08-7.05 (m, 1H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 150.53, 141.50, 139.33, 136.67, 131.17, 130.01, 129.99, 129.83, 129.61, 129.28, 128.01, 98.97, 17.78; HRMS (ESI) calcd for $C_{13}H_{11}INO_2^+$ $[M+H]^+$ 339.9829, found 339.9834.



5-Fluoro-2-iodo-5'-methyl-2'-nitro-1,1'-biphenyl (S4s)

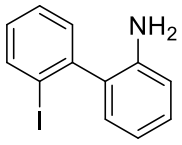
Yellow oil (821.1 mg, 46% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.07 (d, *J* = 8.5 Hz, 1H), 7.83 (dd, *J* = 5.5 Hz, *J* = 9.0 Hz, 1H), 7.38 (dd, *J* = 1.0 Hz, *J* = 8.5 Hz, 1H), 7.06 (d, *J* = 1.0 Hz, 1H), 6.98-6.95 (m, 1H), 6.86-6.83 (m, 1H), 2.48 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 162.74 (d, *J* = 247.5 Hz), 145.70 (d, *J* = 8.0 Hz), 145.44, 144.68, 140.04 (d, *J* = 7.8 Hz), 138.20, 132.51, 129.97, 124.82, 116.68 (d, *J* = 21.5 Hz), 116.39 (d, *J* = 22.8 Hz), 91.16 (d, *J* = 3.8 Hz), 21.42; ^{19}F NMR (470 MHz, $CDCl_3$): -114.05 (s, 1F); HRMS (ESI) calcd for $C_{13}H_{10}FINO_2^+$ $[M+H]^+$ 357.9735, found 357.9745.



2-Iodo-2'-methoxy-5-methyl-6'-nitro-1,1'-biphenyl (S4t)

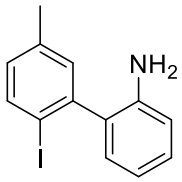
Yellow solid (553.5 mg, 46% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.0 Hz, 1H), 7.58 (dd, *J* = 0.8 Hz, *J* = 8.4 Hz, 1H), 7.53-7.49 (m, 1H), 7.21-7.19 (m, 1H), 6.94 (d, *J* = 1.6 Hz, 1H), 6.89 (dd, *J* = 1.6 Hz, *J* = 8.4 Hz, 1H), 3.81 (s, 3H), 2.30 (s,

3H); ^{13}C NMR (125 MHz, $CDCl_3$): 157.78, 149.71, 138.86, 138.56, 138.13, 130.51, 130.27, 129.62, 127.96, 115.87, 115.40, 95.82, 56.70, 21.05; HRMS (ESI) calcd for $C_{14}H_{13}INO_3^+$ $[M+H]^+$ 369.9935, found 369.9945.



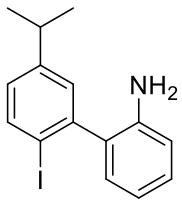
2'-Iodo-[1,1'-biphenyl]-2-amine (S5a)

Colorless oil (354.0 mg, 30% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99-7.97 (m, 1H), 7.45-7.41 (m, 1H), 7.33-7.31 (m, 1H), 7.25-7.20 (m, 1H), 7.09-7.05 (m, 1H), 6.99-6.97 (m, 1H), 6.86-6.84 (m, 1H), 6.78 (d, *J* = 8.4 Hz, 1H), 3.19 (br, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 144.50, 143.57, 139.84, 131.00, 130.74, 130.43, 129.55, 129.49, 129.00, 118.61, 115.87, 100.96; HRMS (ESI) calcd for $C_{12}H_{11}IN^+$ $[M+H]^+$ 295.9931, found 295.9926.



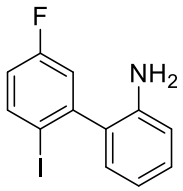
2'-Iodo-5'-methyl-[1,1'-biphenyl]-2-amine (S5b)

Yellow oil (309.0 mg, 40% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.84 (d, *J* = 10.0 Hz, 1H), 7.24-7.20 (m, 1H), 7.15 (d, *J* = 1.0 Hz, 1H), 6.98-6.97 (m, 1H), 6.90 (dd, *J* = 1.2 Hz, *J* = 8.0 Hz, 1H), 6.85-6.82 (m, 1H), 6.78 (d, *J* = 8.0 Hz, 1H), 3.52 (br, 2H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 143.99, 143.32, 139.27, 138.80, 131.58, 130.54, 130.31, 130.12, 129.11, 118.32, 115.56, 96.40, 20.96; HRMS (ESI) calcd for $C_{13}H_{13}IN^+$ $[M+H]^+$ 310.0087, found 310.0076.



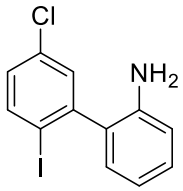
2'-Iodo-5'-isopropyl-[1,1'-biphenyl]-2-amine (S5c)

Colorless oil (674.0 mg, 87% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.0 Hz, 1H), 7.26-7.20 (m, 2H), 7.01-6.94 (m, 2H), 6.86-6.82 (m, 1H), 6.79 (dd, *J* = 0.4 Hz, *J* = 8.0 Hz, 1H), 3.27 (br, 2H), 2.95-2.85 (m, 1H), 1.26 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): 150.09, 144.27, 143.61, 139.61, 130.92, 130.49, 129.37, 129.30, 127.95, 118354, 115.82, 97.00, 34.02, 24.17, 24.10; HRMS (ESI) calcd for $C_{15}H_{17}IN^+$ $[M+H]^+$ 338.0400, found 338.0401.



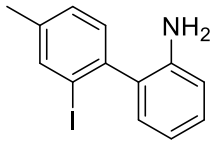
5'-Fluoro-2'-iodo-[1,1'-biphenyl]-2-amine (S5d)

Colorless oil (719.9 mg, 84% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.91-7.88 (m, 1H), 7.23-7.19 (m, 1H), 7.06 (dd, *J* = 3.0 Hz, *J* = 9.0 Hz, 1H), 6.94 (dd, *J* = 1.5 Hz, *J* = 7.5 Hz, 1H), 6.84-6.80 (m, 2H), 6.76 (d, *J* = 8.0 Hz, 1H), 3.33 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.22 (d, *J* = 247.5 Hz), 146.23 (d, *J* = 8.8 Hz), 143.08, 140.75 (d, *J* = 8.8 Hz), 129.74 (d, *J* = 41.6 Hz), 129.36, 118.40, 118.05 (d, *J* = 21.4 Hz), 116.78 (d, *J* = 21.5 Hz), 115.74, 93.59 (d, *J* = 1.3 Hz); ^{19}F NMR (470 MHz, $CDCl_3$): -113.49 (s, 1F); HRMS (ESI) calcd for $C_{12}H_{10}FIN^+$ $[M+H]^+$ 313.9836, found 313.9829.



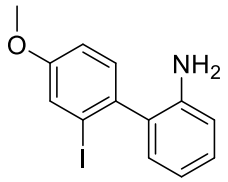
5'-chloro-2'-iodo-[1,1'-biphenyl]-2-amine (S5e)

Colorless oil (590.0 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 0.8 Hz, 1H), 7.45-7.41 (m, 1H), 7.28-7.26 (m, 1H), 7.09-7.05 (m, 1H), 6.89 (d, *J* = 8.0 Hz, 1H), 6.80-6.76 (m, 2H), 3.12 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 144.83, 143.37, 139.98, 134.92, 131.54, 131.03, 129.87, 129.12, 128.93, 118.58, 115.50, 100.81; HRMS (ESI) calcd for $C_{12}H_{10}ClIN^+$ $[M+H]^+$ 329.9541, found 329.9547.



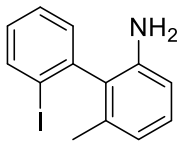
2'-Iodo-4'-methyl-[1,1'-biphenyl]-2-amine (S5f)

Colorless oil (339.9 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (s, 1H), 7.26-7.17 (m, 3H), 6.97-6.95 (m, 1H), 6.84-6.80 (m, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 3.17 (br, 2H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 143.52, 141.21, 140.00, 139.39, 130.40, 130.33, 129.61, 129.11, 118.33, 115.55, 100.55, 20.62; HRMS (ESI) calcd for $C_{13}H_{13}IN^{+}$ $[M+H]^{+}$ 310.0087, found 310.0080.



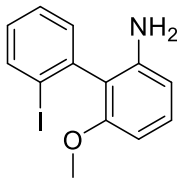
2'-Iodo-4'-methoxy-[1,1'-biphenyl]-2-amine (S5g)

Pale yellow solid (182.3 mg, 57% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.5 (d, *J* = 2.4 Hz, 1H), 7.22-7.18 (m, 2H), 6.99-6.95 (m, 2H), 6.83-6.80 (m, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 3.83 (s, 3H), 3.41 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.31, 143.80, 136.43, 130.89, 130.70, 130.10, 129.10, 124.61, 118.28, 115.48, 114.91, 100.70, 55.66; HRMS (ESI) calcd for $C_{13}H_{13}INO^{+}$ $[M+H]^{+}$ 326.0036, found 326.0036.



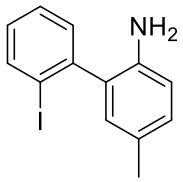
2'-Iodo-6-methyl-[1,1'-biphenyl]-2-amine (S5j)

Colorless oil (1266.9 mg, 91% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.46-7.43 (m, 1H), 7.23 (d, *J* = 7.5 Hz, 1H), 7.12-7.09 (m, 1H), 7.07-7.04 (m, 1H), 6.70 (d, *J* = 7.5 Hz, 1H), 6.63 (d, *J* = 8.0 Hz, 1H), 3.22 (br, 2H), 1.92 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 143.75, 143.68, 140.02, 136.97, 130.94, 130.65, 129.47, 128.99, 120.24, 113.30, 101.69, 20.51; HRMS (ESI) calcd for $C_{13}H_{13}IN^{+}$ $[M+H]^{+}$ 310.0087, found 310.0076.



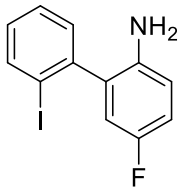
2'-Iodo-6-methoxy-[1,1'-biphenyl]-2-amine (S5k)

Colorless oil (357.5 mg, 44% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.0 Hz, 1H), 7.46-7.42 (m, 1H), 7.28-7.26 (m, 1H), 7.20-7.16 (m, 1H), 7.07-7.03 (m, 1H), 6.43 (dd, *J* = 8.0 Hz, *J* = 13.2 Hz, 2H), 3.71 (s, 3H), 2.58 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 157.46, 144.67, 140.83, 139.50, 131.25, 129.49, 129.07, 128.75, 119.38, 108.51, 102.17, 101.12, 55.76; HRMS (ESI) calcd for $C_{13}H_{13}INO^+$ $[M+H]^+$ 326.0036, found 326.0030.



2'-Iodo-5-methyl-[1,1'-biphenyl]-2-amine (S5l)

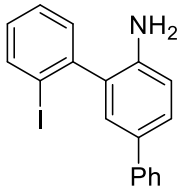
Colorless oil (370.8 mg, 64% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.43-7.40 (m, 1H), 7.30 (dd, *J* = 1.0 Hz, *J* = 7.5 Hz, 1H), 7.07-7.02 (m, 2H), 6.80 (s, 1H), 6.70 (d, *J* = 8.0 Hz, 1H), 3.00 (br, 2H), 2.29 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 144.38, 140.69, 139.40, 130.66, 130.53, 130.45, 129.67, 129.07, 128.59, 127.48, 115.70, 100.53, 20.42; HRMS (ESI) calcd for $C_{13}H_{13}IN^+$ $[M+H]^+$ 310.0087, found 310.0089.



5-Fluoro-2'-iodo-[1,1'-biphenyl]-2-amine (S5m)

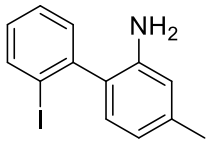
Colorless oil (594.7 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.45-7.41 (m, 1H), 7.30-7.27 (m, 1H), 7.10-7.06 (m, 1H), 6.96-6.91 (m, 1H),

6.74-6.69 (m, 2H), 2.71 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 155.90 (d, *J* = 235.0 Hz), 143.16, 139.55 (d, *J* = 20.0 Hz), 131.19 (d, *J* = 7.5 Hz), 130.51, 129.57, 128.77, 116.59 (d, *J* = 7.5 Hz), 116.46 (d, *J* = 7.5 Hz), 115.72 (d, *J* = 22.1 Hz), 99.92; ^{19}F NMR (470 MHz, $CDCl_3$): -126.82 (s, 1F); HRMS (ESI) calcd for $C_{12}H_{10}FIN^+$ $[M+H]^+$ 313.9836, found 3313.9829.



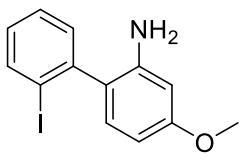
2''-Iodo-[1,1':3',1''-terphenyl]-4'-amine (S5n)

Yellow oil (704.9 mg, 71% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.01 (dd, J = 1.0 Hz, J = 8.0 Hz, 1H), 7.60-7.58 (m, 2H), 7.51-7.49 (m, 1H), 7.47-7.44 (m, 1H), 7.41-7.37 (m, 3H), 7.28-7.26 (m, 2H), 7.10-7.07 (m, 1H), 6.86 (d, J = 8.5 Hz, 1H), 3.35 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 144.12, 142.81, 140.95, 139.71, 131.32, 130.81, 130.64, 129.41, 128.96, 128.78, 128.74, 127.79, 126.46, 126.40, 115.98, 100.70; HRMS (ESI) calcd for $C_{18}H_{15}IN^+$ $[M+H]^+$ 372.0244, found 372.0239.



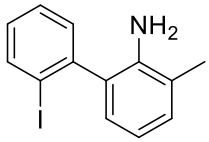
2'-Iodo-4-methyl-[1,1'-biphenyl]-2-amine (S5o)

Colorless oil (741.6 mg, 90% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (dd, *J* = 0.8 Hz, *J* = 8.0 Hz, 1H), 7.44-7.39 (m, 1H), 7.31-7.29 (m, 1H), 7.07-7.03 (m, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 7.6 Hz, 1H), 6.62 (s, 1H), 3.11 (br, 2H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 144.53, 143.30, 139.78, 139.44, 131.19, 130.29, 129.44, 128.97, 128.19, 119.61, 116.57, 101.32, 21.57; HRMS (ESI) calcd for $C_{13}H_{13}IN^+$ $[M+H]^+$ 310.0087, found 310.0077.



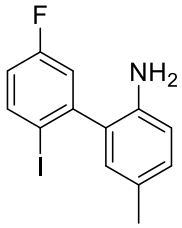
2'-Iodo-5-methoxy-[1,1'-biphenyl]-2-amine (S5p)

Green solid (552.5 mg, 84% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (dd, *J* = 1.2 Hz, *J* = 8.0 Hz, 1H), 7.43-7.39 (m, 1H), 7.31 (dd, *J* = 2.0 Hz, *J* = 7.6 Hz, 1H), 7.07-7.02 (m, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 6.41 (dd, *J* = 2.4 Hz, *J* = 8.4 Hz, 1H), 6.33 (d, *J* = 2.4 Hz, 1H), 3.82 (s, 3H), 3.42 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.61, 144.52, 144.06, 139.54, 131.18, 131.09, 129.15, 128.68, 123.81, 104.00, 101.70, 100.95, 55.20; HRMS (ESI) calcd for $C_{13}H_{13}INO^+$ $[M+H]^+$ 326.0036, found 326.0040.



2'-Iodo-3-methyl-[1,1'-biphenyl]-2-amine (S5r)

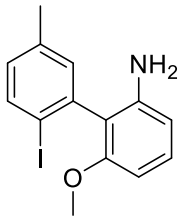
Colorless oil (463.5 mg, 49% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99 (d, *J* = 3.0 Hz, 1H), 7.44-7.41 (m, 1H), 7.32 (dd, *J* = 1.5 Hz, *J* = 7.5 Hz, 1H), 7.13 (d, *J* = 7.5 Hz, 1H), 7.08-7.05 (m, 1H), 6.86 (d, *J* = 7.5 Hz, 1H), 6.79-6.76 (m, 1H), 3.43 (br, 2H), 2.23 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 144.61, 141.54, 139.63, 130.81, 130.27, 130.25, 129.23, 128.75, 127.96, 122.59, 117.88, 100.88, 17.85; HRMS (ESI) calcd for $C_{13}H_{13}IN^+$ $[M+H]^+$ 310.0087, found 310.0083.



5'-Fluoro-2'-iodo-5-methyl-[1,1'-biphenyl]-2-amine (S5s)

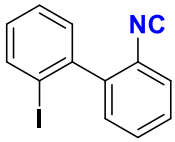
Colorless oil (654.0 mg, 89% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (dd, *J* = 5.5 Hz, *J* = 9.0 Hz, 1H), 7.07-7.03 (m, 2H), 6.85-6.81 (m, 1H), 6.78 (d, *J* = 1.0 Hz, 1H), 6.70 (d, *J* = 8.0 Hz, 1H), 3.25 (br, 2H), 2.29 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.25 (d, *J* = 247.5 Hz), 146.52 (d, *J* = 7.5 Hz), 140.69 (d, *J* = 8.8 Hz), 140.60, 130.22 (d, *J* = 12.5 Hz), 129.58, 127.74, 118.10 (d, *J* = 21.3 Hz), 116.70 (d, *J* = 21.5 Hz), 115.98, 93.53, 20.48; ^{19}F NMR (470 MHz, $CDCl_3$): -113.77 (s, 1F); HRMS (ESI)

calcd for $C_{13}H_{12}FIN^+$ $[M+H]^+$ 327.9993, found 327.9986.



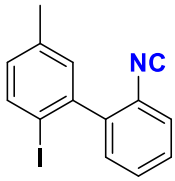
2'-Iodo-6-methoxy-5'-2qmethyl-[1,1'-biphenyl]-2-amine (S5t)

Pale yellow solid (440.7 mg, 85% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.0 Hz, 1H), 7.19-7.15 (m, 1H), 7.10 (d, *J* = 2.0 Hz, 1H), 6.88 (dd, *J* = 2.0 Hz, *J* = 8.0 Hz, 1H), 6.42 (dd, *J* = 8.0 Hz, *J* = 13.0 Hz, 2H), 3.73 (s, 3H), 3.14 (br, 2H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 157.50, 144.77, 140.58, 139.25, 138.80, 132.05, 130.23, 129.43, 119.44, 108.56, 101.19, 98.00, 55.85, 21.03; HRMS (ESI) calcd for $C_{14}H_{15}INO^+$ $[M+H]^+$ 340.0193, found 340.0203.



2-Iodo-2'-isocyano-1,1'-biphenyl (1a)

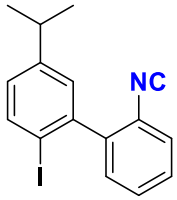
Green solid (244.0 mg, 67% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.0 Hz, 1H), 7.49-7.43 (m, 4H), 7.31-7.27 (m, 2H), 7.15-7.10 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 167.27, 142.57, 141.94, 139.71, 131.11, 130.34, 130.23, 129.46, 129.29, 128.61, 127.30, 125.95, 98.95; HRMS (ESI) calcd for $C_{13}H_9IN^+$ $[M+H]^+$ 305.9774, found 305.9776.



2-Iodo-2'-isocyano-5-methyl-1,1'-biphenyl (1b)

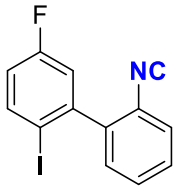
Green solid (191.4 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, *J* = 8.4 Hz, 1H), 7.49-7.41 (m, 3H), 7.29-7.27 (m, 1H), 7.09 (d, *J* = 1.6 Hz, 1H), 6.95 (dd, *J* = 1.6 Hz, *J* = 8.0 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.78, 142.00,

141.67, 139.06, 138.31, 131.00, 130.75, 130.72, 129.06, 128.80, 126.90, 94.42, 20.89; HRMS (ESI) calcd for $C_{14}H_{11}IN^+$ $[M+H]^+$ 319.9931, found 319.9925.



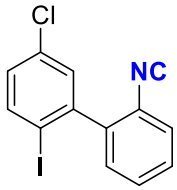
2-Iodo-2'-isocyano-5-isopropyl-1,1'-biphenyl (1c)

Green oil (381.7 mg, 57% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.49-7.42(m, 3H), 7.32 (d, *J* = 7.5 Hz, 1H), 7.14 (s, 1H), 7.00 (d, *J* = 8.0 Hz, 1H), 2.96-2.87 (m, 1H), 1.27 (d, *J* = 1.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 167.18, 149.65, 142.26, 142.14, 139.54, 131.28, 129.36, 129.13, 128.73, 128.67, 127.31, 125.98, 95.06, 34.07, 24.16, 24.05; HRMS (ESI) calcd for $C_{16}H_{15}IN^+$ $[M+H]^+$ 348.0244, found 348.0244.



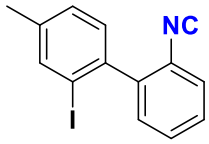
5-Fluoro-2-iodo-2'-isocyano-1,1'-biphenyl (1d)

Green solid (419.9 mg, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (dd, *J* = 5.6 Hz, *J* = 8.8 Hz, 1H), 7.49-7.48 (m, 3H), 7.29-7.26 (m, 1H), 7.04 (dd, *J* = 3.2 Hz, *J* = 8.8 Hz, 1H), 6.93-6.88 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 167.46, 162.74 (d, *J* = 247.5 Hz), 161.75, 143.98 (d, *J* = 7.5 Hz), 140.64 (d, *J* = 8.0 Hz), 140.52, 130.44, 129.33 (d, *J* = 11.3 Hz), 127.04, 117.60 (d, *J* = 15.0 Hz), 117.41 (d, *J* = 16.3 Hz), 91.70 (d, *J* = 3.8 Hz); ^{19}F NMR (470 MHz, $CDCl_3$): -113.61 (s, 1F); HRMS (ESI) calcd for $C_{13}H_8FIN^+$ $[M+H]^+$ 323.9680, found 323.9670.



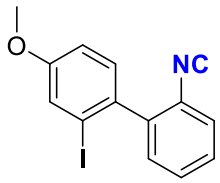
5-chloro-2-iodo-2'-isocyano-1,1'-biphenyl (1e)

Green solid (202.8 mg, 34% yield). ^{1}H NMR (500 MHz, $CDCl_3$): 7.98 (dd, *J* = 1.0 Hz, *J* = 8.0 Hz, 1H), 7.49-7.43(m, 3H), 7.26-7.23 (m, 2H), 7.15-7.12 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 168.94, 141.47, 140.40, 139.82, 134.89, 132.23, 130.65, 130.20, 129.93, 128.73, 127.32, 98.81; HRMS (ESI) calcd for $C_{13}H_8ClIN^+$ $[M+H]^+$ 339.9384, found 339.9379.



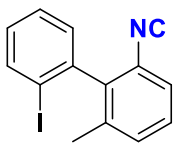
2-Iodo-2'-isocyano-4-methyl-1,1'-biphenyl (1f)

Green oil (159.5 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (s, 1H), 7.47-7.39 (m, 3H), 7.28 (d, J = 8.4 Hz, 1H), 7.24 (d, J = 8.0 Hz, 1H), 7.14 (d, J = 8.0 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.91, 141.65, 140.27, 139.91, 139.36, 131.07, 129.58, 129.19, 129.12, 128.85, 126.97, 125.85, 98.52, 20.72; HRMS (ESI) calcd for $C_{14}H_{11}IN^+$ $[M+H]^+$ 319.9931, found 319.9924.



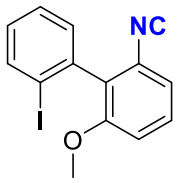
2-Iodo-2'-isocyano-4-methoxy-1,1'-biphenyl (1g)

White solid (100.5 mg, 59% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.50 (s, 1H), 7.47-7.40 (m, 3H), 7.29 (d, *J* = 9.0 Hz, 1H), 7.17 (d, *J* = 7.5 Hz, 1H), 6.99 (d, *J* = 8.5 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.82, 159.83, 141.40, 134.58, 131.37, 130.26, 129.08, 128.81, 126.96, 124.59, 114.47, 98.73, 55.65; HRMS (ESI) calcd for $C_{14}H_{11}INO^+$ $[M+H]^+$ 335.9880, found 335.9882.



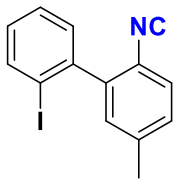
2'-Iodo-2-isocyano-6-methyl-1,1'-biphenyl (1j)

Green solid (638.0 mg, 42% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.0 Hz, 1H), 7.49-7.46 (m, 1H), 7.34-7.32 (m, 3H), 7.19 (d, *J* = 7.5 Hz, 1H), 7.15-7.11 (m, 1H), 2.06 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.47, 142.16, 141.57, 139.75, 138.45, 131.21, 130.18, 129.80, 129.05, 128.96, 126.31, 124.62, 99.30, 20.61; HRMS (ESI) calcd for $C_{14}H_{11}IN^{+}$ $[M+H]^{+}$ 319.9931, found 319.9941.



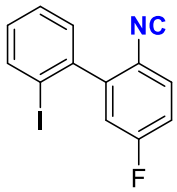
2'-Iodo-2-isocyano-6-methoxy-1,1'-biphenyl (1k)

White solid (201.0 mg, 54% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.48-7.44 (m, 1H), 7.42-7.38 (m, 1H), 7.22 (d, *J* = 6.8 Hz, 1H), 7.14-7.09 (m, 2H), 7.02 (d, *J* = 8.8 Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.52, 157.32, 139.13, 139.11, 130.97, 130.32, 129.75, 128.30, 126.67, 118.92, 112.13, 99.77, 56.18; HRMS (ESI) calcd for $C_{14}H_{11}INO^{+}$ $[M+H]^{+}$ 335.9880, found 335.9887.



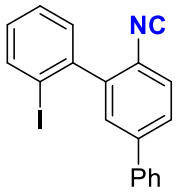
2'-Iodo-2-isocyano-5-methyl-1,1'-biphenyl (1l)

Green solid (223.3 mg, 58% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (dd, *J* = 0.8 Hz, *J* = 8.0 Hz, 1H), 7.46-7.42 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.27-7.22 (m, 2H), 7.13-7.09 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.23, 142.47, 141.42, 139.60, 139.38, 131.29, 129.95, 129.61, 128.29, 126.80, 123.18, 98.73, 21.42; HRMS (ESI) calcd for $C_{14}H_{11}IN^{+}$ $[M+H]^{+}$ 319.9931, found 319.9932.



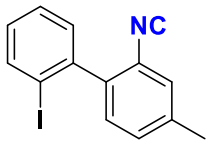
5-Fluoro-2'-iodo-2-isocyano-1,1'-biphenyl (1m)

Green oil (468.4 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.0 Hz, 1H), 7.50-7.45 (m, 2H), 7.28-7.26 (m, 1H), 7.17-7.13 (m, 2H), 7.02 (dd, *J* = 1.6 Hz, *J* = 8.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 167.15, 161.72 (d, *J* = 251.3 Hz), 143.74 (d, *J* = 8.8 Hz), 141.11, 139.46, 130.35, 129.65, 128.82 (d, *J* = 9.3 Hz), 128.35, 121.93, 117.97 (d, *J* = 23.5 Hz), 116.13 (d, *J* = 23.0 Hz), 97.97; ^{19}F NMR (470 MHz, $CDCl_3$): -108.67 (s, 1F); HRMS (ESI) calcd for $C_{13}H_8FIN^+$ $[M+H]^+$ 323.9680, found 323.9672.



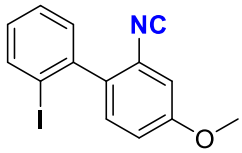
2-Iodo-6'-isocyano-1,1':3',1''-terphenyl (1n)

Green solid (266.7 mg, 37% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.68-7.63 (m, 3H), 7.56 (s, 2H), 7.50-7.47 (m, 3H), 7.43-7.40 (m, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.17-7.14 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 167.53, 142.15, 142.04, 141.84, 139.45, 139.08, 130.09, 129.99, 129.47, 129.06, 128.35, 128.33, 127.42, 127.39, 127.18, 124.44, 98.73; HRMS (ESI) calcd for $C_{19}H_{13}IN^+$ $[M+H]^+$ 382.0087, found 382.0082.



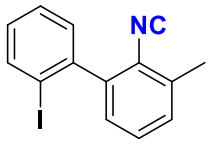
2'-Iodo-2-isocyano-4-methyl-1,1'-biphenyl (1o)

Dark green oil (414.7 mg, 56% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.97 (d, *J* = 1.0 Hz, 1H), 7.45-7.42 (m, 1H), 7.30-7.25 (m, 3H), 7.18 (d, *J* = 7.5 Hz, 1H), 7.12-7.09 (m, 1H), 2.43 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.65, 142.55, 139.63, 139.08, 130.82, 130.38, 130.29, 130.17, 128.55, 127.65, 125.63, 99.32, 21.32; HRMS (ESI) calcd for $C_{14}H_{11}IN^+$ $[M+H]^+$ 319.9931, found 319.9932.



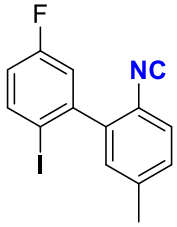
2'-Iodo-2-isocyano-5-methoxy-1,1'-biphenyl (1p)

Green solid (368.5 mg, 68% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (dd, *J* = 0.8 Hz, *J* = 8.0 Hz, 1H), 7.44-7.40 (m, 1H), 7.28-7.25 (m, 1H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.12-7.08 (m, 1H), 7.02-6.98 (m, 2H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 167.03, 159.97, 142.39, 139.66, 134.52, 131.98, 130.63, 130.15, 128.57, 126.54, 115.85, 112.27, 99.92, 56.05; HRMS (ESI) calcd for $C_{14}H_{11}INO^+$ $[M+H]^+$ 335.9880, found 335.9882.



2'-Iodo-2-isocyano-3-methyl-1,1'-biphenyl (1r)

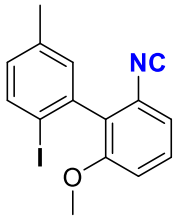
Colorless oil (350.9 mg, 76% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.45-7.42 (m, 1H), 7.37-7.32 (m, 2H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.12-7.09 (m, 2H), 2.50 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 168.92, 142.83, 141.75, 139.39, 135.42, 130.06, 129.91, 128.65, 128.29, 128.12, 98.77, 19.16; HRMS (ESI) calcd for $C_{14}H_{11}IN^+$ $[M+H]^+$ 319.9931, found 319.9931.



5-Fluoro-2-iodo-2'-isocyano-5'-methyl-1,1'-biphenyl (1s)

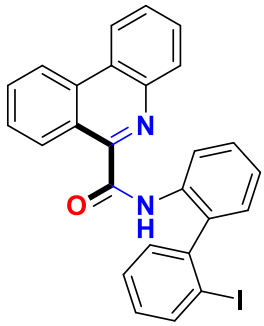
Green oil (438.0 mg, 64% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (dd, *J* = 5.5 Hz, *J* = 9.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.26-7.24 (m, 1H), 7.07 (s, 1H), 7.01 (dd, *J* = 3.0 Hz, *J* = 9.0 Hz, 1H), 6.90-6.86 (m, 1H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.70, 162.81 (d, *J* = 248.8 Hz), 144.26 (d, *J* = 8.8 Hz), 140.65 (d, *J* = 7.9 Hz), 140.37, 139.86, 130.96, 130.04, 126.90, 117.50 (d, *J* = 21.3 Hz), 91.85 (d, *J* = 3.8 Hz), 21.41; ^{19}F NMR (470 MHz, $CDCl_3$): -113.91 (s, 1F);HRMS (ESI) calcd for

$C_{14}H_{10}FIN^+$ $[M+H]^+$ 337.9836, found 337.9839.



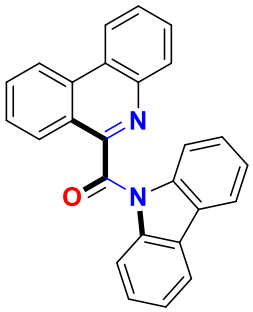
2-Iodo-2'-isocyano-6'-methoxy-5-methyl-1,1'-biphenyl (1t)

Green solid (209.4 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 8.0 Hz, 1H), 7.41-7.37 (m, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.05-7.01 (m, 2H), 6.94 (dd, *J* = 0.8 Hz, *J* = 8.0 Hz, 1H), 3.79 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.44, 157.44, 138.89, 138.39, 131.17, 130.95, 129.71, 126.77, 119.01, 112.20, 95.68, 56.31, 21.06; HRMS (ESI) calcd for $C_{15}H_{13}INO^+$ $[M+H]^+$ 350.0036, found 350.0031.



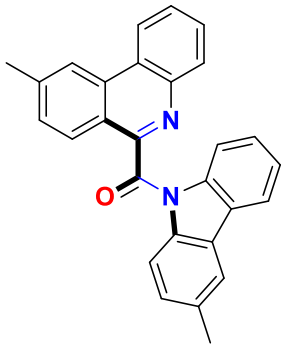
N-(2'-iodo-[1,1'-biphenyl]-2-yl)phenanthridine-6-carboxamide (**2a**)

White solid (16.3 mg, 65% yield). Mp 219-221 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.45 (s, 1H), 9.85 (d, *J* = 10.0 Hz, 1H), 8.75 (d, *J* = 8.0 Hz, 1H), 8.61 (d, *J* = 8.0 Hz, 1H), 8.54-8.53 (m, 1H), 8.14 (d, *J* = 7.5 Hz, 1H), 7.87-7.84 (m, 1H), 7.77-7.74 (m, 1H), 7.70-7.69 (m, 2H), 7.62-7.56 (m, 3H), 7.46 (d, *J* = 7.0 Hz, 1H), 7.29-7.26 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.20, 147.79, 143.33, 141.39, 139.73, 135.54, 134.93, 134.00, 131.19, 131.04, 130.43, 129.79, 129.76, 129.31, 129.09, 128.88, 128.84, 128.72, 128.15, 125.73, 124.60, 123.86, 122.10, 121.89, 120.12, 100.92; IR (cm^{-1}) 3284, 3114, 1682, 1628, 1579, 1456, 1251, 869, 804, 785, 772, 490; HRMS (ESI) calcd for $C_{26}H_{18}IN_2O^+$ $[M+H]^+$ 501.0458, found 501.0437.



(9H-carbazol-9-yl)(phenanthridin-6-yl)methanone (3a)

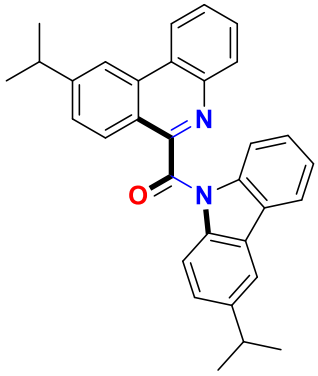
White solid (16.7 mg, 90% yield). Mp 202-205 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.09 (d, J = 8.5 Hz, 1H), 9.01 (d, J = 8.0 Hz, 1H), 8.24 (d, J = 7.5 Hz, 2H), 8.16 (d, J = 8.0 Hz, 1H), 8.11-8.08 (m, 2H), 7.94-7.87 (m, 2H), 7.83-7.80 (m, 1H), 7.42-7.36 (m, 3H), 7.30 (br, 3H) ; ^{13}C NMR (125 MHz, DMSO-d_6): 167.00, 155.26, 143.28, 138.60, 134.00, 133.39, 130.86, 130.72, 129.95, 129.88, 128.47, 127.19, 126.99, 125.42, 125.10, 124.25, 124.15, 123.21, 121.45, 116.29; IR (cm^{-1}) 3379, 2059, 1675, 1610, 1581, 1489, 1443, 876, 848, 762, 736; HRMS (ESI) calcd for $C_{26}H_{17}N_2O^+$ $[M+H]^+$ 373.1335, found 373.1338.



(3-Methyl-9H-carbazol-9-yl)(9-methylphenanthridin-6-yl)methanone (3b)

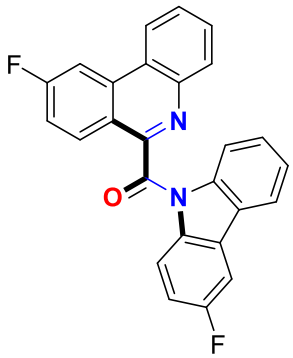
White solid (19.0 mg, 95% yield). Mp 285-290 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.97 (d, J = 7.6 Hz, 1H), 8.89 (s, 1H), 8.18 (d, J = 7.6 Hz, 1H), 8.07 (d, J = 8.0 Hz, 1H), 8.02 (s, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.89-7.85 (m, 2H), 7.71-7.62 (m, 3H), 7.38 (br, 1H), 7.27 (br, 1H), 7.09 (br, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.66, 154.98, 143.39, 142.43, 138.79, 136.63, 133.88, 133.77, 130.80, 130.06, 129.19, 128.38, 128.23, 127.14, 126.99, 126.89, 126.61, 124.46, 124.12, 122.26, 122.15, 121.40, 119.88, 119.64, 22.47, 21.23; IR (cm^{-1}) 3440, 2956, 2851, 1671, 1583, 1486,

1464, 1447, 1379, 878, 824, 760; HRMS (ESI) calcd for $C_{28}H_{21}N_2O^+$ $[M+H]^+$ 401.1648, found 401.1644.



(3-Isopropyl-9H-carbazol-9-yl)(9-isopropylphenanthridin-6-yl)methanone (3c)

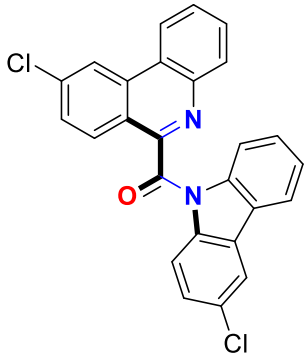
Pale yellow solid (17.3 mg, 76% yield). Mp 175-179 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.05 (d, J = 7.2 Hz, 1H), 8.89 (s, 1H), 8.23 (d, J = 8.0 Hz, 1H), 8.08-8.05 (m, 2H), 8.01 (d, J = 8.4 Hz, 1H), 7.91-7.82 (m, 2H), 7.71-7.68 (m, 1H), 7.41-7.37 (m, 2H), 7.29 (br, 1H), 7.10 (br, 2H), 3.28-3.20 (m, 1H), 2.99-2.93 (m, 1H), 1.36 (d, J = 6.8 Hz, 6H), 1.21 (d, J = 6.8 Hz, 6H); ^{13}C NMR (125 MHz, DMSO-d_6): 165.92, 154.20, 153.29, 144.92, 142.45, 137.92, 135.85, 133.23, 129.80, 129.52, 128.58, 127.91, 127.31, 126.24, 126.18, 126.11, 125.94, 124.34, 124.12, 123.23, 120.76, 120.34, 120.12, 117.78, 115.46, 114.95, 34.12, 33.16, 23.87, 23.42; IR (cm^{-1}) 3362, 2958, 2865, 1634, 1582, 1512, 1460, 1448, 1357, 885, 851, 692; HRMS (ESI) calcd for $C_{32}H_{29}N_2O^+$ $[M+H]^+$ 457.2274, found 457.2260.



(3-Fluoro-9H-carbazol-9-yl)(9-fluorophenanthridin-6-yl)methanone (3d)

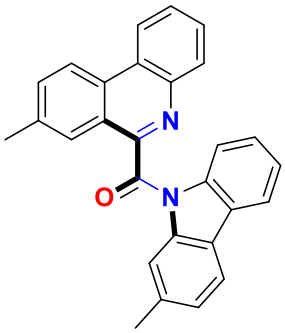
Pale yallow solid (18.8 mg, 92% yield). Mp 181-185 °C. ^{1}H NMR (400 MHz,

DMSO-d_6): δ 9.01-8.99 (m, 1H), 8.95 (dd, J = 2.4 Hz, J = 10.8 Hz, 1H), 8.32 (dd, J = 4.8 Hz, J = 9.2 Hz, 1H), 8.26 (d, J = 6.8 Hz, 1H), 8.16 (dd, J = 2.4 Hz, J = 8.4 Hz, 1H), 8.11-8.08 (m, 1H), 7.93-7.90 (m, 2H), 7.73-7.68 (m, 1H), 7.42-7.38 (m, 2H), 7.28-7.23 (m, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 165.68, 164.20 (d, J = 352.0 Hz), 159.42 (d, J = 239.1 Hz), 153.49, 142.53, 138.43, 135.96 (d, J = 10.1 Hz), 134.26, 130.56, 130.11 (d, J = 7.3 Hz), 130.01, 129.14, 128.23, 127.80 (d, J = 9.9 Hz), 125.56 (d, J = 3.4 Hz), 124.54, 124.03 (d, J = 4.3 Hz), 123.90, 121.17, 119.60, 118.22 (d, J = 24.3 Hz), 117.17, 115.34, 114.87 (d, J = 24.6 Hz), 108.93 (d, J = 22.9 Hz), 106.95 (d, J = 24.4 Hz); ^{19}F NMR (470 MHz, $CDCl_3$): -103.64 (s, 1F), -117.74 (s, 1F); IR (cm^{-1}) 3392, 2956, 2920, 1674, 1597, 1583, 1459, 1447, 1392, 894, 836, 744, 698; HRMS (ESI) calcd for $C_{26}H_{15}F_2N_2O^+$ $[M+H]^+$ 409.1147, found 409.1144.



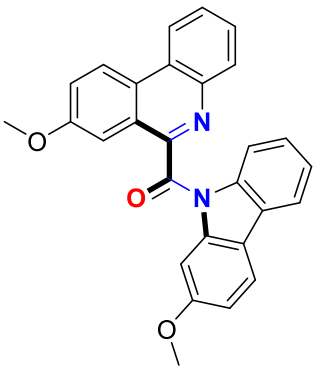
(3-chloro-9H-carbazol-9-yl)(9-chlorophenanthridin-6-yl)methanone (3e)

Pale yellow solid (15.0 mg, 68% yield). Mp 223-227 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.75 (s, 1H), 8.65-8.63 (m, 1H), 8.17-8.15 (m, 1H), 8.09 (d, J = 8.8 Hz, 1H), 7.96-7.94 (m, 2H), 7.86-7.84 (m, 2H), 7.63 (d, J = 9.2 Hz, 1H), 7.36-7.21 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): 116.11, 153.86, 143.36, 138.62, 136.90, 134.93, 130.95, 130.22, 129.15, 129.12, 128.33, 128.01, 127.36, 125.78, 124.53, 123.58, 122.49, 122.42, 121.42, 120.15, 119.78, 117.61, 116.13, 138.82, 130.10, 129.94; IR (cm^{-1}) 3065, 2921, 2851, 1674, 1442, 1323, 881, 849, 788, 764, 746, 706; HRMS (ESI) calcd for $C_{26}H_{15}Cl_2N_2O^+$ $[M+H]^+$ 441.0556, found 441.0551.



(2-Methyl-9H-carbazol-9-yl)(8-methylphenanthridin-6-yl)methanone (3f)

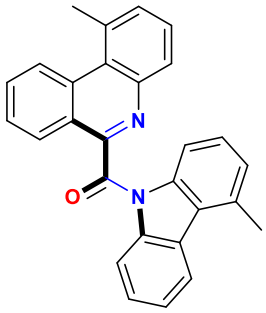
White solid (18.8 mg, 94% yield). Mp 181-183 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.00-8.95 (m, 2H), 8.16 (d, J = 7.6 Hz, 1H), 8.11 (d, J = 8.0 Hz, 1H), 8.08-8.06 (m, 1H), 7.98-7.84 (m, 4H), 7.55 (br, 1H), 7.35-7.31 (m, 1H), 7.29 (d, J = 8.0 Hz, 1H), 7.14 (s, 1H), 6.81 (br, 1H), 3.35 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 167.01, 154.80, 142.96, 139.29, 138.65, 138.48, 137.74, 133.71, 131.66, 130.84, 128.94, 128.50, 127.16, 126.65, 126.15, 125.63, 124.77, 124.58, 124.06, 123.53, 122.51, 122.18, 119.61, 119.40, 117.42, 115.94, 22.22, 21.70; IR (cm^{-1}) 3424, 3057, 2955, 1679, 1602, 1568, 1499, 1459, 877, 826, 742, 703; HRMS (ESI) calcd for $C_{28}H_{21}N_2O^+$ $[M+H]^+$ 401.1648, found 401.1652.



(2-Methoxy-9H-carbazol-9-yl)(8-methoxyphenanthridin-6-yl)methanone (3g)

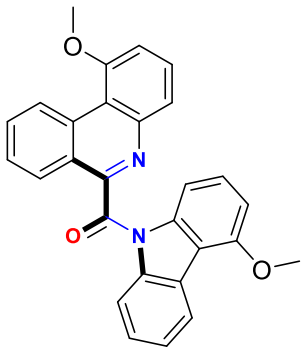
White solid (20.5 mg, 95% yield). Mp 170-173 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.03 (d, J = 9.6 Hz, 1H), 8.92 (d, J = 8.4 Hz, 1H), 8.12 (d, J = 8.8 Hz, 2H), 8.04 (d, J = 8.0 Hz, 1H), 7.80-7.86 (m, 1H), 7.82-7.78 (m, 1H), 7.75 (dd, J = 9.2 Hz, J = 2.4 Hz, 1H), 7.53 (d, J = 2.4 Hz, 1H), 7.37-7.34 (m, 2H), 7.19 (br, 2H), 7.04 (d, J = 8.8 Hz, 1H), 3.84 (s, 3H), 3.48 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 166.26, 159.20, 159.08, 153.21, 141.56, 139.14, 137.87, 129.90, 129.17, 128.80, 127.56, 126.20,

126.14, 125.31, 124.43, 124.39, 123.82, 123.01, 122.72, 121.22, 119.70, 119.44, 115.34, 111.87, 106.13, 100.89, 55.68, 55.08; IR (cm^{-1}) 3393, 3058, 2921, 1646, 1602, 1500, 1463, 1145, 883, 834, 757, 743, 702; HRMS (ESI) calcd for $C_{28}H_{21}N_2O_3^+$ $[M+H]^+$ 433.1574, found 433.1554.



(4-Methyl-9H-carbazol-9-yl)(1-methylphenanthridin-6-yl)methanone (3j)

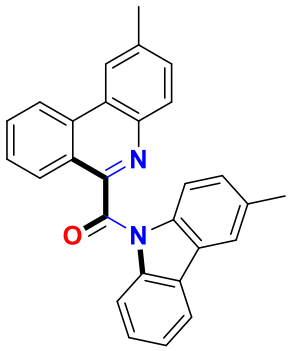
Pale yellow solid (14.2 mg, 71% yield). Mp 210-215 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.18 (d, J = 8.4 Hz, 1H), 8.26 (d, J = 8.0 Hz, 1H), 8.22 (d, J = 8.0 Hz, 1H), 8.15-8.11 (m, 1H), 8.01-7.99 (m, 1H), 7.89-7.85 (m, 1H), 7.82-7.77 (m, 2H), 7.49-7.35 (m, 3H), 7.23 (br, 3H), 3.25 (s, 3H), 2.86 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 167.27, 155.34, 144.88, 138.82, 138.68, 136.78, 134.91, 134.12, 133.92, 132.76, 129.85, 129.79, 129.12, 128.19, 128.03, 127.82, 127.53, 127.36, 127.16, 125.46, 125.07, 124.53, 124.16, 123.72, 116.11, 113.76, 27.09, 21.41; IR (cm^{-1}) 3363, 2957, 2850, 2921, 2850, 1666, 1598, 1583, 1497, 1450, 1347, 781, 740, 670; HRMS (ESI) calcd for $C_{28}H_{21}N_2O^+$ $[M+H]^+$ 401.1648, found 401.1659.



(4-Methoxy-9H-carbazol-9-yl)(1-methoxyphenanthridin-6-yl)methanone (3k)

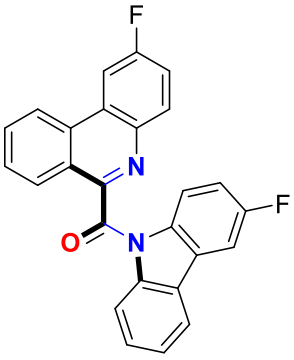
Yellow solid (15.3 mg, 71% yield). Mp 214-222 °C. ^{1}H NMR (500 MHz, DMSO-d_6):

δ 9.74 (d, *J* = 8.5 Hz, 1H), 8.31 (d, *J* = 8.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.11-8.08 (m, 1H), 7.88-7.85 (m, 1H), 7.83-7.80 (m, 1H), 7.77-7.69 (m, 2H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.45-7.42 (m, 1H), 7.32-7.26 (m, 3H), 7.04 (d, *J* = 8.0 Hz, 1H), 4.26 (s, 3H), 4.08 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 167.05, 158.23, 155.84, 155.64, 145.31, 139.71, 137.81, 133.55, 131.55, 128.77, 128.37, 127.90, 127.53, 126.32, 126.23, 126.17, 124.23, 123.60, 123.52, 123.15, 115.86, 115.69, 115.38, 109.46, 108.88, 105.51, 56.01, 55.58; IR (cm^{-1}) 3365, 2957, 2921, 2850, 1600, 1573, 1487, 1450, 1137, 783, 742, 725; HRMS (ESI) calcd for $C_{28}H_{21}N_2O_3^+$ $[M+H]^+$ 433.1547, found 433.1557.



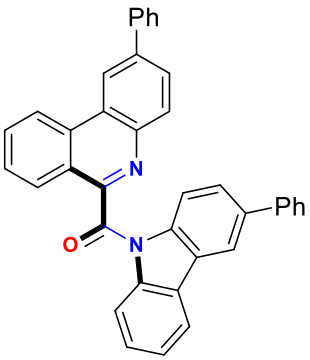
(3-Methyl-9H-carbazol-9-yl)(2-methylphenanthridin-6-yl)methanone (3l)

White solid (19.6 mg, 98% yield). Mp 214-218 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.05 (d, *J* = 8.5 Hz, 1H), 8.81 (s, 1H), 8.19 (d, *J* = 7.5 Hz, 1H), 8.10-8.03 (m, 3H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.80-7.77 (m, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.40-7.10 (m, 5H), 2.68 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 166.10, 155.52, 140.78, 139.15, 137.98, 135.89, 133.95, 132.82, 132.27, 131.49, 129.76, 129.66, 128.87, 128.57, 127.47, 126.28, 126.16, 124.52, 124.11, 123.34, 122.71, 122.45, 120.51, 120.47, 115.47, 115.18, 21.58, 20.78; IR (cm^{-1}) 3367, 2919, 2851, 1671, 1634, 1585, 1486, 1446, 875, 846, 755, 699; HRMS (ESI) calcd for $C_{28}H_{21}N_2O^+$ $[M+H]^+$ 401.1648, found 401.1643.



(3-Fluoro-9H-carbazol-9-yl)(2-fluorophenanthridin-6-yl)methanone (3m)

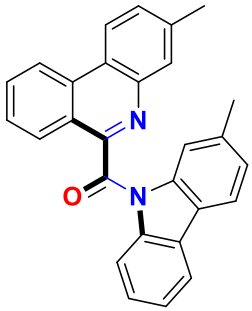
Pale yellow solid (14.3 mg, 70% yield). Mp 199-204 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.09 (d, J = 8.4 Hz, 1H), 8.87 (dd, J = 2.4 Hz, J = 6.4 Hz, 1H), 8.26 (d, J = 8.0 Hz, 1H), 8.20-8.14 (m, 3H), 8.13-8.09 (m, 1H), 7.88-7.84 (m, 1H), 7.79-7.74 (m, 1H), 7.42-7.38 (m, 2H), 7.28-7.23 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.23. 162.43 (d, J = 248.4 Hz), 160.03 (d, J = 241.4 Hz), 153.91 (d, J = 3.0 Hz), 139.91, 139.12, 134.82, 133.14 (d, J = 9.3 Hz), 133.09 (d, J = 4.3 Hz), 131.89, 129.04, 128.28 (d, J = 9.4 Hz), 127.84, 126.82, 126.23, 126.18 (d, J = 4.8 Hz), 124.26, 123.23, 122.79, 120.14, 118.56 (d, J = 24.3 Hz), 117.74, 116.07, 114.63 (d, J = 24.4 Hz), 107.44 (d, J = 23.4 Hz), 106.04 (d, J = 24.1 Hz); ^{19}F NMR (470 MHz, $CDCl_3$): -109.62 (s, 1F), -117.83 (s, 1F); IR (cm^{-1}) 3360, 3050, 2921, 2851, 1666, 1631, 1598, 1581, 1485, 1447, 895, 833, 764, 707; HRMS (ESI) calcd for $C_{26}H_{15}F_2N_2O^+$ $[M+H]^+$ 409.1147, found 409.1163.



(3-Phenyl-9H-carbazol-9-yl)(2-phenylphenanthridin-6-yl)methanone (3n)

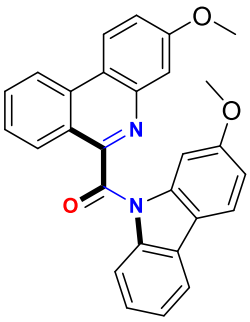
White solid (23.8 mg, 91% yield). Mp > 350 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.33 (d, J = 8.4 Hz, 1H), 9.27 (s, 1H), 8.60 (d, J = 1.2 Hz, 1H), 8.38 (d, J = 7.6 Hz,

1H), 8.20-8.19 (m, 3H), 8.14-8.10 (m, 1H), 8.04 (d, *J* = 7.2 Hz, 2H), 7.87-7.83 (m, 1H), 7.77 (d, *J* = 7.6 Hz, 2H), 7.62-7.58 (m, 3H), 7.51-7.45 (m, 5H), 7.39-7.35 (m, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 166.10, 154.26, 141.85, 140.76, 139.56, 139.35, 138.24, 137.13, 136.70, 133.28, 132.50, 130.66, 129.19, 129.14, 128.93, 128.71, 128.22, 127.85, 127.60, 127.46, 126.94, 126.85, 126.37, 126.28, 124.72, 124.67, 123.90, 122.63, 120.95, 118.58, 115.81, 115.60; IR (cm^{-1}) 3439, 2957, 2920, 2851, 1674, 1629, 1468, 1450, 987, 933, 531, 526; HRMS (ESI) calcd for $C_{38}H_{25}N_2O^+$ $[M+H]^+$ 525.1961, found 525.1992.



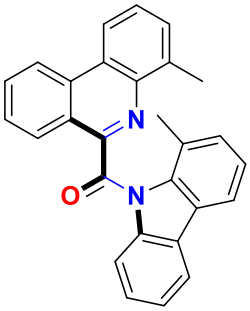
(2-Methyl-9H-carbazol-9-yl)(3-methylphenanthridin-6-yl)methanone (3o)

White solid (18.0 mg, 90% yield). Mp 220-225 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.03 (d, *J* = 8.4 Hz, 1H), 8.89 (d, *J* = 8.4 Hz, 1H), 8.16-8.04 (m, 4H), 7.91 (s, 1H), 7.79-7.42 (m, 2H), 7.56 (br, 1H), 7.34-7.28 (m, 2H), 7.12 (br, 1H), 6.79 (br, 1H), 2.56 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 166.21, 154.42, 142.59, 139.85, 138.33, 137.52, 137.38, 133.15, 132.44, 130.76, 129.36, 128.55, 126.92, 126.24, 126.19, 125.79, 124.34, 123.80, 123.16, 123.06, 122.06, 121.90, 120.33, 120.19, 116.28, 114.93, 21.77, 21.02; IR (cm^{-1}) 3361, 3032, 2920, 2851, 1678, 1600, 1581, 1499, 1458, 889, 844, 746, 696; HRMS (ESI) calcd for $C_{28}H_{21}N_2O^+$ $[M+H]^+$ 401.1648, found 401.1696.



(3-Methoxy-9H-carbazol-9-yl)(2-methoxyphenanthridin-6-yl)methanone (3p)

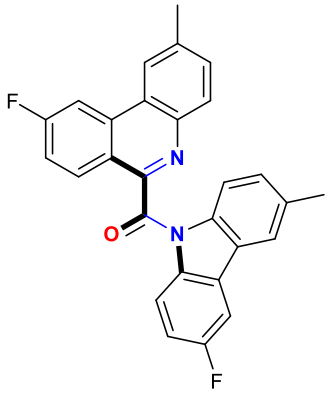
White solid (21.2 mg, 98% yield). Mp 200-205 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.97 (d, J = 8.5 Hz, 1H), δ 8.89 (d, J = 9.0 Hz, 1H), 8.12-8.08 (m, 3H), 8.05-8.02 (m, 1H), 7.74-7.71 (m, 1H), 7.60 (s, 1H), 7.53 (d, J =9.0 Hz, 1H), 7.36-7.02 (m, 4H), 3.92 (s, 3H), 3.48 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 166.23, 160.47, 159.13, 154.79, 144.32, 138.98, 137.73, 133.36, 132.56, 127.91, 126.27, 126.25, 126.15, 124.57, 124.53, 122.84, 121.37, 121.30, 119.80, 119.77, 119.49, 118.18, 115.32, 111.93, 110.08, 100.88, 55.67, 55.09; IR (cm^{-1}) 3388, 3365, 2920, 1667, 1616, 1583, 1459, 1439, 1121, 886, 853, 765, 699; HRMS (ESI) calcd for $C_{28}H_{21}N_2O_3^+$ $[M+H]^+$ 433.1547, found 433.1549.



(1-Methyl-9H-carbazol-9-yl)(4-methylphenanthridin-6-yl)methanone (3r)

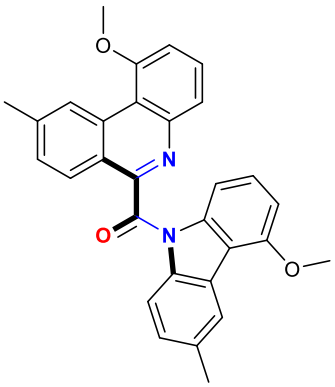
Pale yellow solid (17.6 mg, 88% yield). Mp 183-186 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.01 (d, J = 8.5 Hz, 1H), 8.74 (d, J = 8.0 Hz, 2H), 8.23 (d, J = 7.5 Hz, 1H), 8.11-8.06 (m, 2H), 7.95-7.91 (m, 1H), 7.74-7.71 (m, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 7.0 Hz, 1H), 7.42-7.31 (m, 3H), 7.08 (d, J = 7.5 Hz, 1H), 2.01 (s, 3H), 1.72 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 167.39, 149.98, 140.17, 140.00, 139.54, 138.18, 133.71, 131.81, 130.01, 129.48, 129.41, 128.82, 127.32, 126.83,

126.50, 126.11, 125.34, 124.58, 123.94, 123.33, 122.92, 120.78, 120.48, 117.95, 114.11, 20.34, 16.72; IR (cm^{-1}) 3365, 2957, 2920, 2851, 1678, 1595, 1543, 1493, 1468, 1446, 1374, 788, 766; HRMS (ESI) calcd for $C_{28}H_{21}N_2O^+$ $[M+H]^+$ 401.1648, found 401.1649.



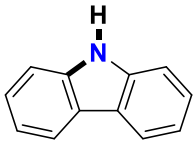
(9-Fluoro-2-methylphenanthridin-6-yl)(3-fluoro-6-methyl-9H-carbazol-9-yl)methanone (3s)

White solid (18.1 mg, 83% yield). Mp 234-236 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.86 (d, J = 10.5 Hz, 1H), 8.79 (s, 1H), 8.23 (s, 3H), 8.05-7.96 (m, 4H), 7.72-7.65 (m, 3H), 7.18-7.05 (m, 3H), 2.64 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 165.59, 164.01 (d, J = 250.0 Hz), 159.37 (d, J = 238.8 Hz), 152.55, 140.83, 139.23, 136.55, 135.56 (d, J = 9.9 Hz), 134.46, 133.88, 132.12, 129.86 (d, J = 9.9 Hz), 129.72, 129.14, 127.77 (d, J = 9.9 Hz), 125.67 (d, J = 3.3 Hz), 123.84 (d, J = 3.8 Hz), 123.26, 120.95, 119.67, 118.02 (d, J = 24.4 Hz), 117.15, 115.01, 114.65 (d, J = 24.5 Hz), 108.76 (d, J = 22.8 Hz), 106.75 (d, J = 24.4 Hz), 21.48, 20.70; ^{19}F NMR (470 MHz, $CDCl_3$): -104.25 (s, 1F), -117.95 (s, 1F); IR (cm^{-1}) 3429, 2951, 2919, 2852, 1679, 1620, 1585, 1457, 1274, 859, 831, 815; HRMS (ESI) calcd for $C_{28}H_{19}F_2N_2O^+$ $[M+H]^+$ 437.1460, found 437.1461.



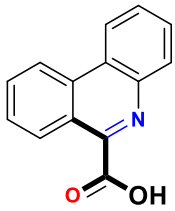
(3-Methoxy-5-methyl-9H-carbazol-9-yl)(1-methoxy-9-methylphenanthridin-6-yl) methanone (3t)

Yellow solid (21.2 mg, 92% yield). Mp 238-241 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.49 (s, 1H), 8.07 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.81-7.77 (m, 1H), 7.70-7.68 (m, 1H), 7.60 (dd, *J* = 1.2 Hz, *J* = 8.4 Hz, 1H), 7.49 (d, *J* = 7.6 Hz, 2H), 7.19-6.97 (m, 4H), 4.21 (s, 3H), 4.03 (s, 3H), 2.64 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): 166.24, 158.01, 155.38, 154.96, 144.65, 142.55, 139.03, 135.12, 133.81, 132.95, 129.66, 129.47, 128.44, 127.66, 127.51, 125.80, 125.46, 122.93, 122.48, 120.80, 114.72, 114.57, 114.18, 110.27, 107.85, 106.31, 56.28, 55.84, 22.39, 20.88; IR (cm^{-1}) 3392, 3185, 2920, 2850, 1635, 1585, 1506, 1452, 1034, 880, 812, 782, 770, 751; HRMS (ESI) calcd for $C_{30}H_{25}N_2O_3^+$ $[M+H]^+$ 461.1860, found 461.1864.



9H-carbazole (**4**)

Yellow solid (15.0 mg, 90% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.22 (s, 1H), 8.10 (d, *J* = 10.0 Hz, 2H), 7.47 (d, *J* = 10.5 Hz, 2H), 7.39-7.35 (m, 2H), 7.17-7.13 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): 139.68, 125.45, 122.35, 120.08, 118.43, 110.88; HRMS (ESI) calcd for $C_{12}H_{10}N^+$ $[M+H]^+$ 168.0808, found 168.0807.



Phenanthridine-6-carboxylic acid (**5**)

Yellow solid (20.5 mg, 92% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.74 (d, *J* = 5.0 Hz, 1H), 8.69 (d, *J* = 5.0 Hz, 1H), 8.64 (s, 1H), 8.21 (s, 1H), 7.97-7.94 (m, 1H), 7.84-7.82 (m, 3H), 6.73 (br, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): 163.99, 144.46, 140.50, 134.36, 132.05, 130.17, 129.96, 129.60, 129.01, 128.92, 126.69, 124.13, 122.46, 122.12; HRMS (ESI) calcd for $C_{14}H_{10}NO_2^+$ $[M+H]^+$ 224.0706, found 224.0708.

6. References

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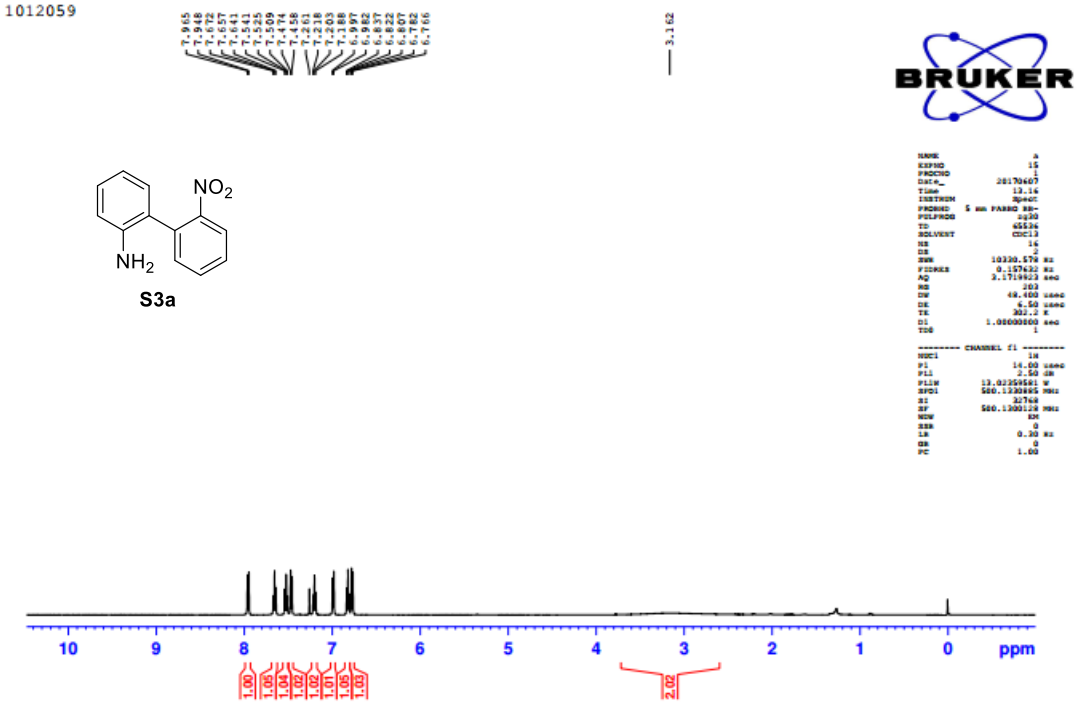
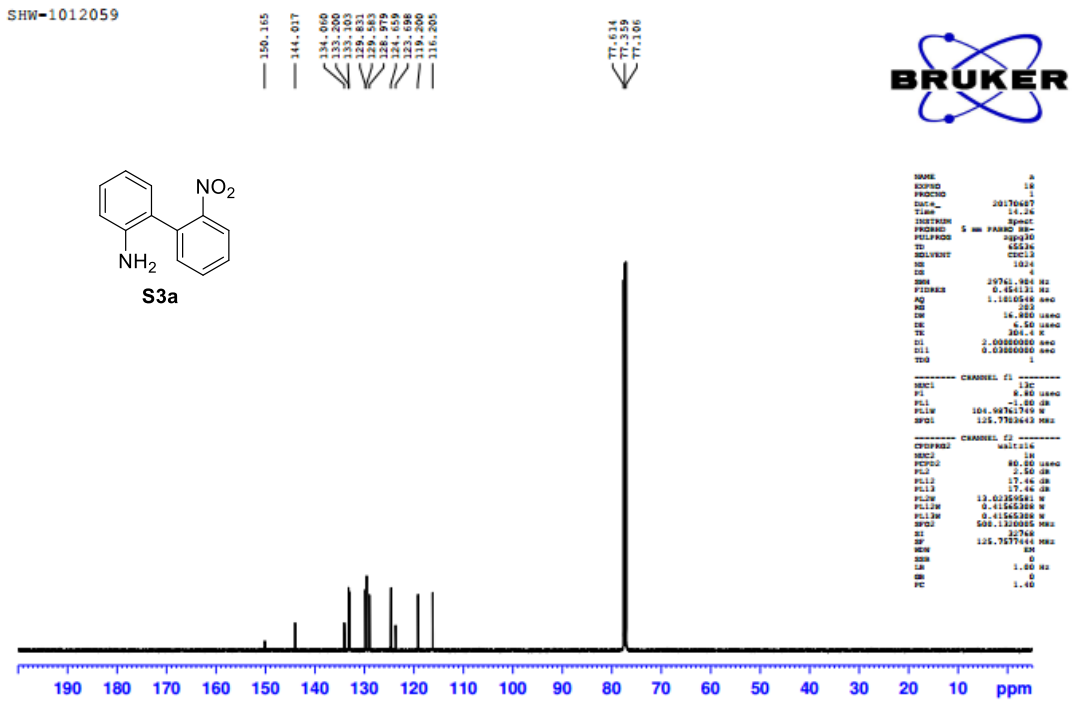
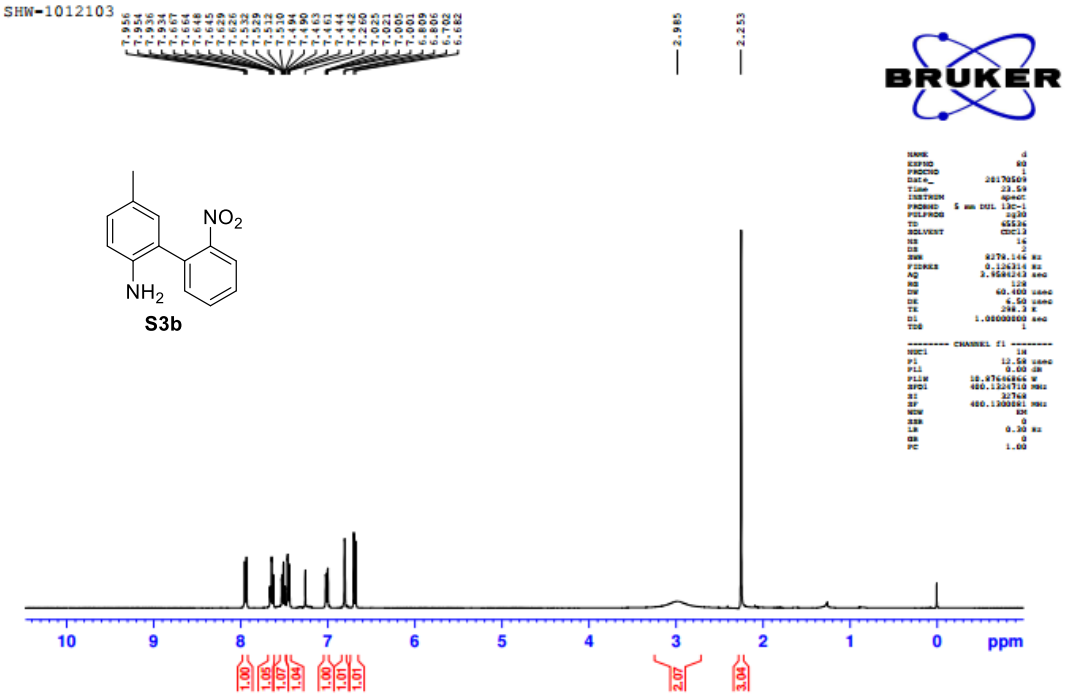
7. Copies of ^{1}H and ^{13}C NMR Spectra



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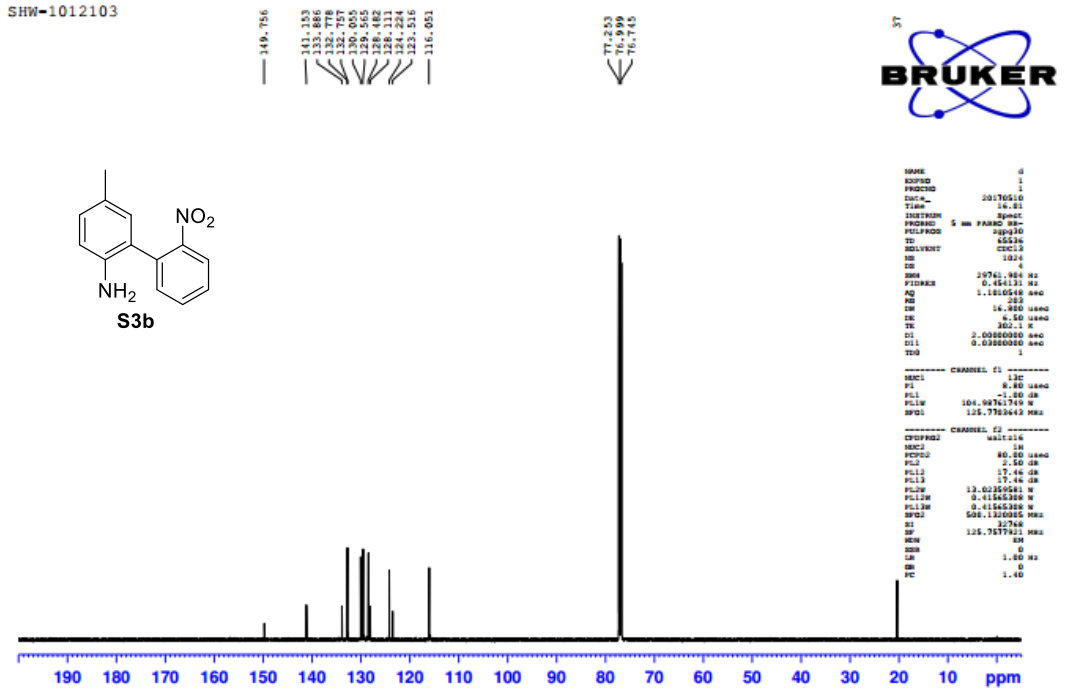
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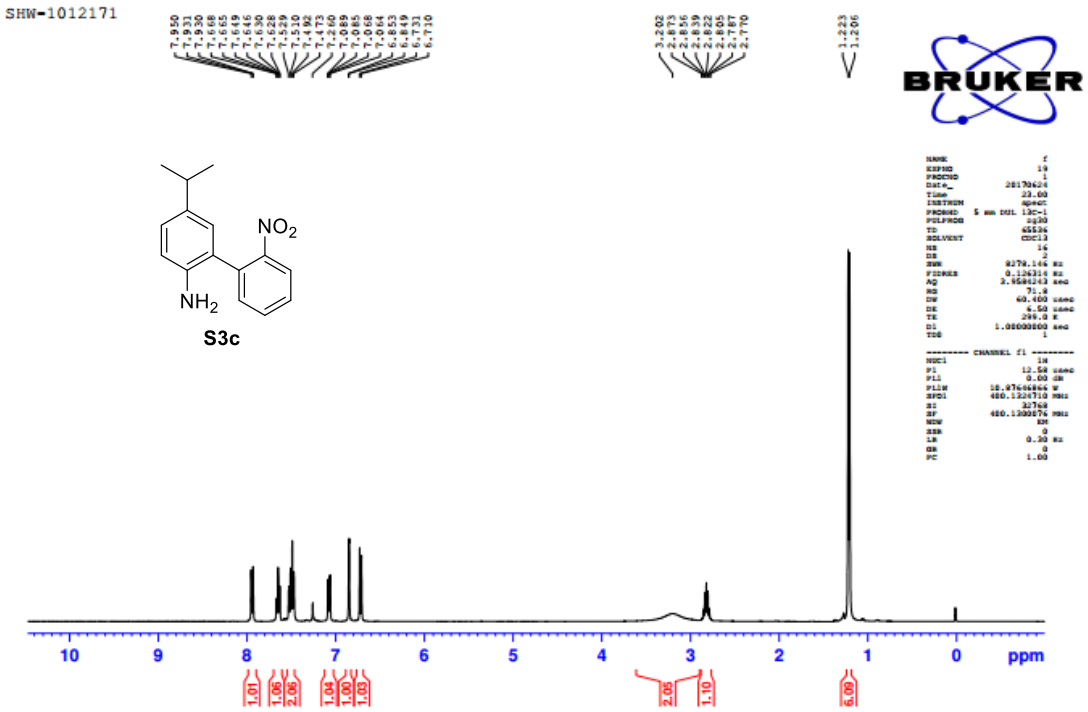
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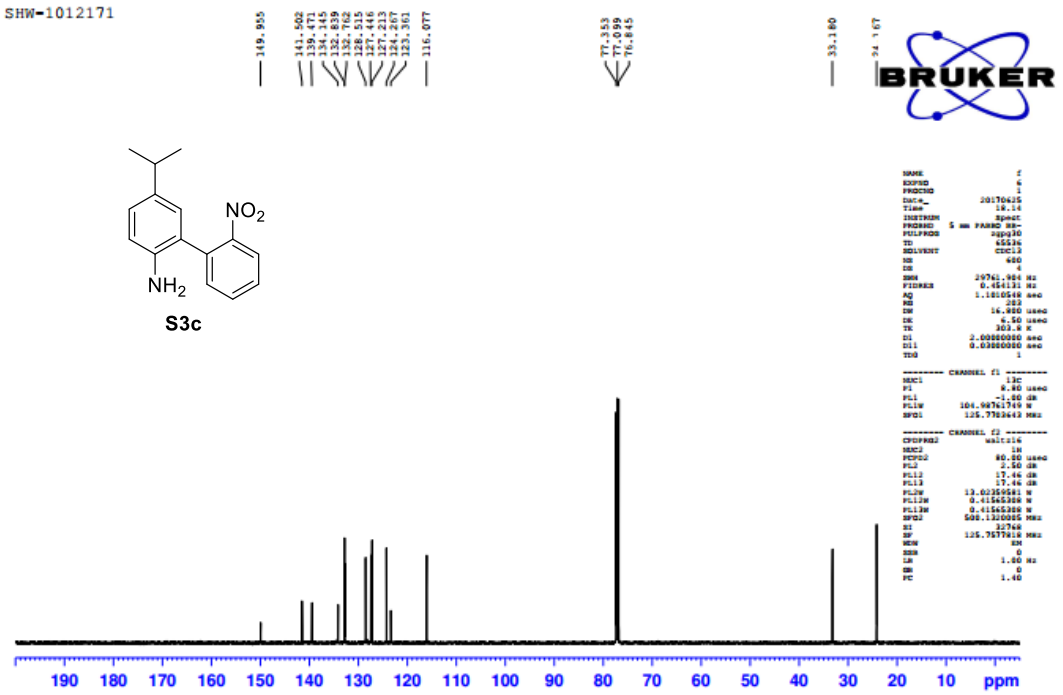
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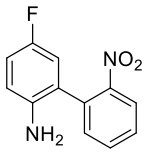

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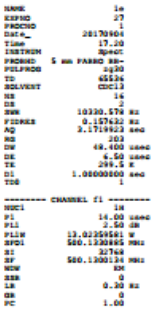

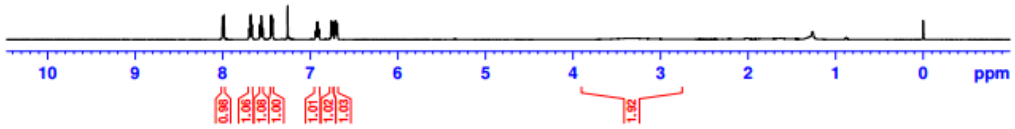

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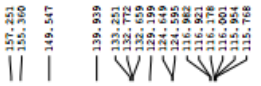

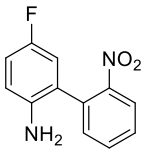

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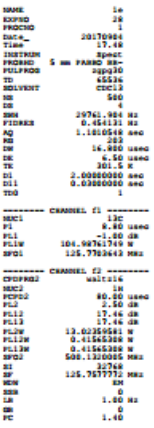

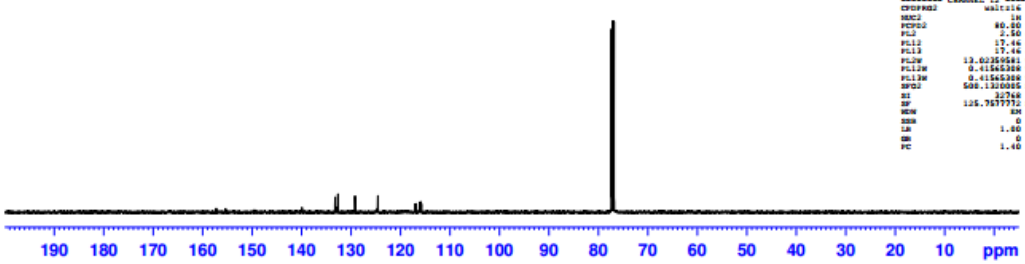

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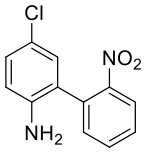

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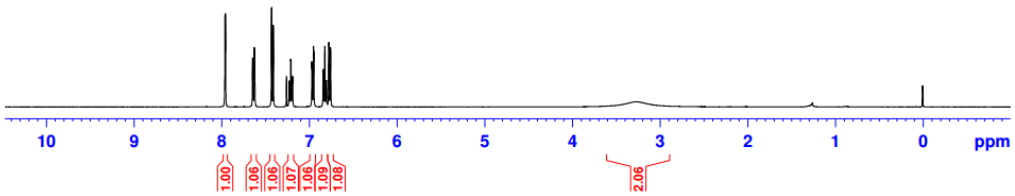
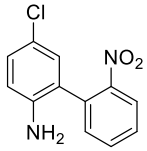
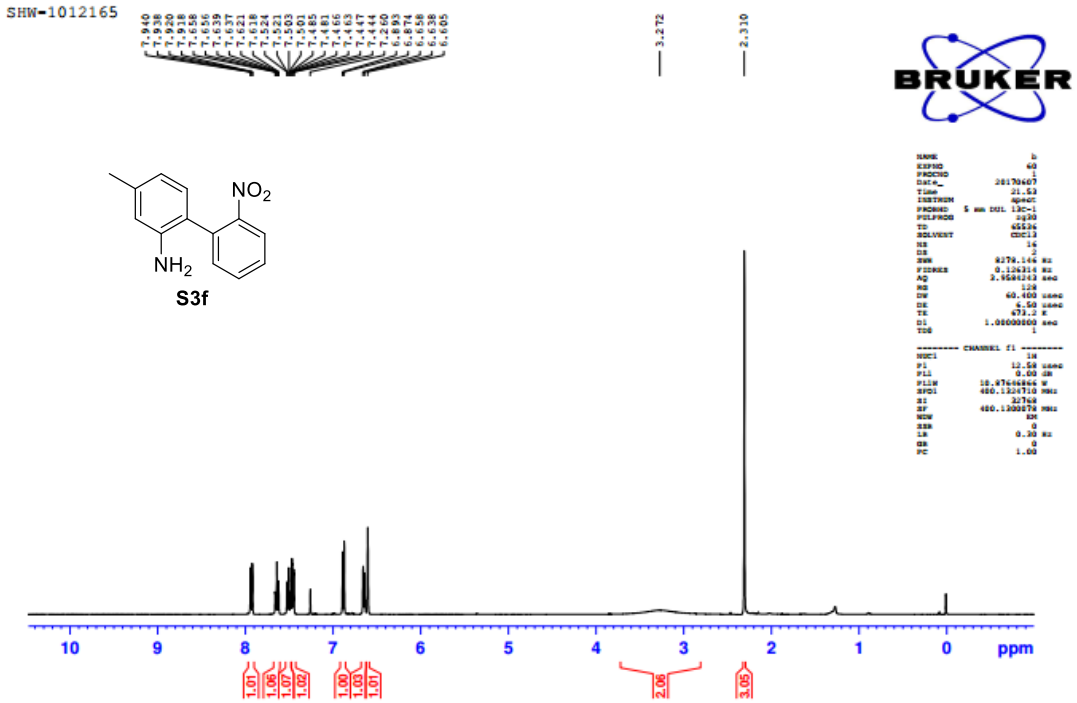
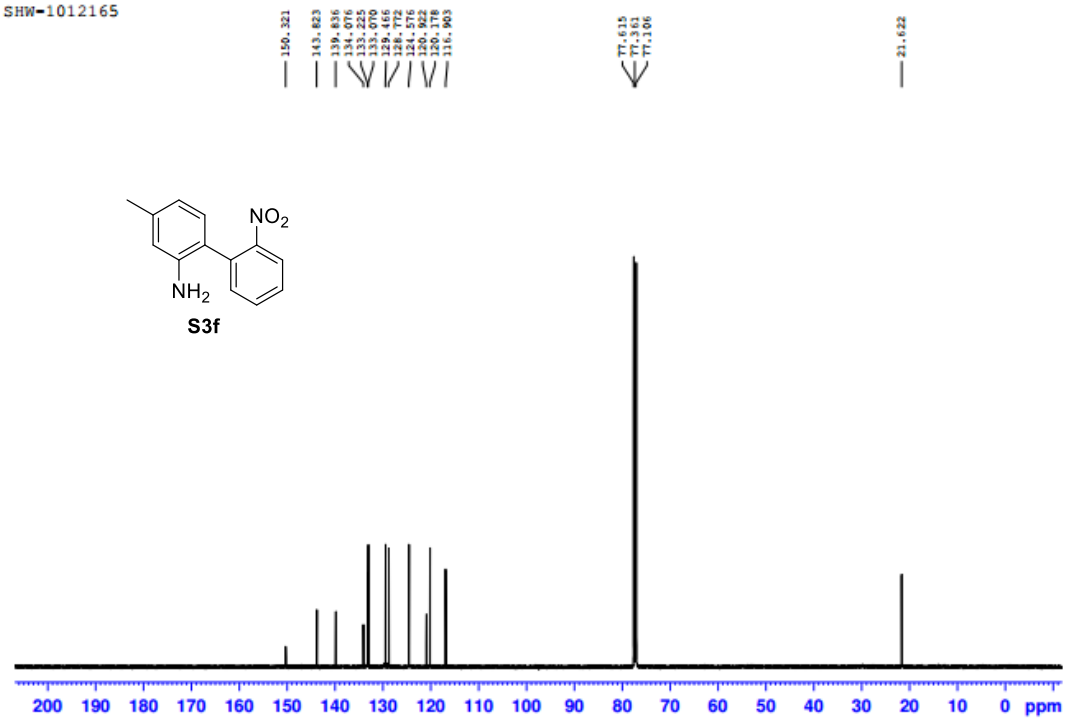


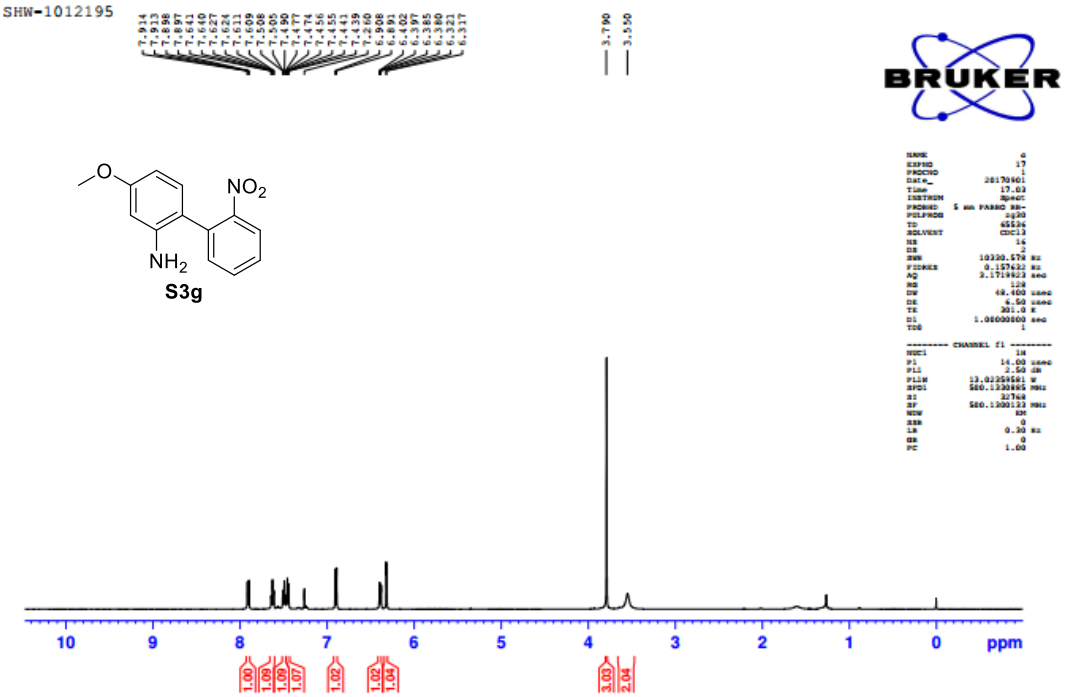
1012052



S3e


SHW-1012165
7.940
7.938
7.920
7.918
7.658
7.656
7.639
7.637
7.621
7.618
7.524
7.521
7.503
7.501
7.485
7.483
7.466
7.463
7.447
7.444
7.260
7.255
6.874
6.658
6.638
6.605
3.272
2.330
BRUKER
NO2
NH2
S3f
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.06
1.07
1.02
1.00
1.03
1.01
2.06
3.05


SHW-1012165
150.321
143.823
139.836
134.076
133.225
133.070
129.466
128.772
124.575
120.922
120.178
116.903
77.615
77.363
77.106
21.622
NO2
NH2
S3f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


SHW-1012195
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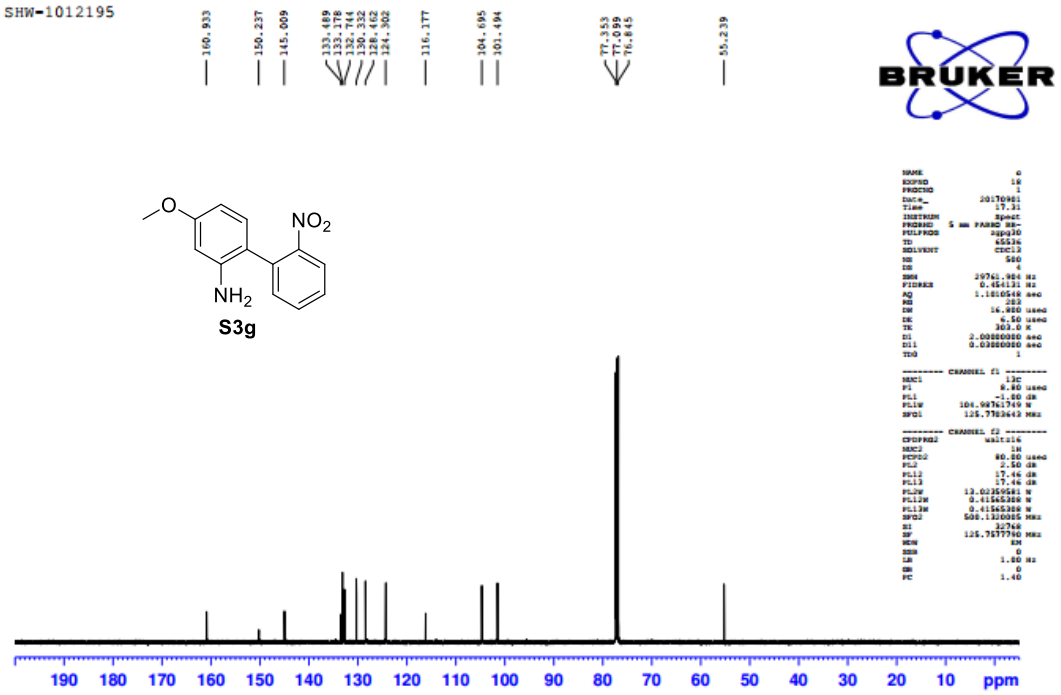
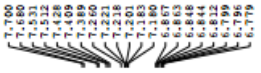
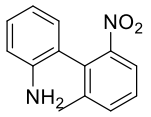
7.913
7.898
7.897
7.641
7.640
7.627
7.624
7.611
7.609
7.508
7.505
7.490
7.477
7.474
7.456
7.455
7.441
7.439
7.260
6.898
6.881
6.402
6.397
6.385
6.380
6.321
6.317
3.790
3.550
BRUKER
O
NO2
NH2
S3g
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.08
1.09
1.07
1.02
1.02
1.04
3.03
2.04

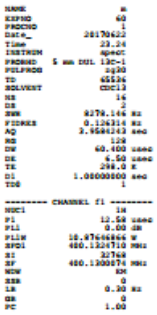

SHW-1012195
160.933
150.237
145.009
133.489
133.178
132.744
130.332
126.468
124.902
116.177
104.695
101.494
77.353
77.099
76.845
55.239
BRUKER
O
NO2
NH2
S3g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

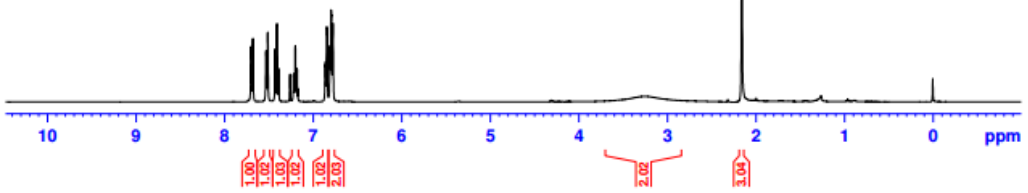
SHW-1012174



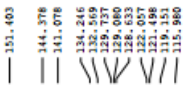


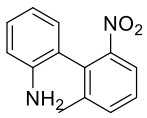
S3j



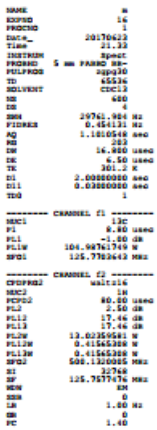


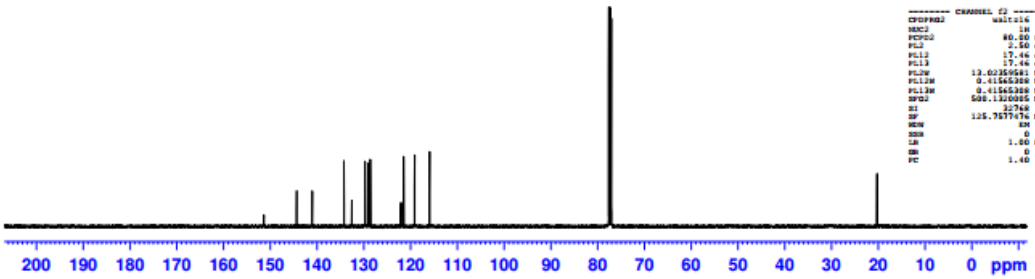
SHW-1012174

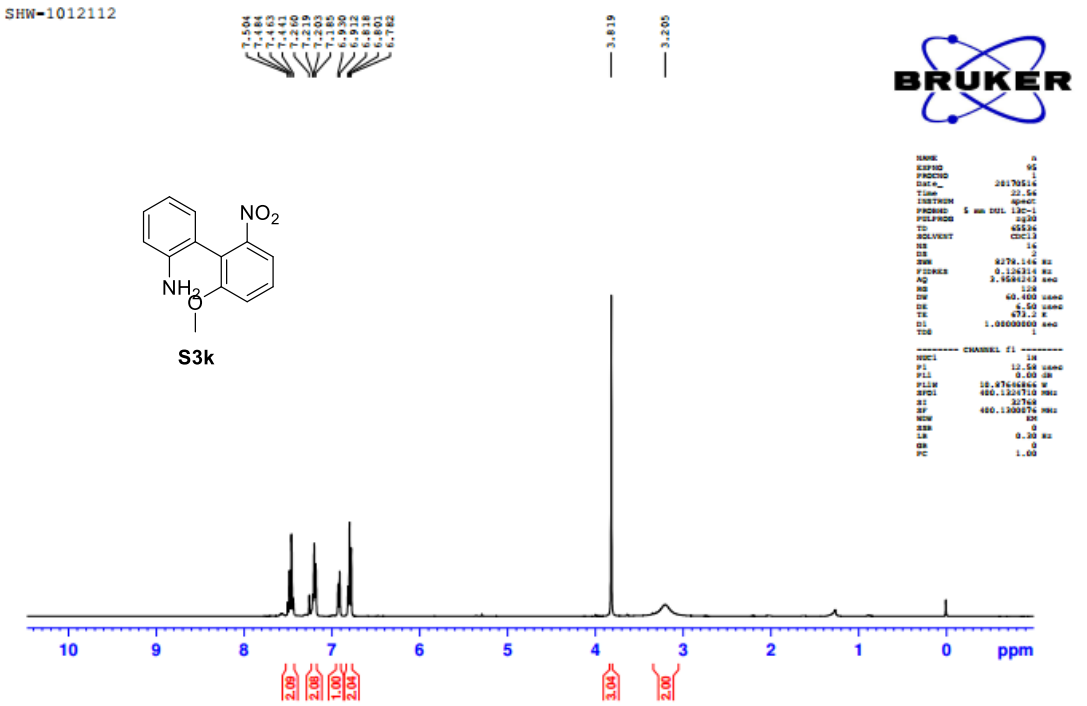


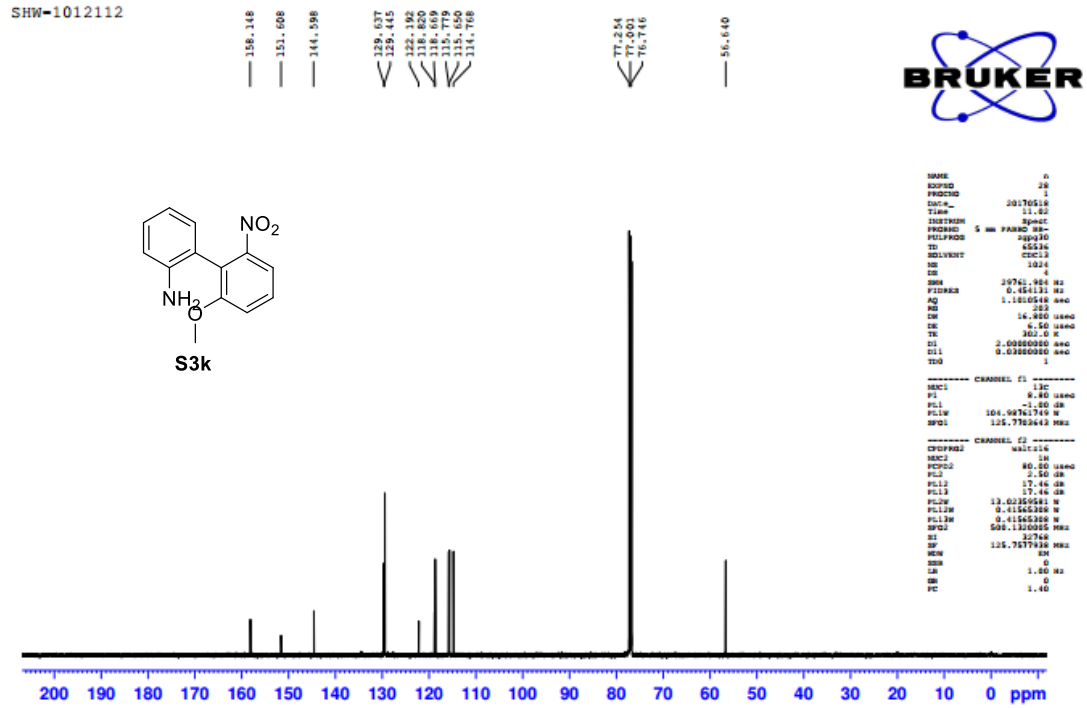


S3j

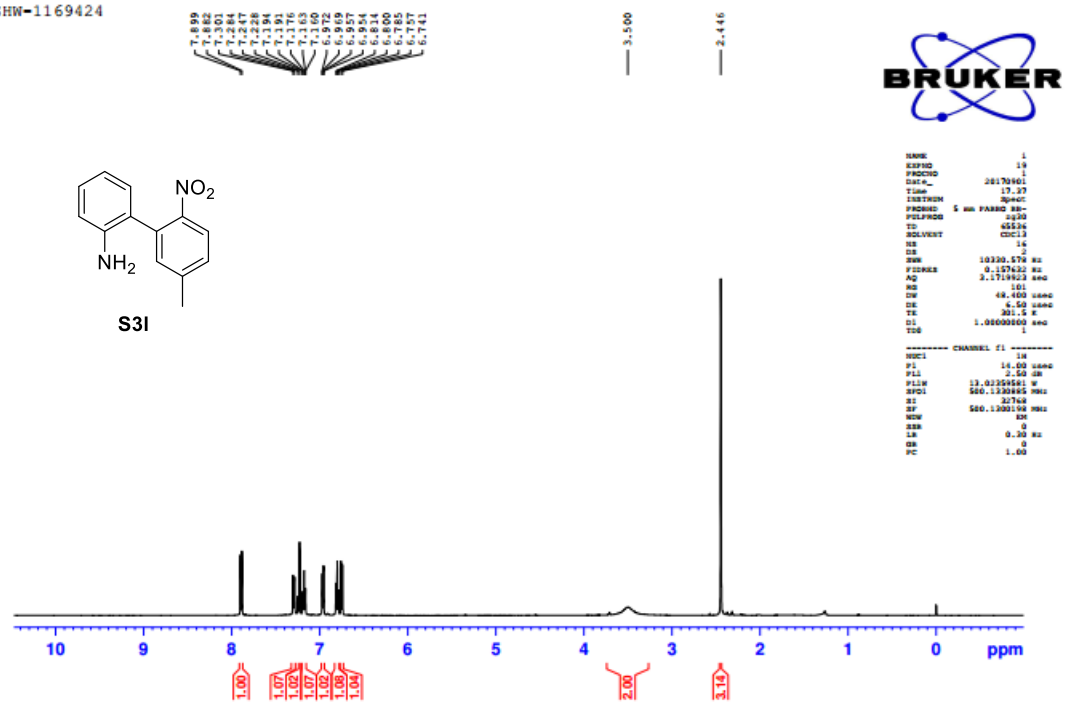




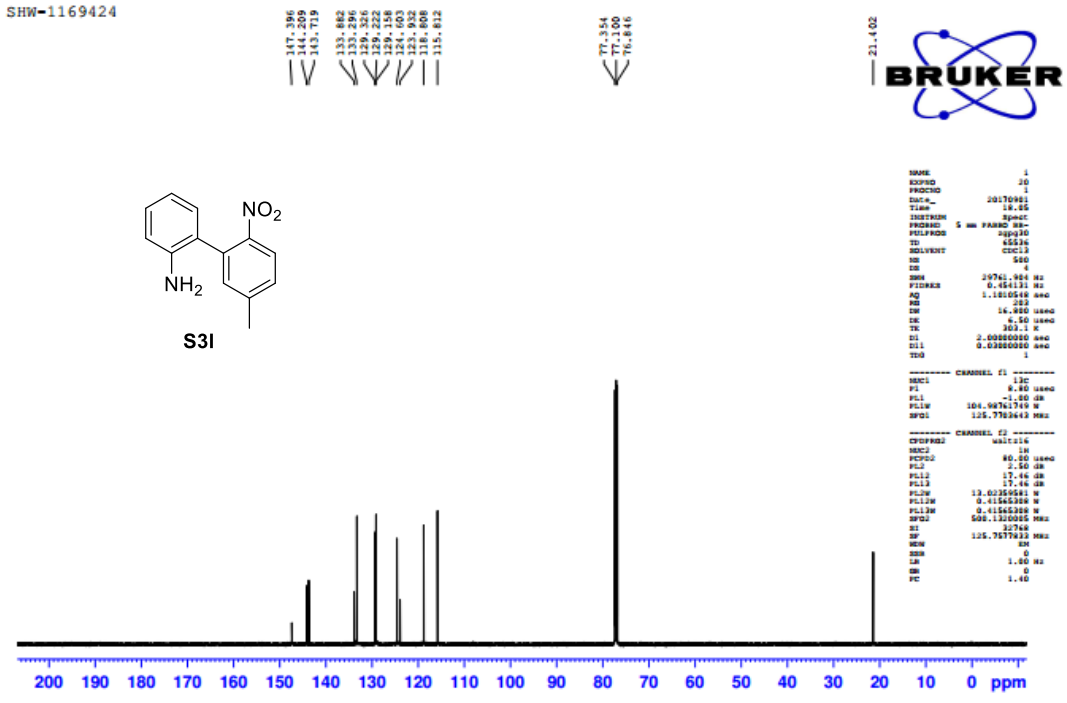

SHW-1012112
7.504
7.484
7.463
7.441
7.260
7.219
7.203
7.185
6.932
6.912
6.818
6.801
6.782
3.819
3.205
BRUKER
NO2
NH2
O
S3k
10
9
8
7
6
5
4
3
2
1
0
ppm
2.08
2.08
1.00
2.04
3.04
2.00


SHW-1012112
158.148
151.608
144.598
129.637
129.445
122.192
118.820
118.669
115.779
115.650
114.768
77.254
77.001
76.746
56.640
BRUKER
NO2
NH2
O
S3k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

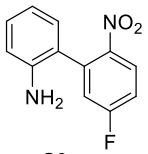
SHW-1169424



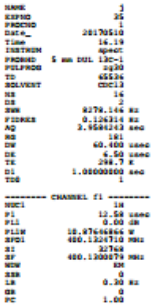
SHW-1169424

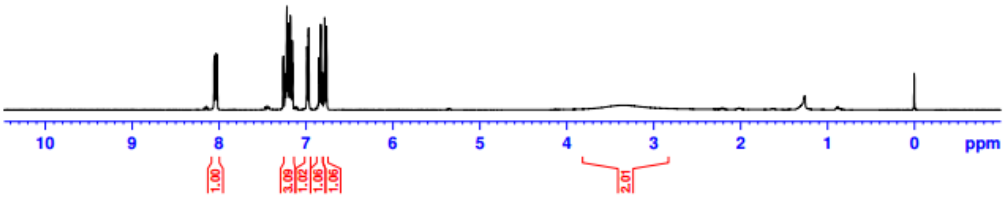


SHW-1012113

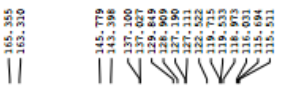


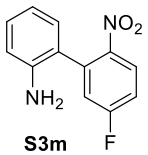
S3m



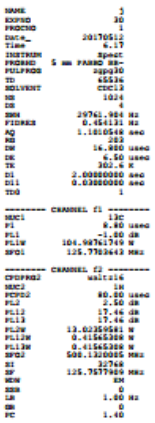


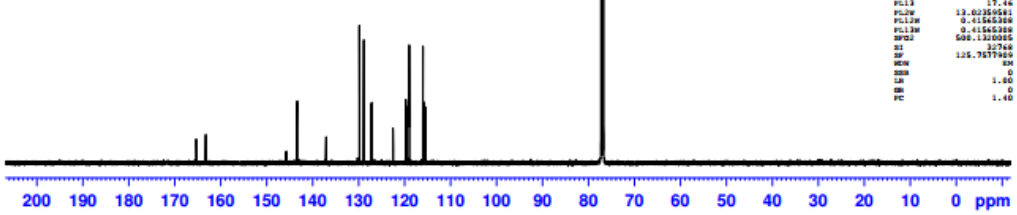
SHW-1012113

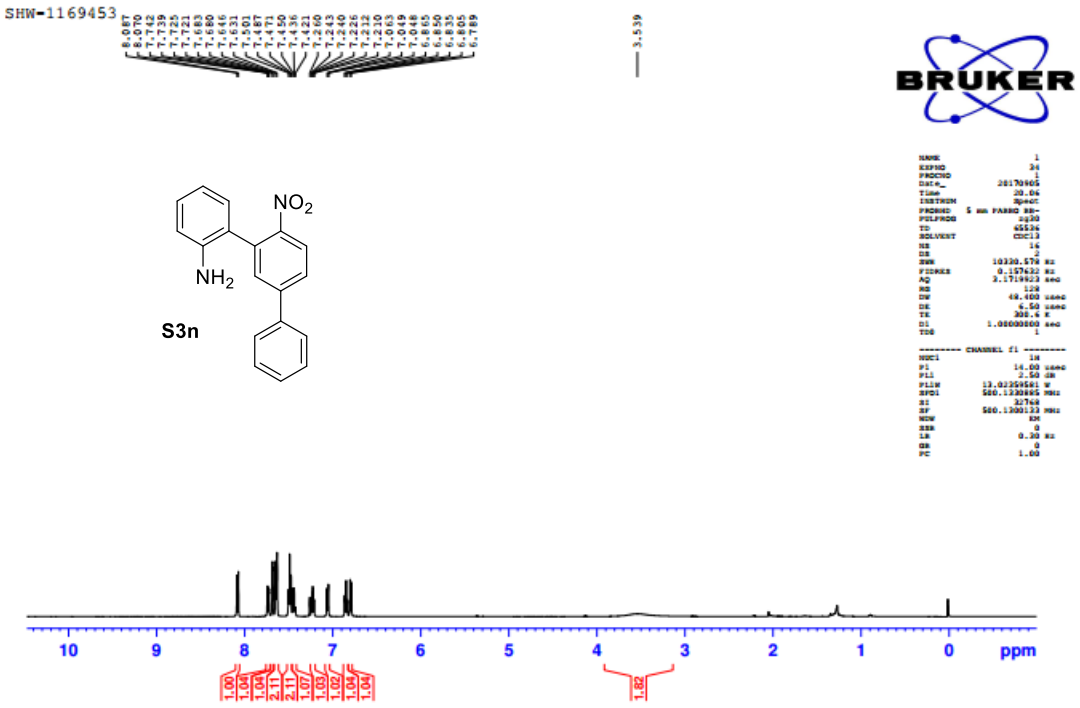


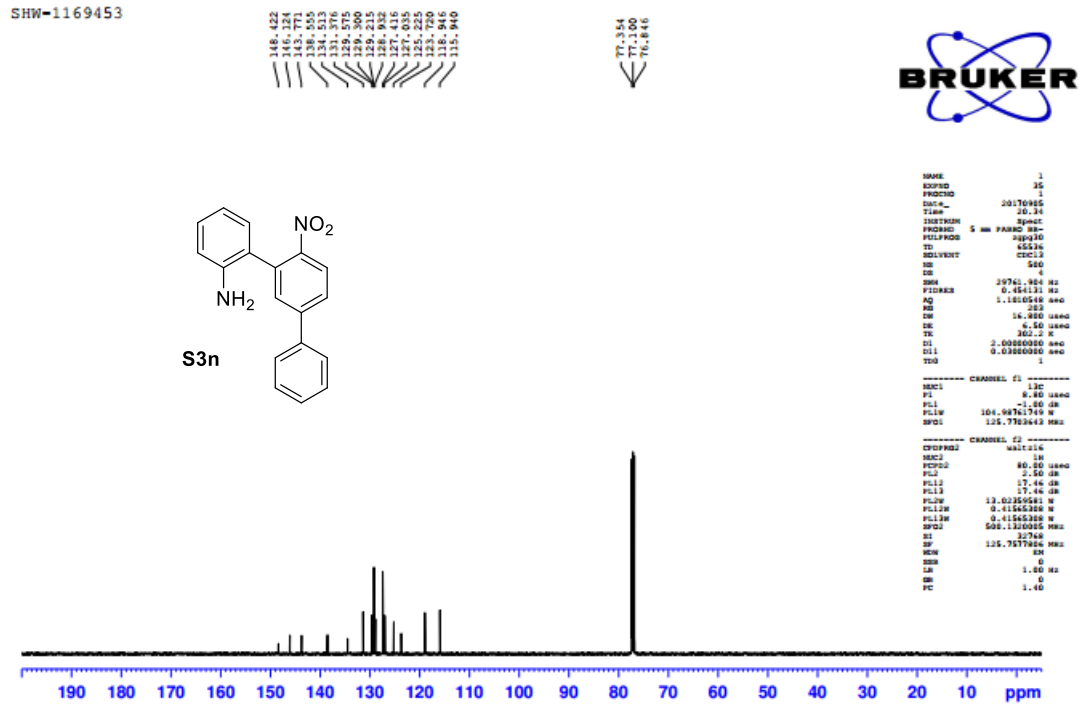


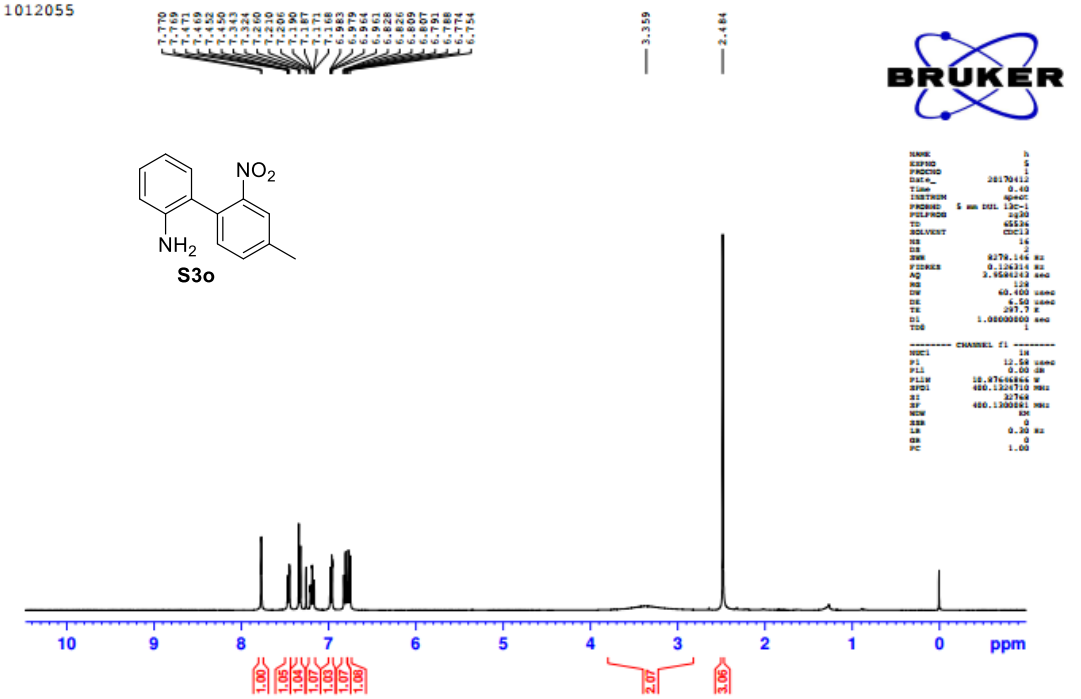
S3m






SHW-1169453
S3n
ppm


SHW-1169453
S3n
ppm


1012055
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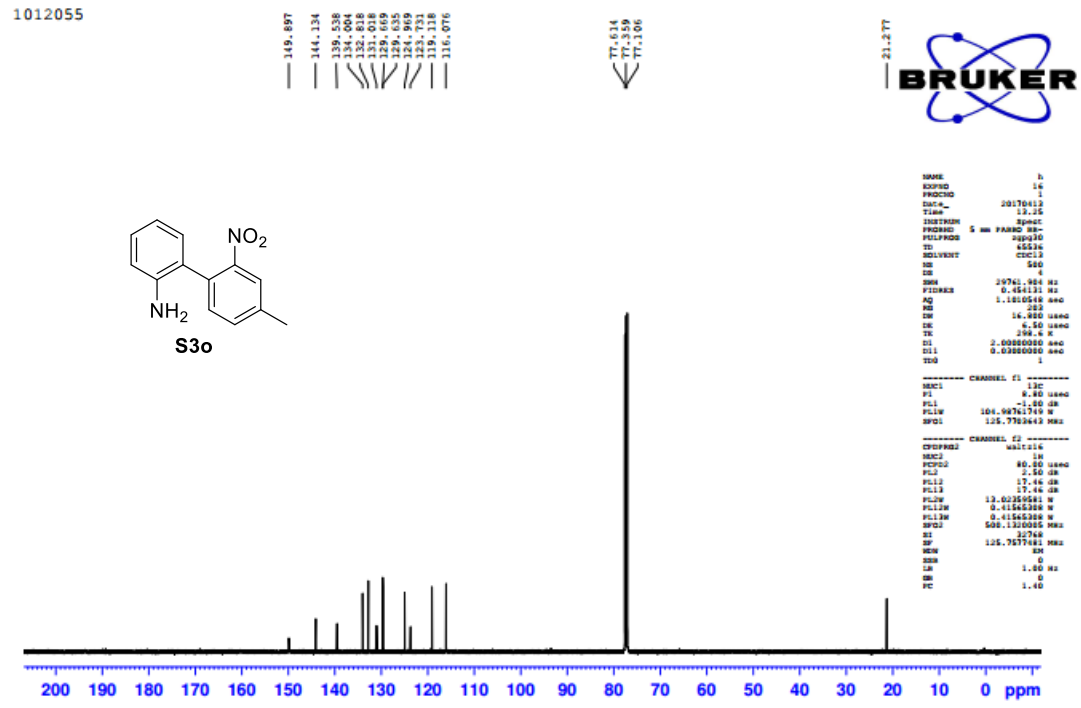
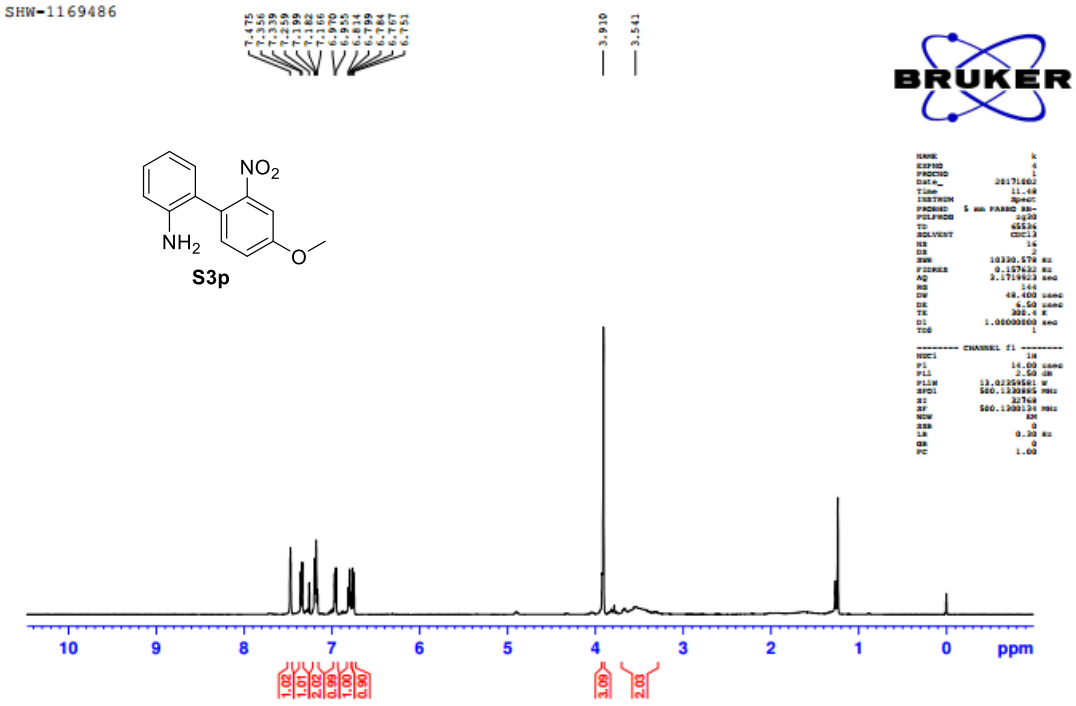
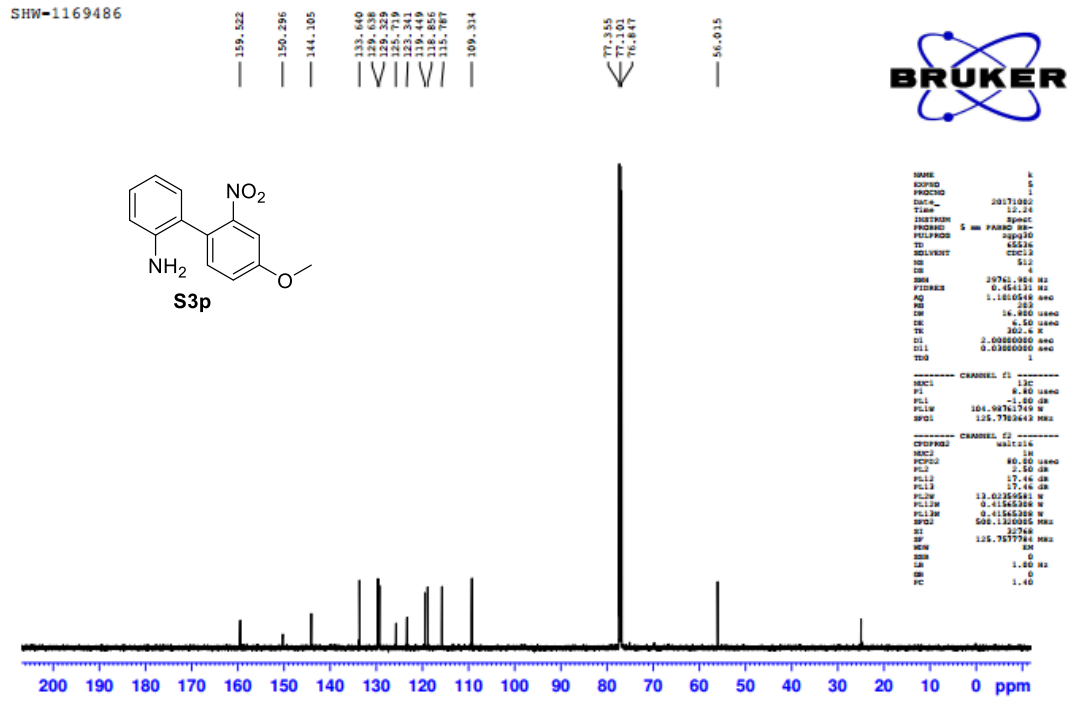
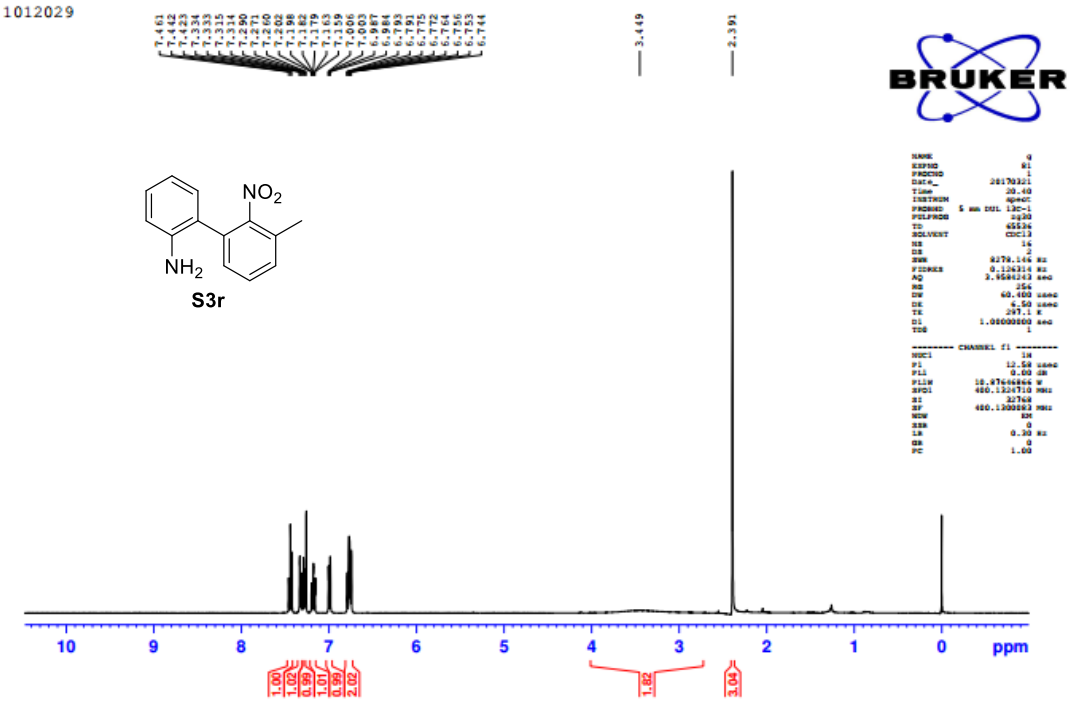
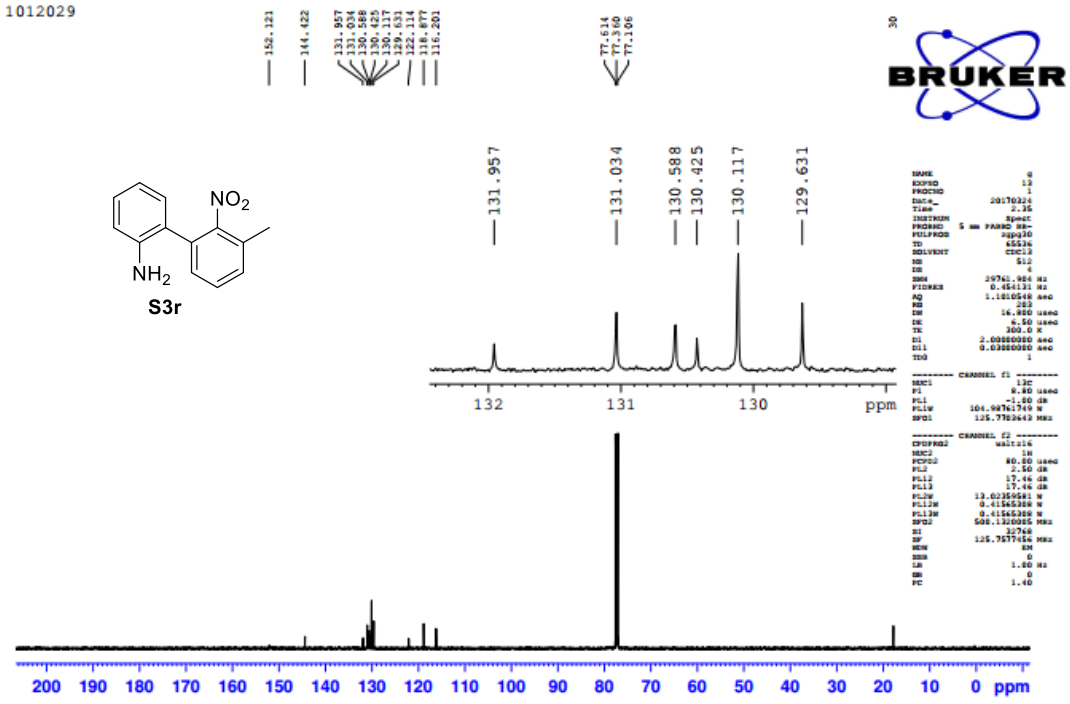
7.769
7.471
7.469
7.452
7.450
7.343
7.324
7.260
7.230
7.206
7.190
7.187
7.171
7.168
6.983
6.979
6.964
6.961
6.828
6.826
6.809
6.807
6.791
6.788
6.774
6.754
3.359
2.484
BRUKER
NO2
NH2
S3o
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.05
1.04
1.07
1.03
1.07
1.08
2.07
3.06

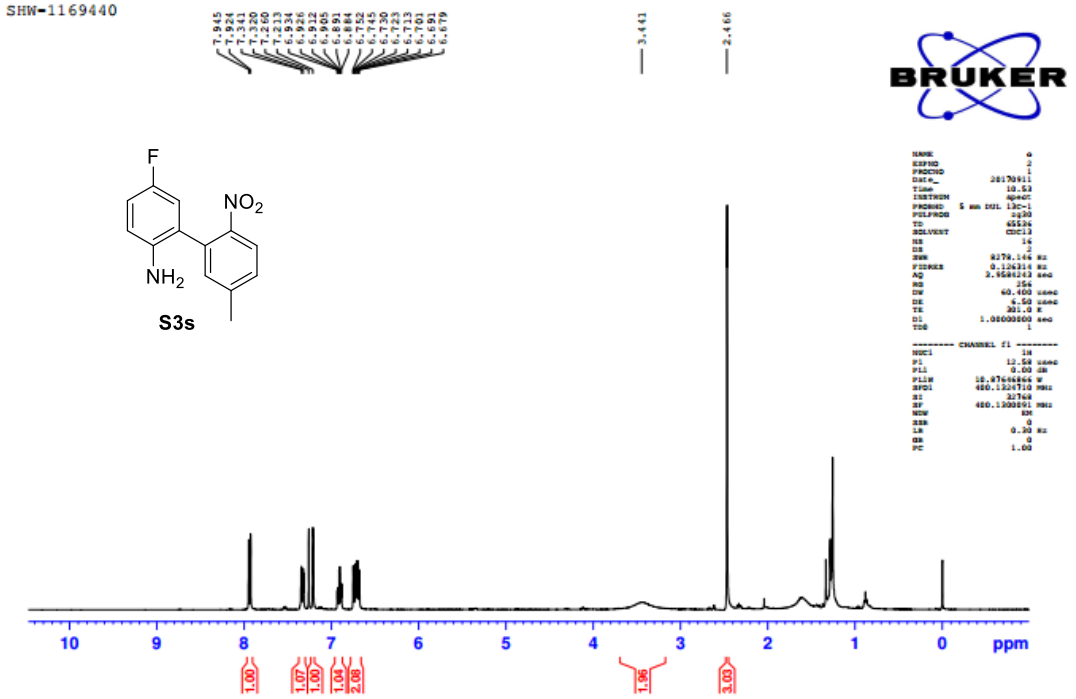

1012055
149.897
144.134
139.538
134.004
132.818
131.018
129.669
129.635
124.969
123.731
119.118
116.076
77.634
77.359
77.106
21.277
BRUKER
NO2
NH2
S3o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

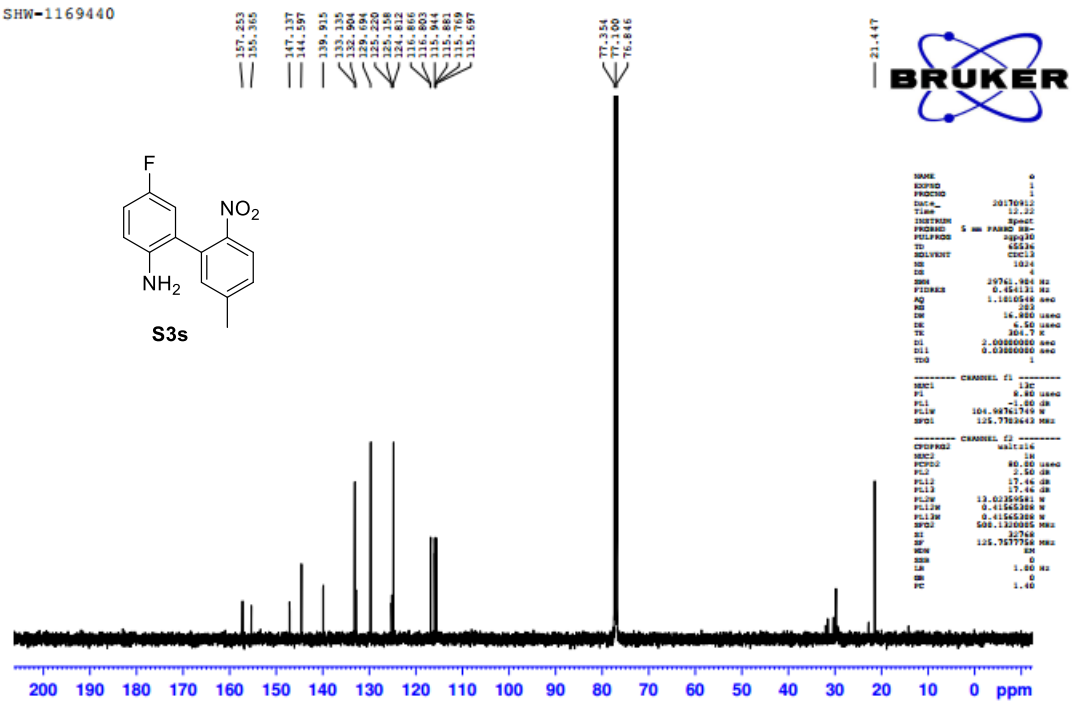

SHW-1169486
7.475
7.356
7.339
7.334
7.199
7.182
7.166
6.970
6.955
6.914
6.787
6.784
6.767
6.751
3.930
3.541
BRUKER
NO2
NH2
O
S3p
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
2.02
0.98
1.00
0.90
3.00
2.03

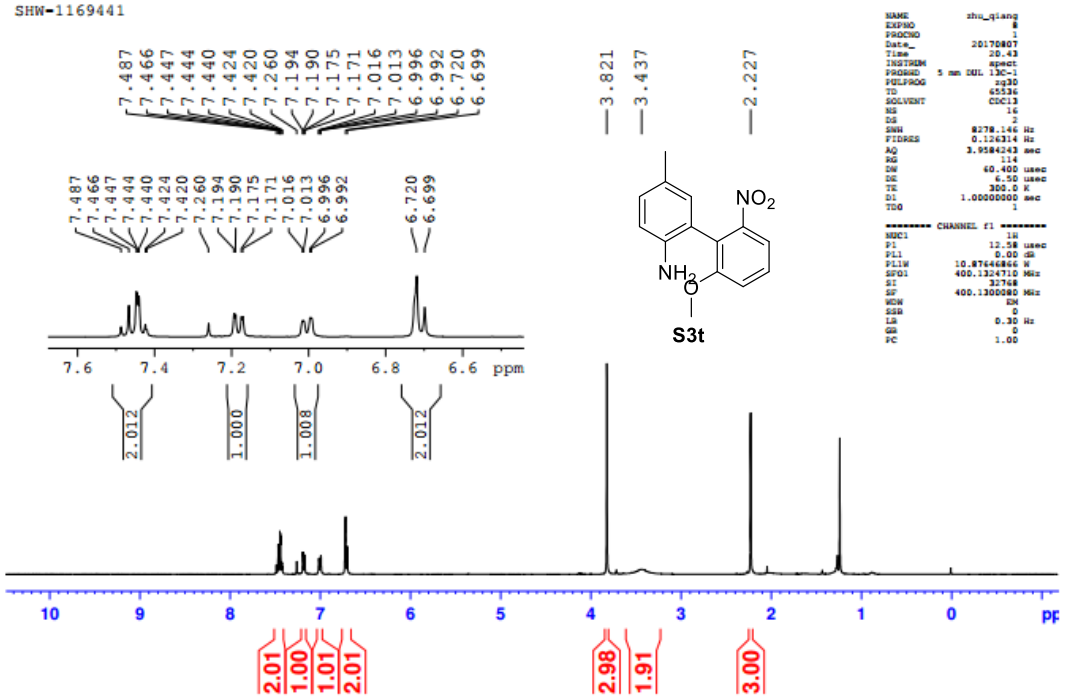

SHW-1169486
159.522
150.296
144.305
133.640
129.638
128.239
125.719
123.341
119.449
118.856
115.787
109.334
77.355
77.101
76.847
56.035
BRUKER
NO2
NH2
O
S3p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

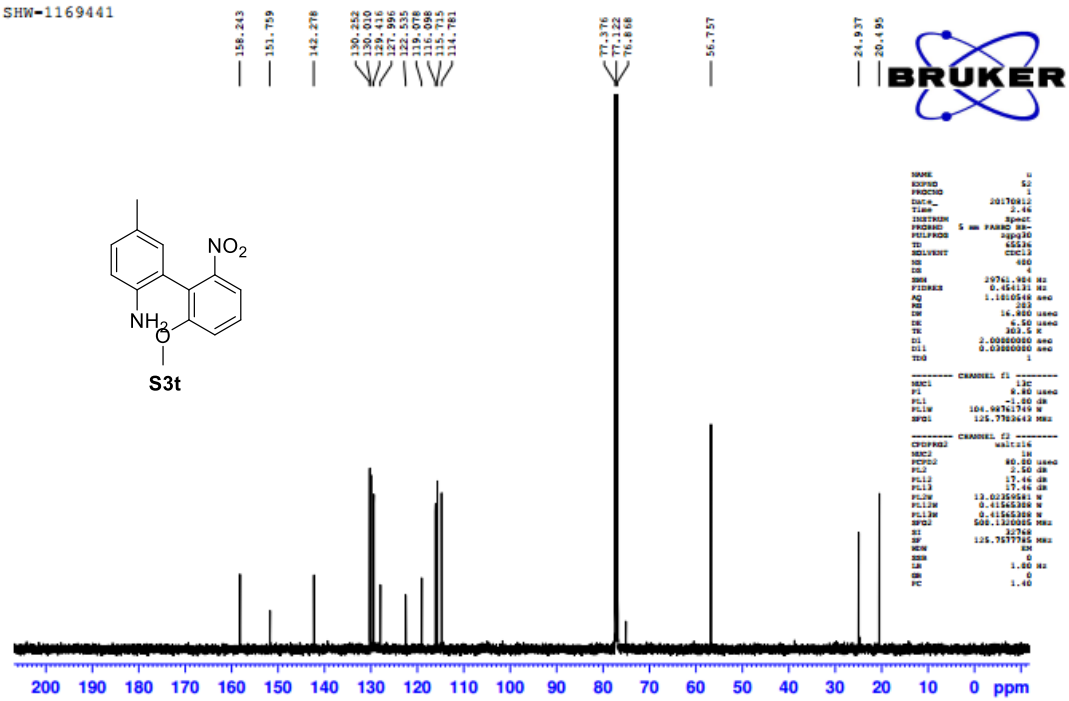

1012029
NO2
NH2
S3r
ppm


1012029
NO2
NH2
S3r
131.957
131.034
130.588
130.425
130.117
129.631
ppm

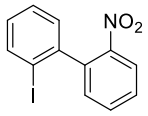

SHW-1169440
F
NO2
NH2
S3s
ppm


SHW-1169440
F
NO2
NH2
S3s
ppm

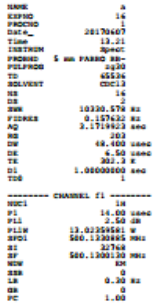

SHW-1169441
7.487
7.466
7.447
7.444
7.440
7.424
7.420
7.260
7.194
7.190
7.175
7.171
7.016
7.013
6.996
6.992
6.720
6.699
3.821
3.437
2.227
NO2
NH2
O
S3t
7.6
7.4
7.2
7.0
6.8
6.6 ppm
2.012
1.000
1.008
2.012
10
9
8
7
6
5
4
3
2
1
0
2.01
1.00
1.01
2.01
2.98
1.91
3.00

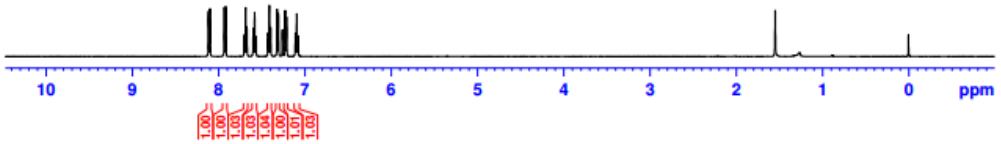

SHW-1169441
158.243
151.759
142.278
130.252
130.010
129.416
127.996
122.535
119.078
116.698
115.715
114.781
77.376
77.122
76.868
56.757
24.937
20.495
BRUKER
NO2
NH2
O
S3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

SHW-1012160

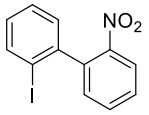


S4a

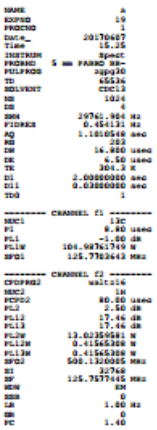


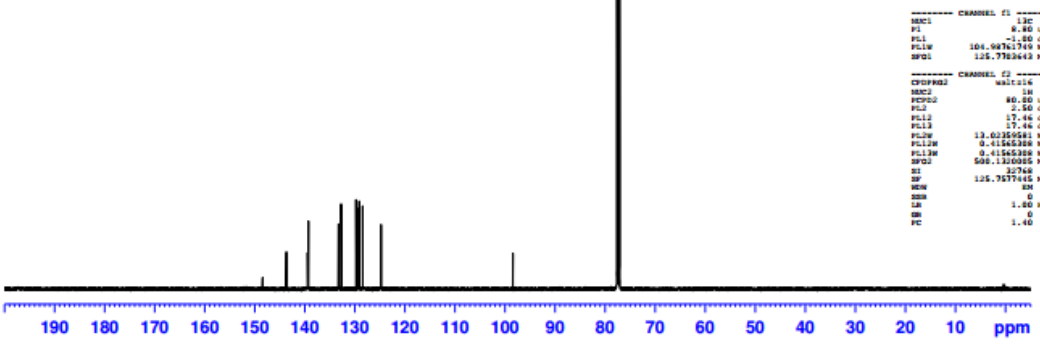


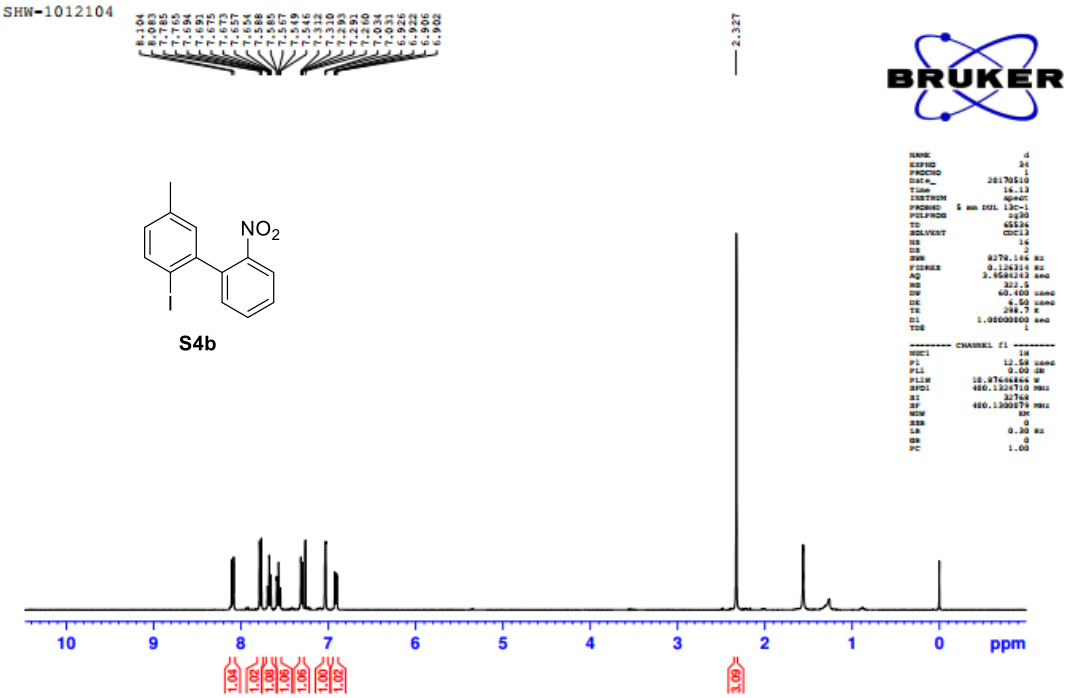
SHW-1012160

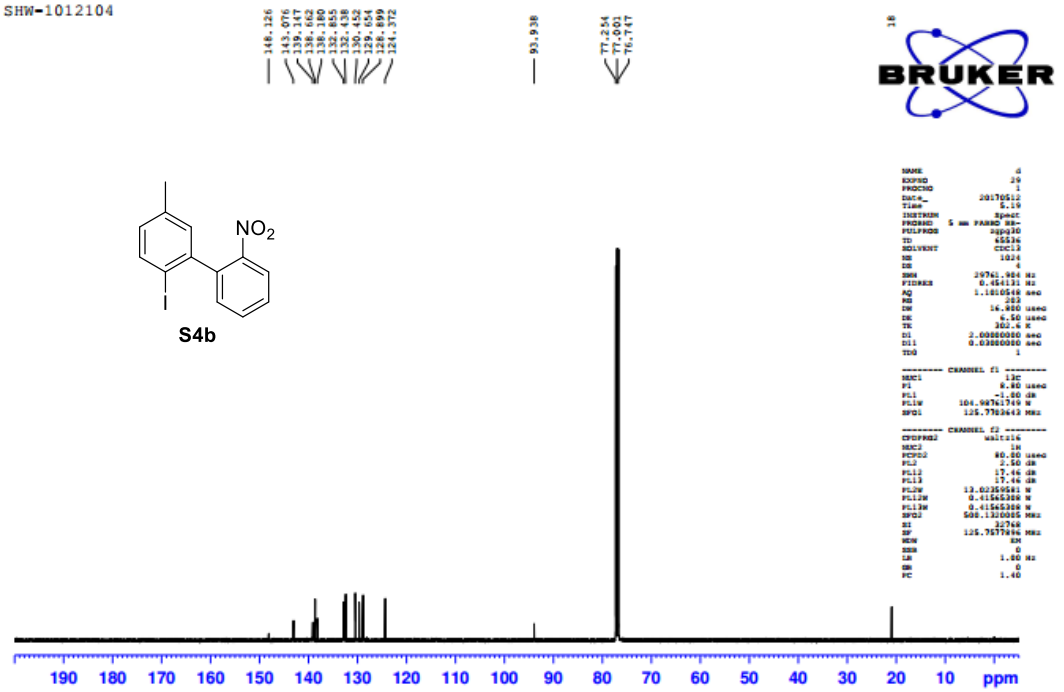


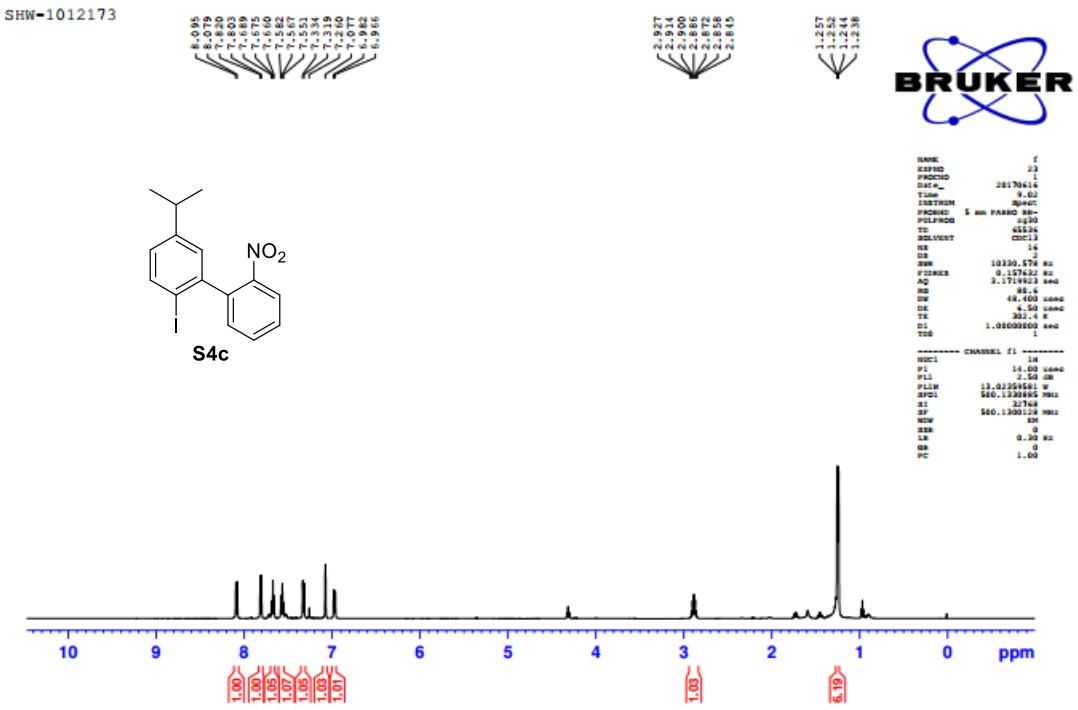
S4a






SHW-1012104
NO2
I
S4b
ppm


SHW-1012104
NO2
I
S4b
ppm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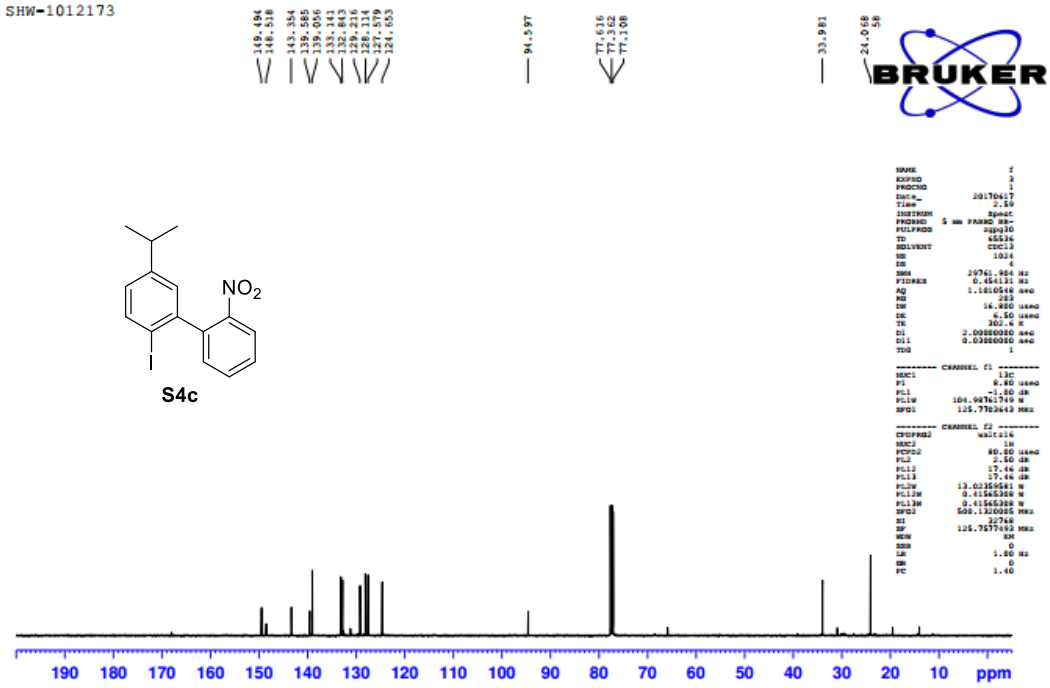
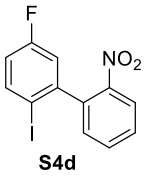
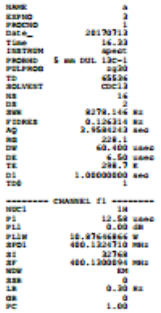
8.079
7.820
7.803
7.689
7.673
7.660
7.582
7.567
7.551
7.334
7.319
7.301
7.077
6.982
6.966
2.927
2.914
2.900
2.886
2.872
2.858
2.845
1.257
1.252
1.244
1.238
BRUKER
NO2
I
S4c
ppm

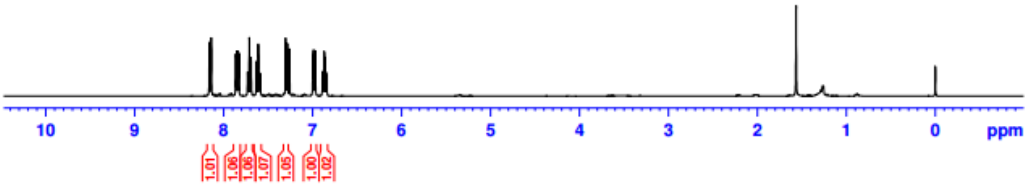

SHW-1012173
149.494
148.518
143.354
139.585
139.066
133.141
132.843
129.216
128.334
127.579
124.653
94.597
77.616
77.302
77.188
33.981
24.068
BRUKER
NO2
I
S4c
ppm

shw-1169412

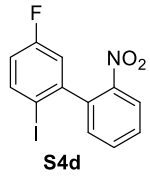


S4d

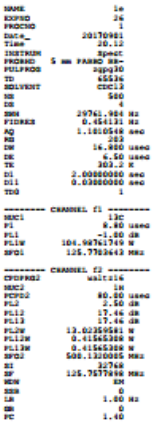


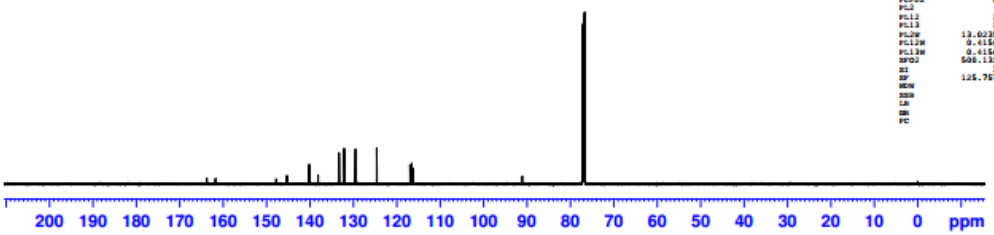


SHW-1169412

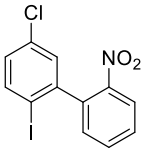


S4d

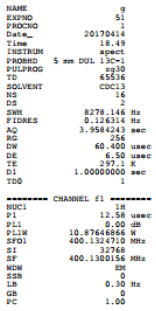


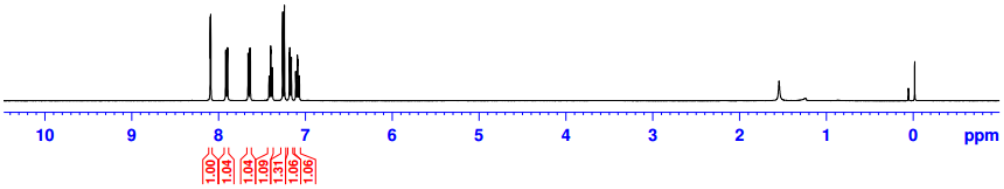


1012064



S4e





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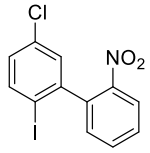
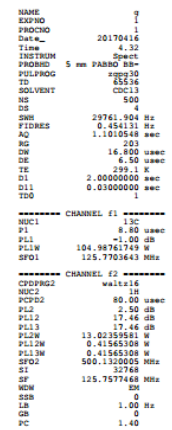
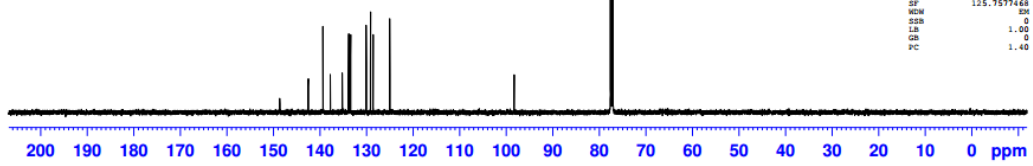
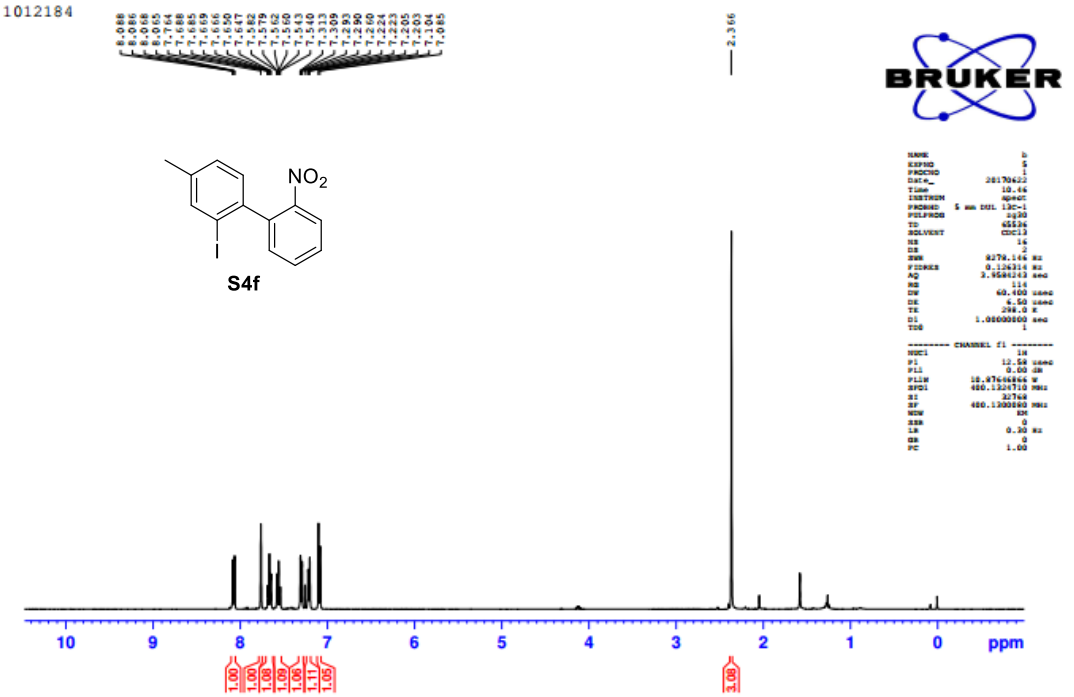
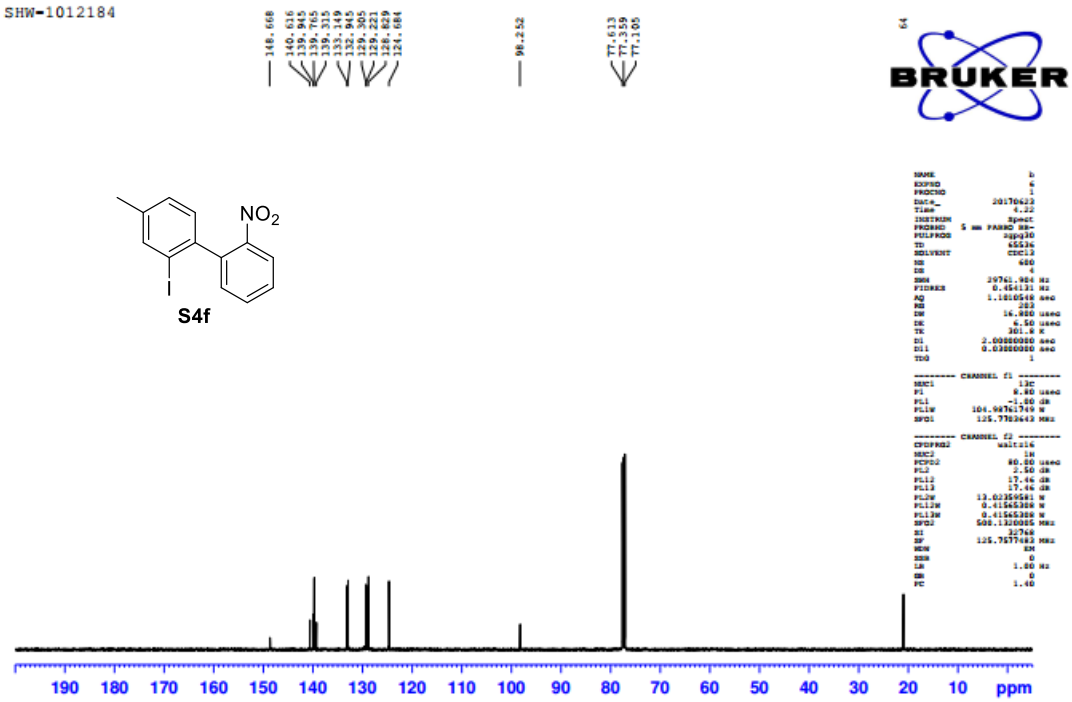


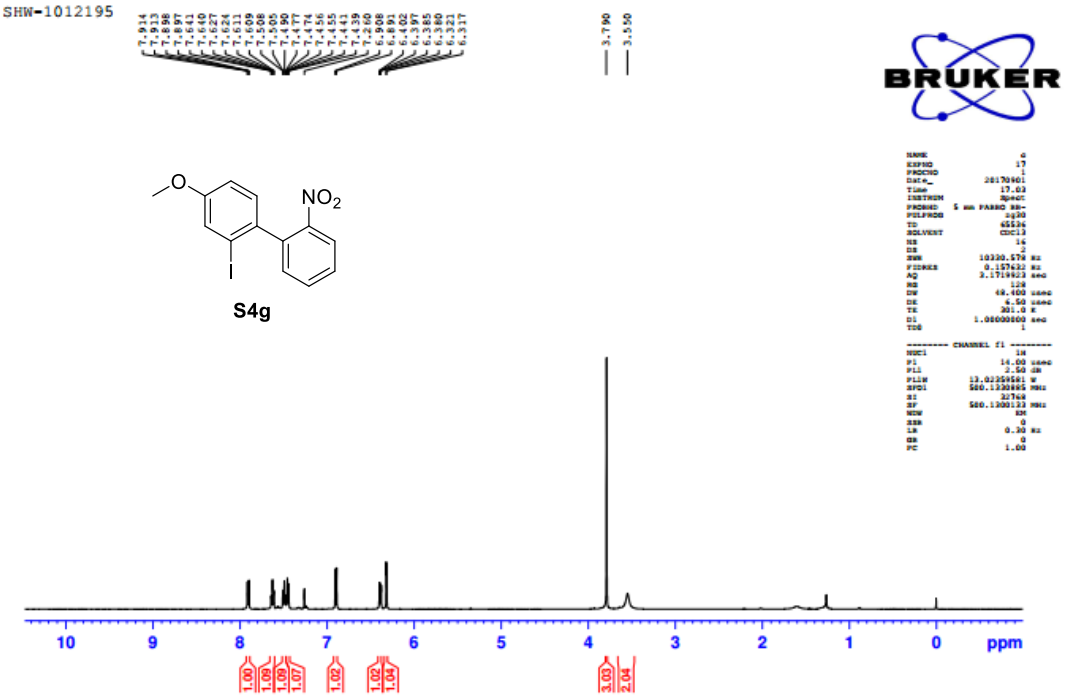
S4e






1012184
NO2
S4f
BRUKER
10
9
8
7
6
5
4
3
2
1
0
ppm


SHW-1012184
NO2
S4f
BRUKER
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


SHW-1012195
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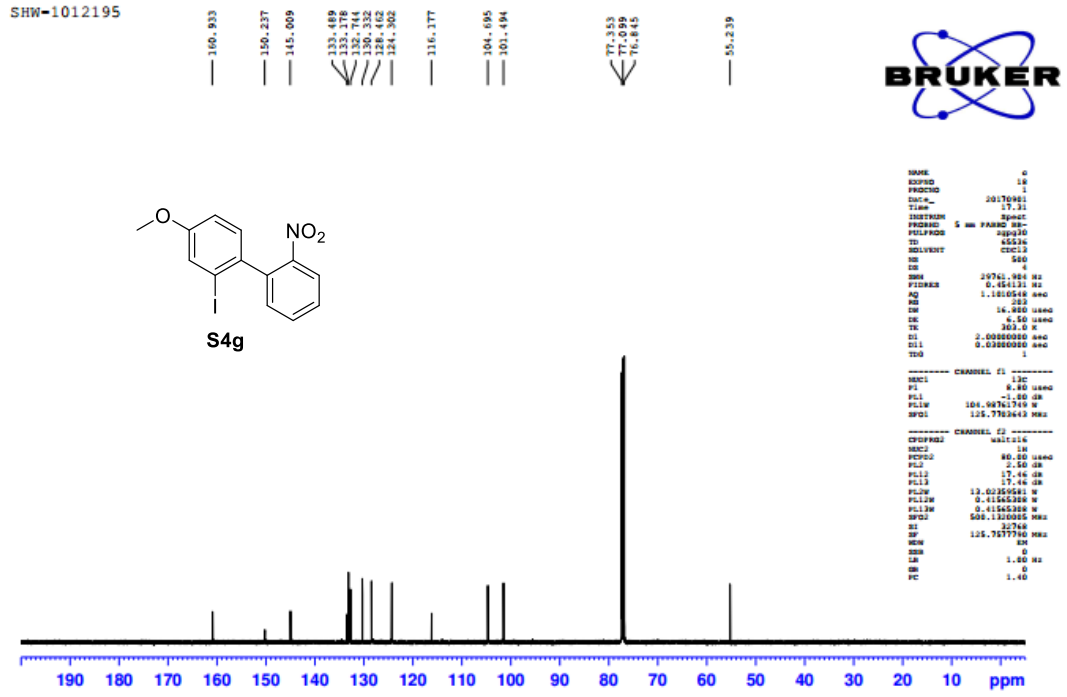
7.913
7.898
7.897
7.641
7.640
7.627
7.624
7.611
7.609
7.508
7.505
7.490
7.477
7.476
7.456
7.455
7.441
7.439
7.260
6.898
6.881
6.402
6.397
6.385
6.380
6.321
6.317
3.790
3.550
BRUKER
O
NO2
I
S4g
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.08
1.09
1.07
1.02
1.02
1.04
3.03
2.04


SHW-1012195
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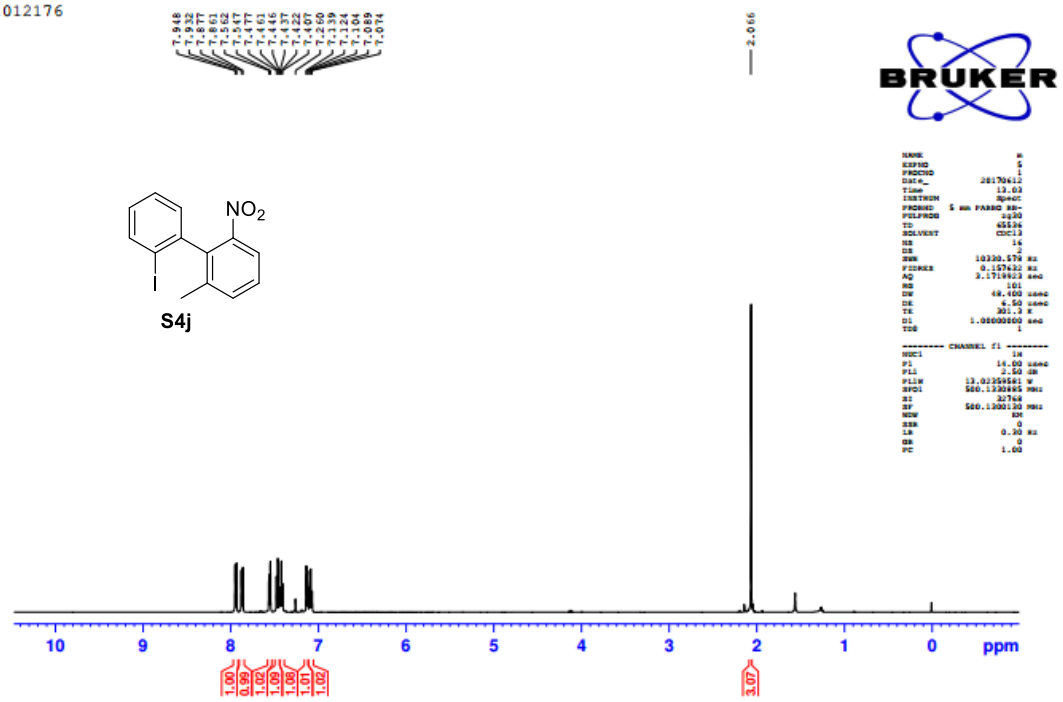
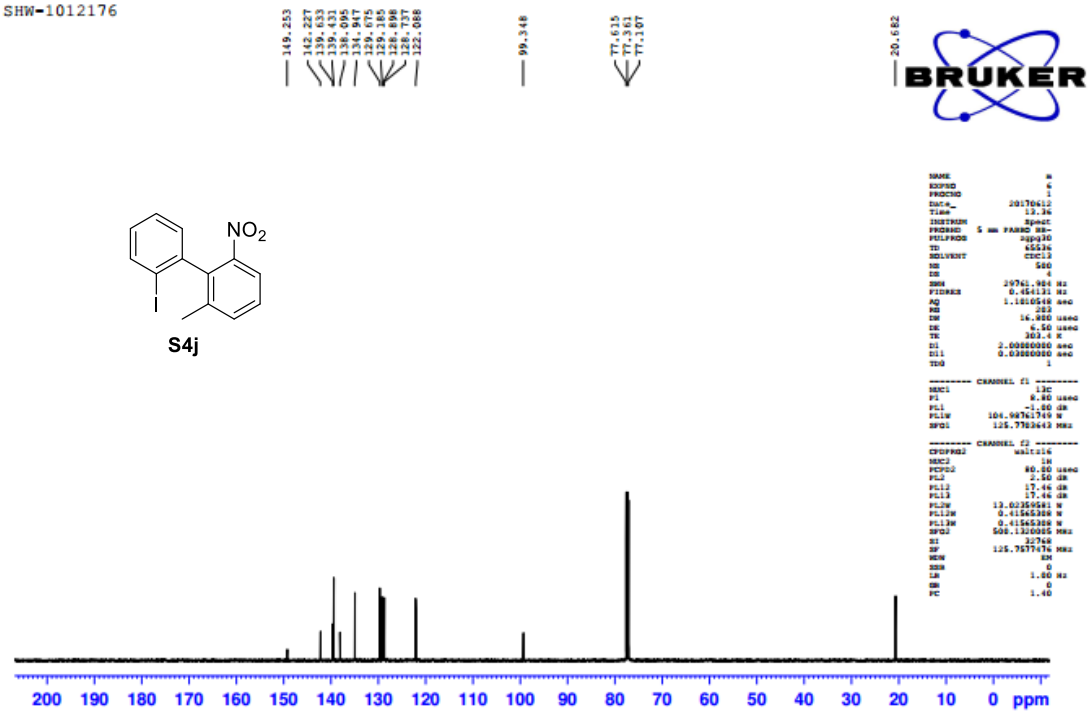
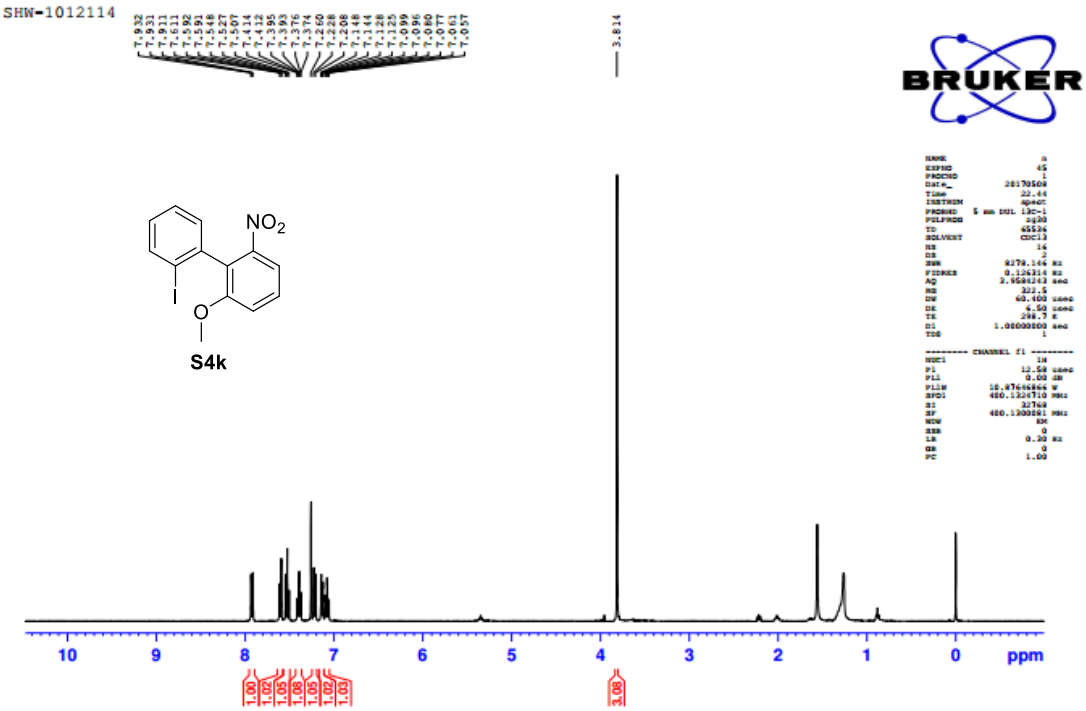
150.237
145.009
133.489
133.178
132.744
130.332
126.468
124.902
116.177
104.695
101.494
77.353
77.099
76.845
55.239
BRUKER
O
NO2
I
S4g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

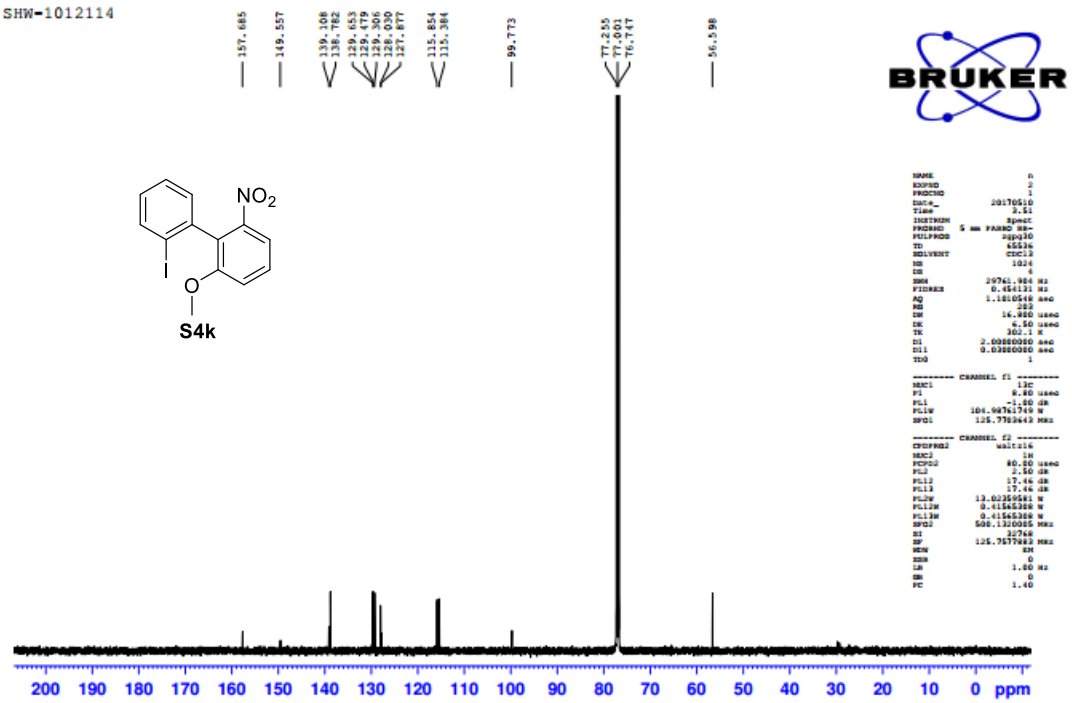
1012176

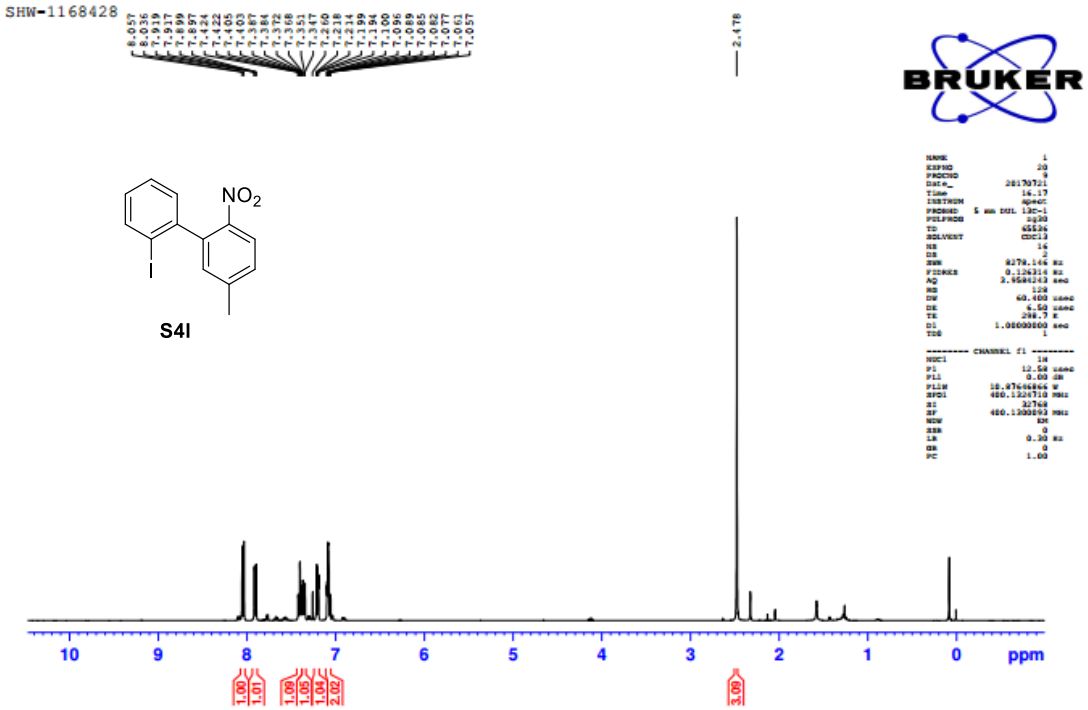


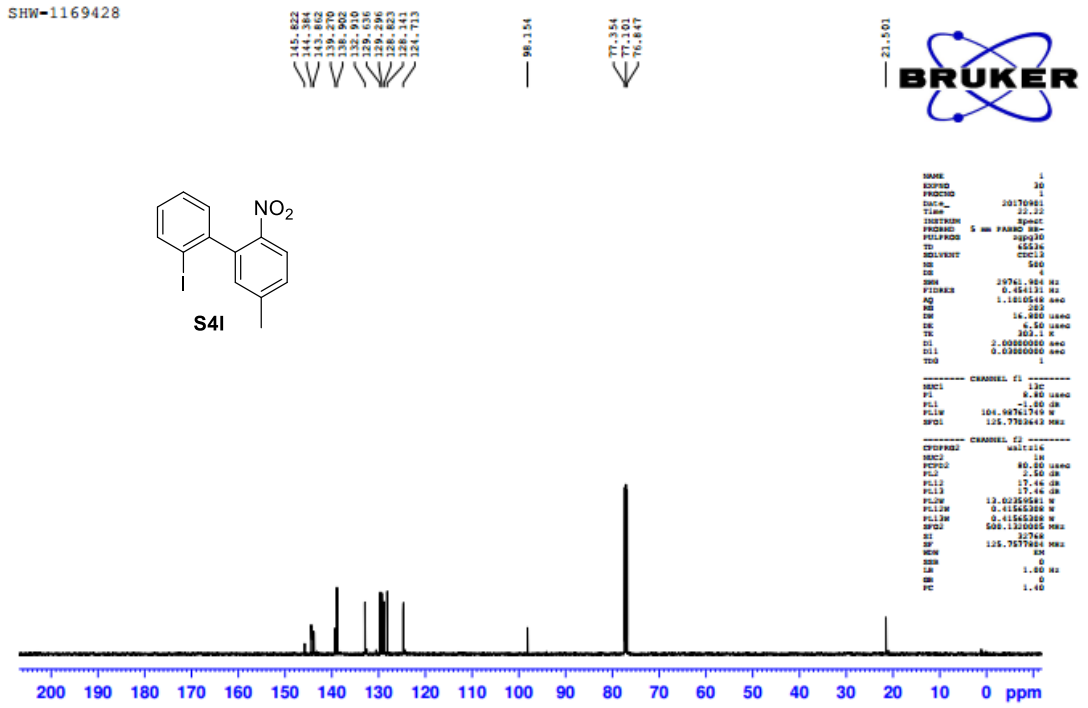
SHW-1012176



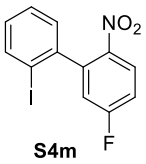

SHW-1012114
NO2
I
O
S4k
ppm

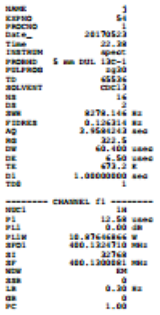

SHW-1012114
NO2
I
O
S4k
ppm

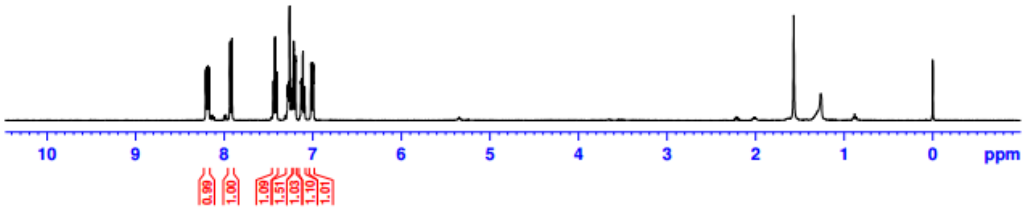

SHW-1168428
NO2
I
S4l
2.478
BRUKER
10
9
8
7
6
5
4
3
2
1
0
ppm


SHW-1169428
NO2
I
S4l
98.154
77.354
77.101
76.847
21.501
BRUKER
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

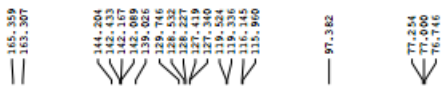
SHW-1012115

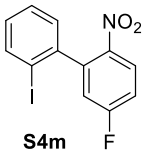


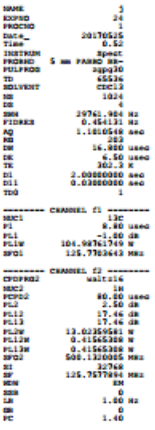


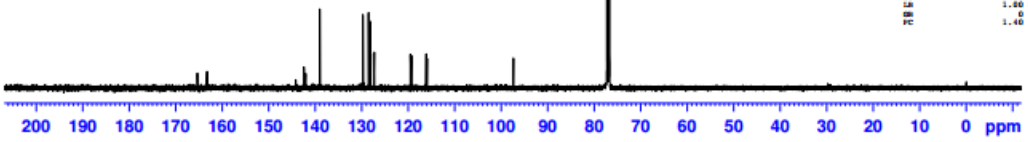


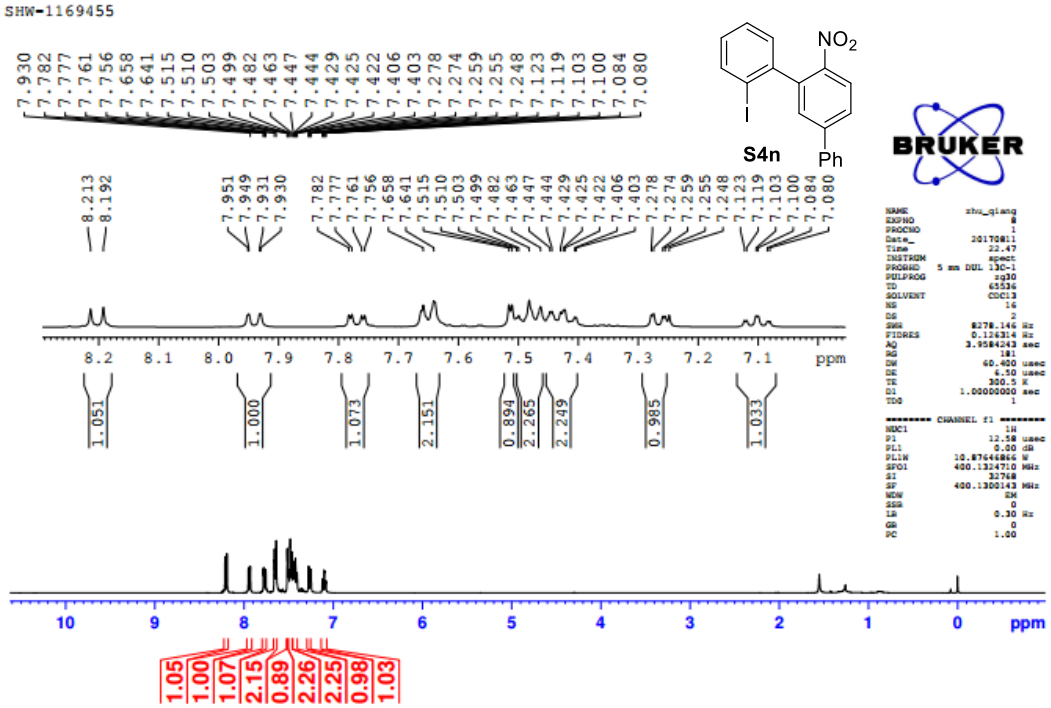
SHW-1012115

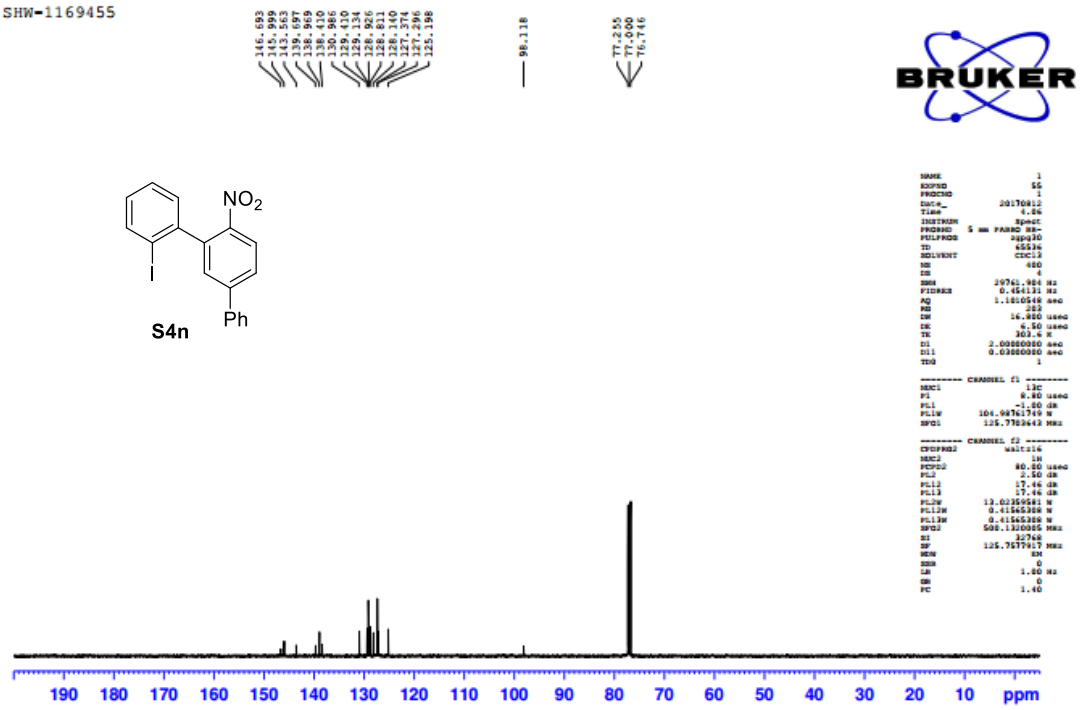




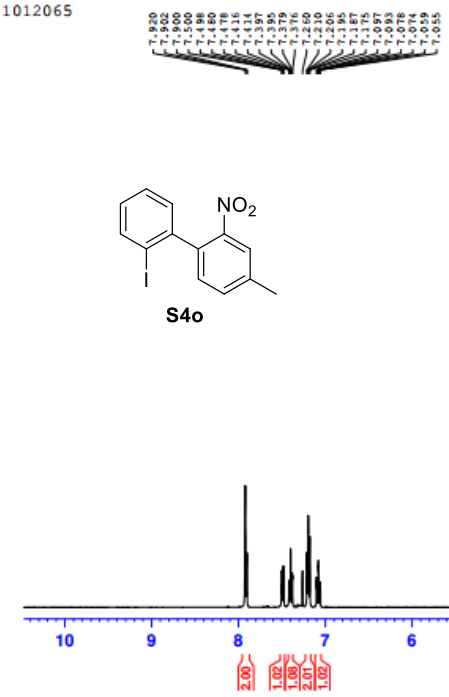




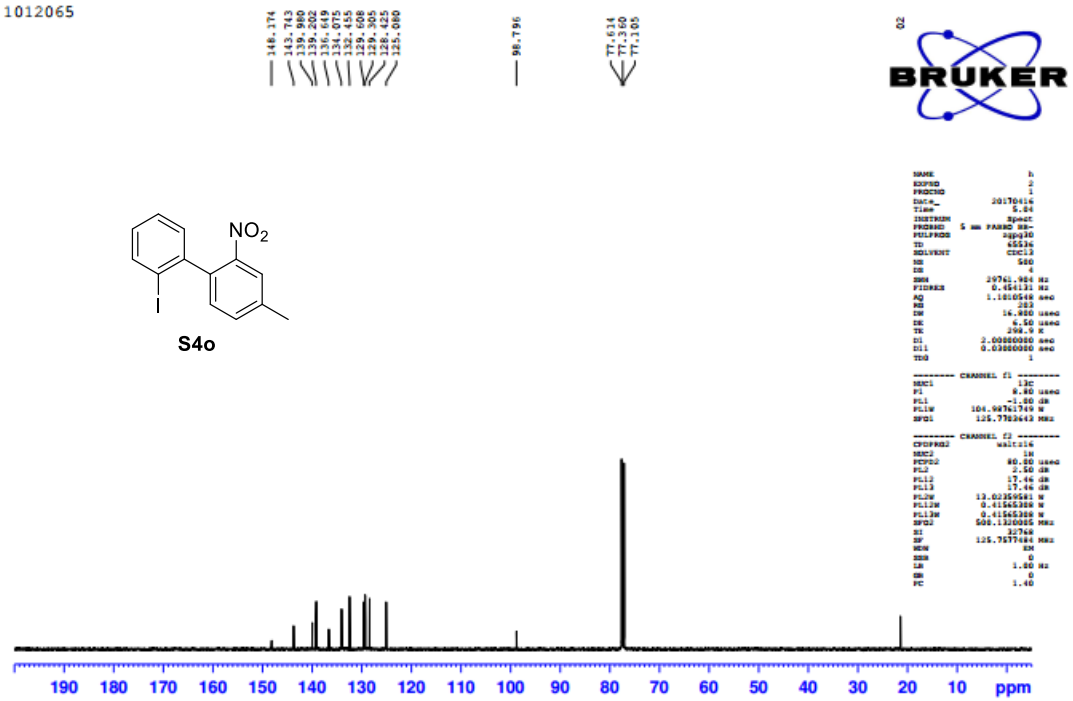

SHW-1169455
S4n
BRUKER
ppm


SHW-1169455
S4n
BRUKER
ppm

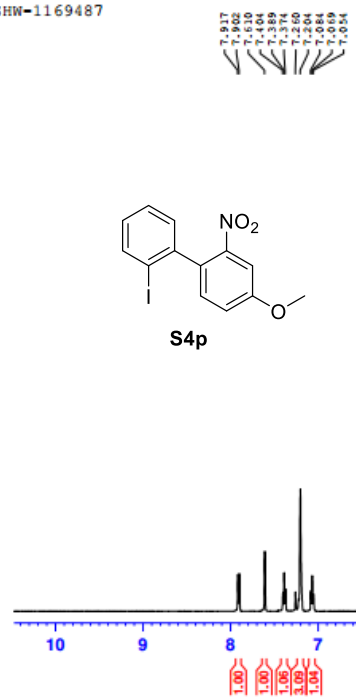
1012065



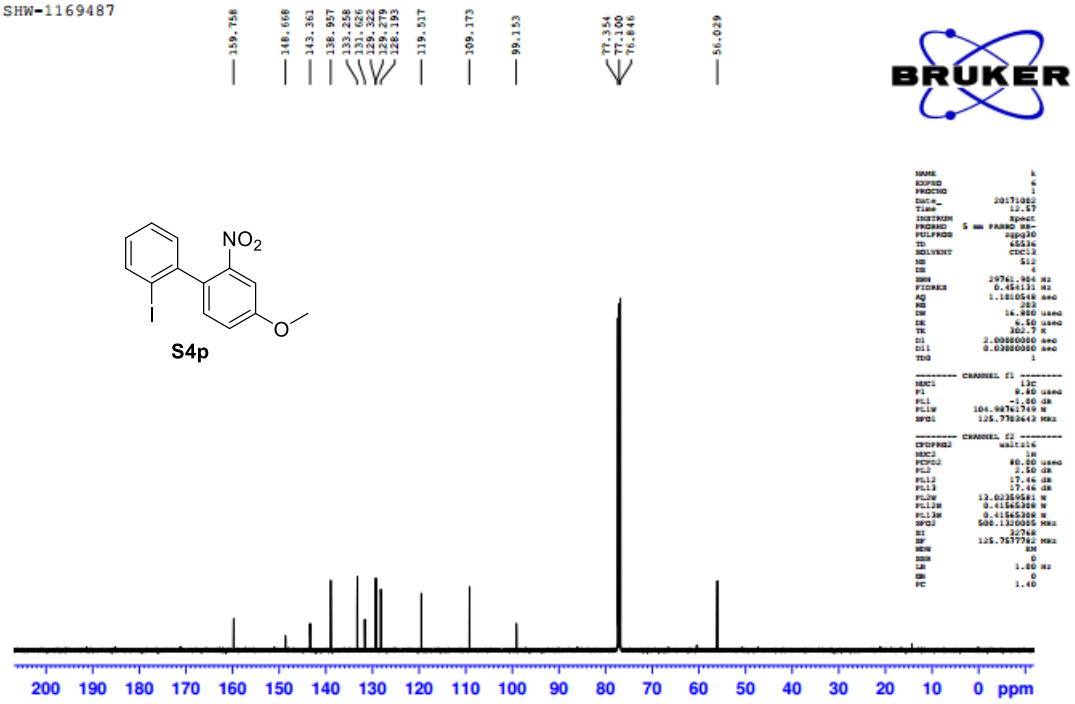
1012065



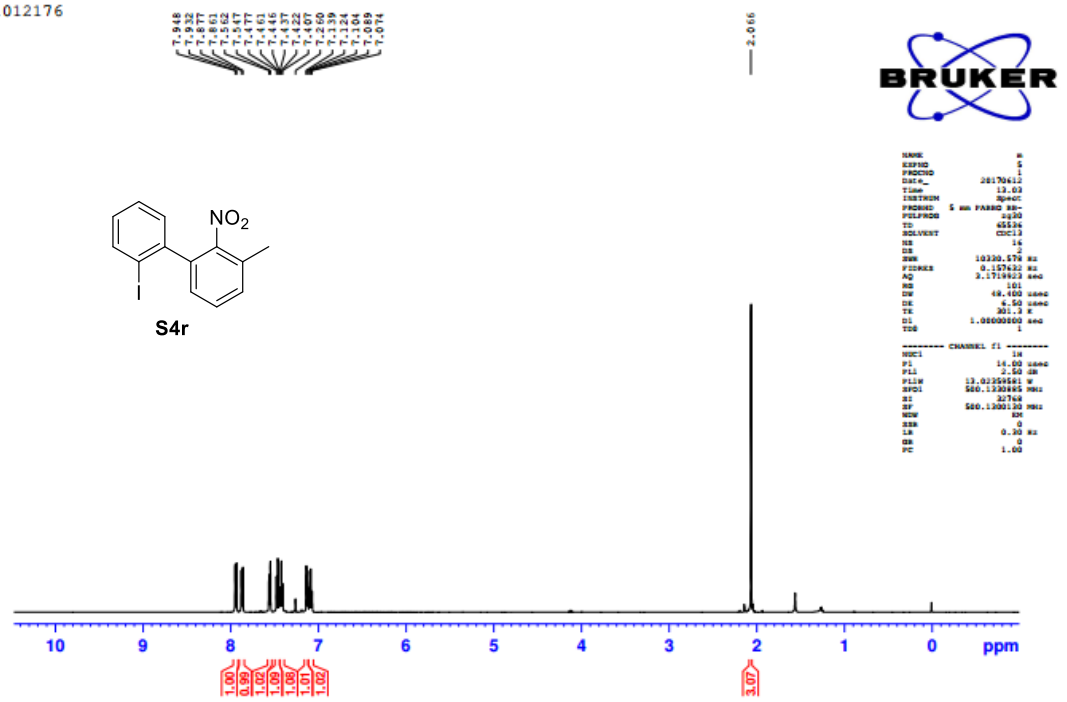
SHW-1169487



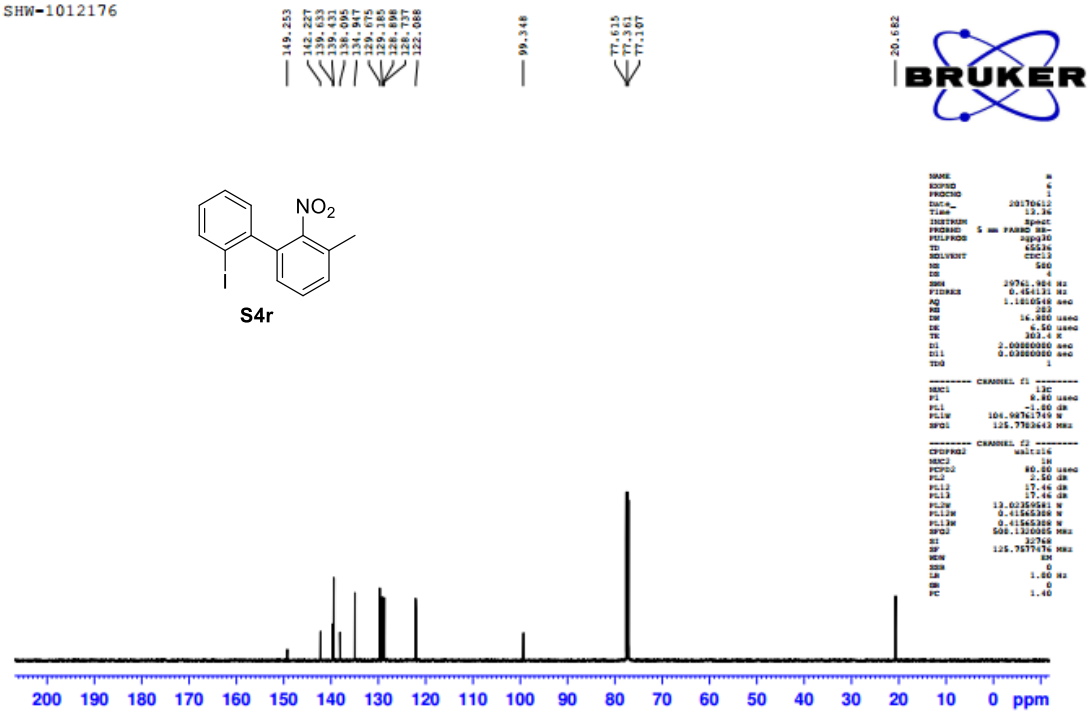
SHW-1169487

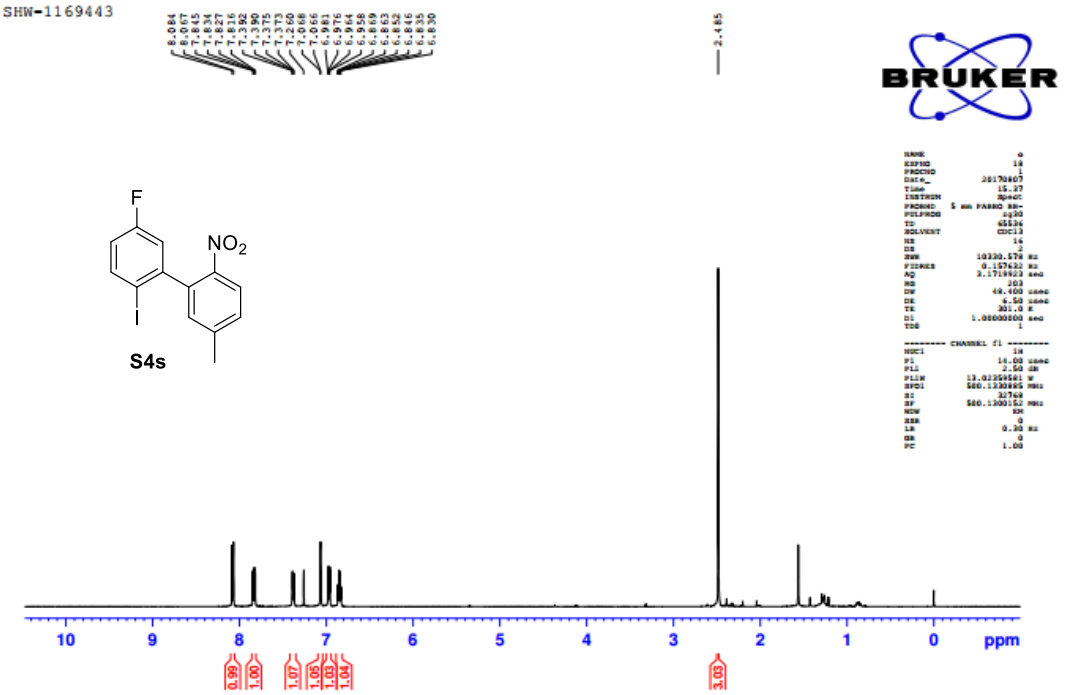


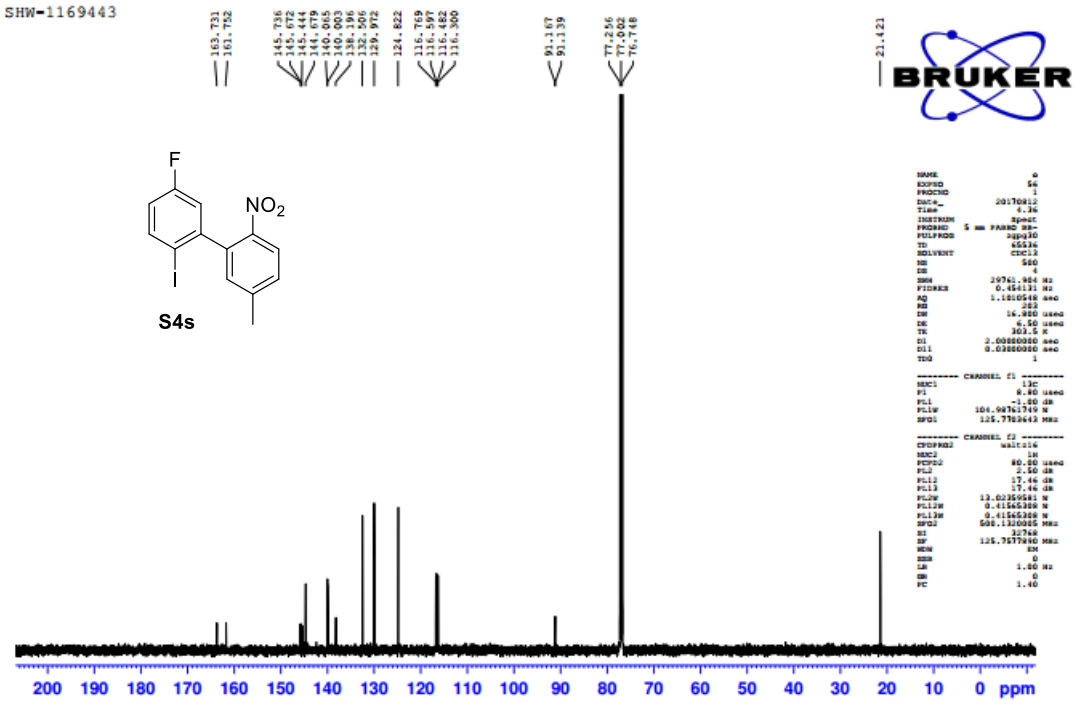
1012176

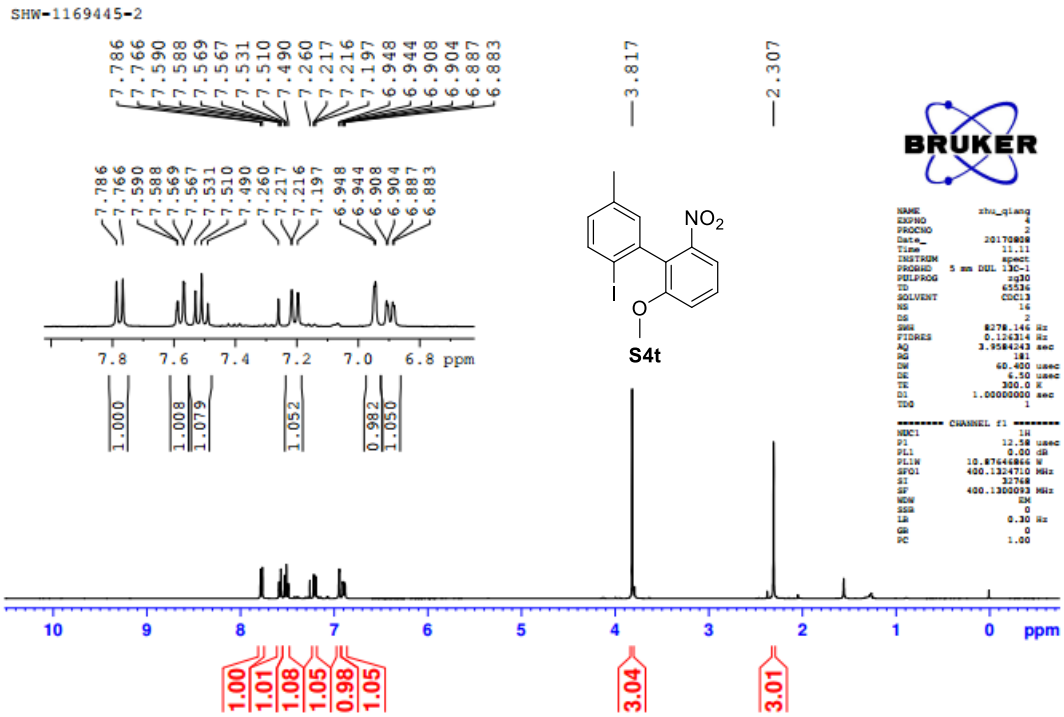


SHW-1012176




SHW-1169443
F
NO2
I
S4s
ppm


SHW-1169443
F
NO2
I
S4s
ppm


SHW-1169445-2
7.786
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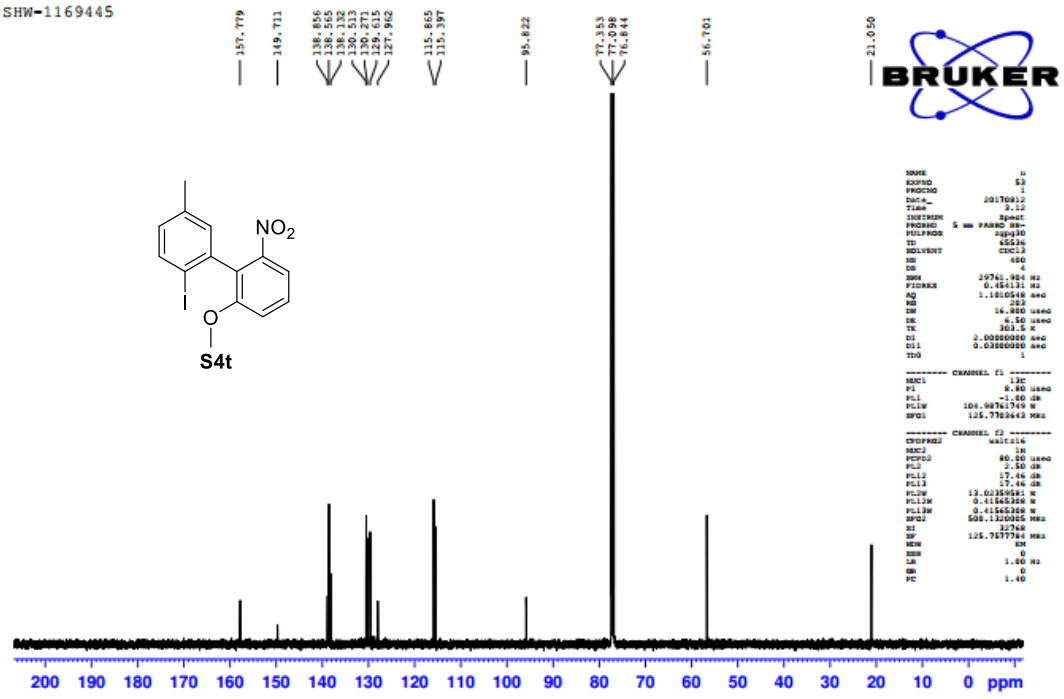
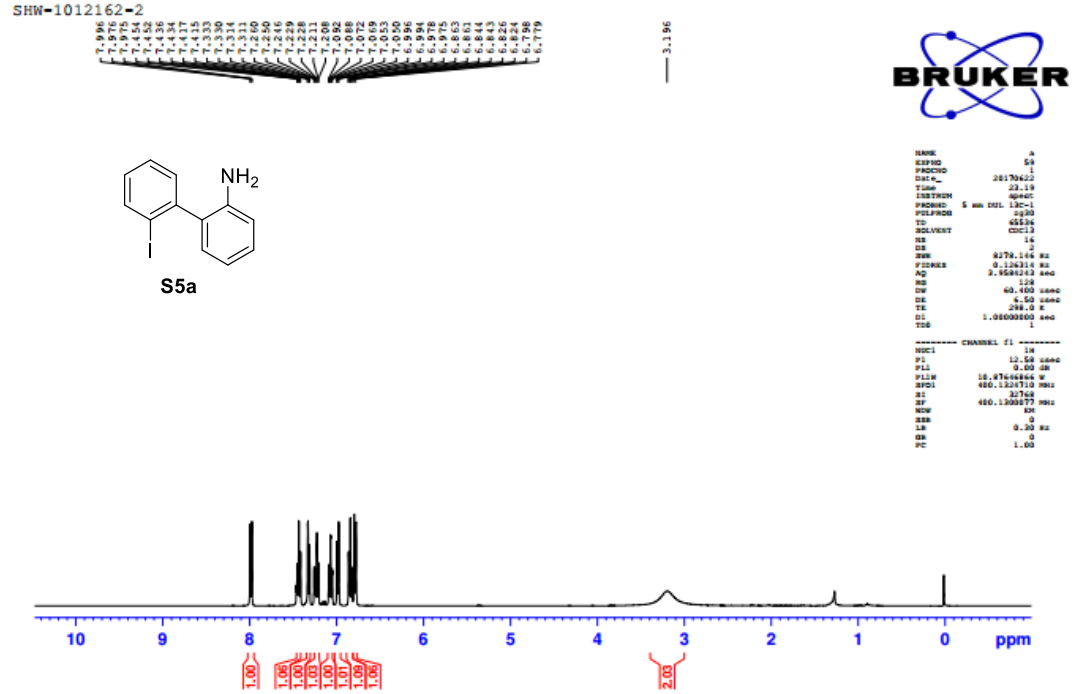
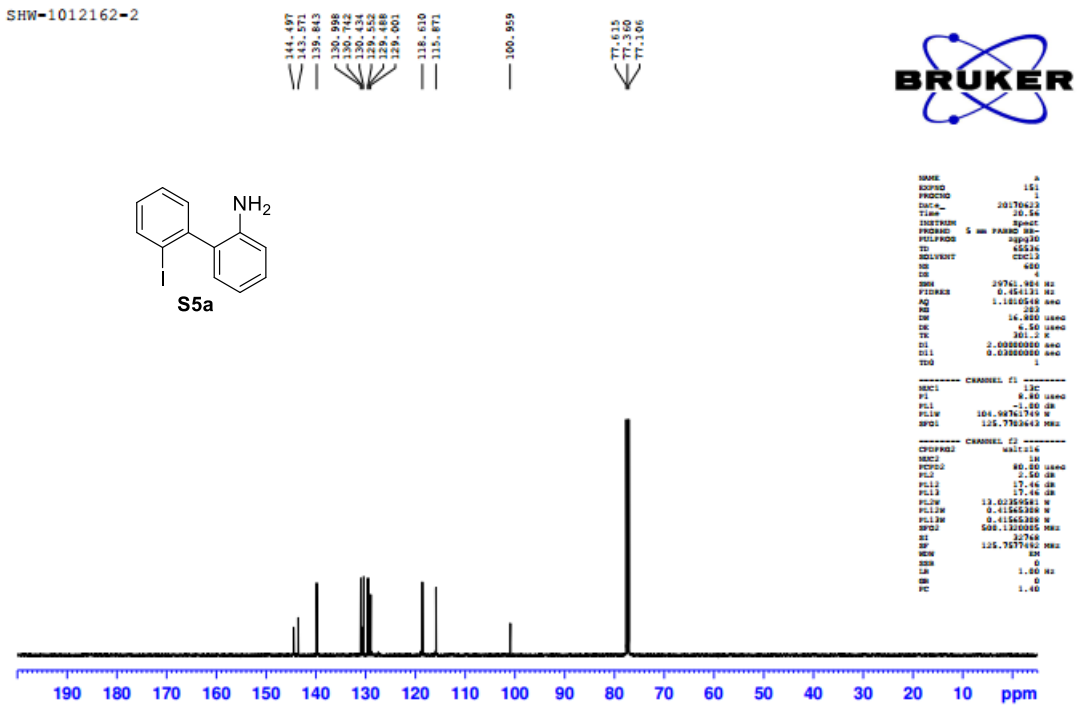
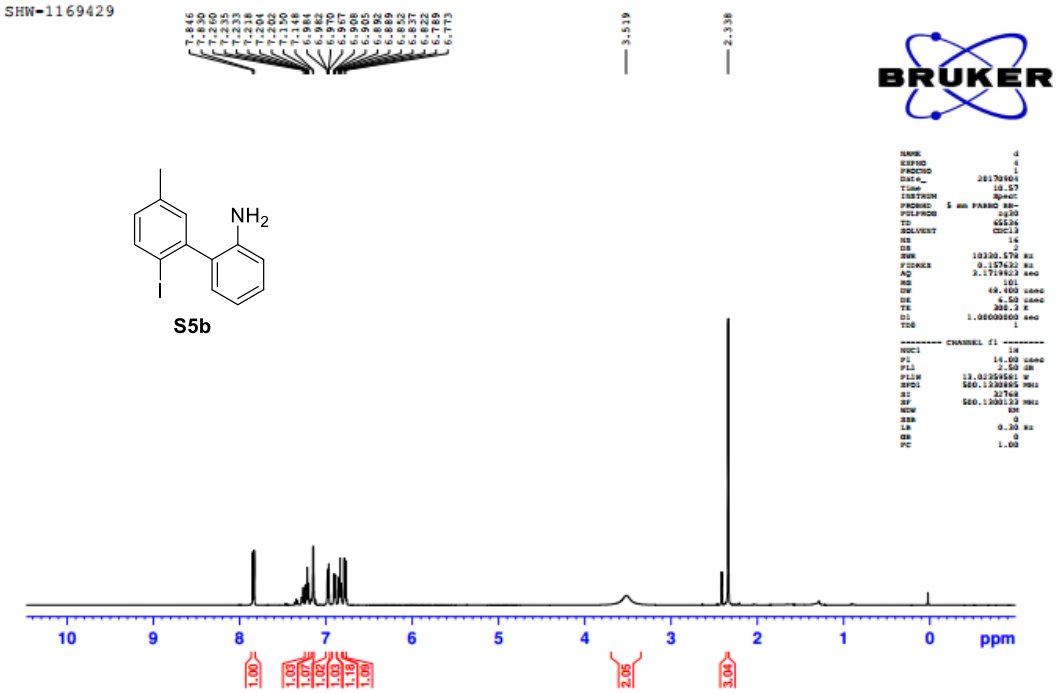
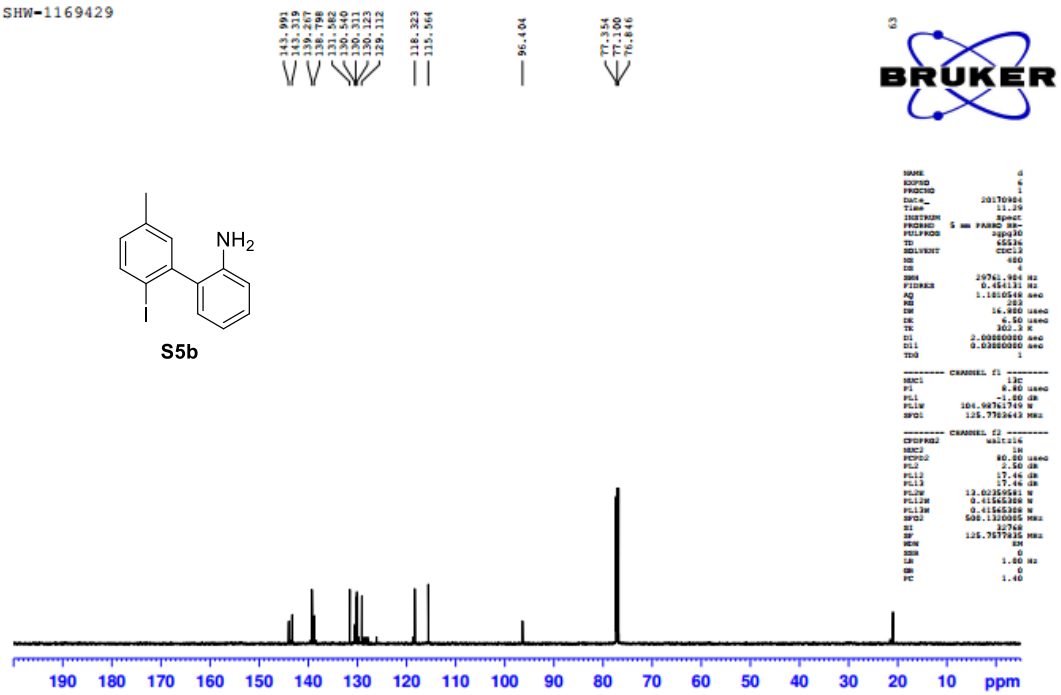
7.590
7.588
7.569
7.567
7.531
7.510
7.490
7.260
7.217
7.216
7.197
6.948
6.944
6.908
6.904
6.887
6.883
3.817
2.307
NO2
I
O
S4t
BRUKER
7.8
7.6
7.4
7.2
7.0
6.8 ppm
1.000
1.008
1.079
1.052
0.982
1.050
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.08
1.05
0.98
1.05
3.04
3.01

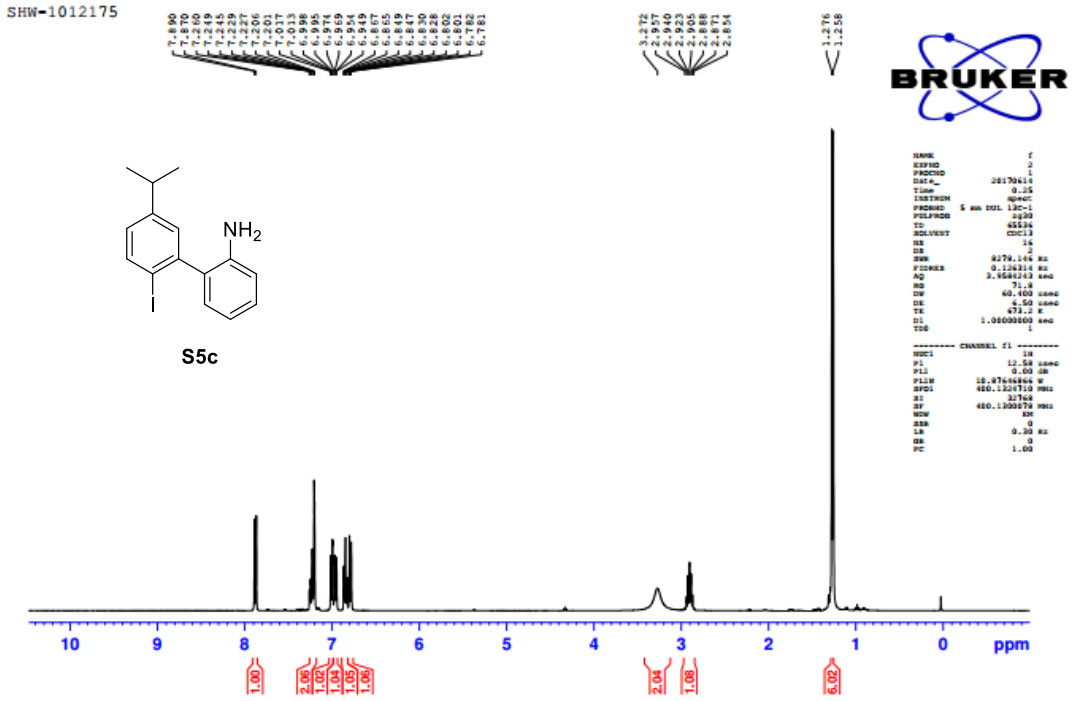

SHW-1169445
157.779
149.711
138.856
138.565
138.132
130.513
130.271
129.515
127.962
115.865
115.397
95.822
77.353
77.098
76.844
56.701
21.050
NO2
I
O
S4t
BRUKER
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

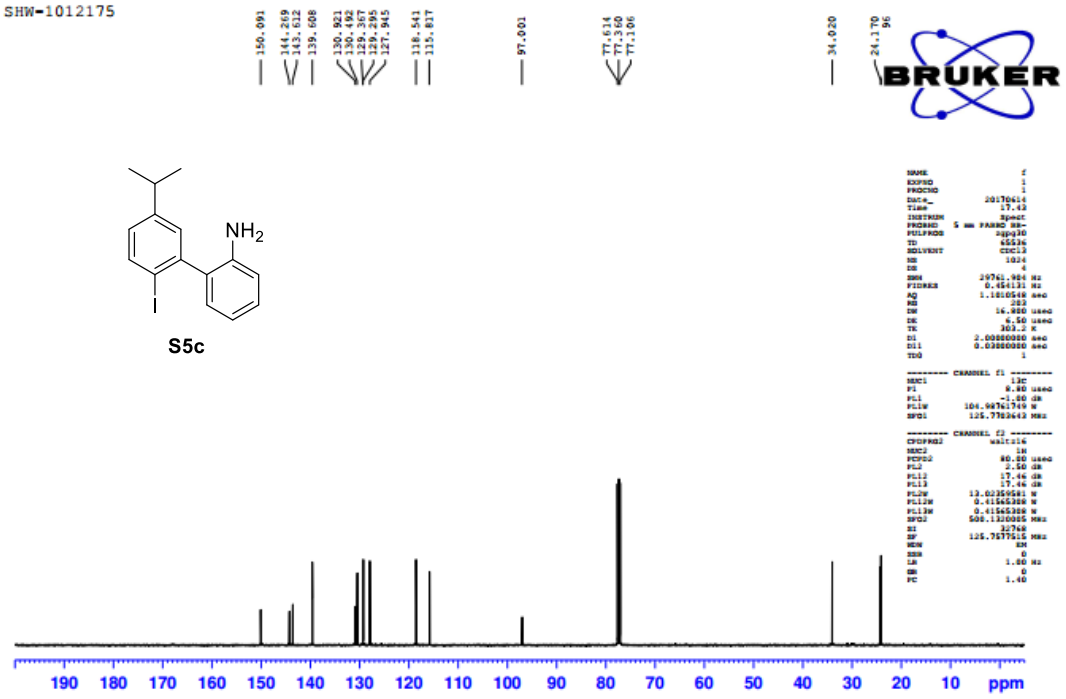

SHW-1012162-2
NH2
I
S5a
10
9
8
7
6
5
4
3
2
1
0
ppm


SHW-1012162-2
NH2
I
S5a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

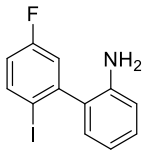

SHW-1169429
7.846
7.840
7.260
7.235
7.233
7.218
7.204
7.200
7.150
7.148
6.984
6.982
6.970
6.967
6.908
6.905
6.892
6.889
6.852
6.837
6.822
6.789
6.773
3.539
2.338
BRUKER
NH2
I
S5b
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
1.07
1.02
1.03
1.18
1.09
2.05
3.04


SHW-1169429
143.991
143.339
139.267
136.798
131.582
130.560
130.311
130.123
129.132
118.323
115.564
96.404
77.354
77.100
76.846
BRUKER
NH2
I
S5b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

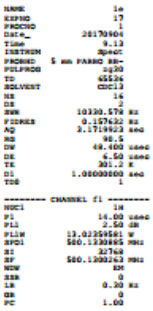

SHW-1012175
BRUKER
NH2
I
S5c
ppm

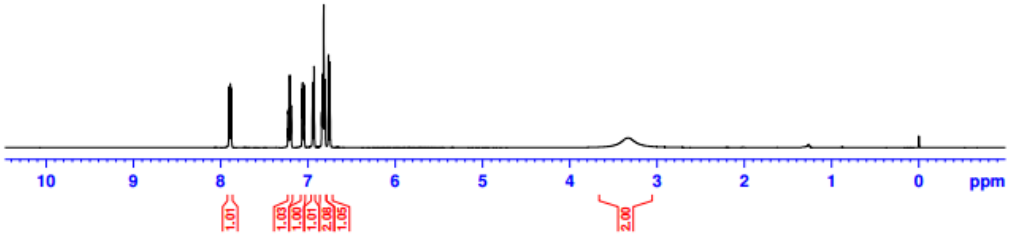

SHW-1012175
BRUKER
NH2
I
S5c
ppm

SHW-1169414

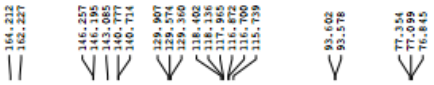


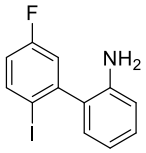
S5d



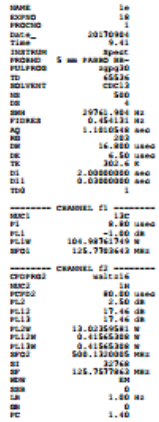


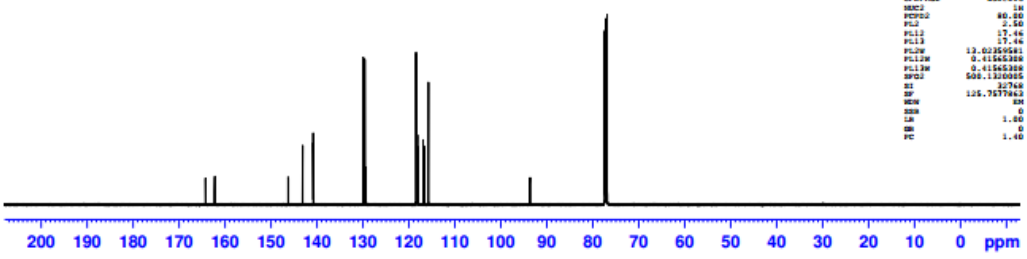
SHW-1169414



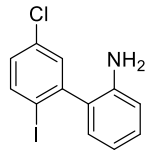


S5d



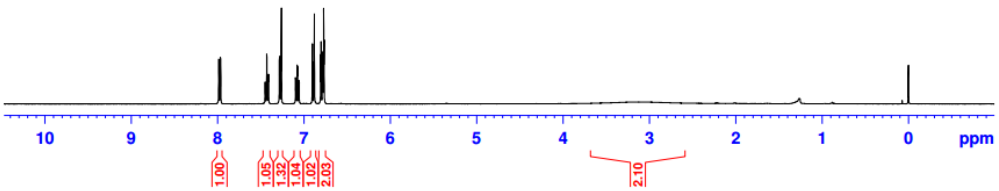


1012066

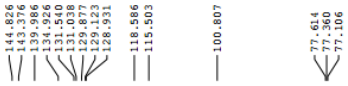


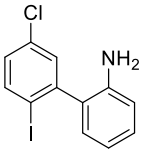
S5e

```
NAME                  g
EXPNO                53
PROCNO                1
Date_          20170414
Time              18.59
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.9584243 sec
RG                 256
DW               60.400 usec
DE                6.50 usec
TE              297.0 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                12.58 usec
PL1                0.00 dB
PL1W        10.87644866 W
SFO1        400.1324710 MHz
SI                32768
SF          400.1300083 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



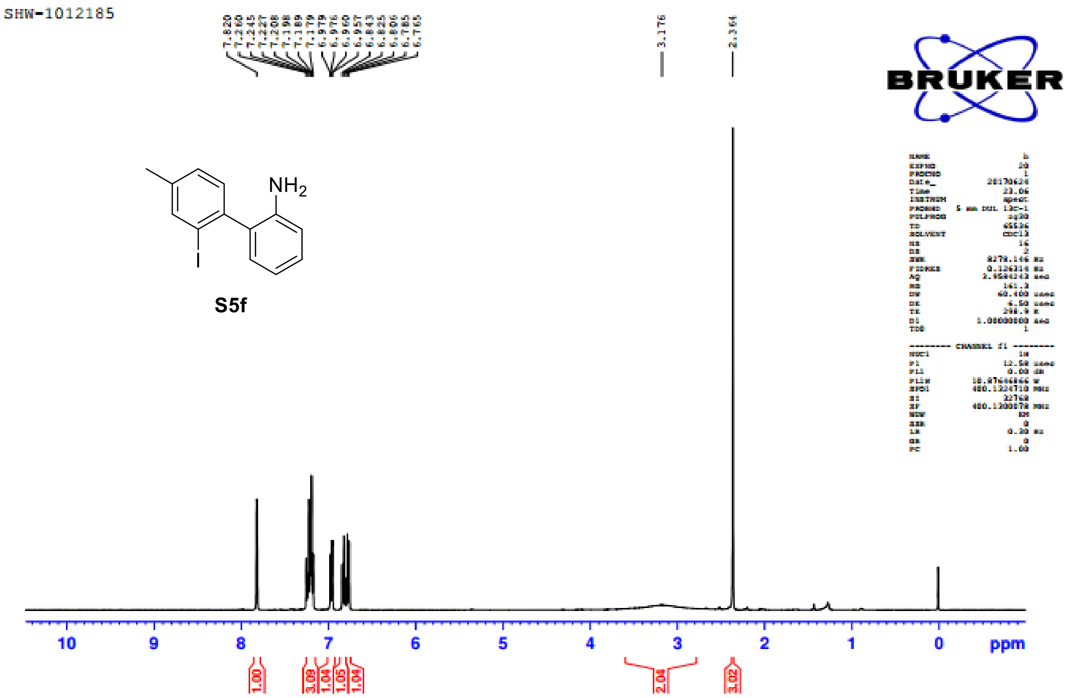
1012066

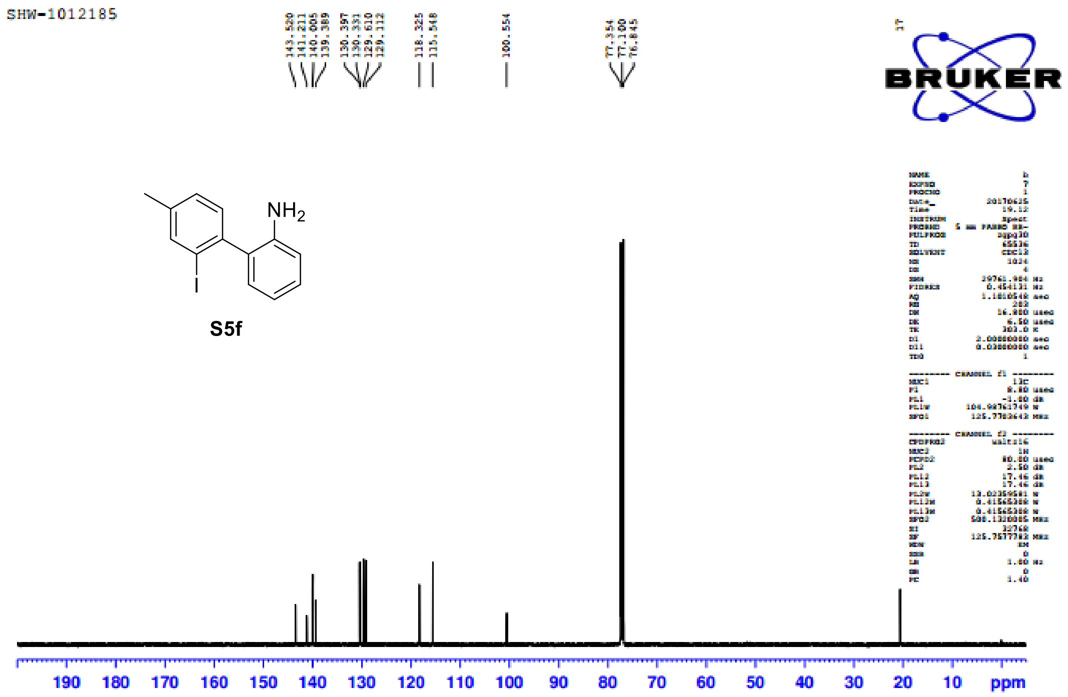


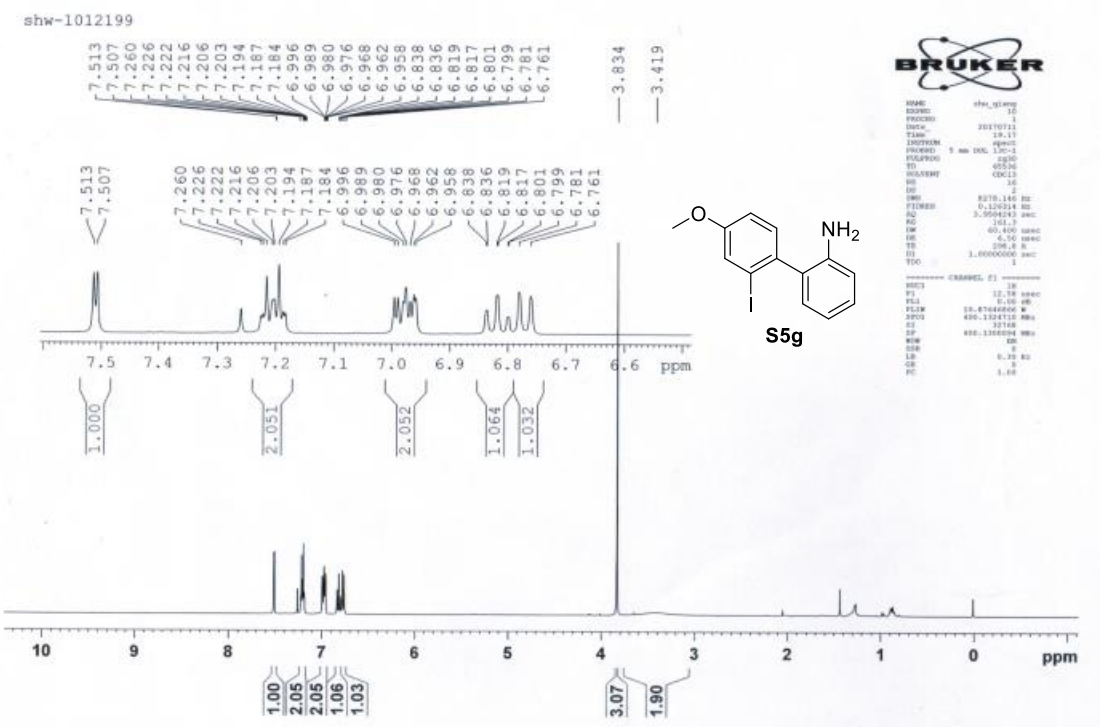


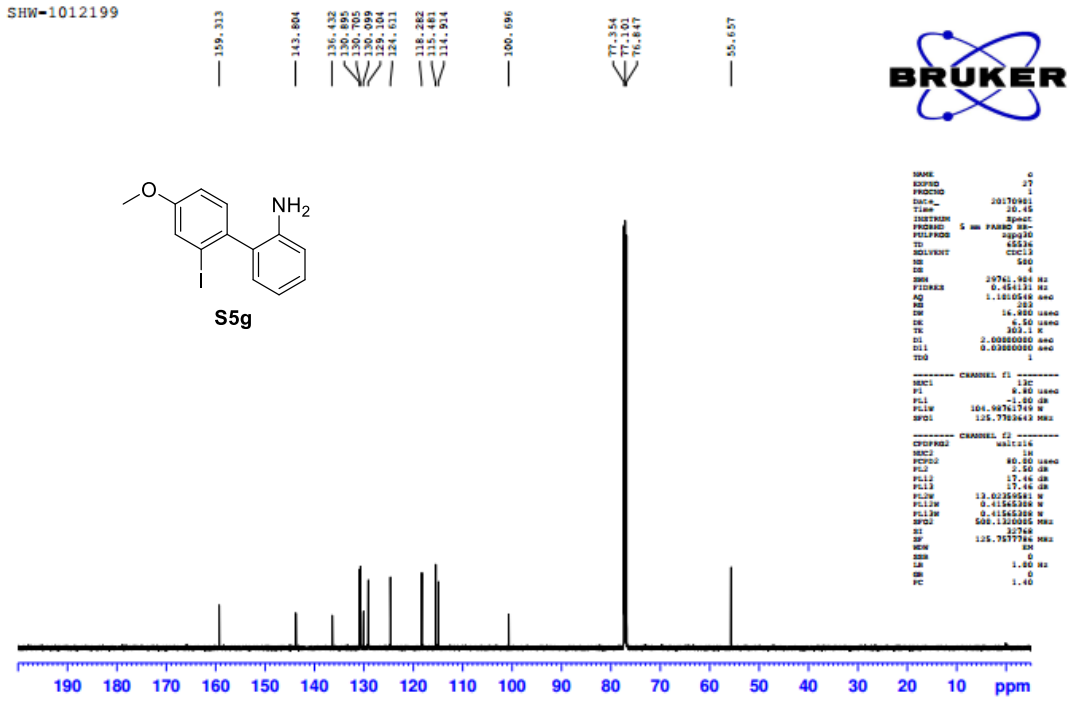
S5e

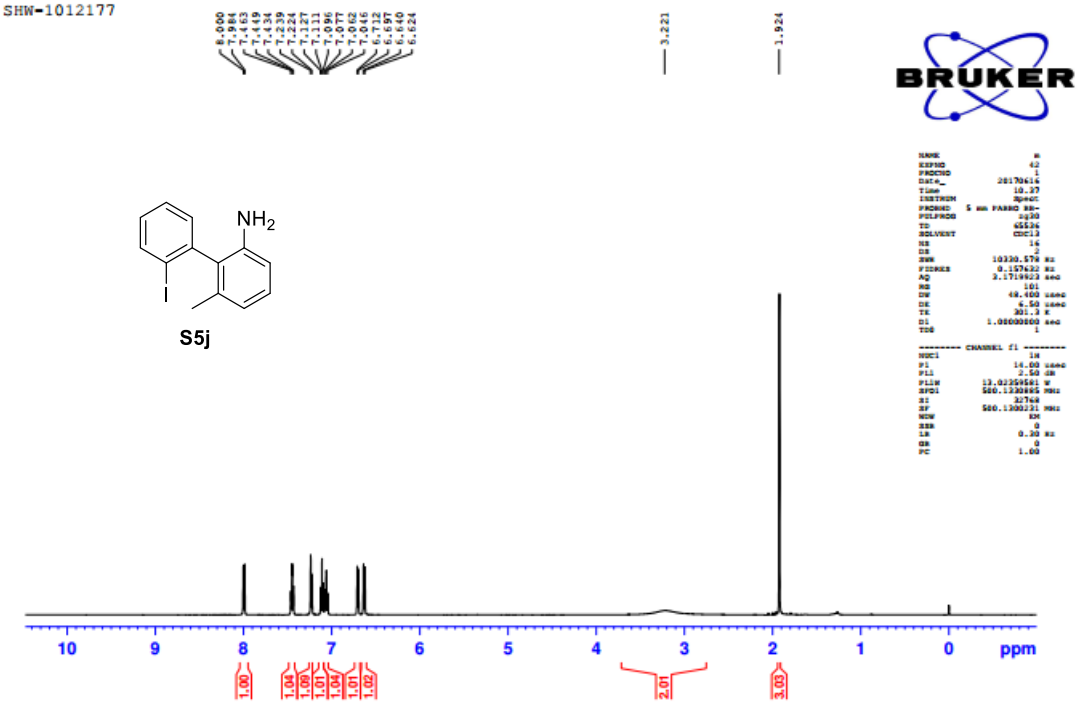
```
NAME                  g
EXPNO                 3
PROCNO                1
Date_          20170416
Time              5.35
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD               65536
SOLVENT          CDCl3
NS                  500
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG                  203
DW               16.800 usec
DE                6.50 usec
TE              298.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                8.80 usec
PL1               +1.00 dB
PL1W       104.98761749 W
SFO1       125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               2.50 dB
PL12              17.46 dB
PL13              17.46 dB
PL2W       13.02359581 W
PL12W       0.41565308 W
PL13W       0.41565308 W
SFO2       500.1320005 MHz
SI                32768
SF         125.7577466 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

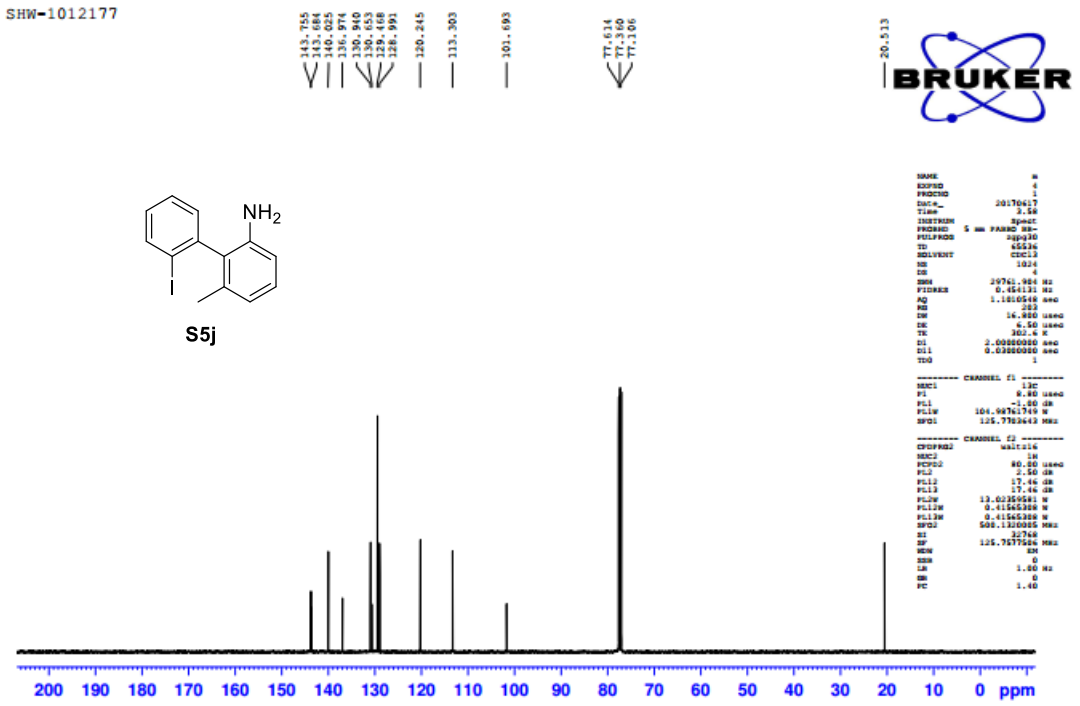

SHW-1012185
NH2
I
S5f
ppm

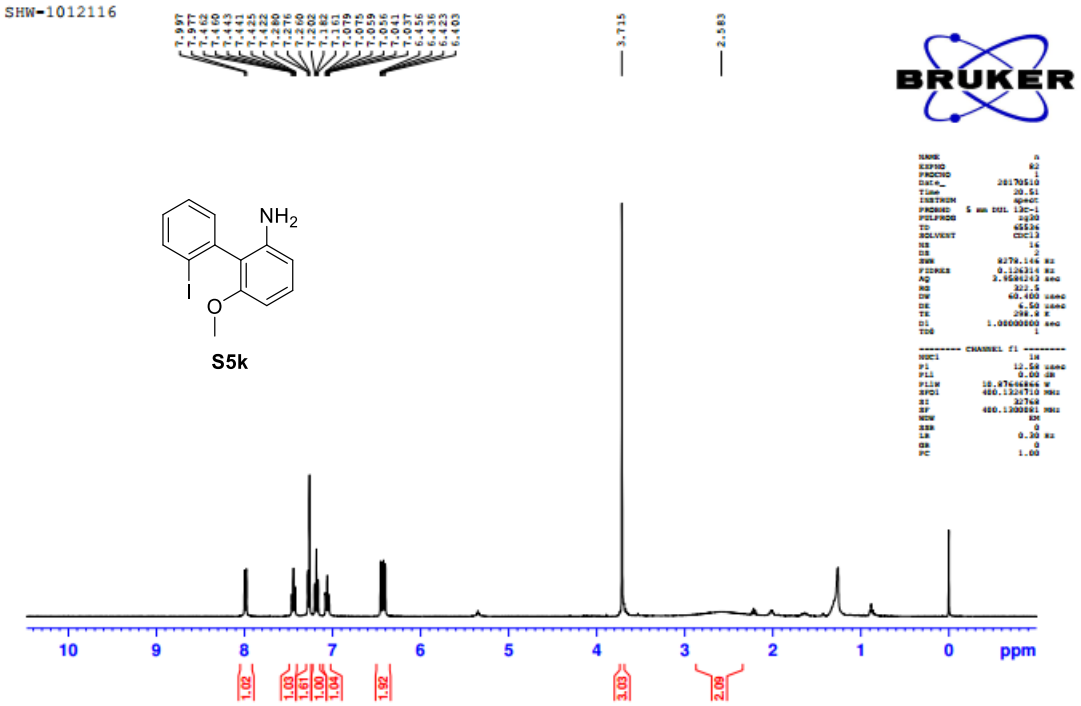

SHW-1012185
NH2
I
S5f
ppm

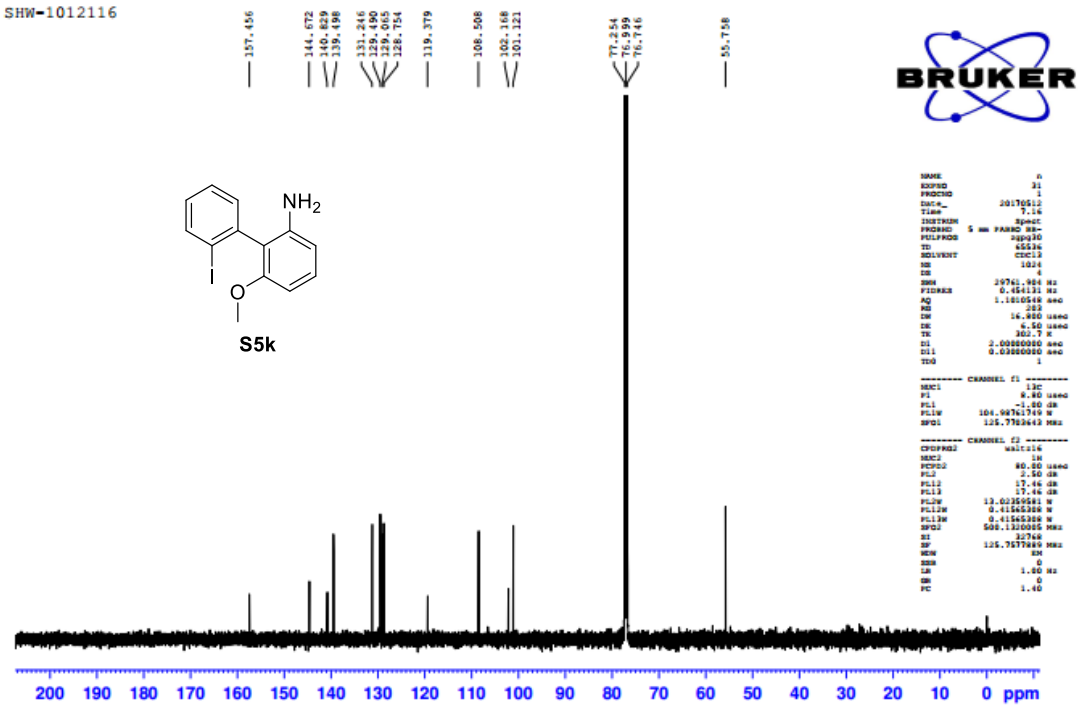

shw-1012199
BRUKER
7.513
7.507
7.260
7.226
7.222
7.216
7.206
7.203
7.194
7.187
7.184
6.996
6.989
6.980
6.976
6.968
6.962
6.958
6.838
6.836
6.819
6.817
6.801
6.799
6.781
6.761
3.834
3.419
O
NH2
I
S5g
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
ppm
1.000
2.051
2.052
1.064
1.032
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.05
2.05
1.06
1.03
3.07
1.90

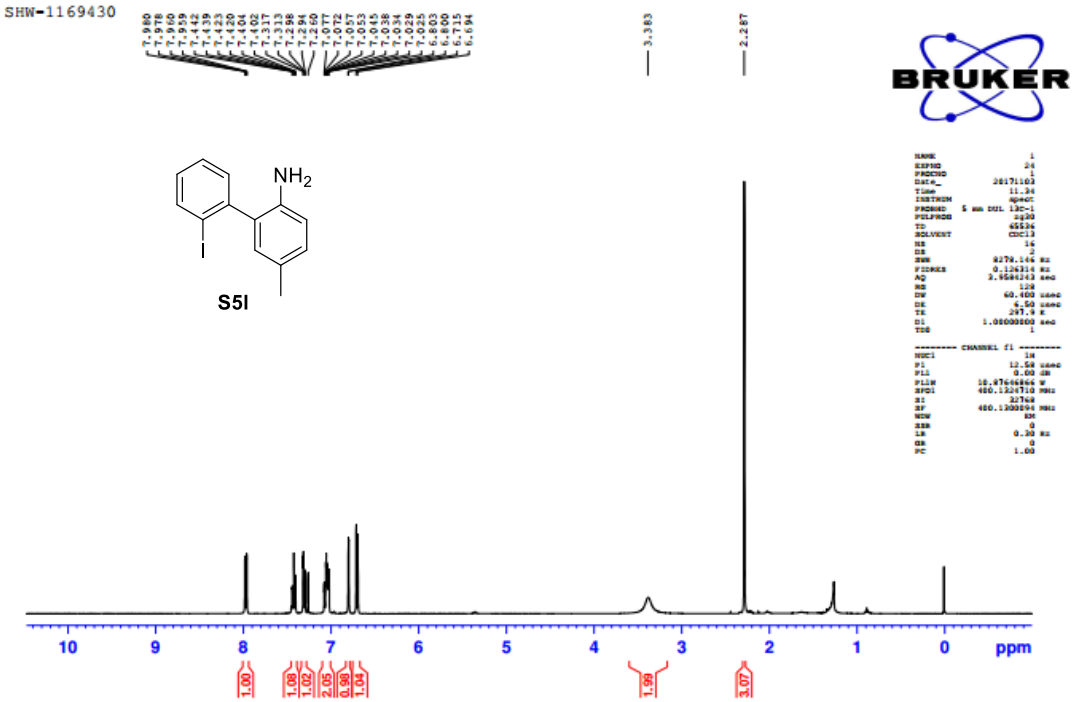

SHW-1012199
159.333
143.804
136.432
130.895
130.705
130.569
129.304
124.611
118.282
115.481
114.934
100.696
77.354
77.101
76.847
55.657
BRUKER
O
NH2
I
S5g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

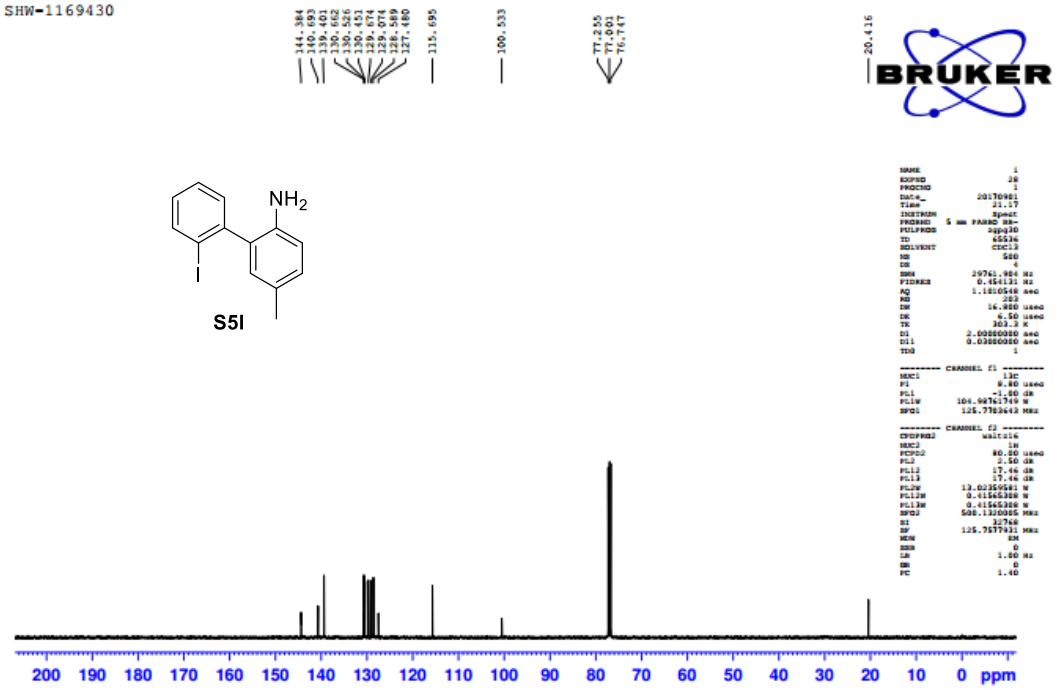

SHW-1012177
8.000
7.984
7.463
7.449
7.434
7.239
7.224
7.127
7.111
7.096
7.077
7.062
7.046
6.712
6.697
6.640
6.624
3.221
1.924
BRUKER
NH2
I
S5j
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.04
1.08
1.01
1.04
1.01
1.02
2.01
3.03

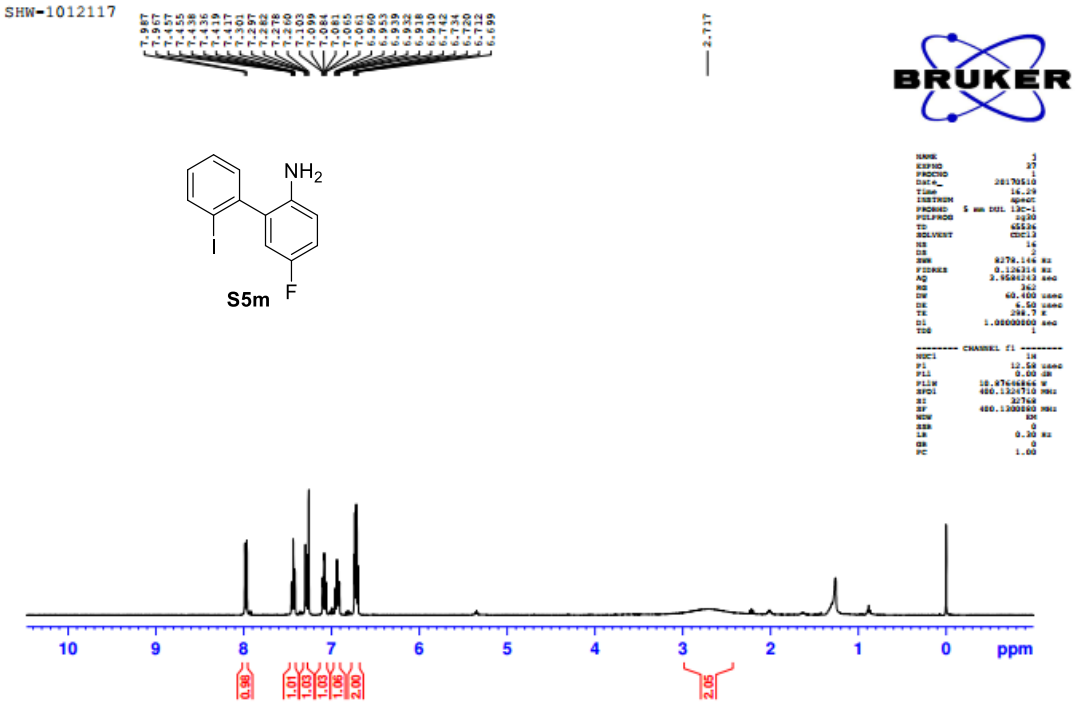

SHW-1012177
143.755
143.684
140.025
136.974
130.940
130.653
129.468
128.991
120.245
113.303
101.693
77.634
77.360
77.106
20.513
BRUKER
NH2
I
S5j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

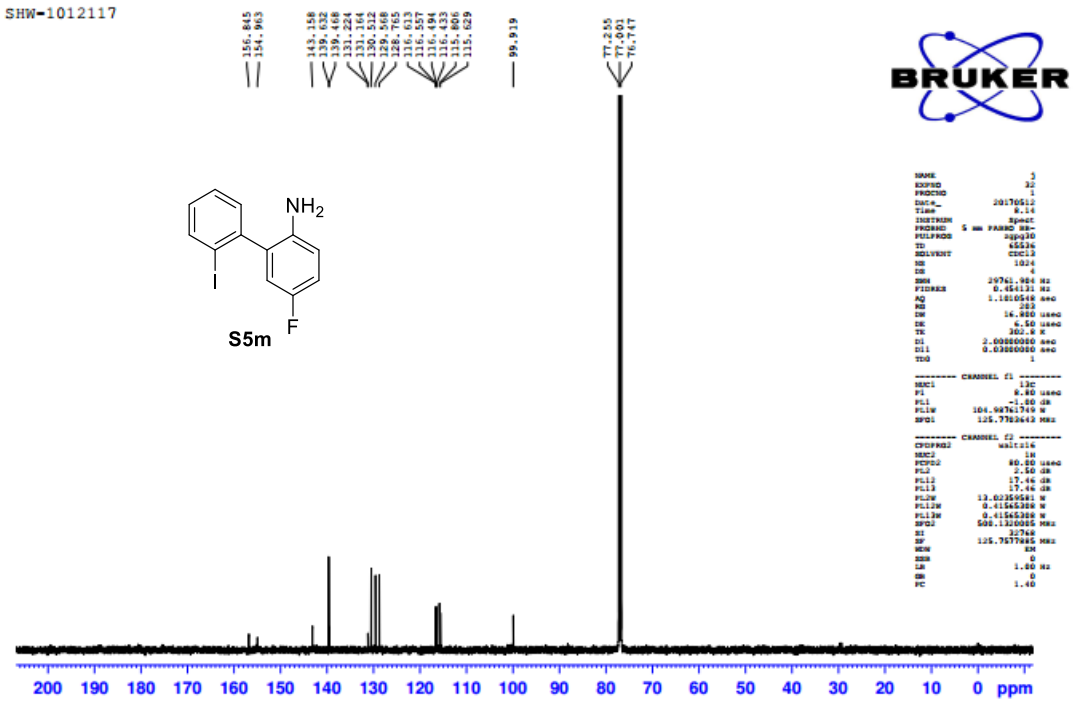

SHW-1012116
7.997
7.977
7.462
7.460
7.443
7.441
7.425
7.422
7.280
7.276
7.260
7.258
7.182
7.161
7.079
7.075
7.059
7.056
7.041
7.037
6.456
6.436
6.423
6.403
3.715
2.583
BRUKER
NH2
O
I
S5k
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
1.03
1.61
1.00
1.04
1.92
3.03
2.09


SHW-1012116
157.456
144.672
140.829
139.498
131.246
129.490
129.065
128.754
119.379
108.508
102.168
101.121
77.254
76.999
76.746
55.758
BRUKER
NH2
O
I
S5k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

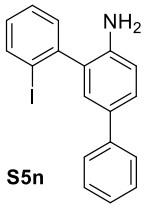

SHW-1169430
7.980
7.978
7.960
7.959
7.442
7.439
7.423
7.420
7.404
7.402
7.317
7.313
7.298
7.294
7.260
7.077
7.072
7.057
7.053
7.045
7.038
7.034
7.029
7.025
6.803
6.800
6.715
6.694
3.383
2.287
BRUKER
NH2
I
S5I
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.08
1.02
2.05
0.98
1.04
1.99
3.07


SHW-1169430
144.384
140.693
139.401
130.662
130.526
130.451
129.574
129.074
128.589
127.480
115.695
100.533
77.255
77.001
76.747
20.416
BRUKER
NH2
I
S5I
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

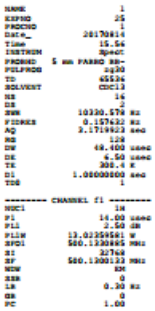

SHW-1012117
7.987
7.967
7.457
7.455
7.438
7.436
7.419
7.417
7.301
7.297
7.282
7.278
7.260
7.103
7.099
7.084
7.081
7.065
7.061
6.960
6.955
6.939
6.932
6.918
6.910
6.742
6.734
6.720
6.712
6.699
2.717
BRUKER
NH2
I
F
S5m
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.01
1.03
1.03
1.05
2.00
2.05

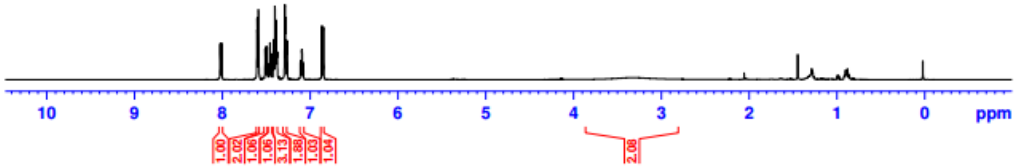

SHW-1012117
156.845
154.963
143.158
139.632
139.468
131.224
131.164
130.512
129.568
128.765
116.613
116.557
116.434
116.153
115.806
115.629
99.919
77.255
77.001
76.747
BRUKER
NH2
I
F
S5m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

SHW-1169457

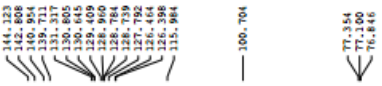


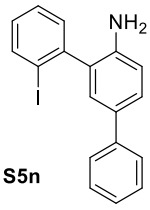
S5n



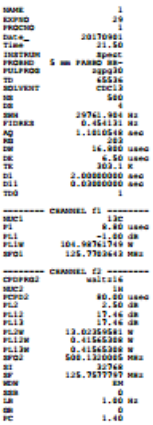


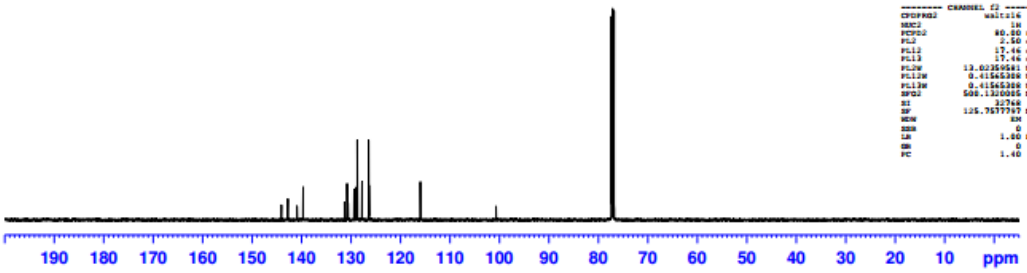
SHW-1169457



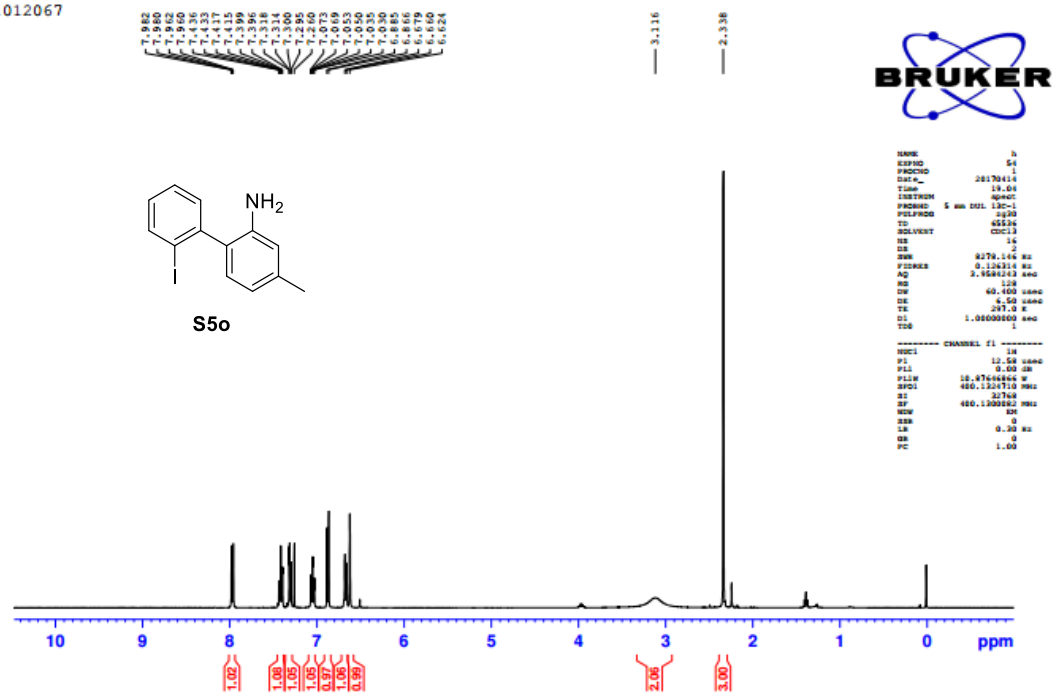


S5n

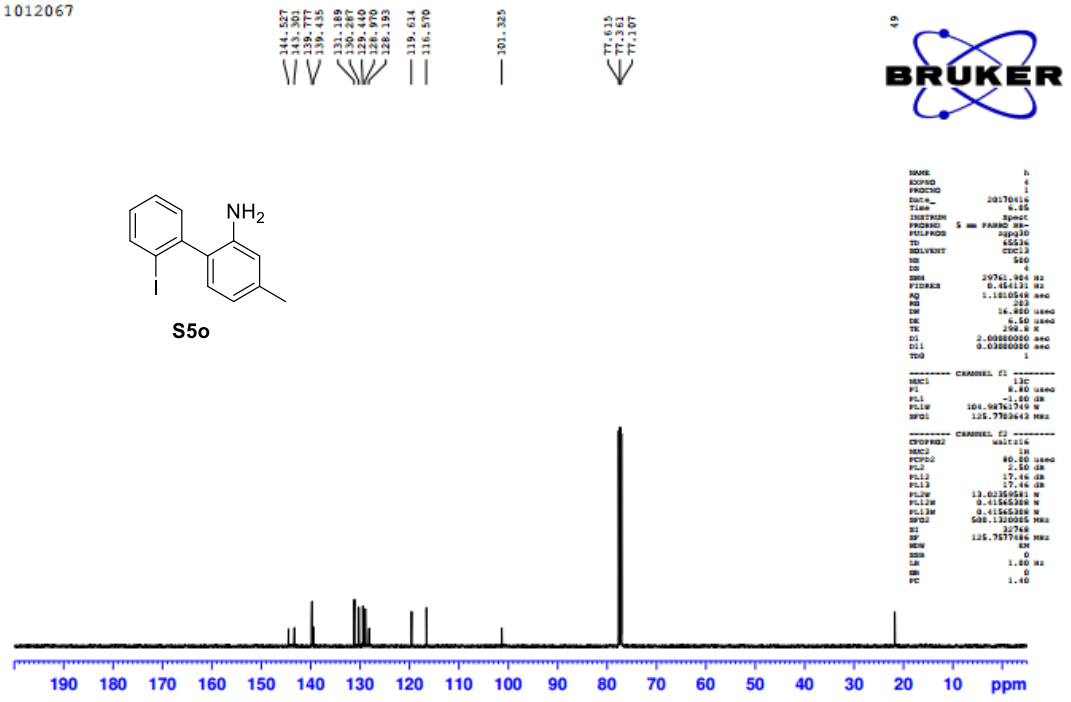


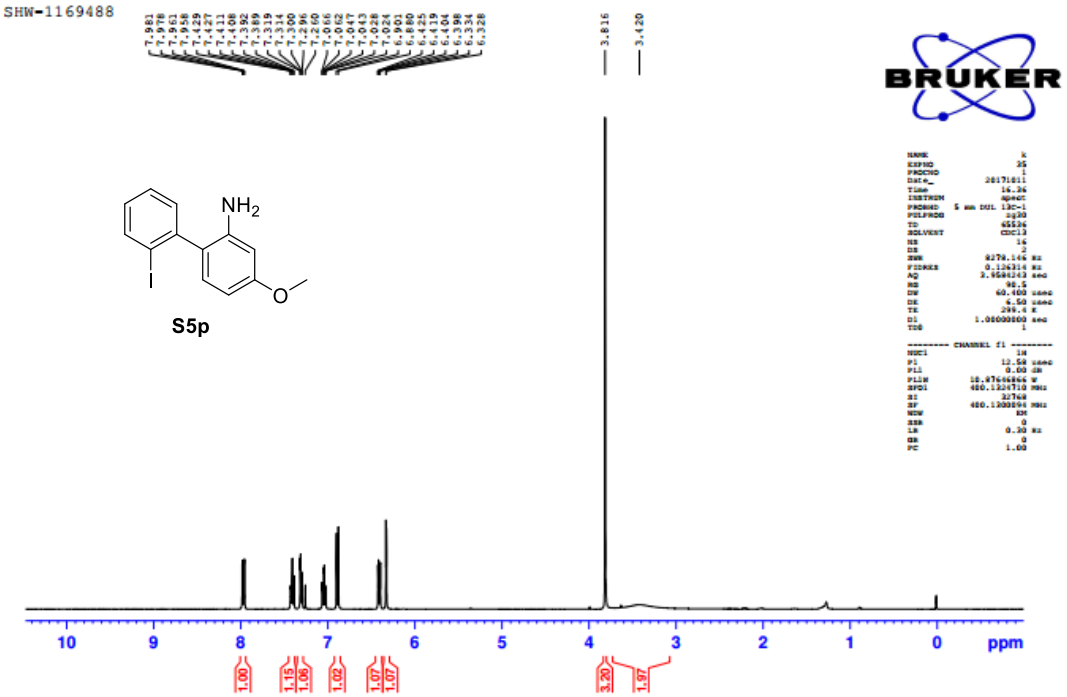


1012067



1012067

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7.958
7.429
7.427
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7.408
7.392
7.389
7.319
7.314
7.300
7.296
7.260
7.066
7.062
7.047
7.043
7.028
7.024
6.901
6.880
6.425
6.419
6.404
6.398
6.334
6.328
3.816
3.420
NH2
I
O
S5p
BRUKER
10
9
8
7
6
5
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1
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ppm
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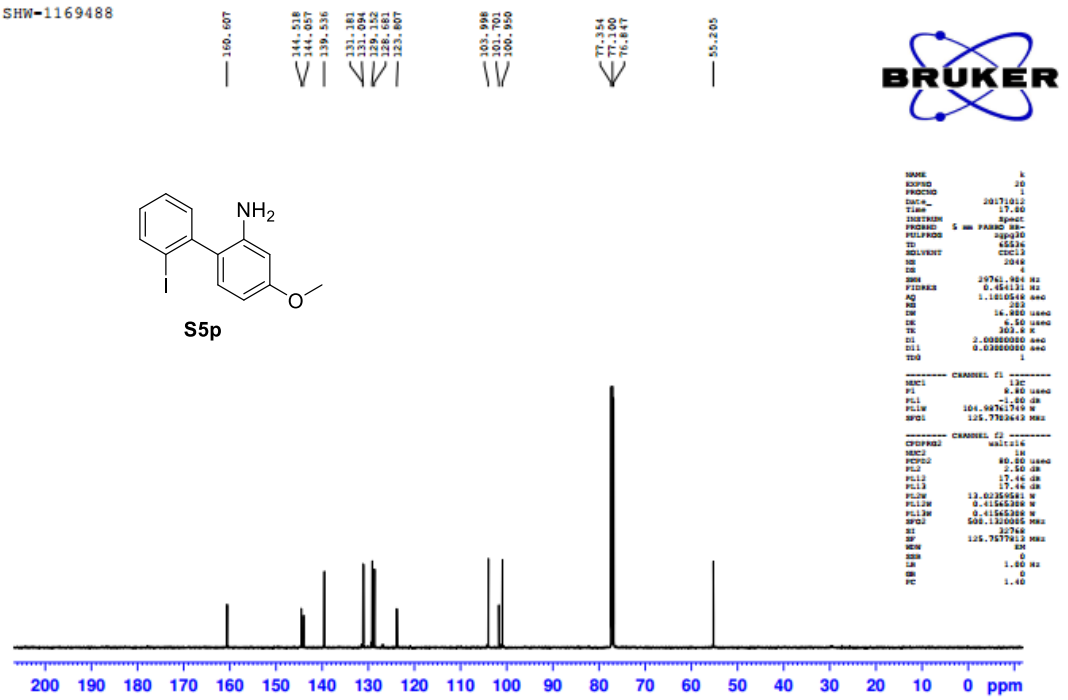
1.15
1.06
1.02
1.07
1.07
3.20
1.97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139.536
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123.807
103.998
101.701
100.950
77.354
77.100
76.847
55.205
NH2
I
O
S5p
BRUKER
200
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140
130
120
110
100
90
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60
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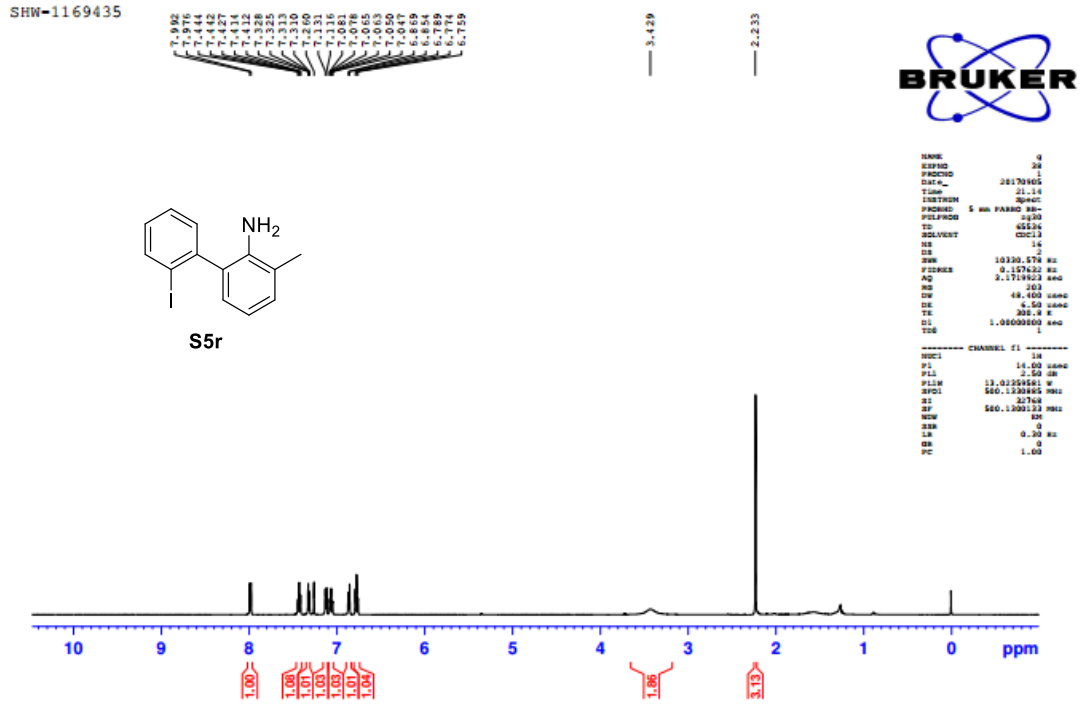
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7.442
7.427
7.414
7.412
7.328
7.325
7.313
7.310
7.260
7.131
7.116
7.081
7.078
7.065
7.063
7.050
7.047
6.869
6.854
6.789
6.774
6.759
3.429
2.233
BRUKER
NH2
I
S5r
10
9
8
7
6
5
4
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1
0
ppm
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1.07
1.03
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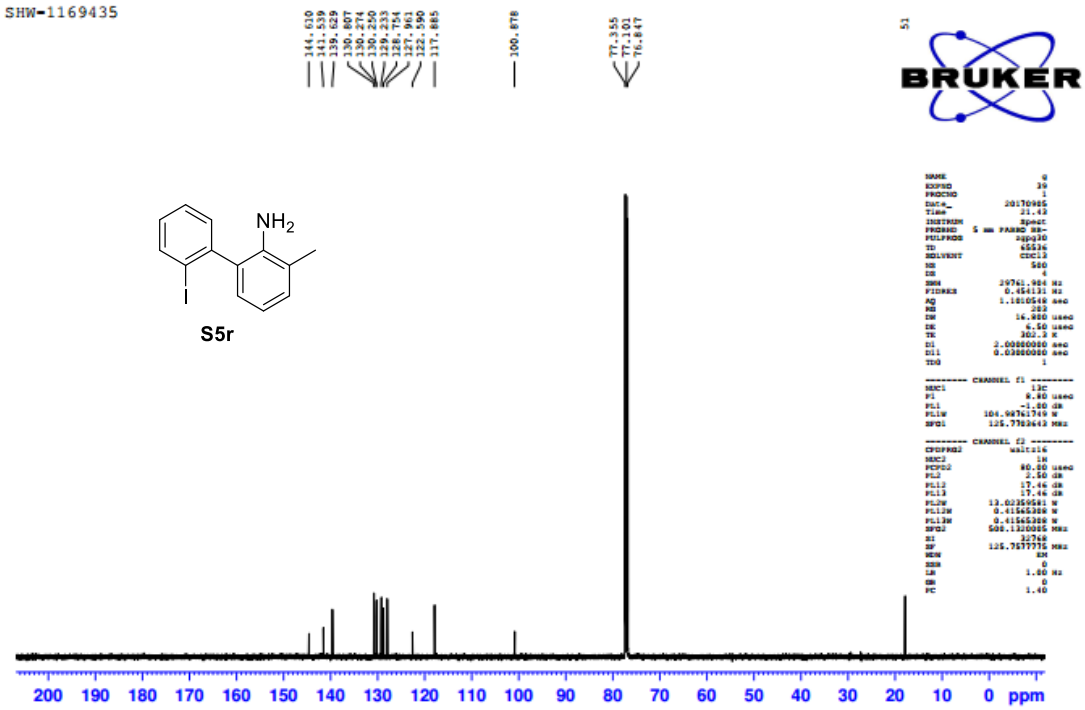
1.04
1.86
3.13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139.629
130.897
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129.233
128.754
127.961
122.590
117.885
100.878
77.355
77.101
76.847
BRUKER
NH2
I
S5r
200
190
180
170
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140
130
120
110
100
90
80
70
60
50
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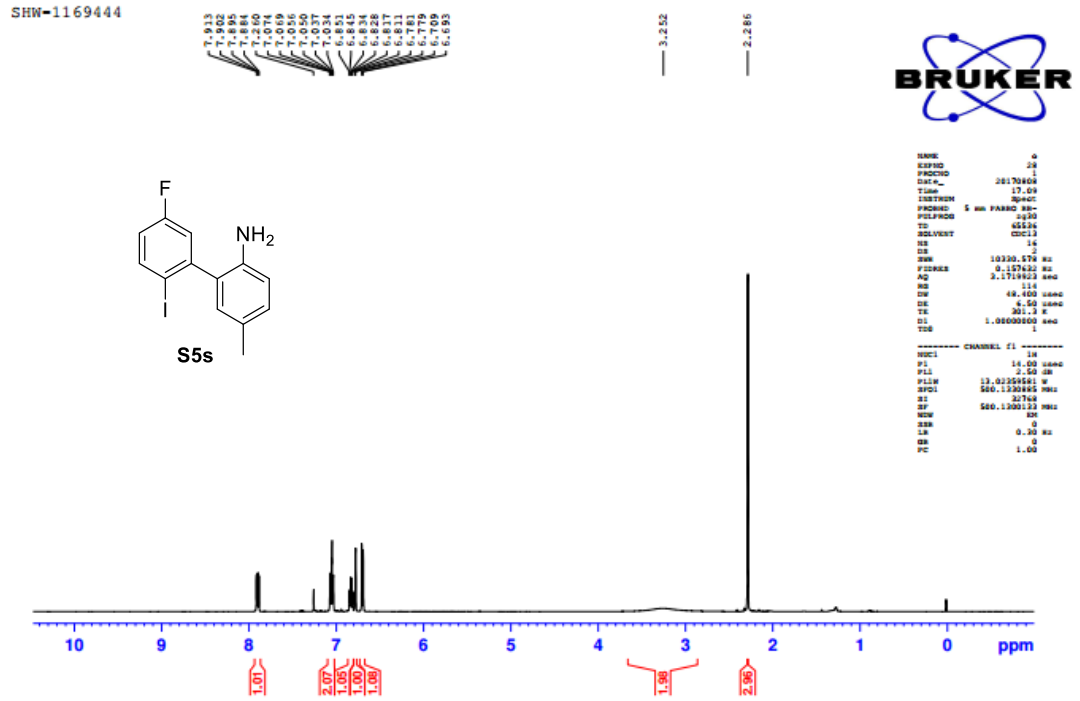
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7.895
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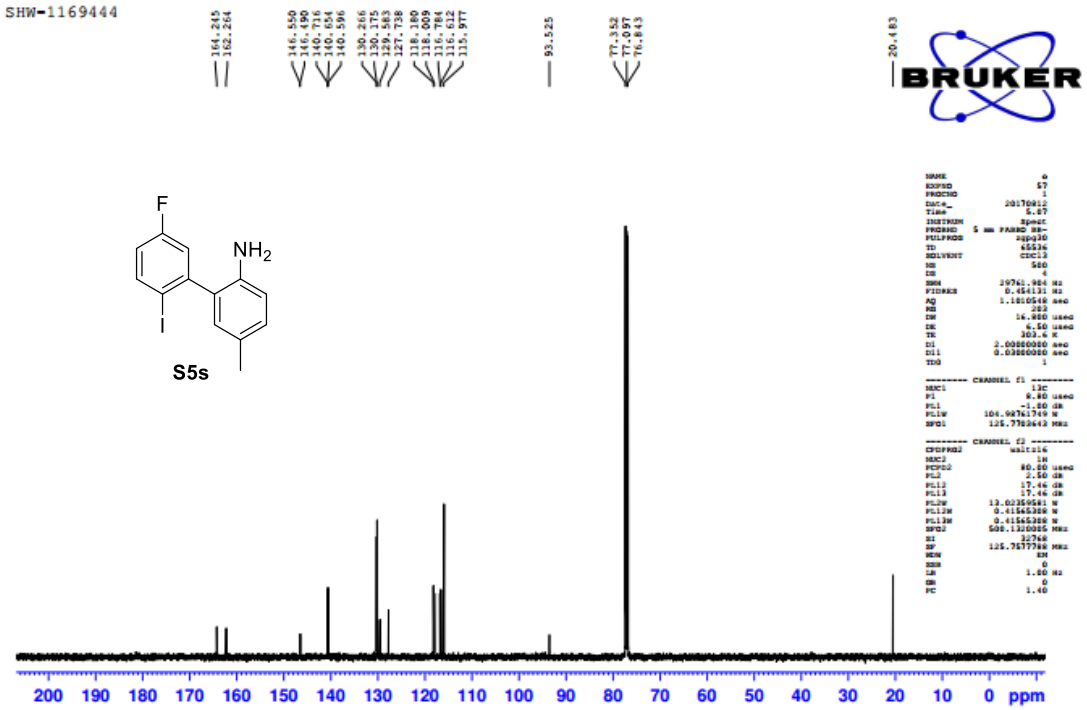
7.860
7.074
7.069
7.056
7.050
7.037
7.034
6.851
6.845
6.834
6.828
6.817
6.811
6.779
6.709
6.693
3.252
2.286
BRUKER
F
NH2
I
S5s
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
2.07
1.05
1.00
1.08
1.98
2.96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146.490
146.376
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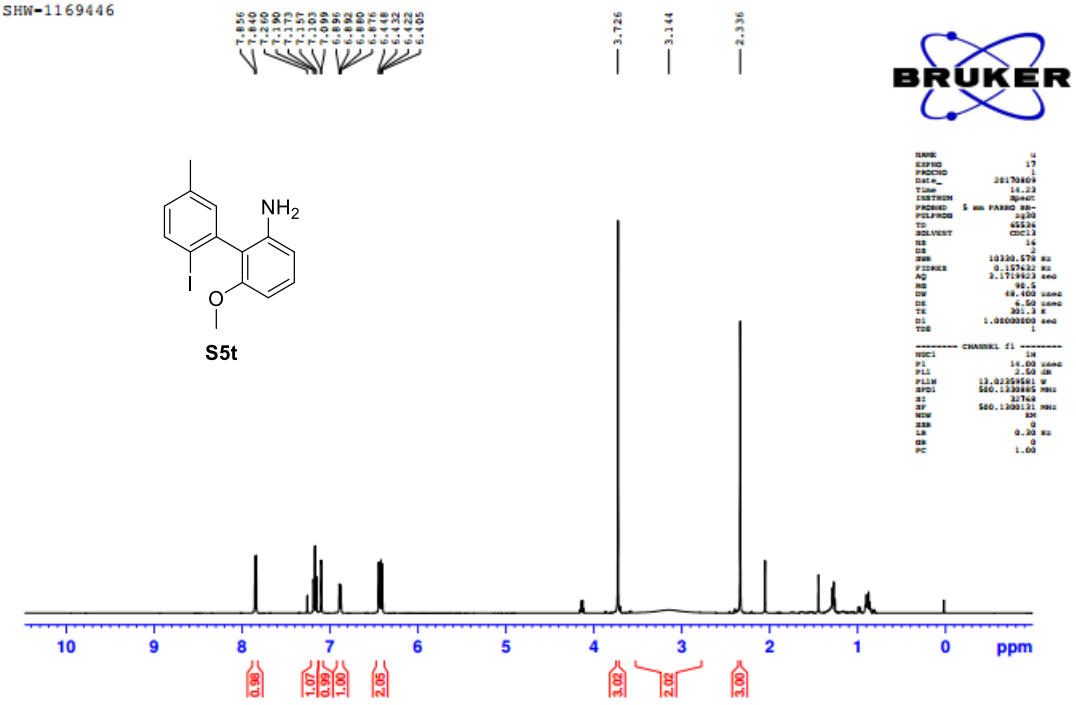
140.596
130.266
130.175
129.583
127.758
118.180
118.089
116.784
116.632
115.977
93.525
77.352
77.097
76.843
20.483
BRUKER
F
NH2
I
S5s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

SHW-1169446



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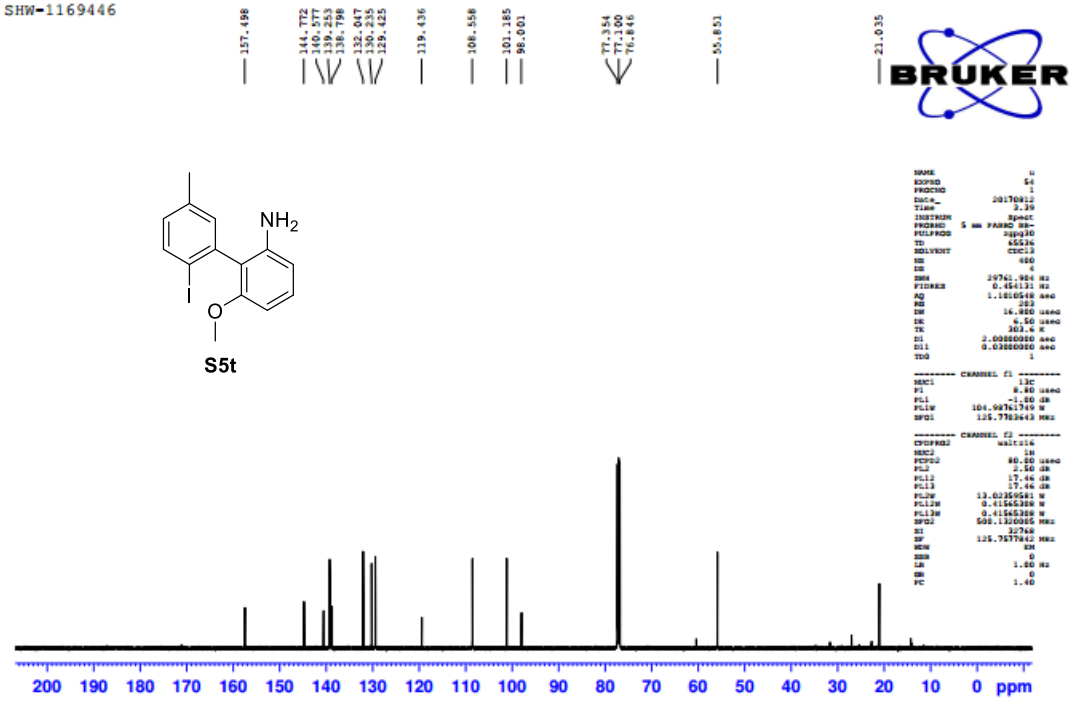

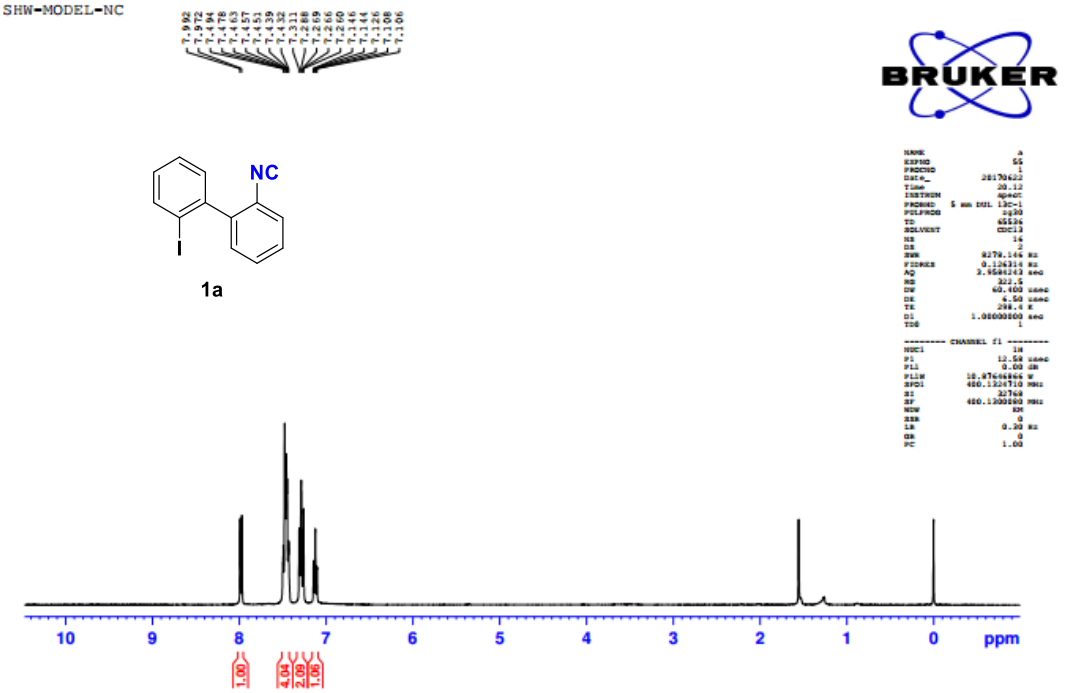
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7.463
7.457
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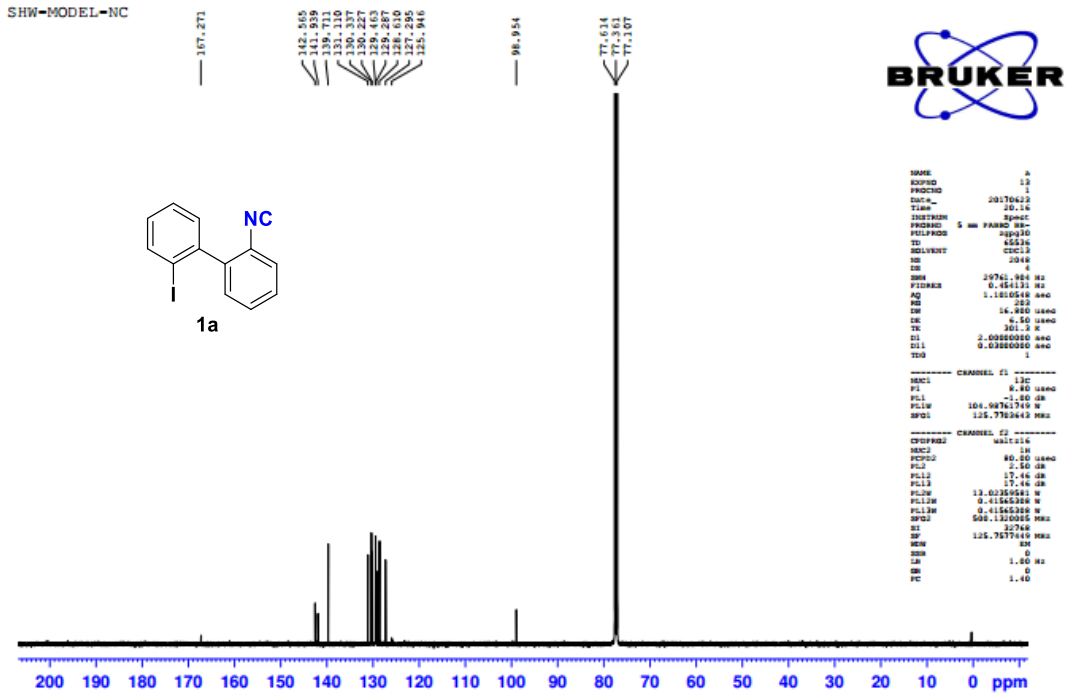
7.439
7.432
7.311
7.288
7.269
7.260
7.146
7.144
7.126
7.108
7.106
NC
1a
BRUKER
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
4.04
2.09
1.06


SHW-MODEL-NC
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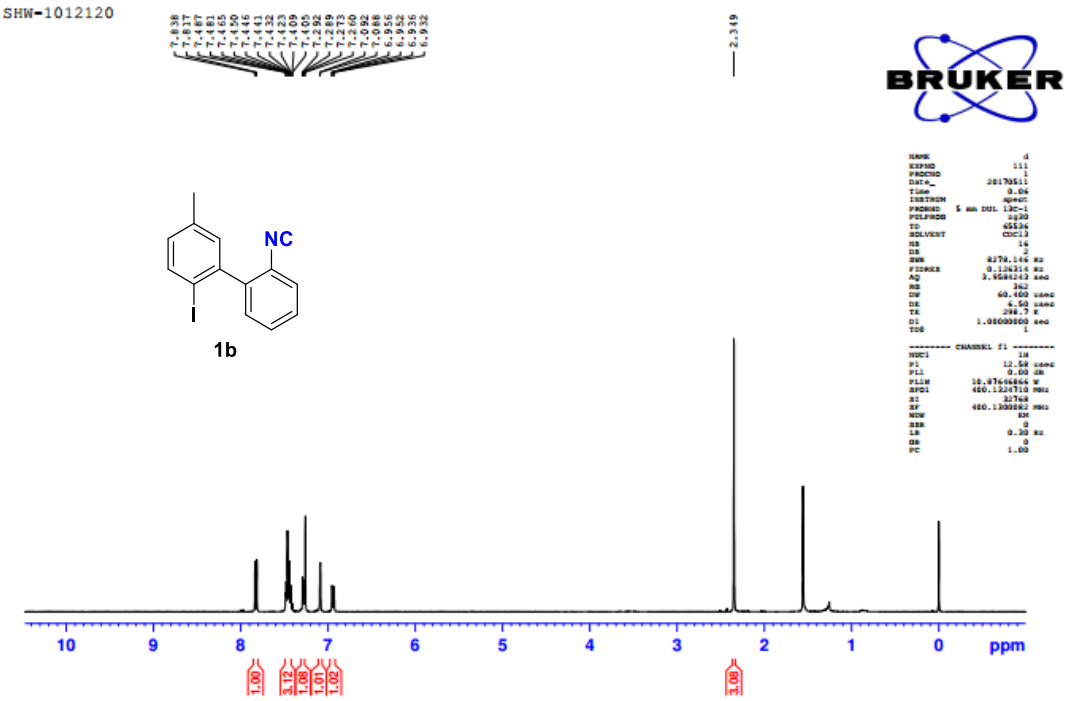
142.565
141.959
139.711
131.130
130.327
130.227
129.463
129.287
128.610
127.295
125.946
98.954
77.634
77.361
77.107
NC
1a
BRUKER
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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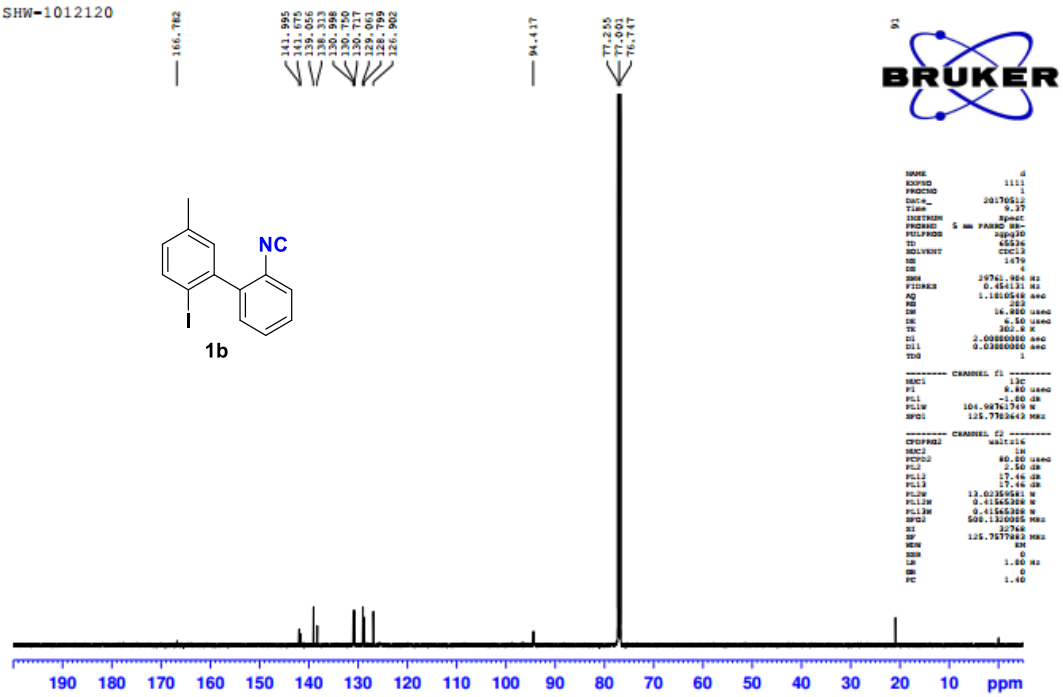
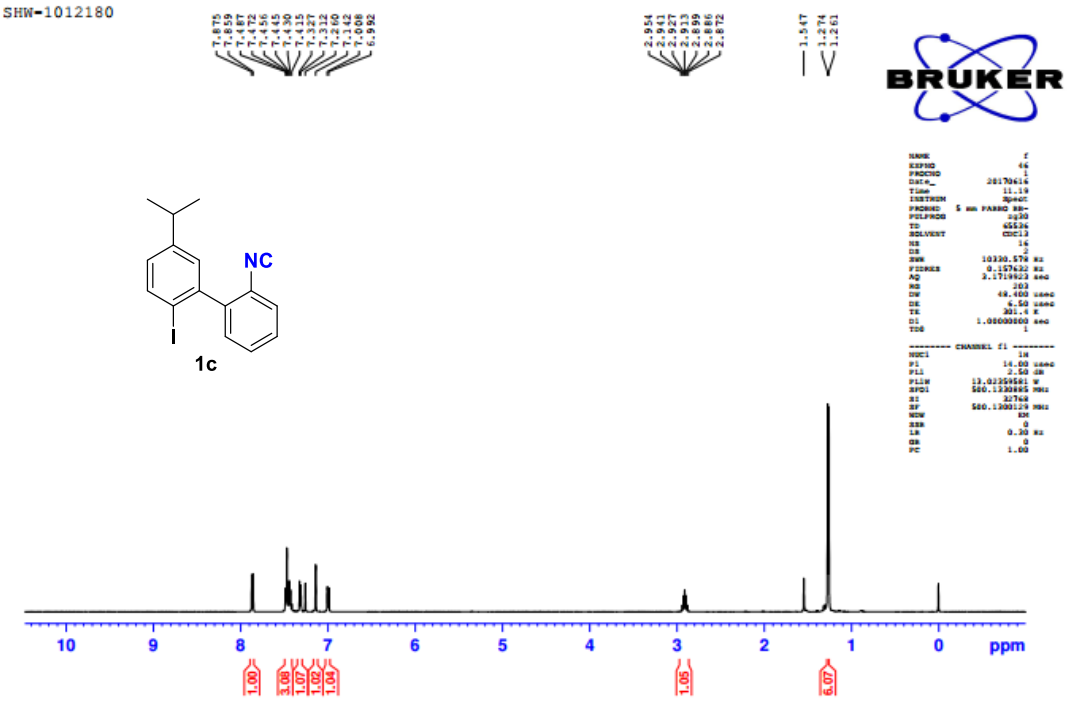
NC
1b
ppm


SHW-1012120
NC
1b
ppm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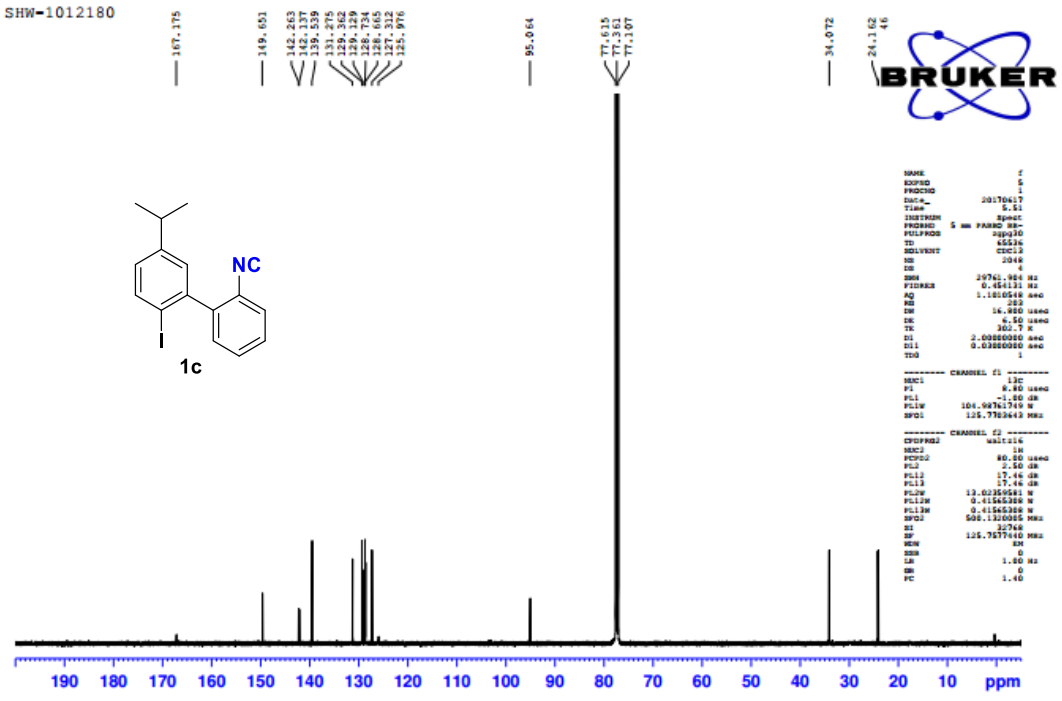
7.453
7.456
7.445
7.430
7.415
7.327
7.322
7.260
7.142
7.008
6.992
2.954
2.941
2.927
2.913
2.899
2.886
2.872
1.547
1.274
1.261
BRUKER
NC
I
1c
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
3.08
1.07
1.02
1.04
1.06
6.07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129.362
129.259
128.734
128.665
127.312
125.976
95.064
77.615
77.361
77.107
34.072
24.162
BRUKER
NC
I
1c
190
180
170
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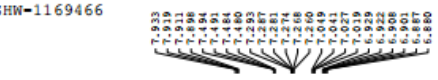
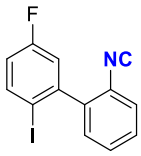
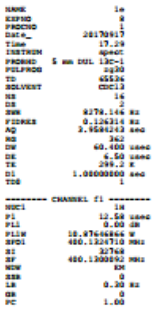
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

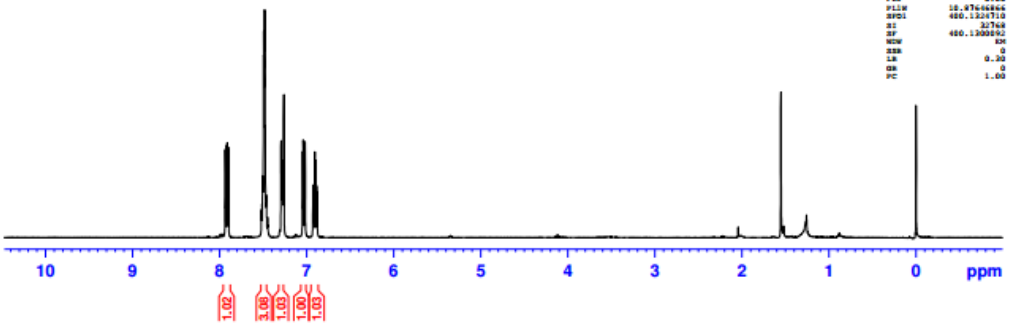
SHW-1169466



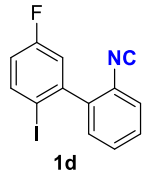


1d

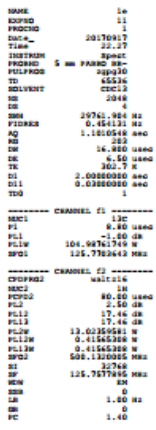


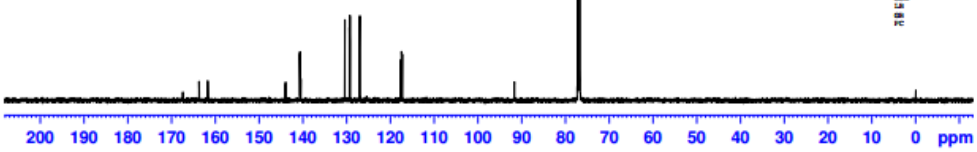


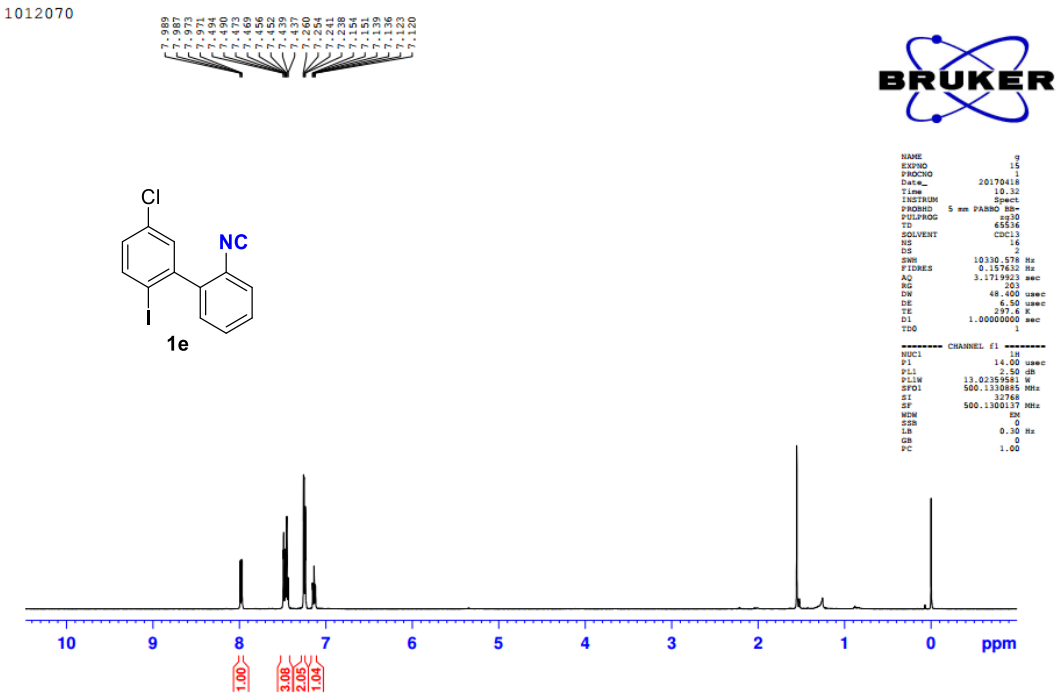
SHW-1169466



1d



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7.452
7.439
7.437
7.260
7.254
7.241
7.238
7.154
7.151
7.139
7.136
7.123
7.120
BRUKER
Cl
NC
I
1e
10
9
8
7
6
5
4
3
2
1
0
ppm
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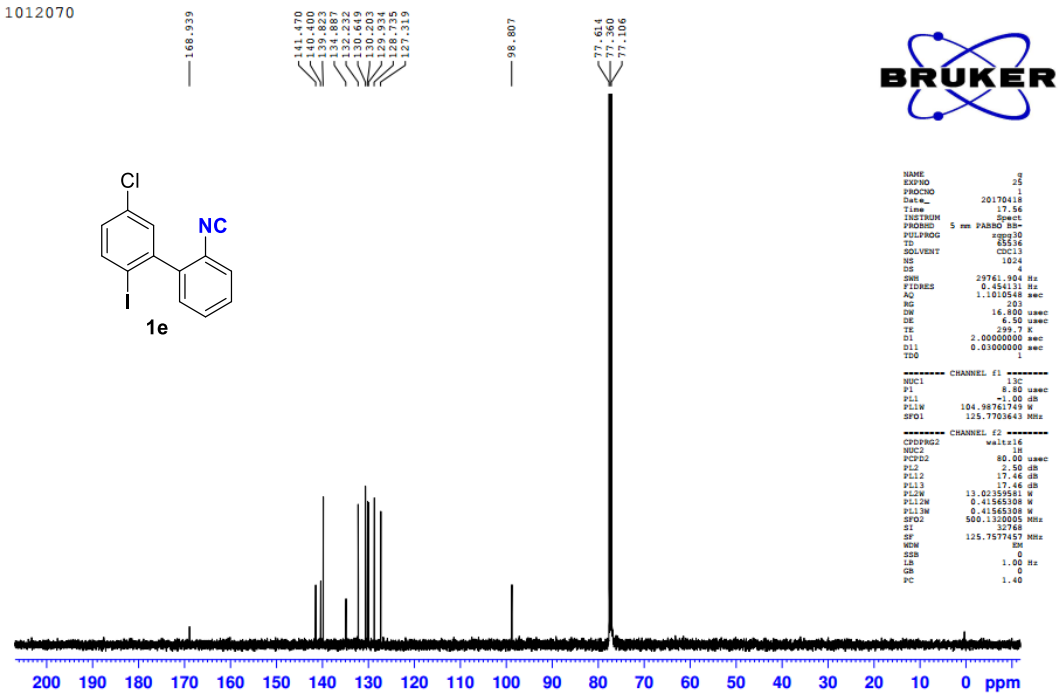
3.08
2.05
1.04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134.887
132.232
130.649
130.203
129.934
128.735
127.319
98.807
77.614
77.360
77.106
BRUKER
Cl
NC
I
1e
200
190
180
170
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140
130
120
110
100
90
80
70
60
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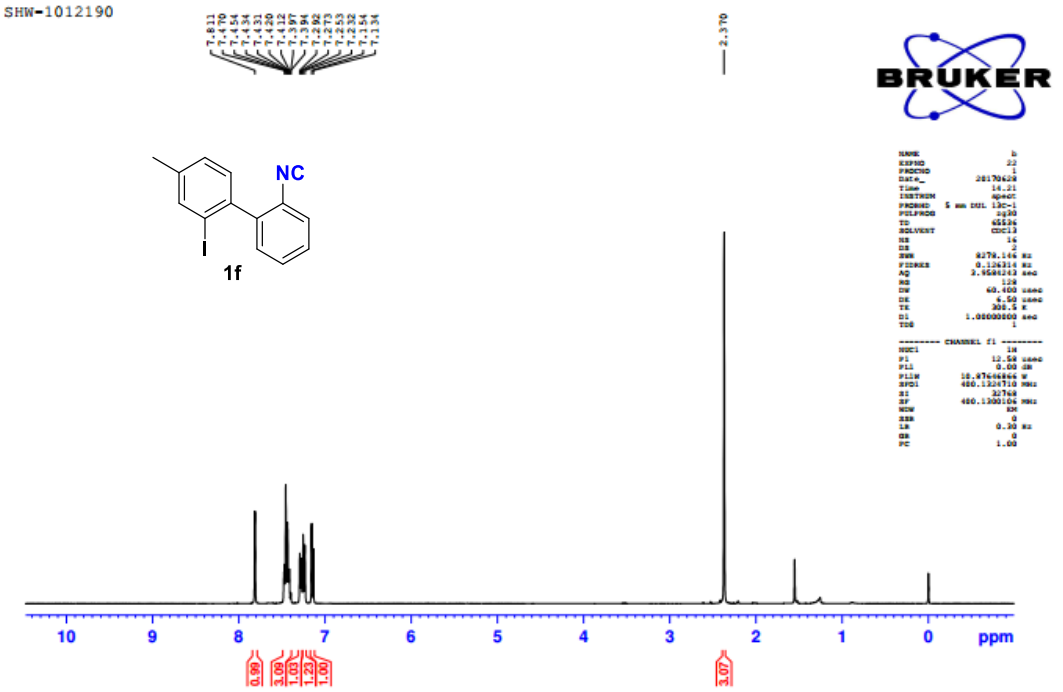
20
10
0
ppm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7.428
7.412
7.397
7.394
7.292
7.273
7.253
7.232
7.154
7.134
2.370
BRUKER
NC
I
1f
10
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4
3
2
1
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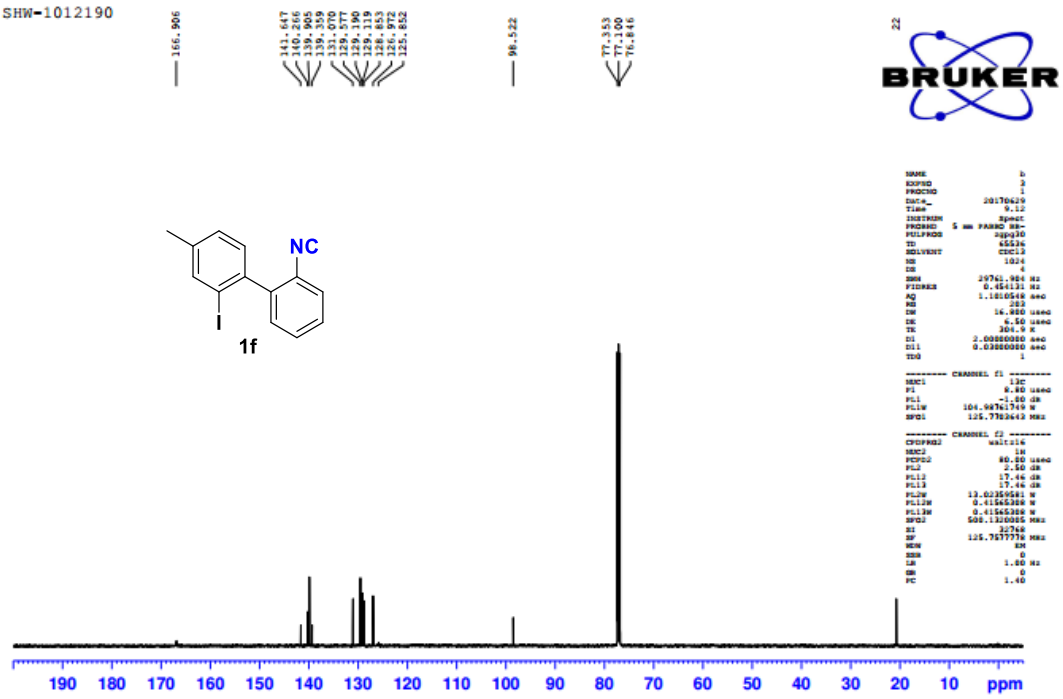
1.23
1.00
3.07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126.972
125.852
98.522
77.353
77.100
76.846
22
BRUKER
NC
I
1f
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150
140
130
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110
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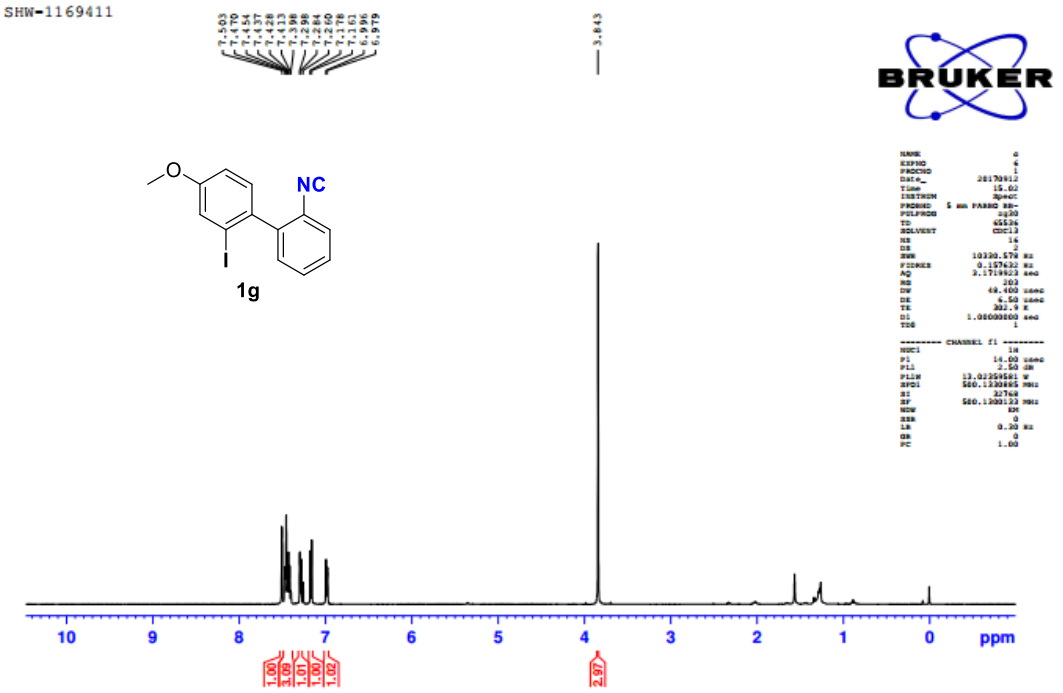
20
10
ppm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6.996
6.979
3.843
BRUKER
NC
O
I
1g
10
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4
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ppm
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3.09
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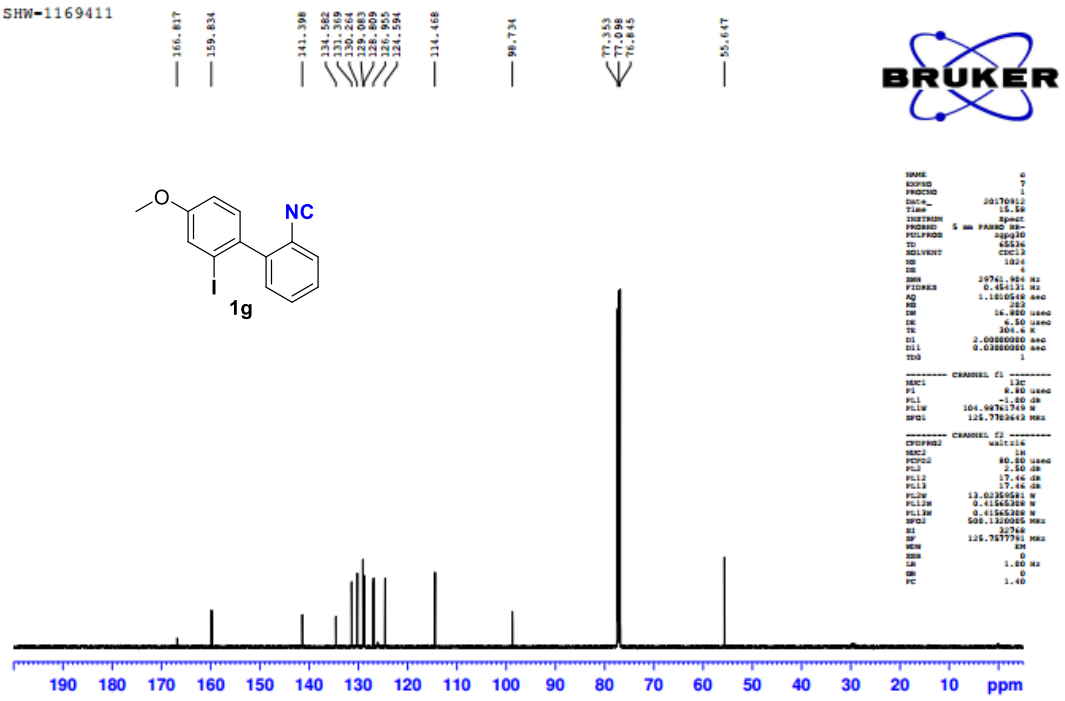
1.00
1.02
2.97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124.594
114.468
96.734
77.353
77.098
76.845
55.647
BRUKER
NC
O
I
1g
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150
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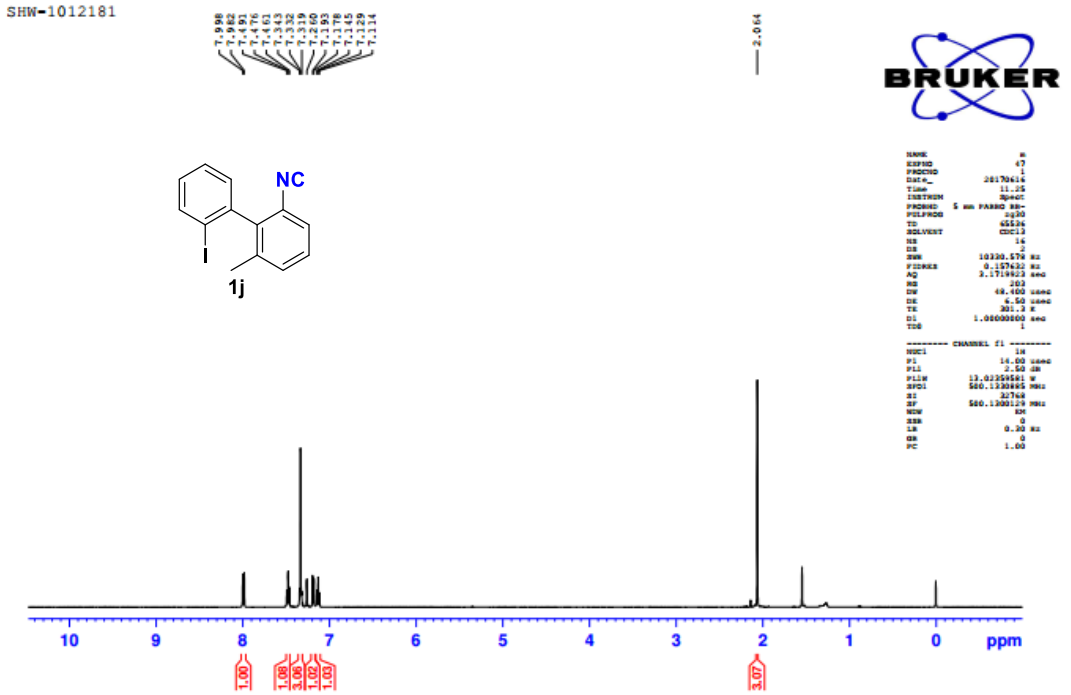
10
ppm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7.319
7.260
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7.178
7.145
7.139
7.134
2.064
BRUKER
NC
I
1j
10
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4
3
2
1
0
ppm
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1.00
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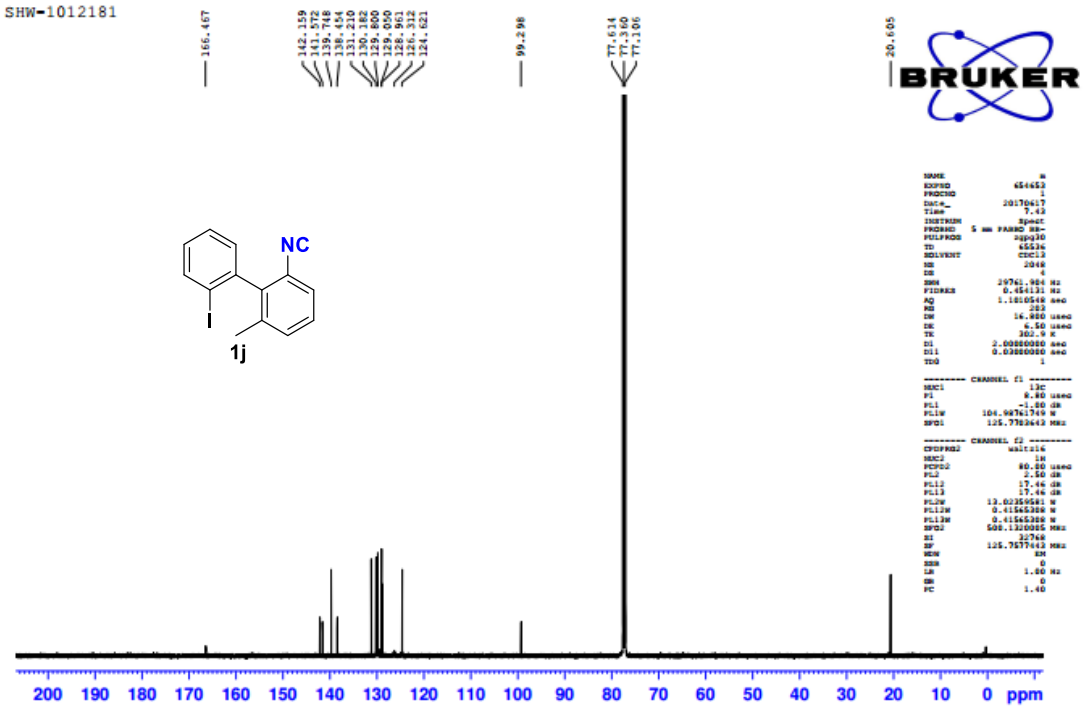
1.00
3.07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126.332
124.621
99.298
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77.360
77.106
20.605
BRUKER
NC
I
1j
200
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130
120
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100
90
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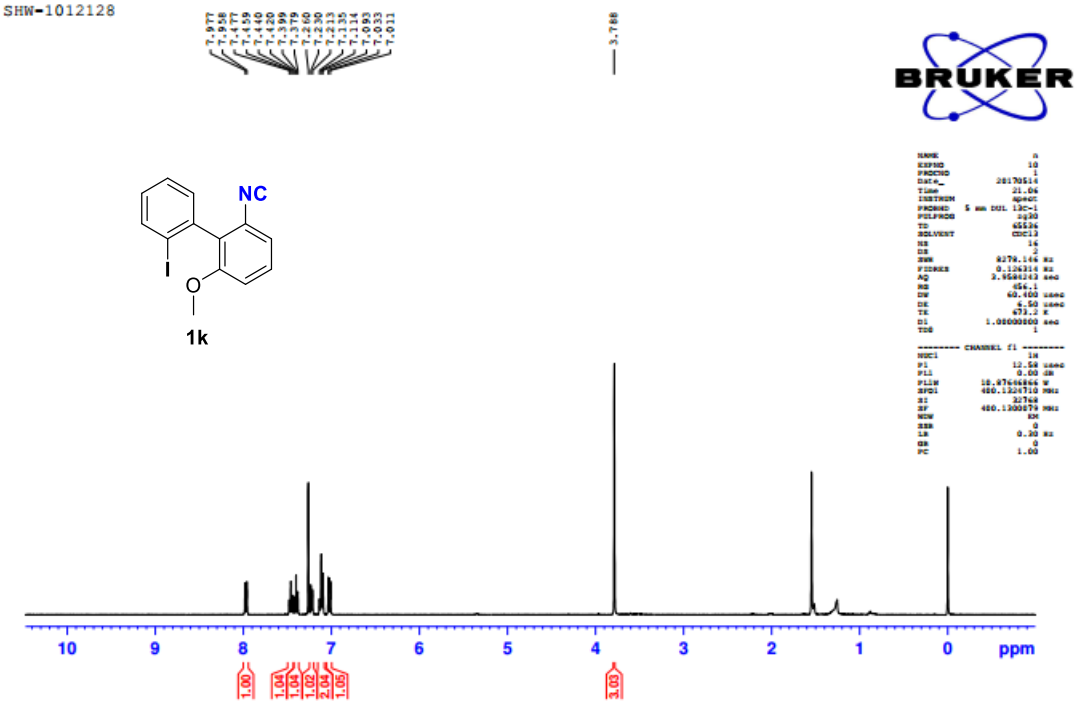
10
0
ppm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7.260
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7.033
7.011
3.788
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I
O
1k
10
9
8
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1.04
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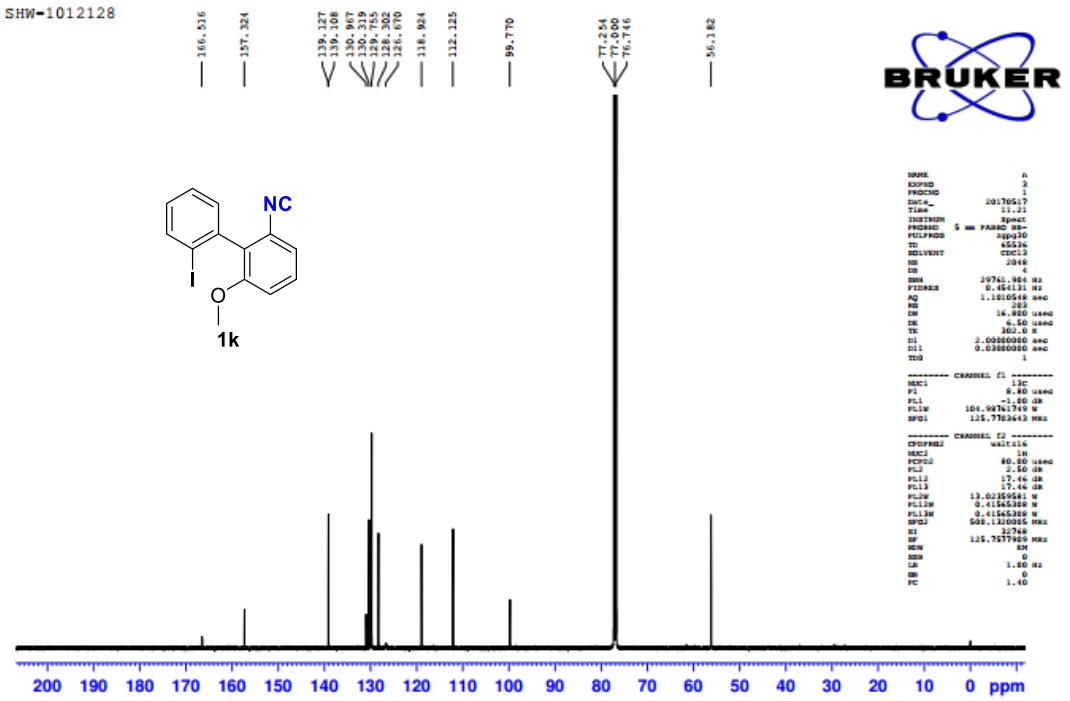
1.00
3.03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139.108
130.967
130.319
128.705
128.302
126.670
118.924
112.125
99.770
77.254
77.000
76.746
56.182
NC
I
O
1k
200
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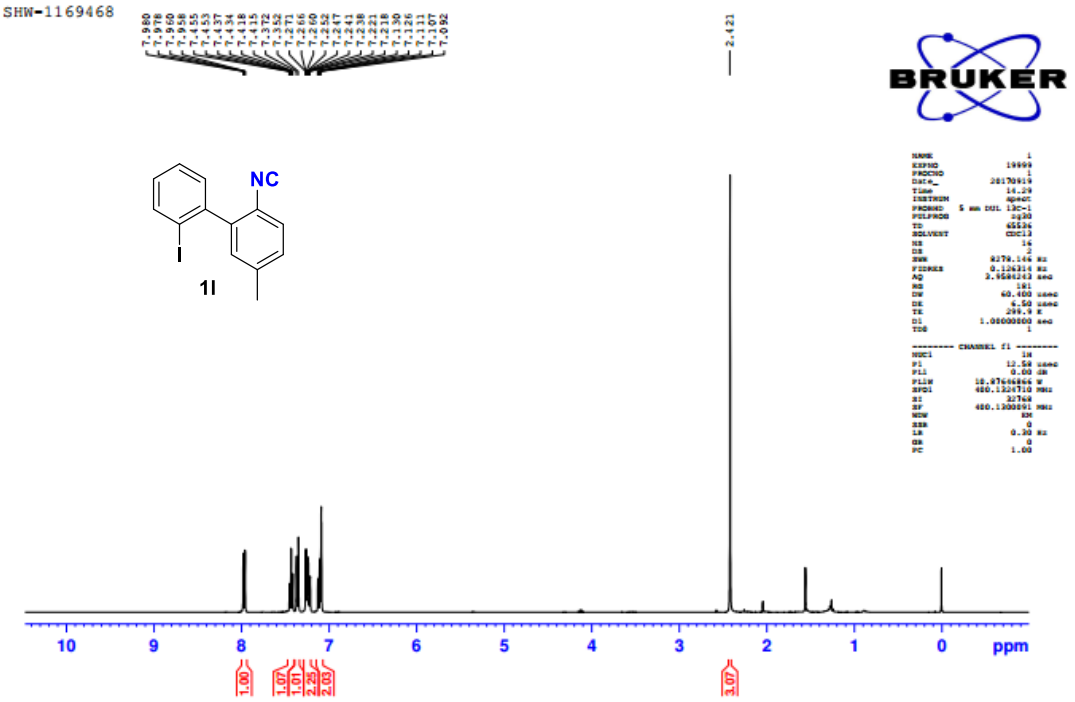
20
10
0
ppm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7.978
7.960
7.958
7.455
7.453
7.437
7.434
7.418
7.415
7.372
7.352
7.271
7.266
7.260
7.252
7.247
7.241
7.238
7.221
7.218
7.130
7.126
7.111
7.107
7.092
2.421
BRUKER
NC
I
1l
10
9
8
7
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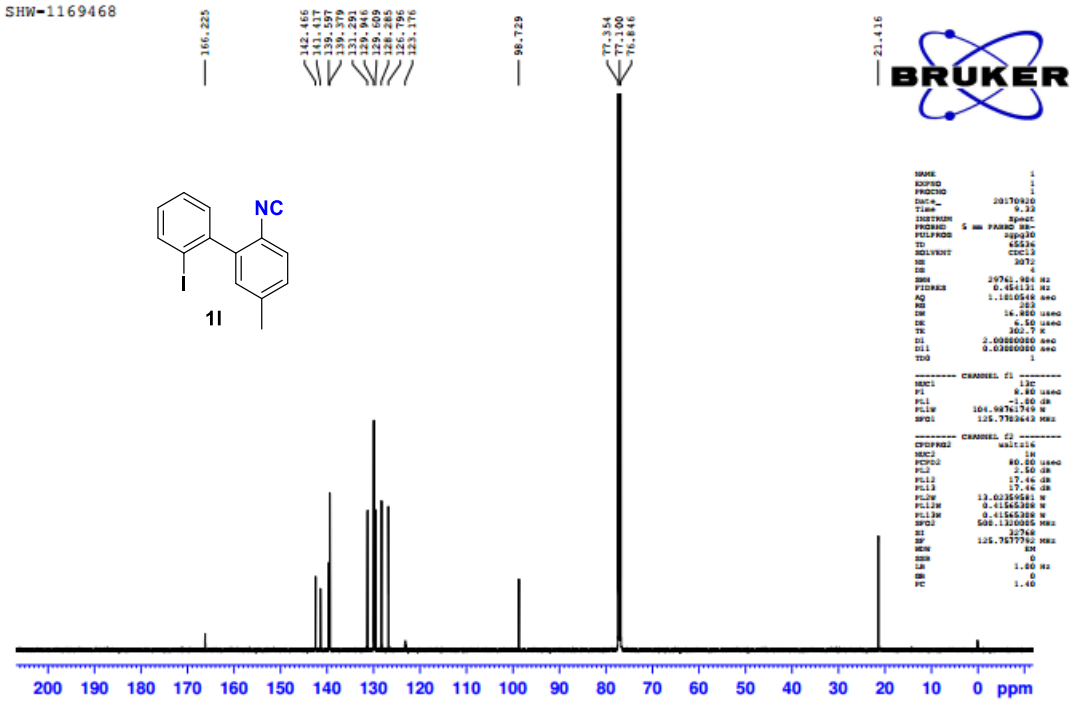
5
4
3
2
1
0
ppm
1.00
1.07
1.01
2.25
2.03
3.07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129.689
128.545
126.796
123.176
98.729
77.354
77.100
76.846
21.416
BRUKER
NC
I
1l
200
190
180
170
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110
100
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80
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30
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10
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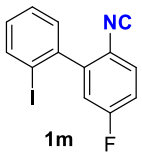
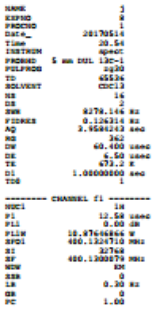
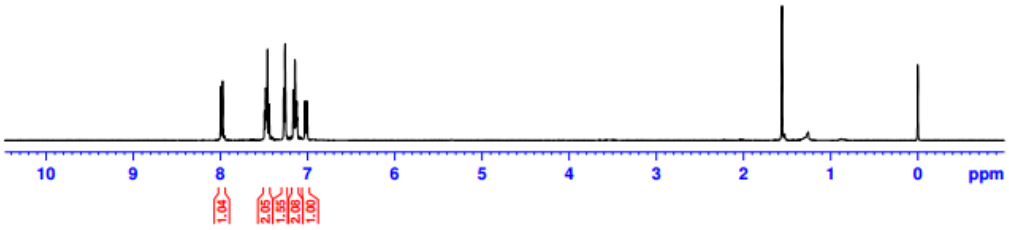
ppm

SHW-1012127







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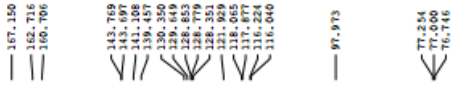
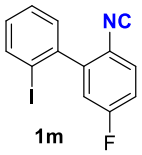
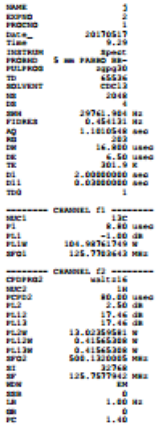
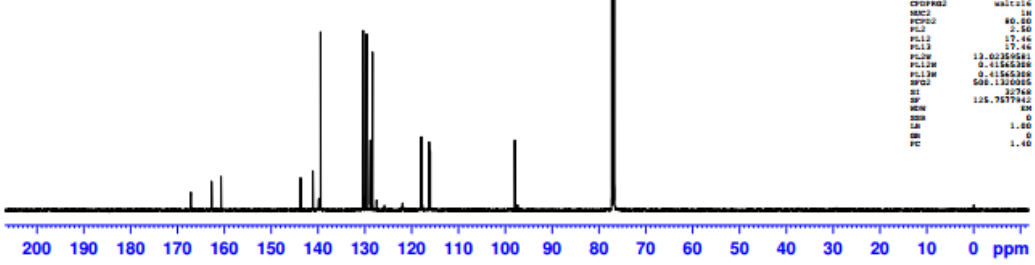
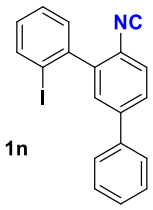


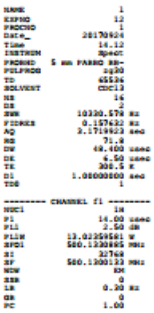


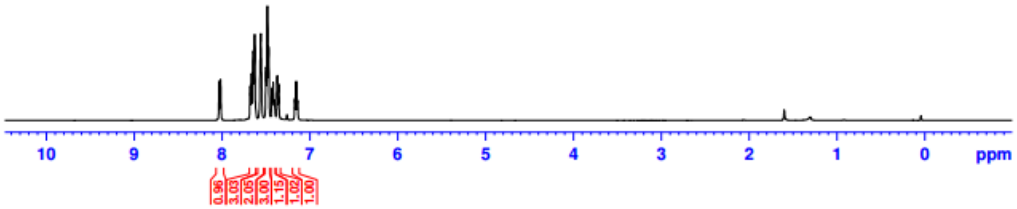




SHW-1169475







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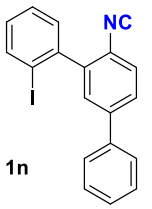

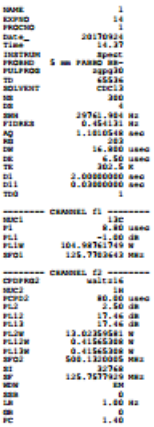

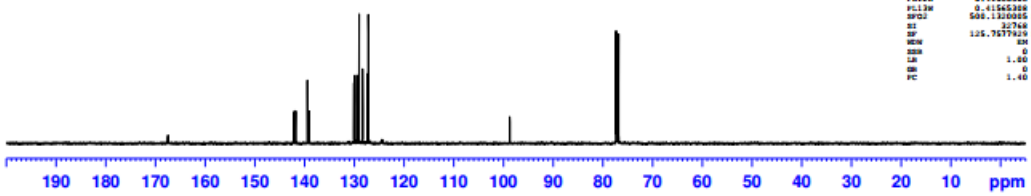

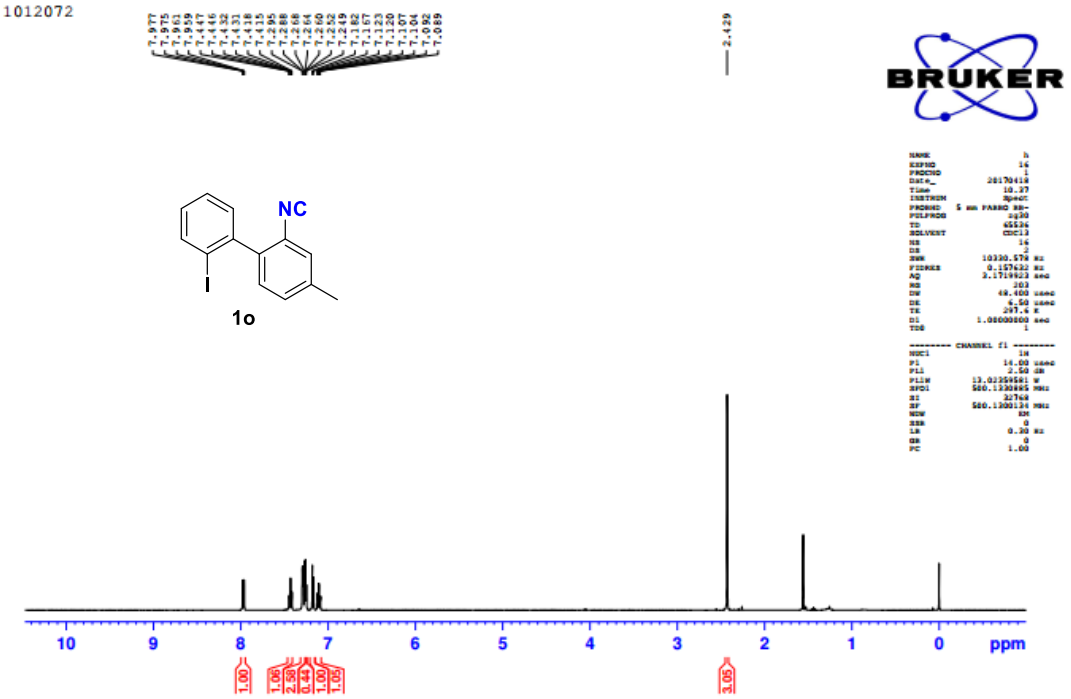
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7.975
7.961
7.959
7.447
7.446
7.432
7.431
7.418
7.415
7.295
7.288
7.266
7.264
7.260
7.252
7.249
7.182
7.167
7.123
7.120
7.107
7.104
7.092
7.089
2.429
BRUKER
NC
I
1o
10
9
8
7
6
5
4
3
2
1
0
ppm
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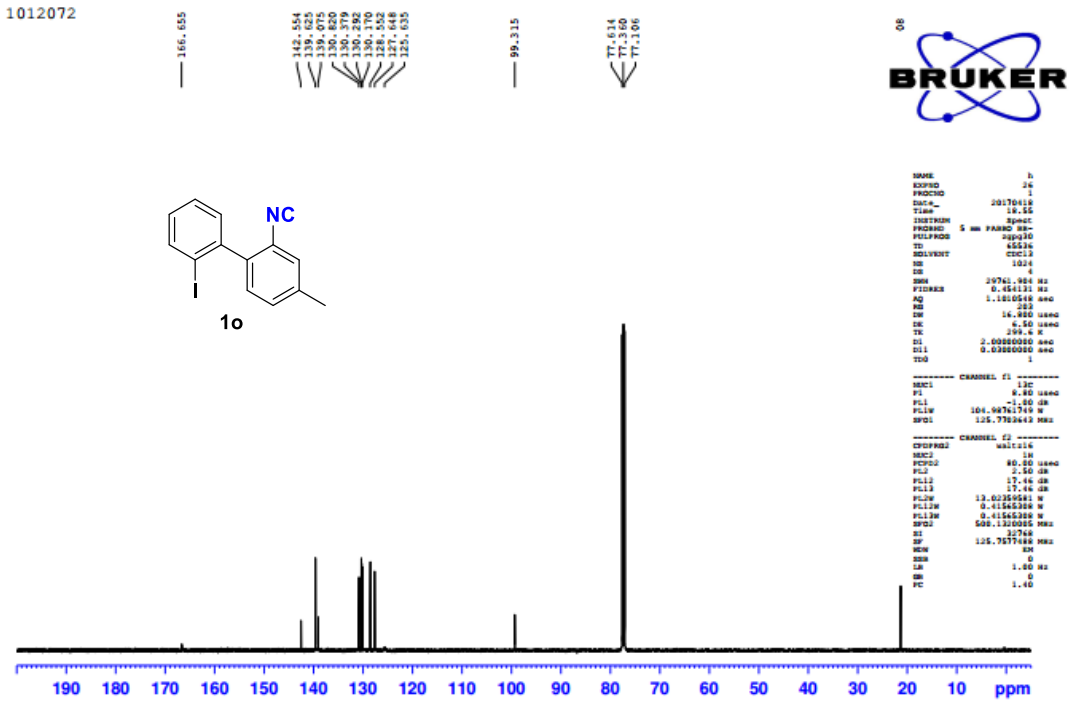
1.06
2.58
0.44
1.00
1.06
3.05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130.379
130.292
130.170
128.552
127.648
125.635
99.315
77.614
77.360
77.106
08
BRUKER
NC
I
1o
190
180
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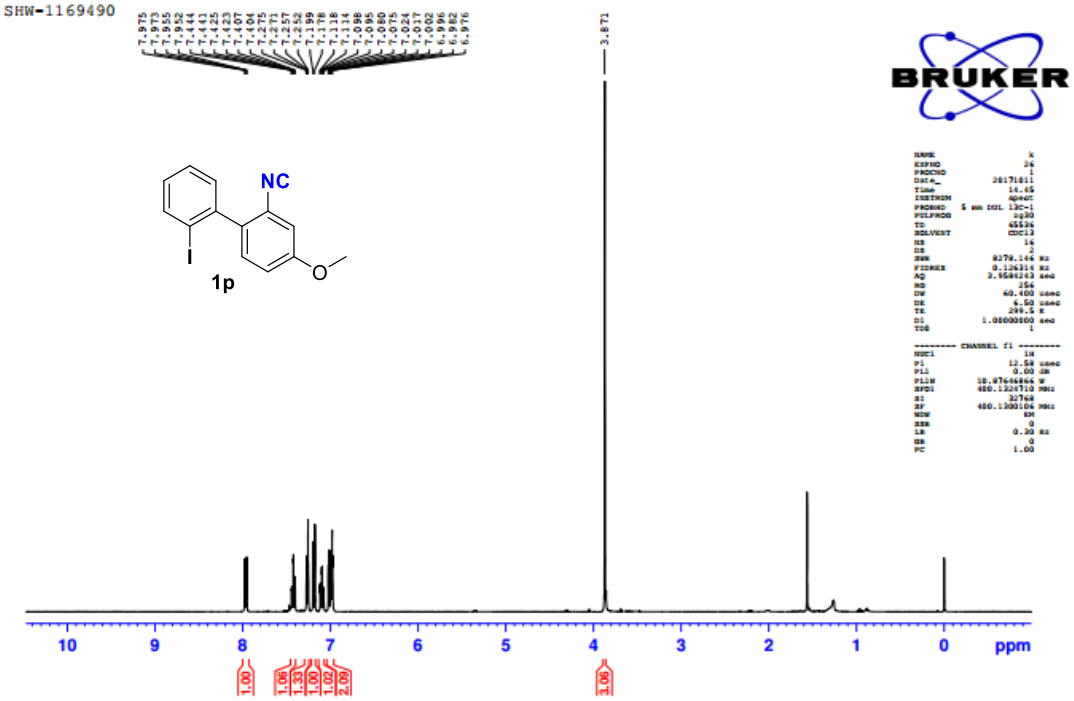
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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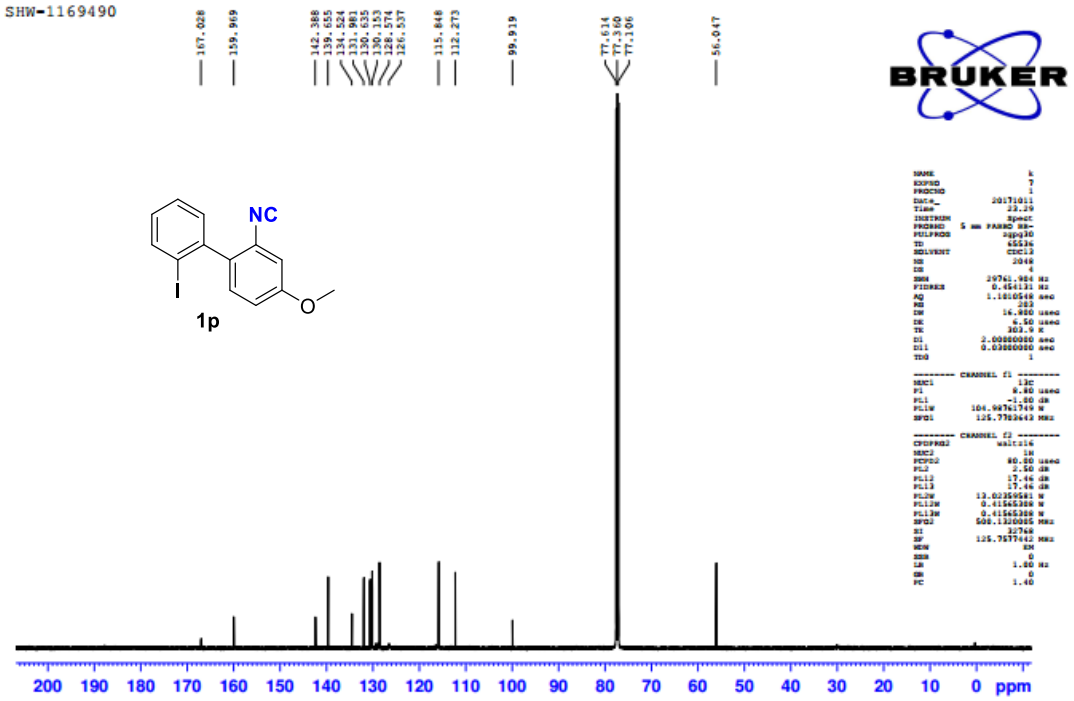
I
O
1p
ppm


SHW-1169490
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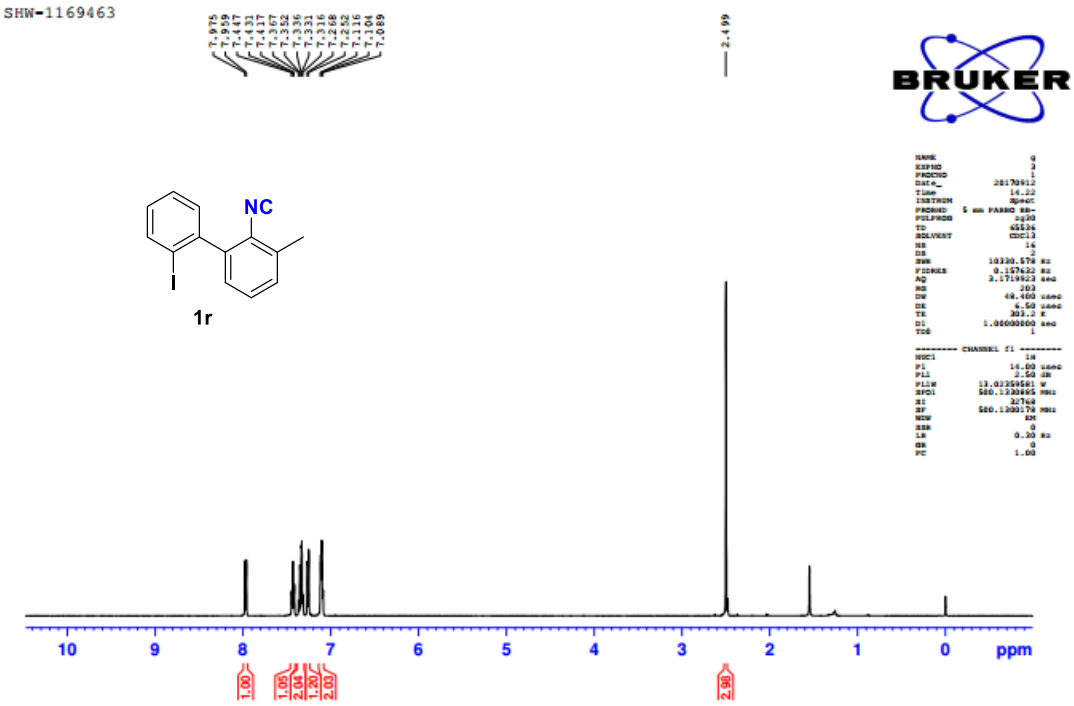
I
O
1p
ppm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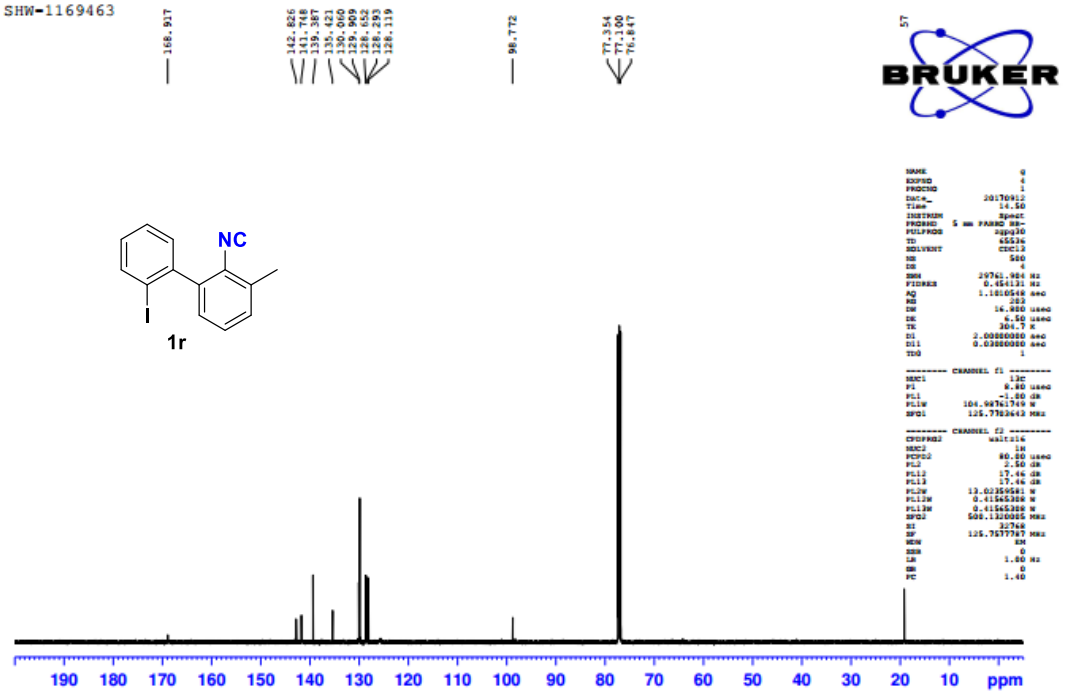
7.431
7.417
7.367
7.352
7.336
7.331
7.316
7.268
7.252
7.116
7.104
7.089
2.499
BRUKER
NC
I
1r
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.05
2.04
1.20
2.03
2.98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135.421
130.060
129.909
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128.293
128.139
98.772
77.354
77.100
76.847
BRUKER
NC
I
1r
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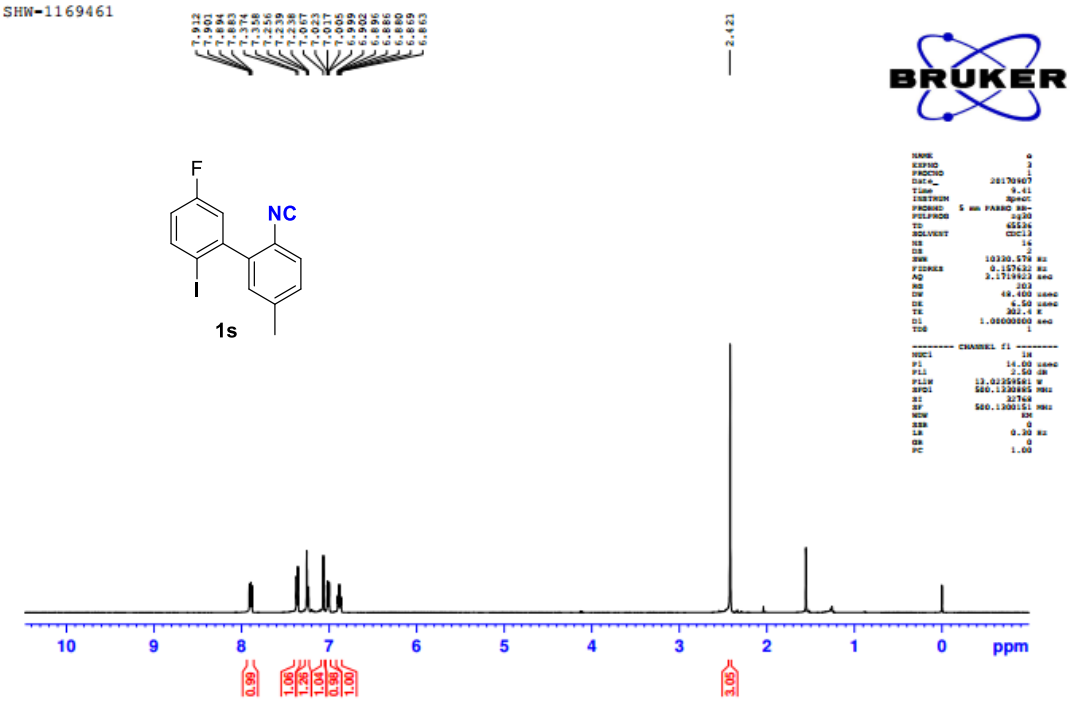
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.883
7.374
7.358
7.356
7.239
7.238
7.067
7.023
7.017
7.005
6.999
6.992
6.896
6.886
6.880
6.869
6.863
2.421
BRUKER
F
NC
I
1s
10
9
8
7
6
5
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3
2
1
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ppm
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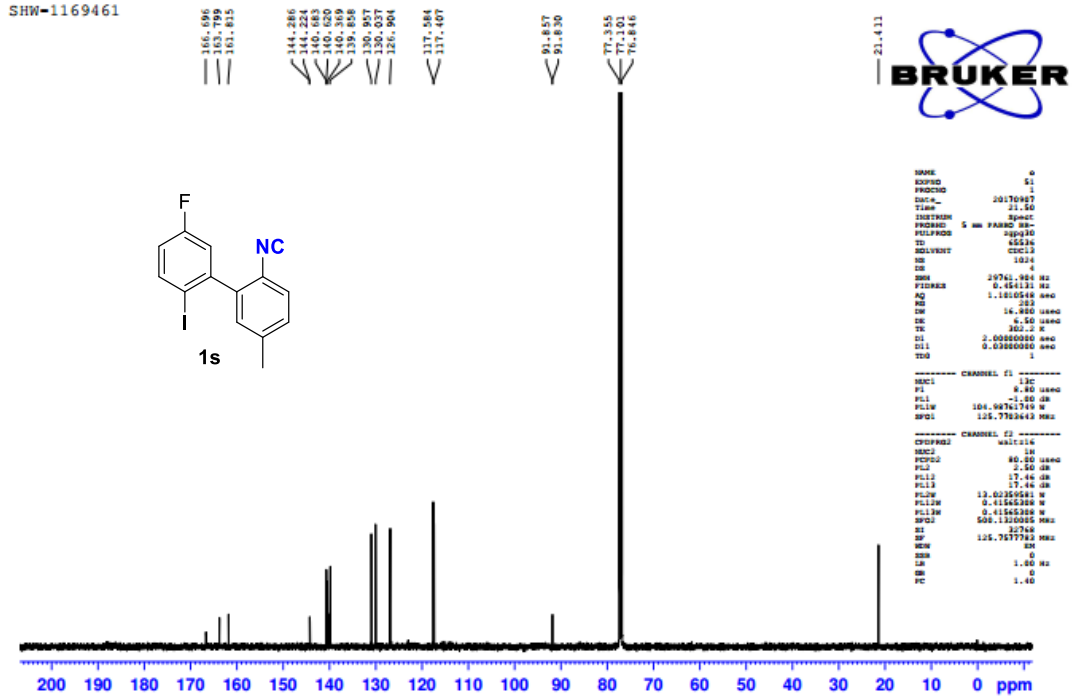
1.28
1.04
0.98
1.00
3.00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161.815
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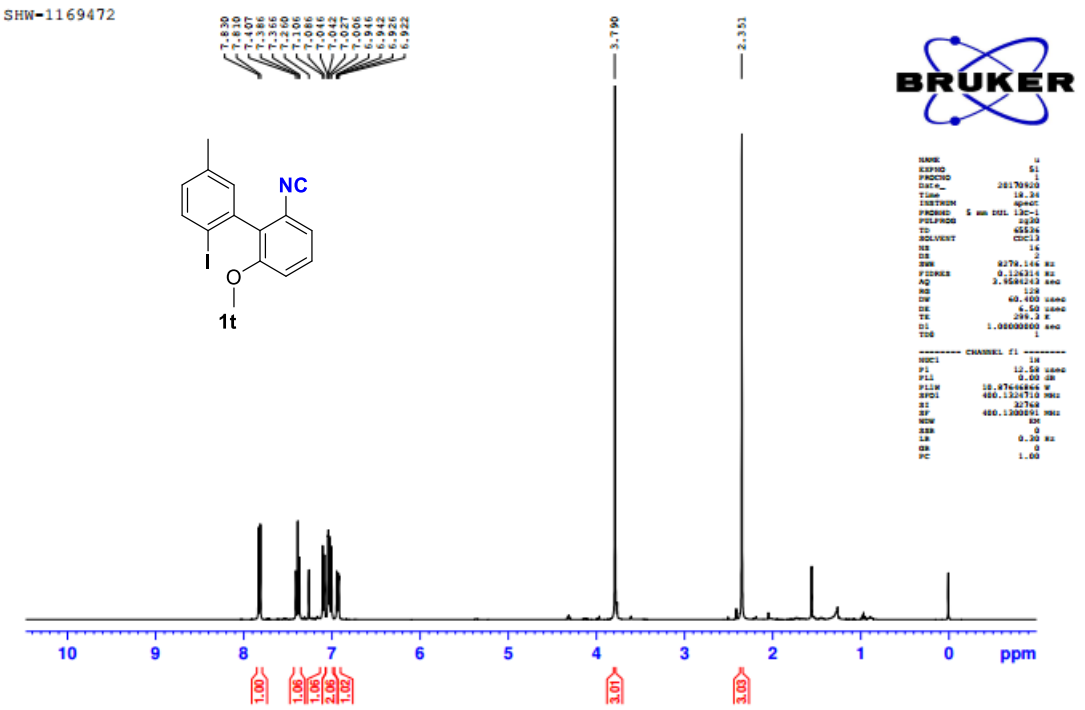
144.224
140.683
140.620
140.369
139.858
130.957
130.857
126.904
117.584
117.407
91.857
91.830
77.355
77.101
76.846
21.411
BRUKER
F
NC
I
1s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.407
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7.366
7.260
7.106
7.086
7.046
7.042
7.027
7.006
6.946
6.926
6.922
3.790
2.351
NC
I
O
1t
BRUKER
10
9
8
7
6
5
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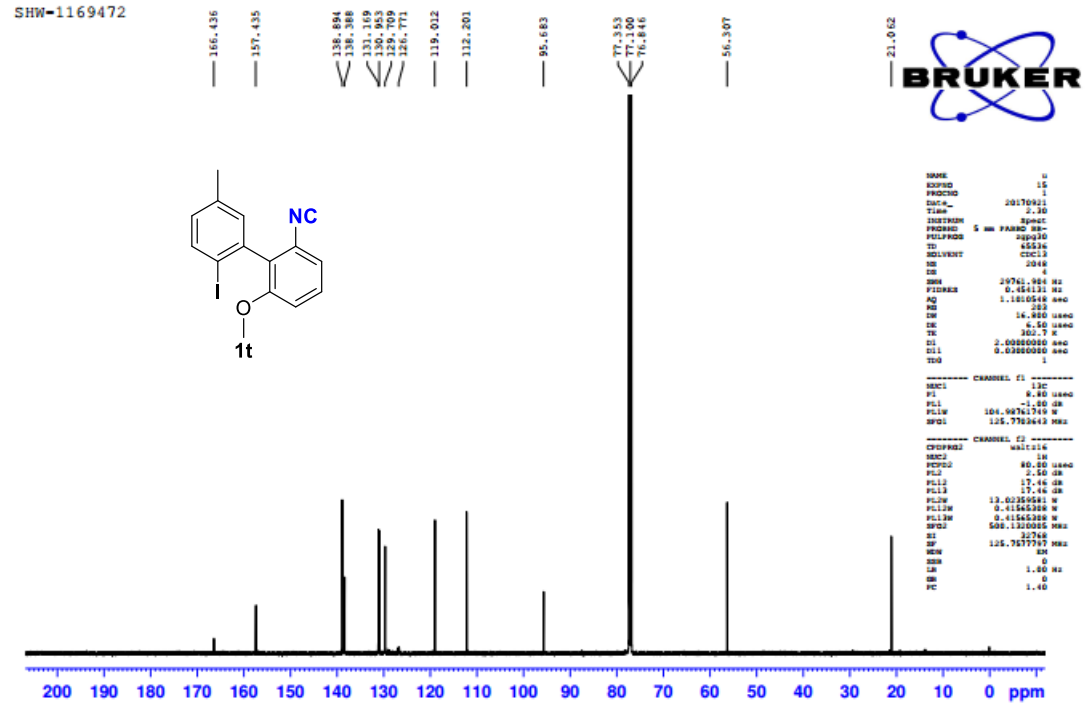
3
2
1
0
ppm
1.00
1.06
1.06
2.06
1.02
3.01
3.03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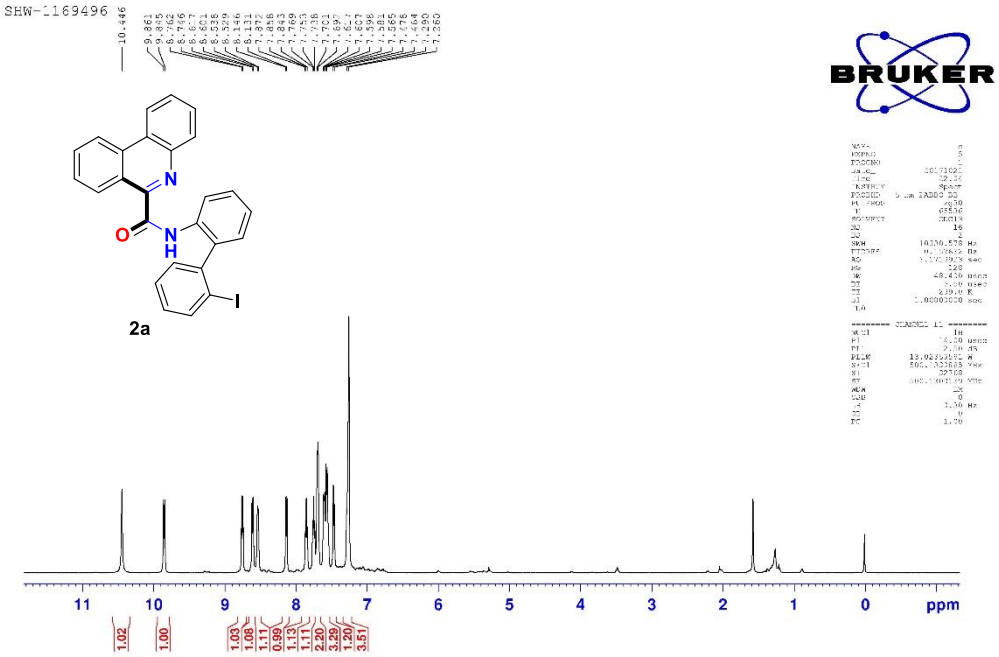
130.953
129.709
126.771
119.012
112.201
95.683
77.353
77.100
76.846
56.307
21.062
NC
I
O
1t
BRUKER
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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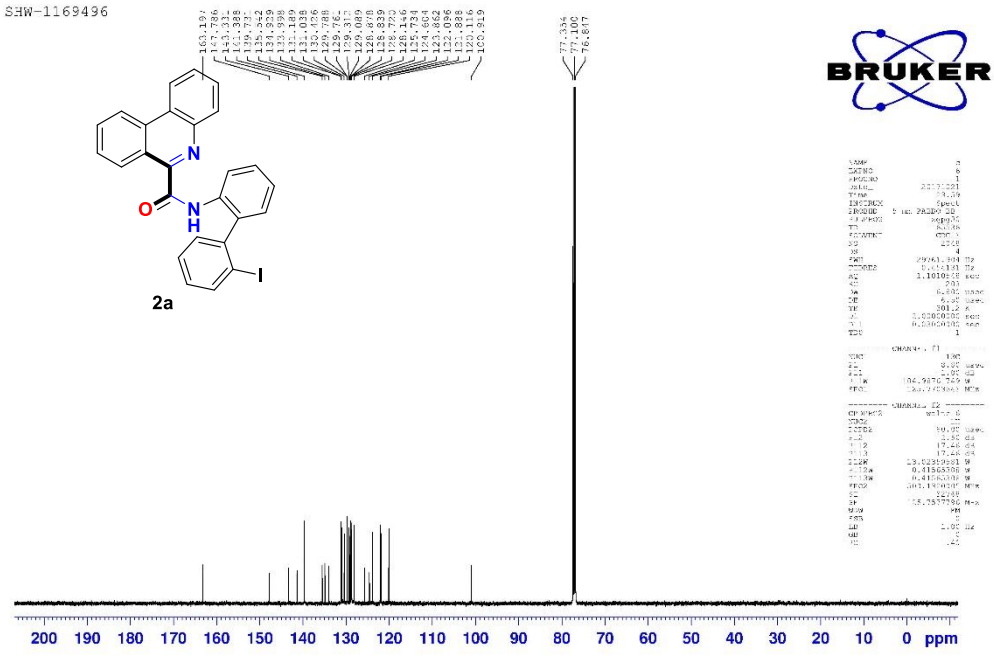
ppm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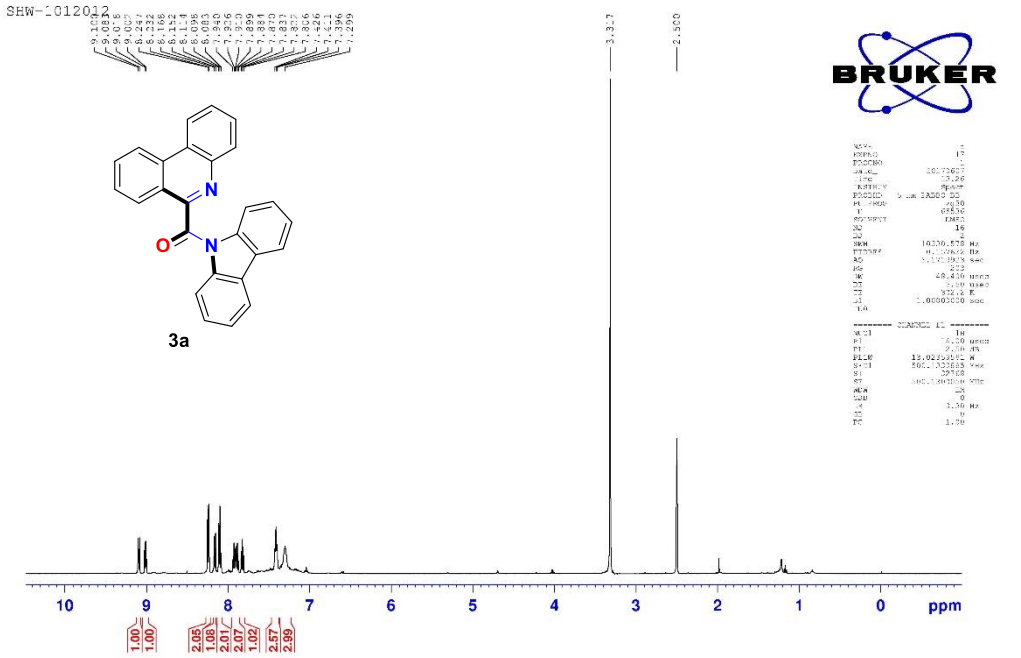
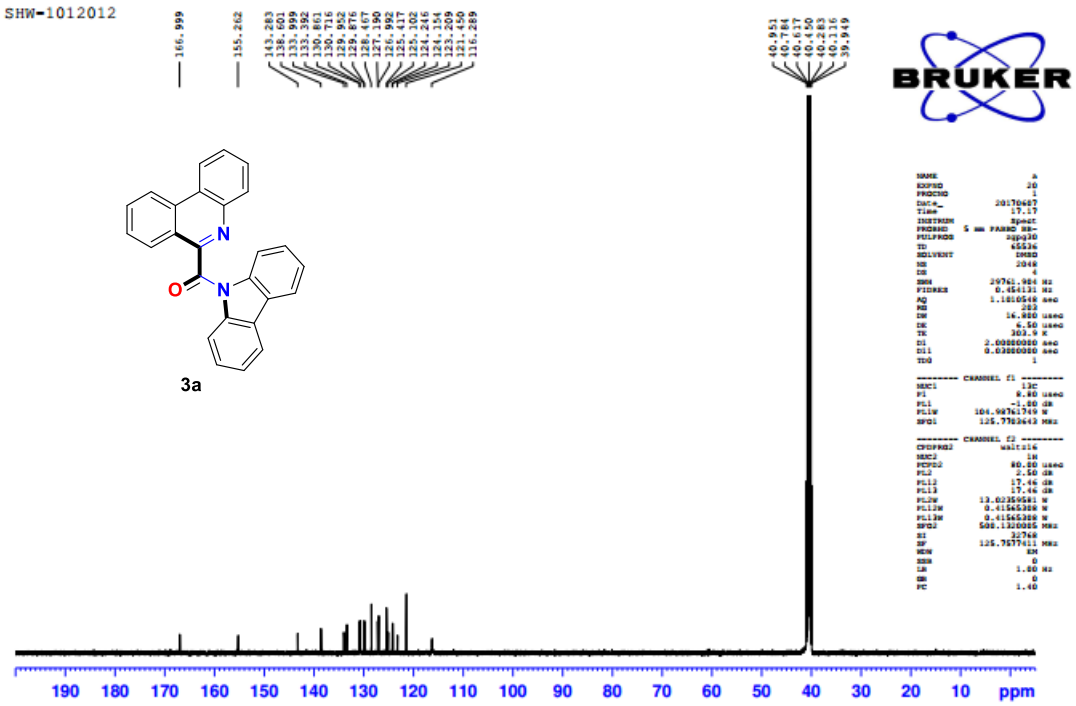
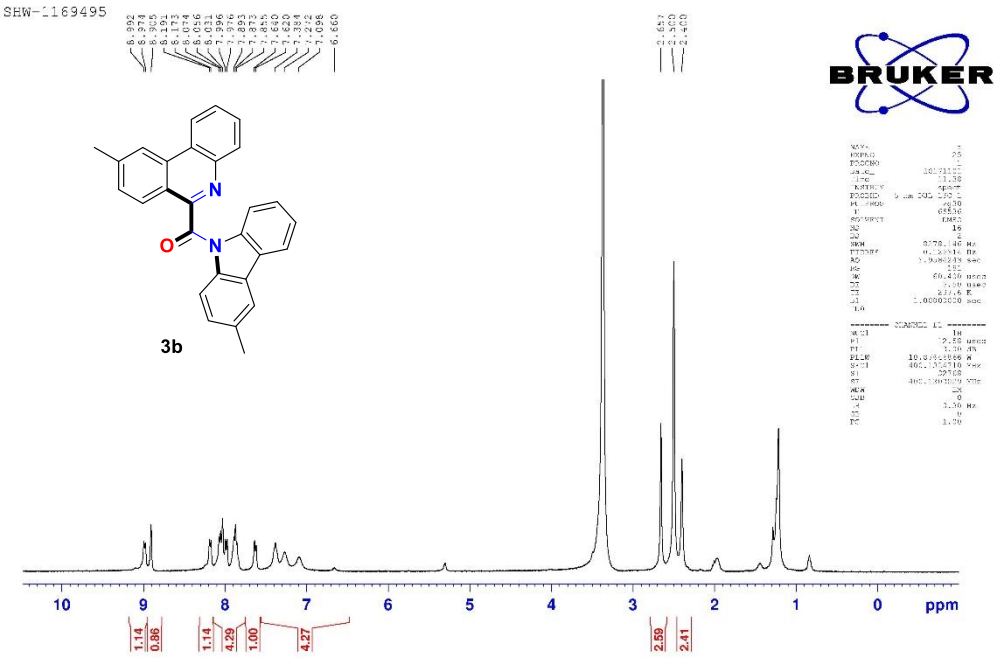
2a
ppm


SHW-1012012
3a
ppm


SHW-1012012
3a
ppm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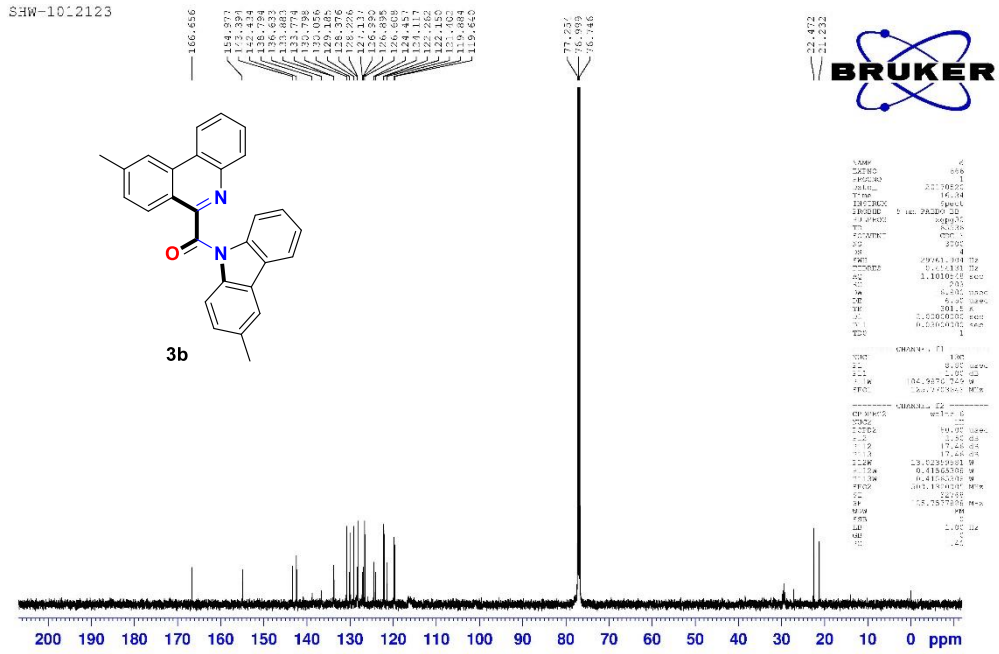
10
9
8
7
6
5
4
3
2
1
0
ppm


SHW-1012123
3b
200
190
180
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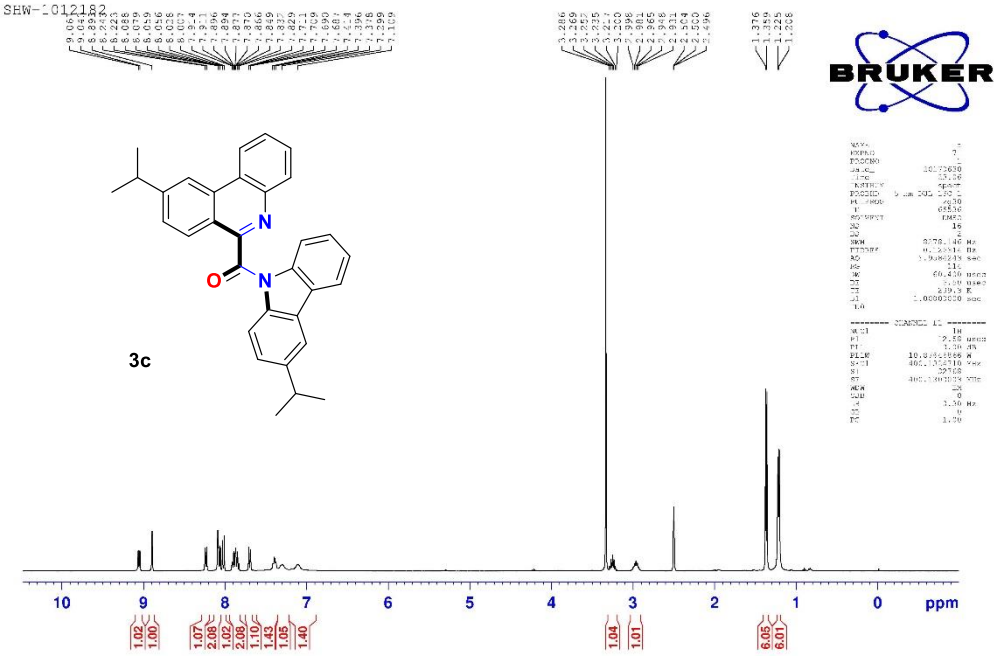
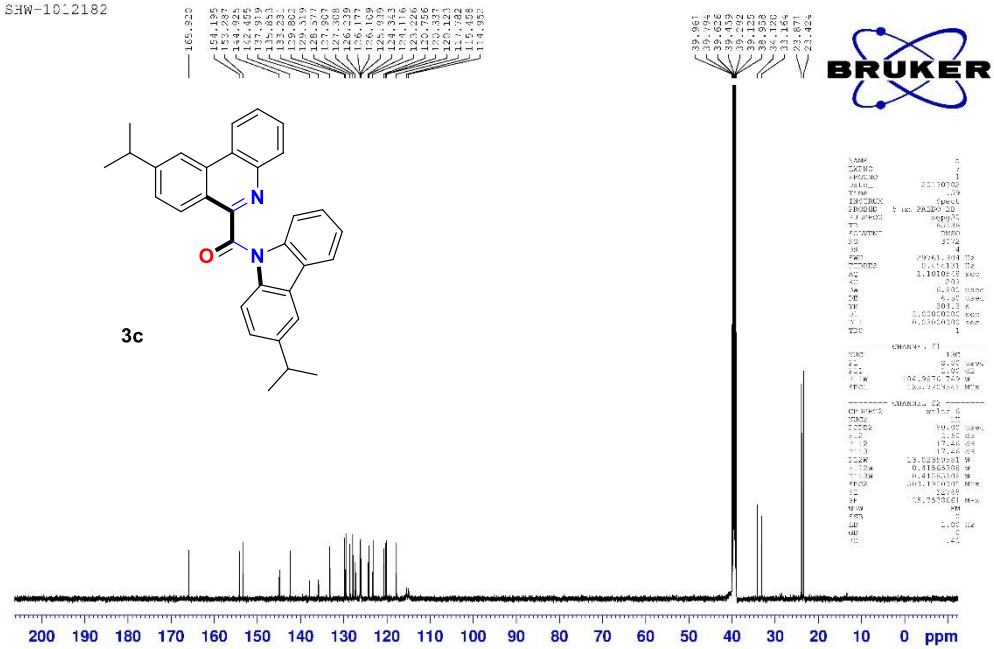
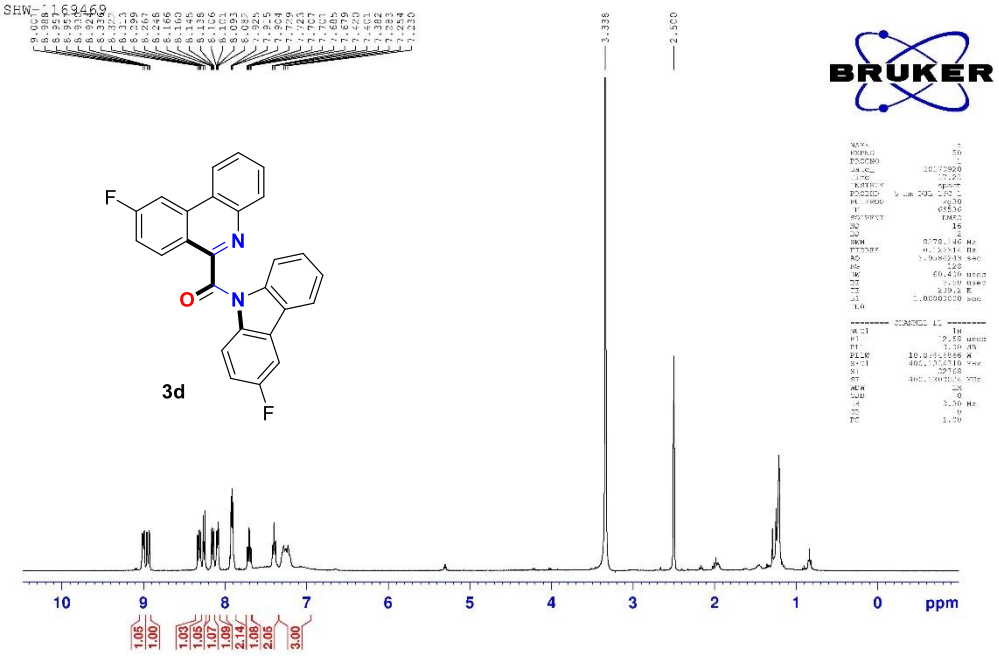
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


SHW-1012182
3c
BRUKER
10
9
8
7
6
5
4
3
2
1
0
ppm


SHW-1012182
3c
BRUKER
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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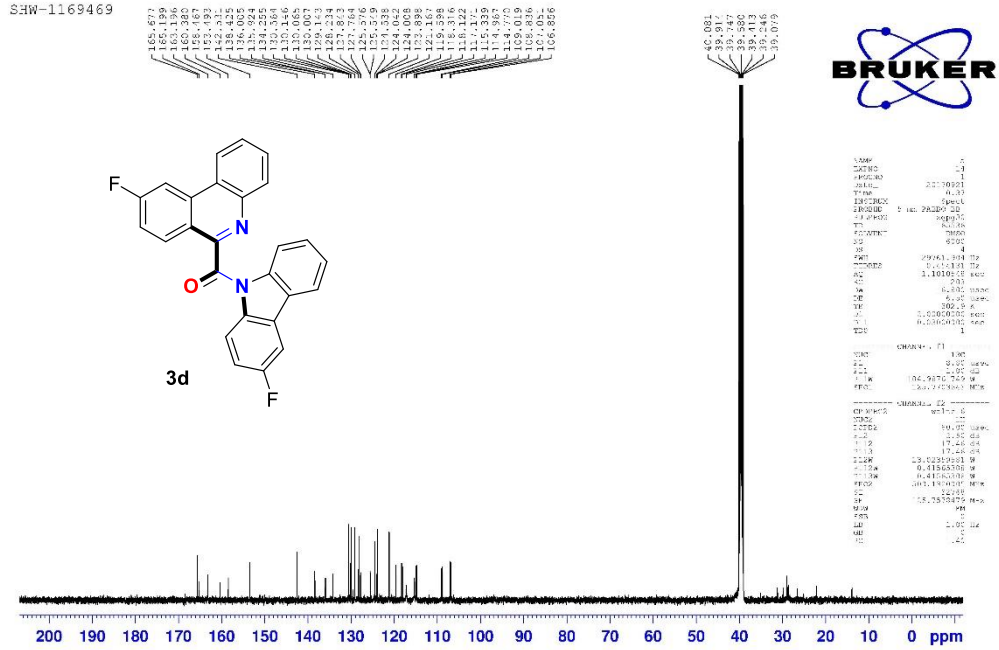
3d
10 9 8 7 6 5 4 3 2 1 0 ppm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3d
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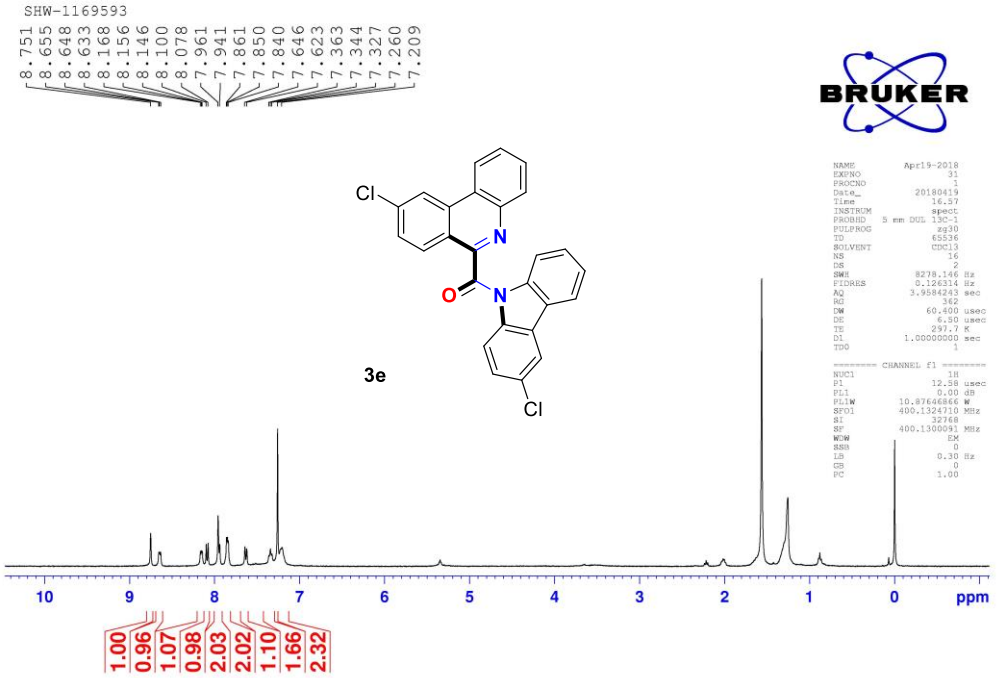
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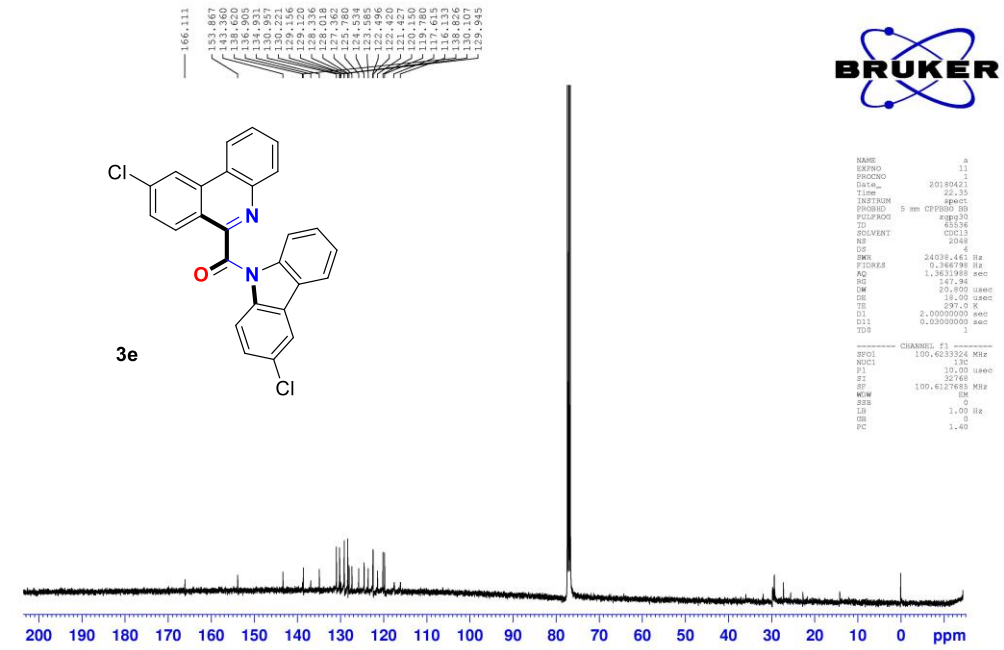
8.168
8.156
8.146
8.100
8.078
7.961
7.941
7.861
7.850
7.840
7.646
7.623
7.363
7.344
7.327
7.260
7.209
BRUKER
Cl
N
O
N
Cl
3e
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.96
1.07
0.98
2.03
2.02
1.10
1.66
2.32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143.360
138.620
136.905
134.951
130.221
129.156
129.120
128.786
128.018
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125.780
124.534
123.885
122.496
122.420
121.427
120.150
119.780
117.615
116.133
138.826
130.107
129.945
BRUKER
Cl
N
O
N
Cl
3e
200
190
180
170
160
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140
130
120
110
100
90
80
70
60
50
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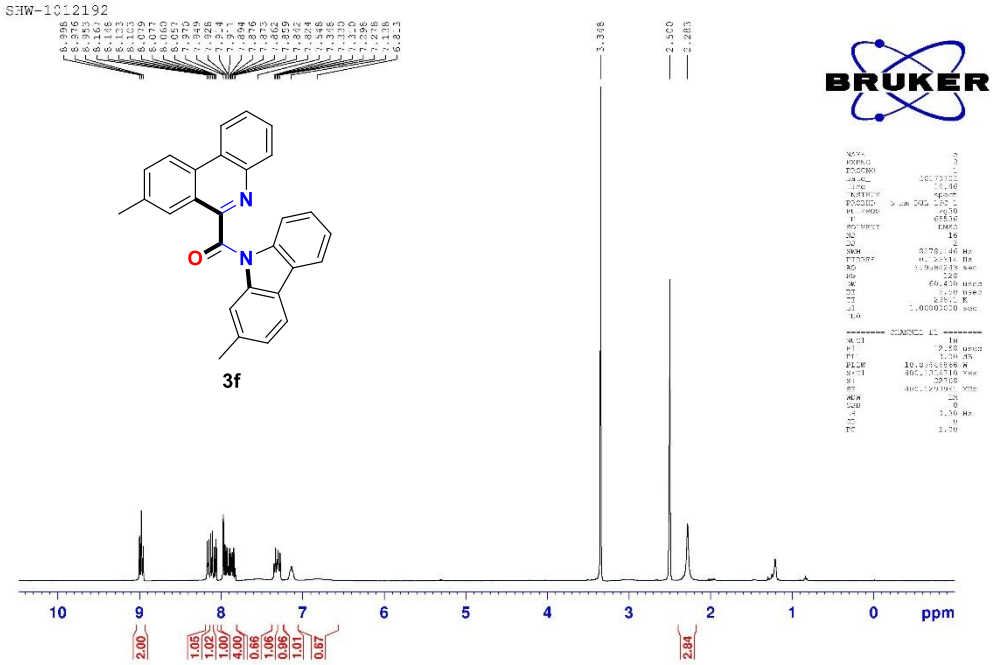
30
20
10
0
ppm


SHW-1012192
3f
10
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8
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6
5
4
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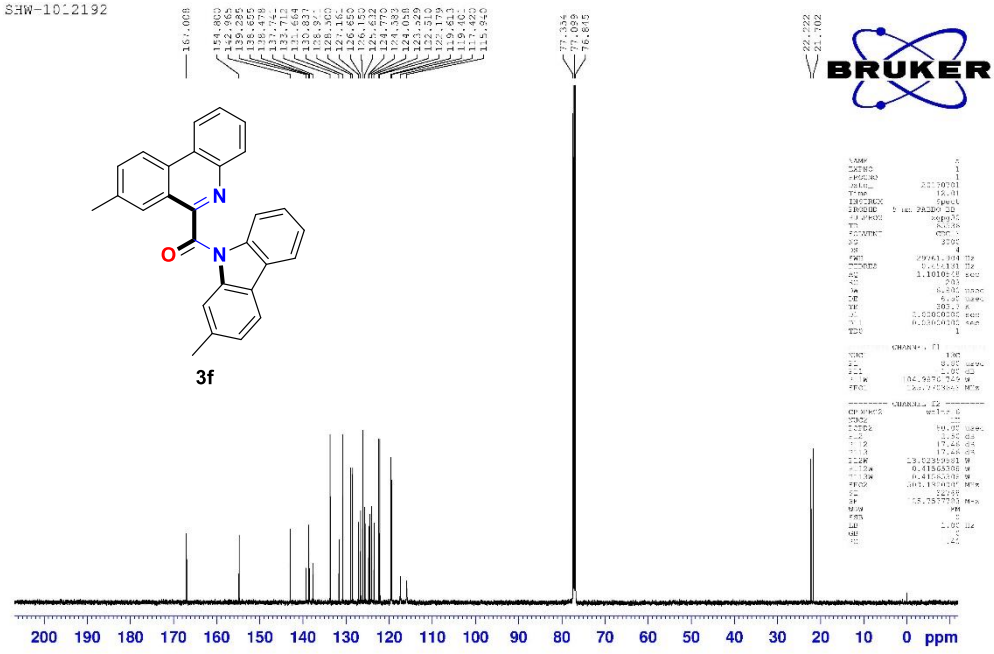
2
1
0
ppm


SHW-1012192
3f
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60
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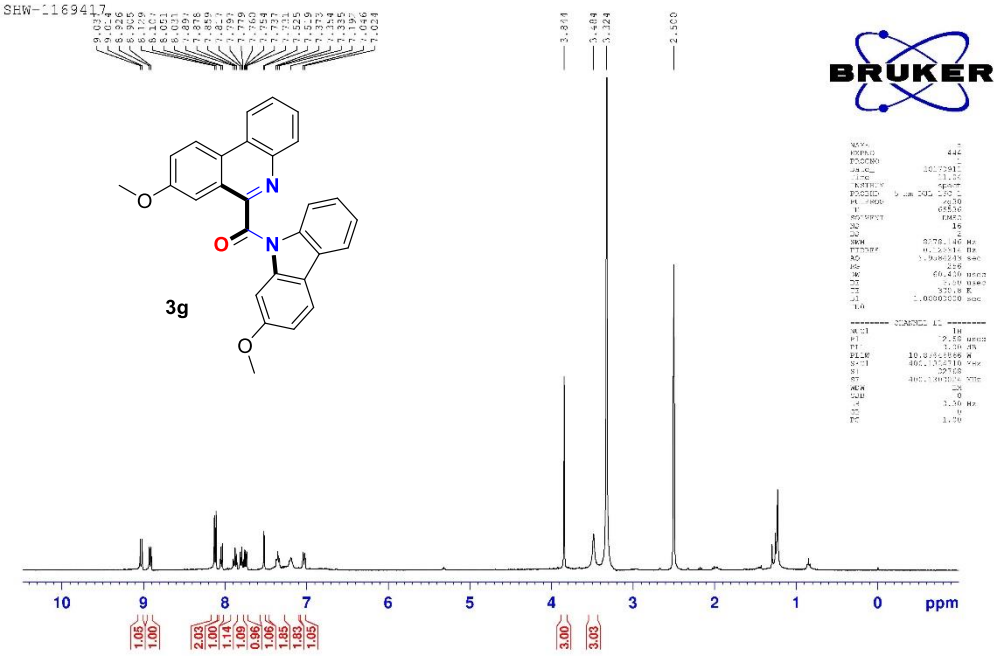
30
20
10
0
ppm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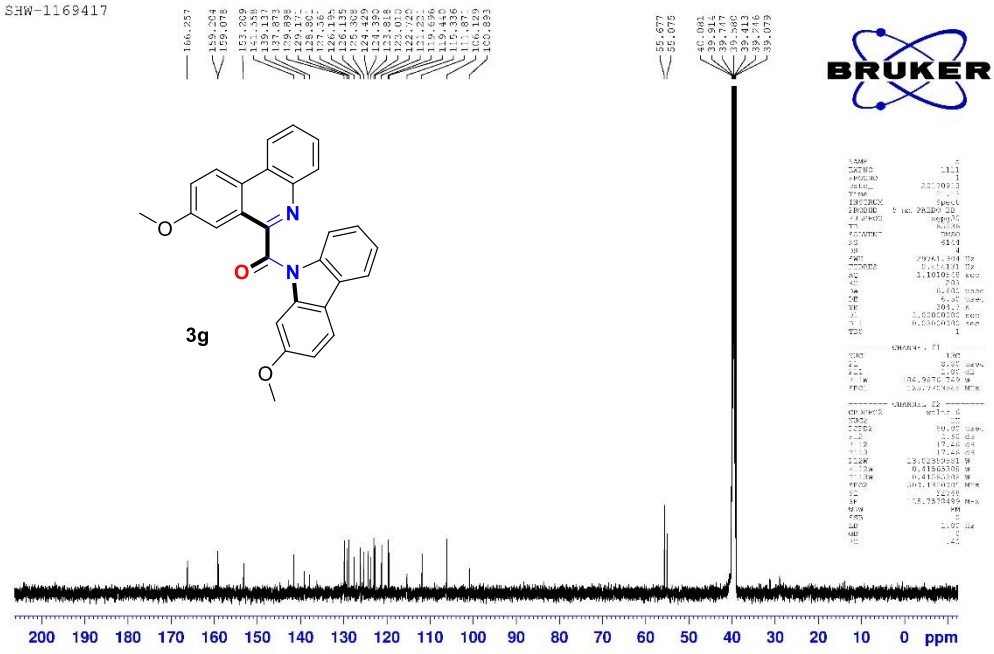
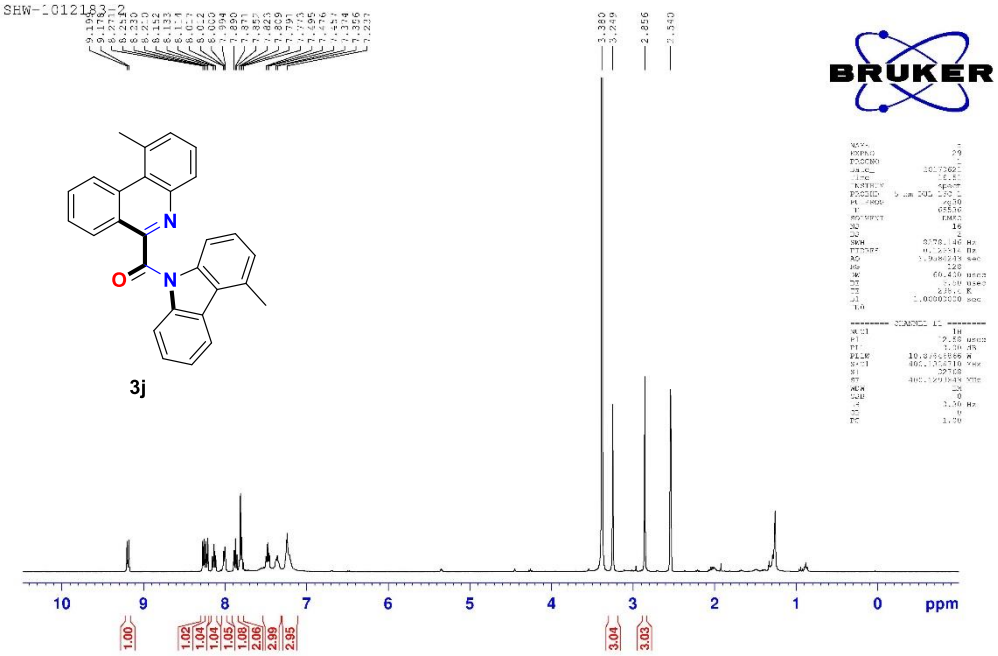
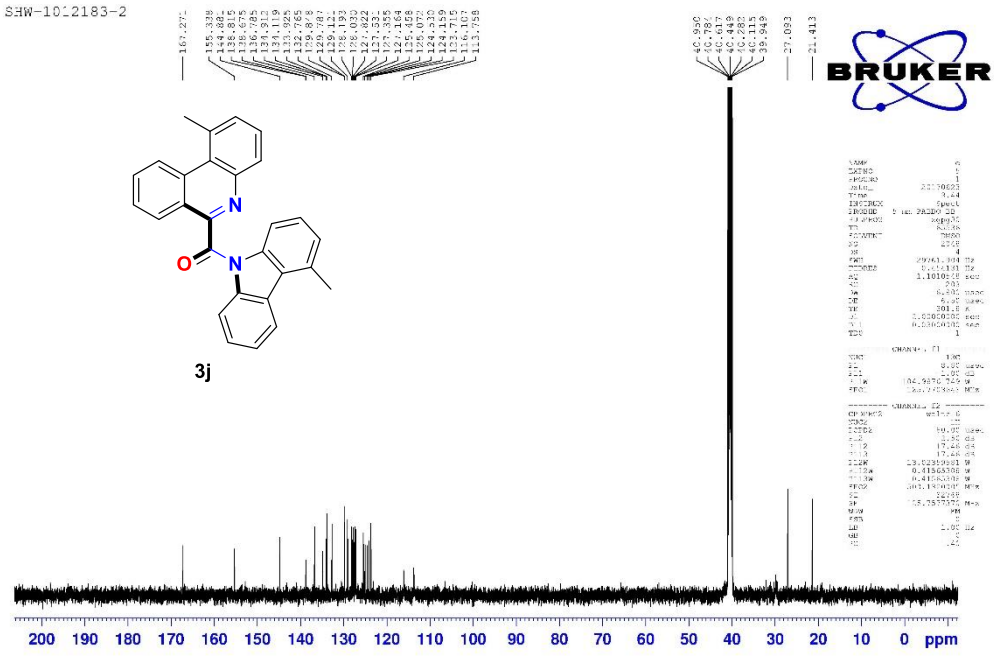
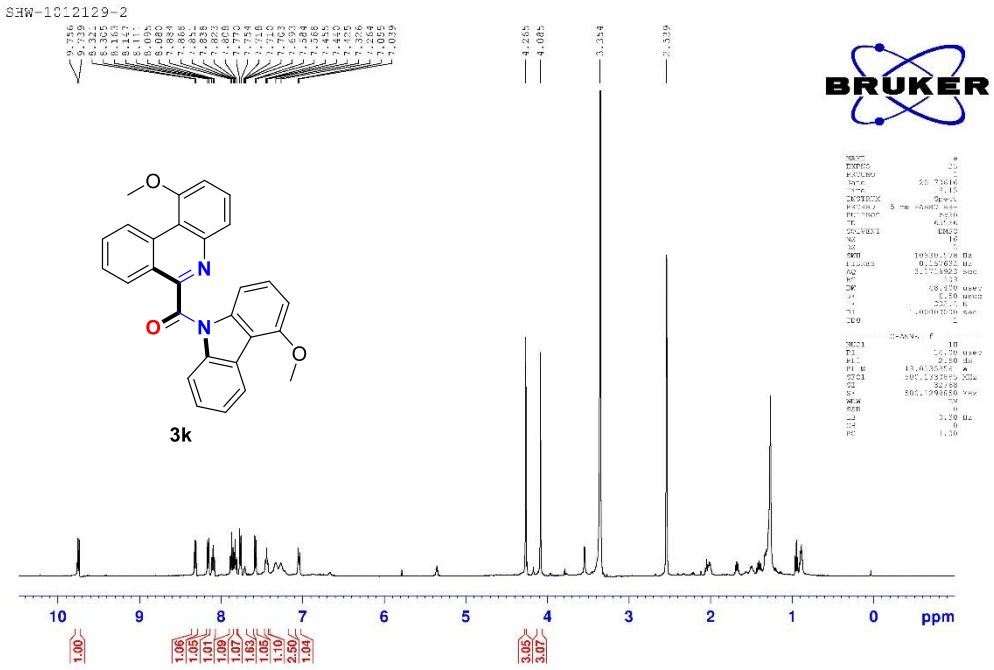
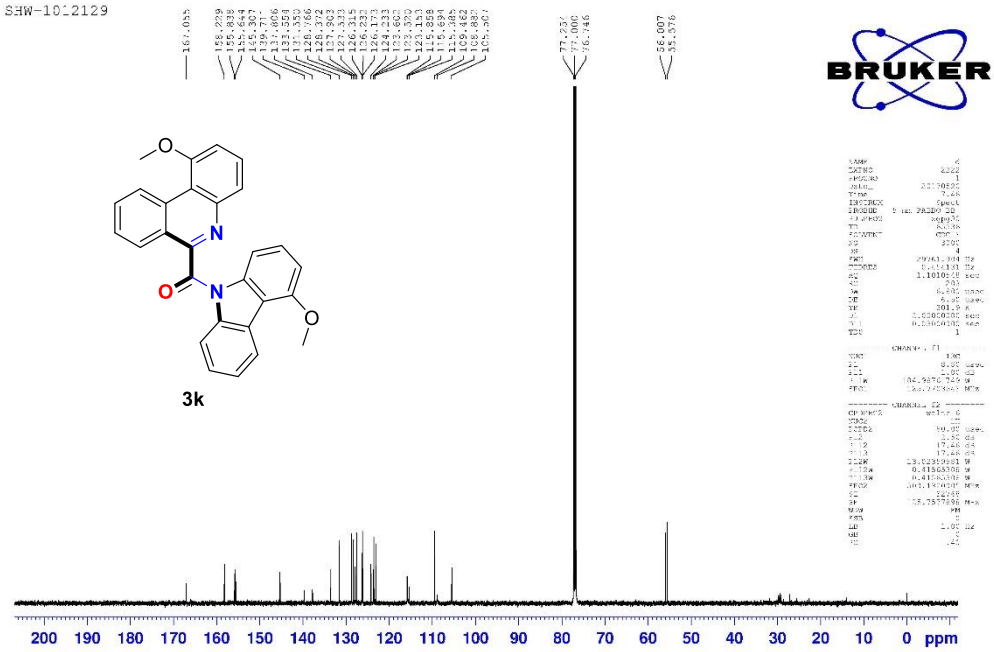
3g
BRUKER
10 9 8 7 6 5 4 3 2 1 0 ppm

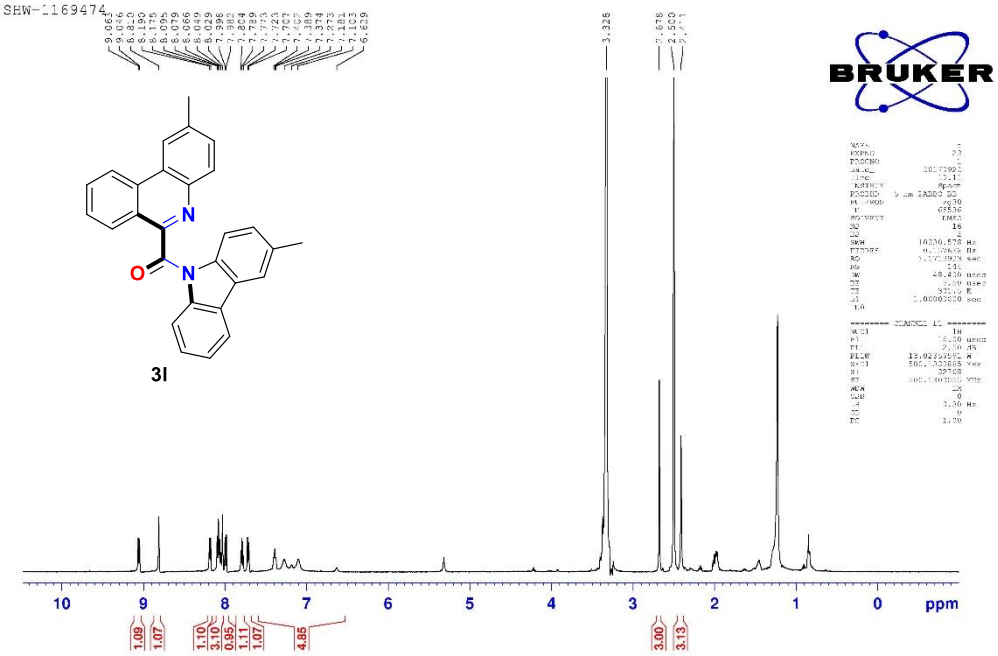

SHW-1169417
3g
BRUKER
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

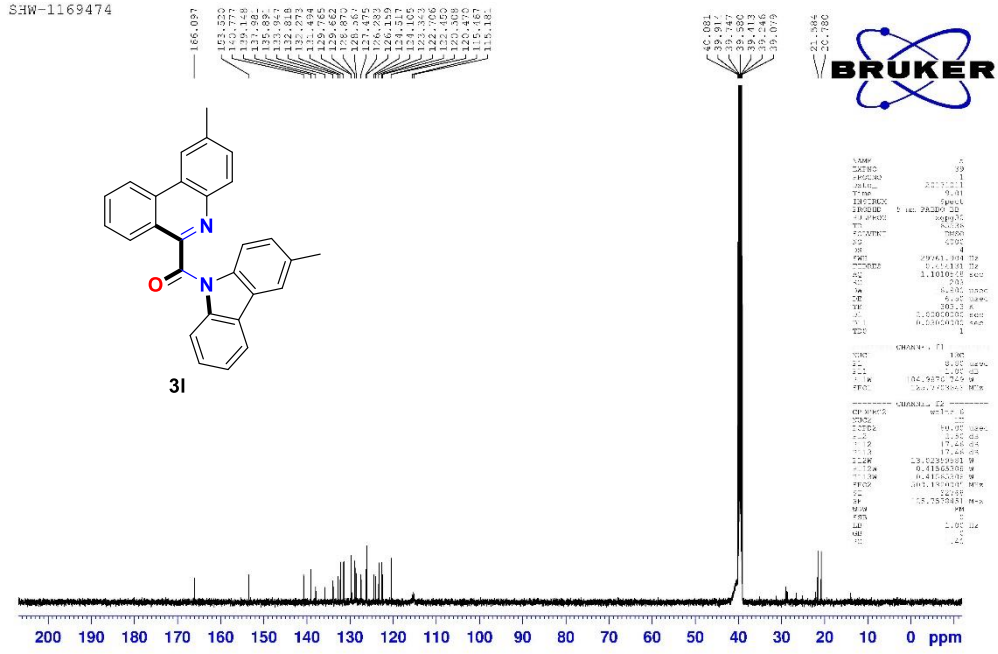

SHW-1012183-2
3j
BRUKER
10
9
8
7
6
5
4
3
2
1
0
ppm

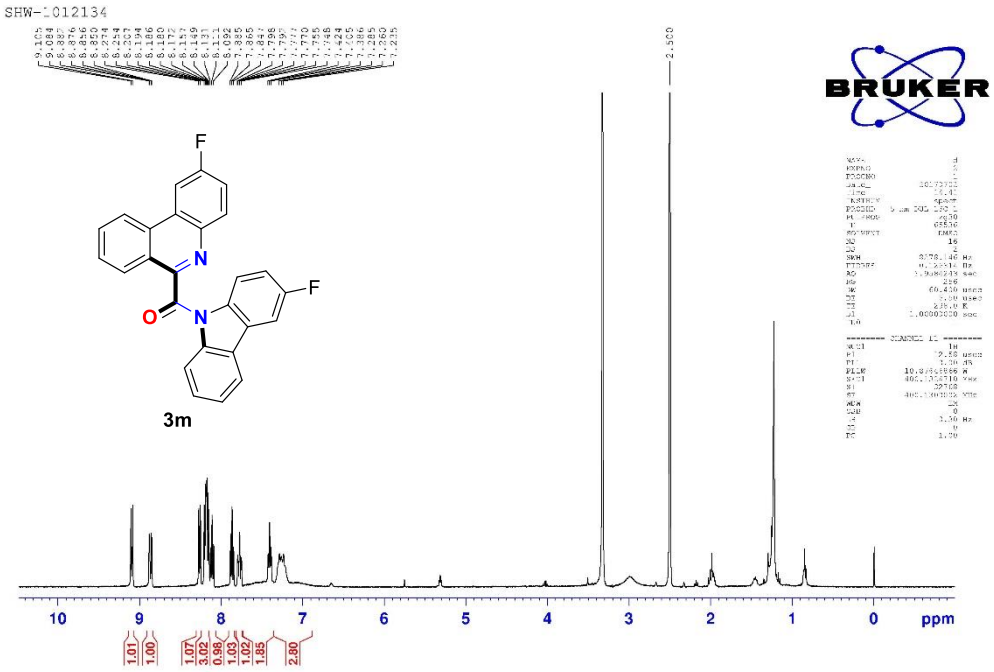

SHW-1012183-2
3j
BRUKER
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

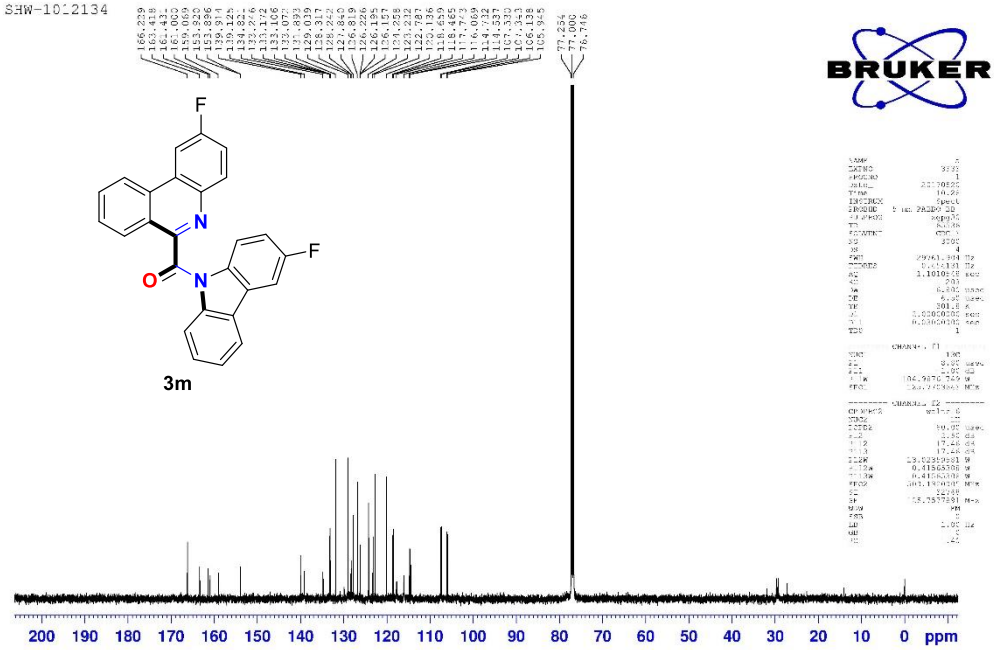

SHW-1012129-2
3k
10
9
8
7
6
5
4
3
2
1
0
ppm

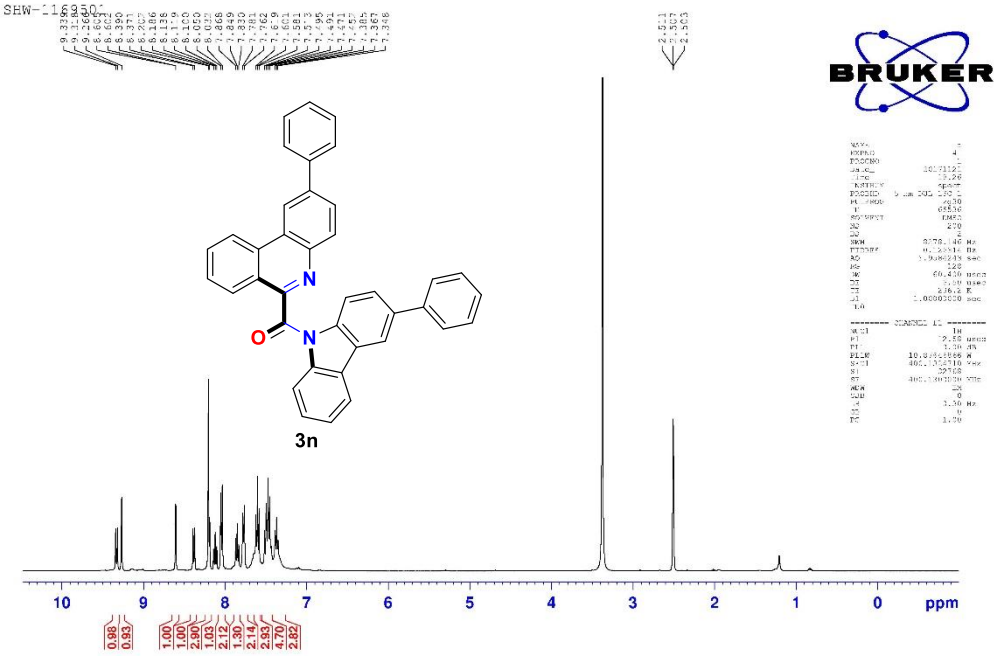

SHW-1012129
3k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

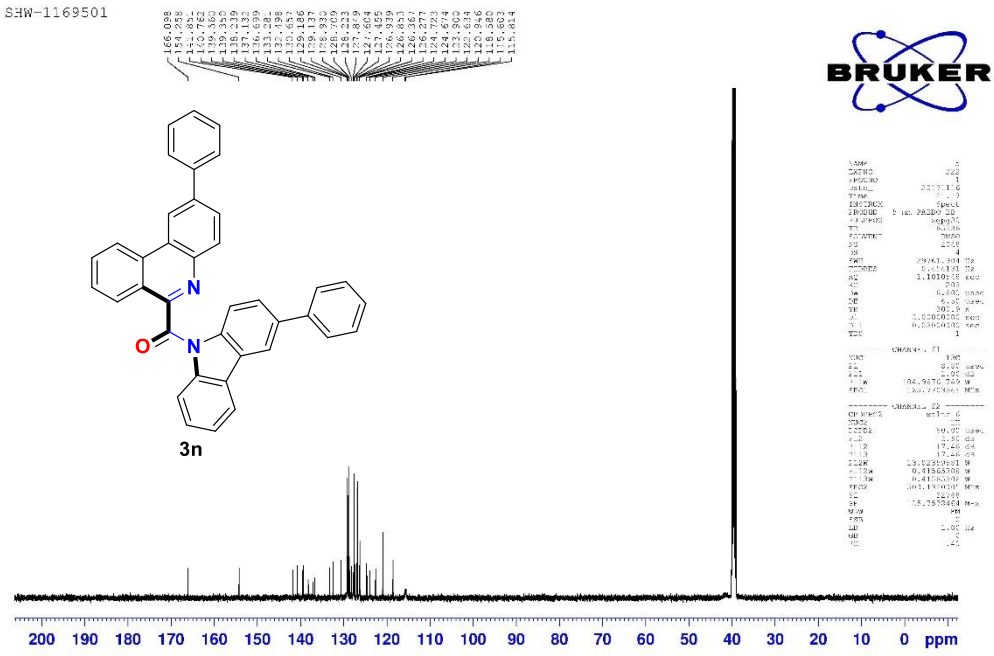

SHW-1169474
3l
BRUKER
10 9 8 7 6 5 4 3 2 1 0 ppm

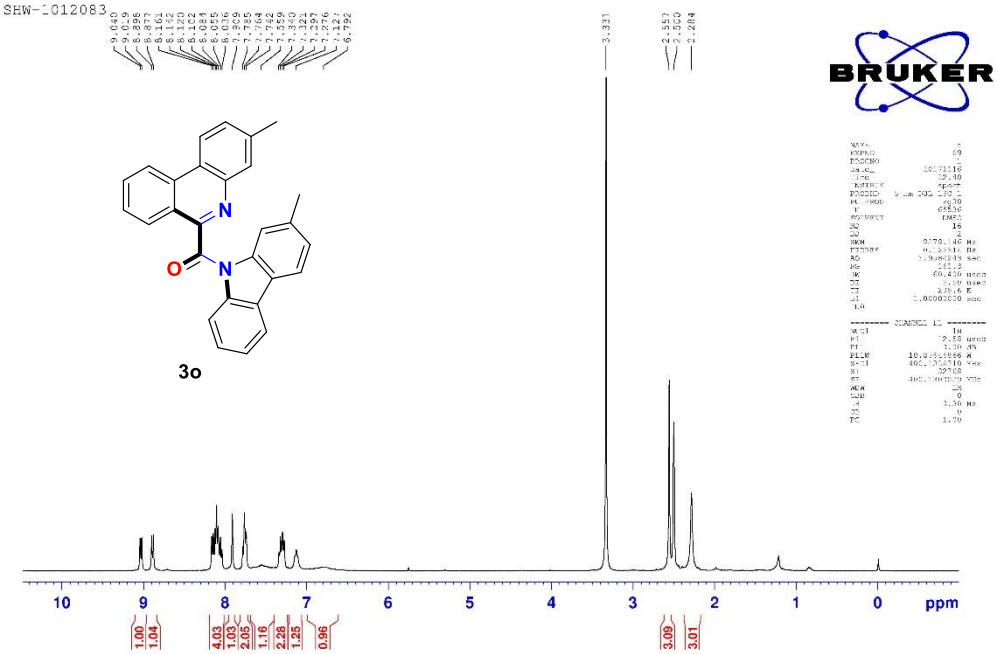

SHW-1169474
3l
BRUKER
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

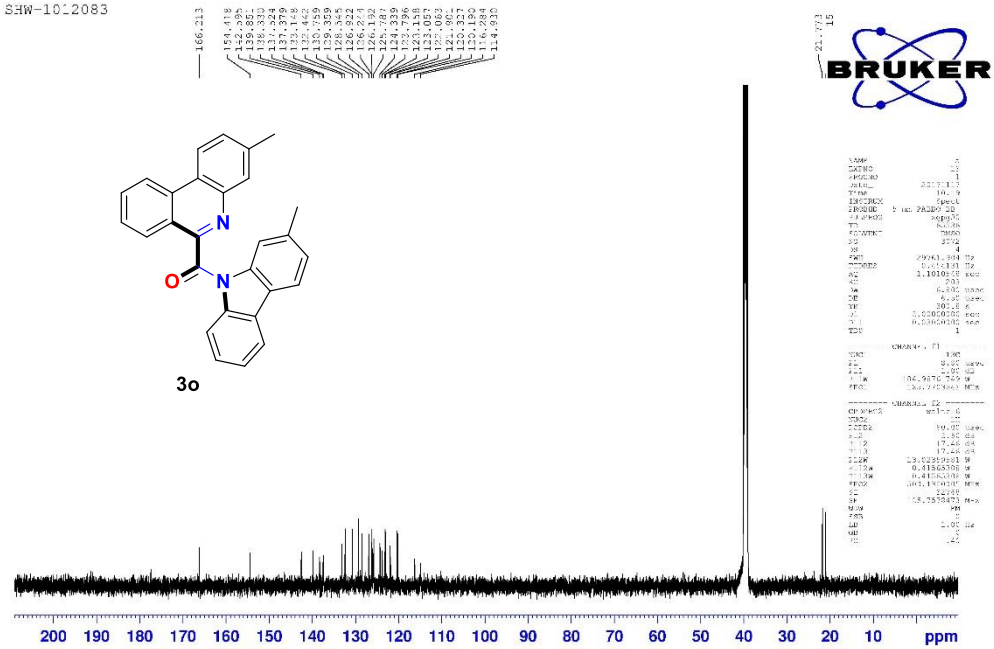

SHW-1012134
F
N
O
N
F
3m
2.960
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.00
1.07
3.02
0.98
1.03
1.02
1.85
2.80

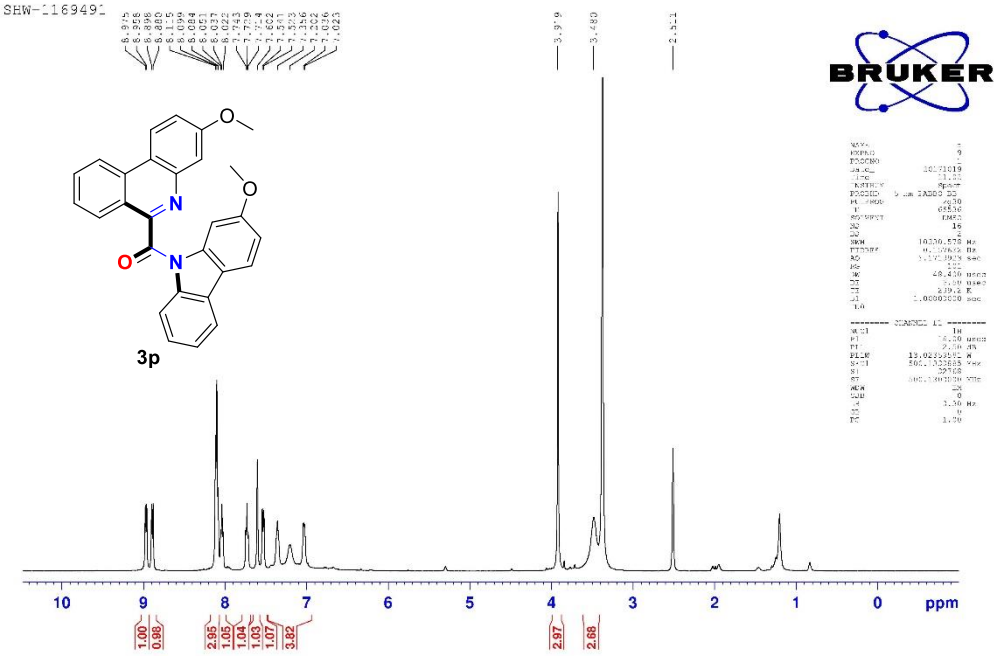

SHW-1012134
F
N
O
N
F
3m
77.254
77.000
76.746
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

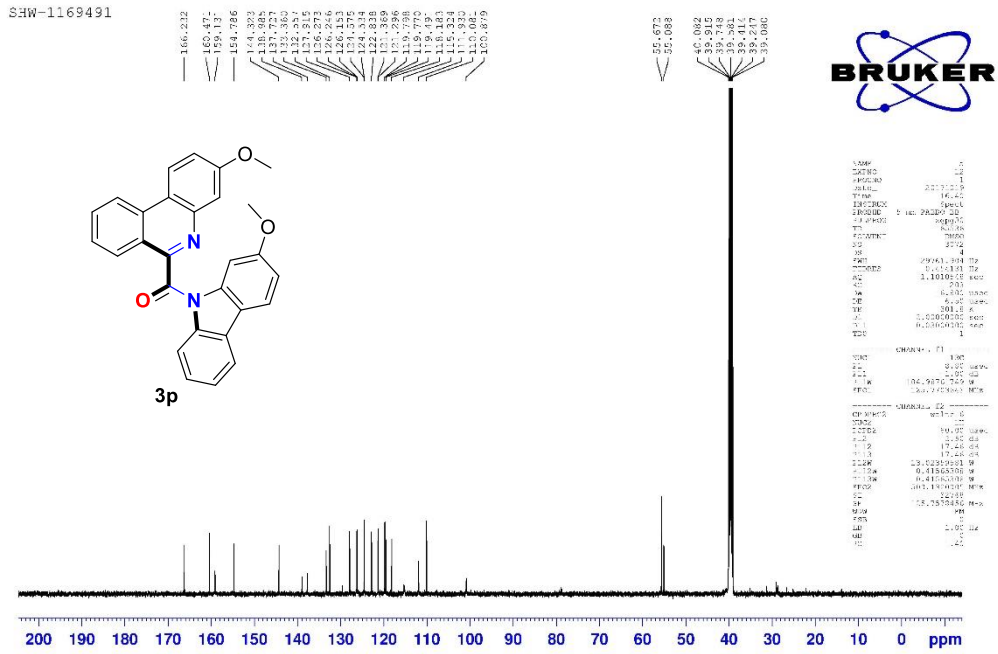

3n
ppm

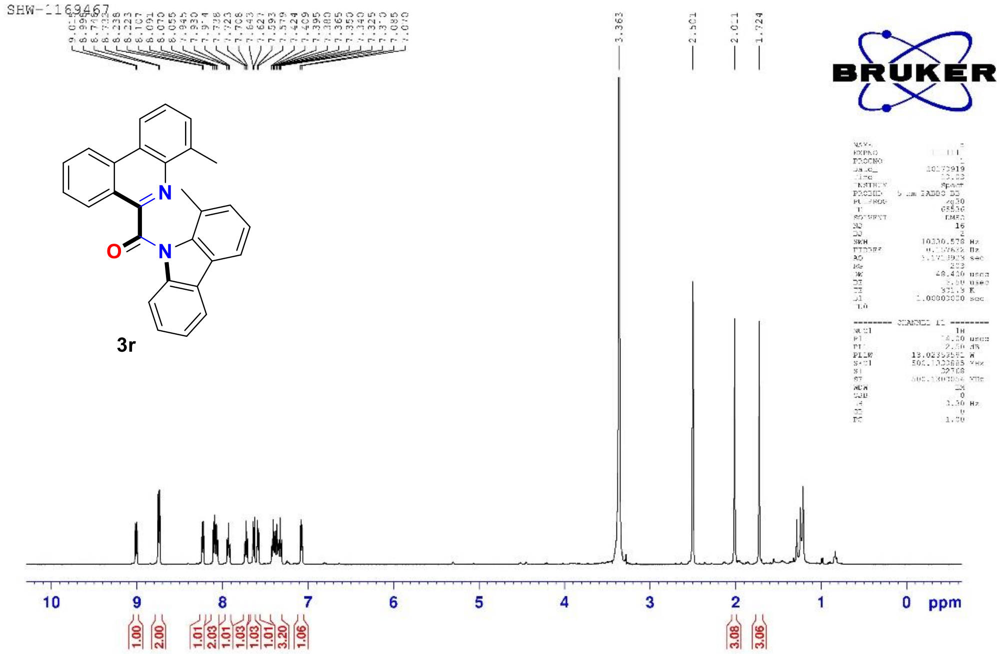

SHW-1169501
3n
ppm

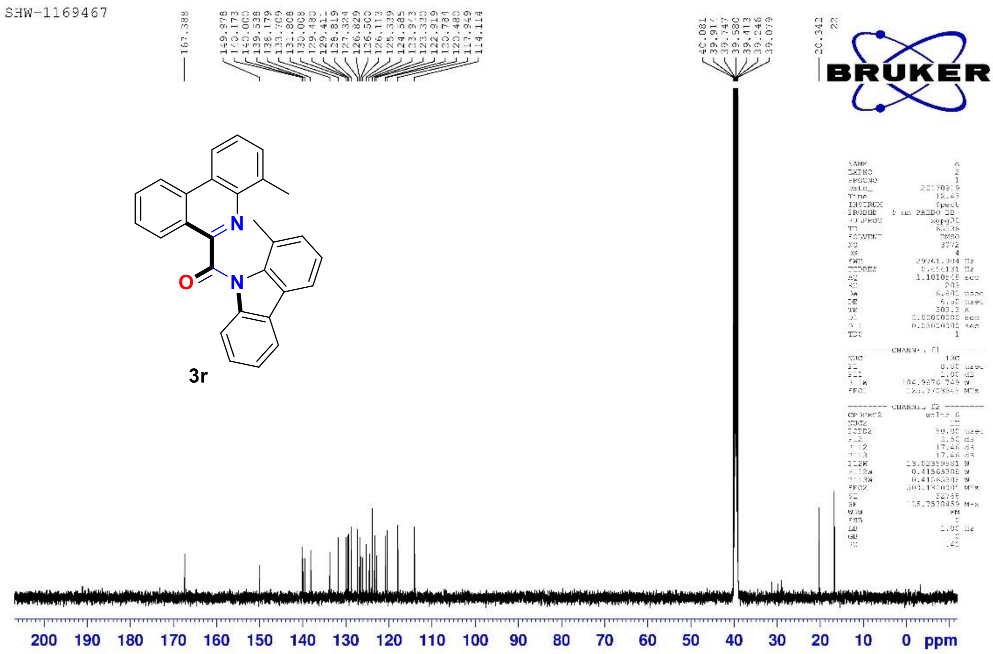

SHW-1012083
3o
ppm

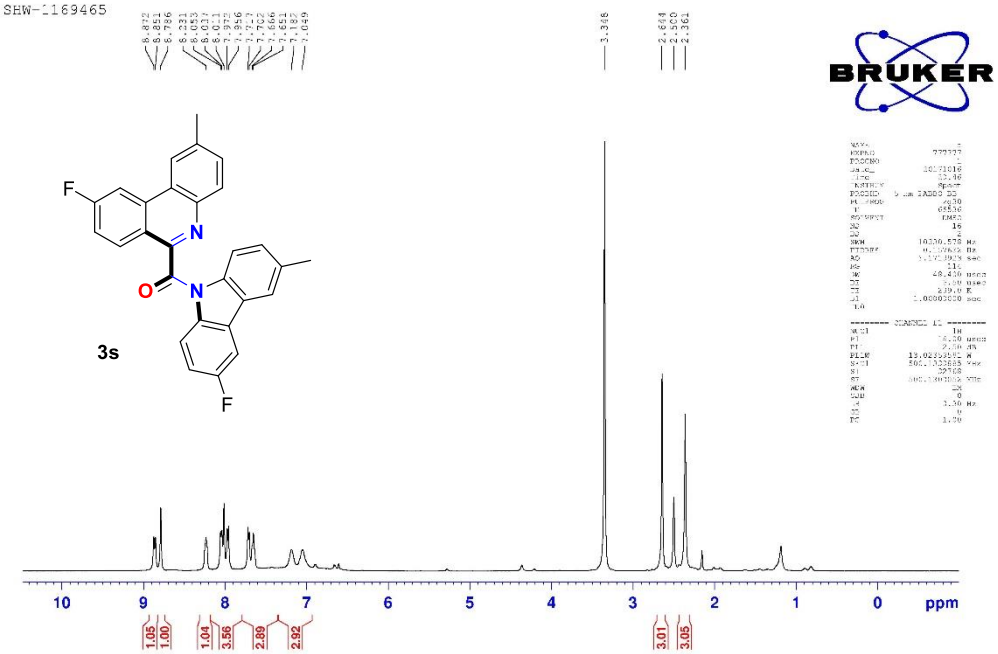

SHW-1012083
3o
ppm

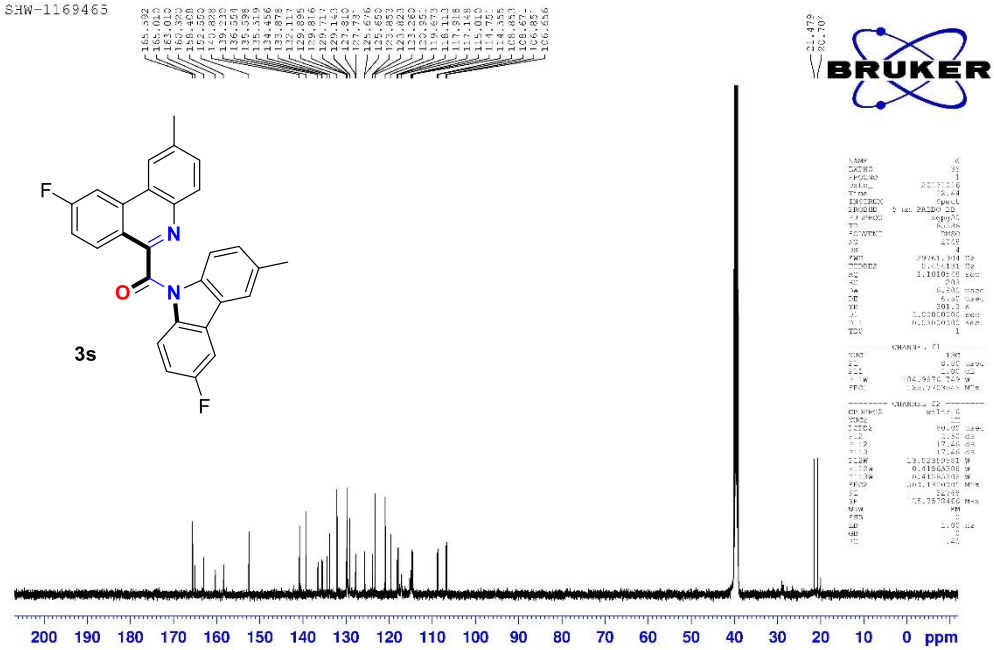

SHW-1169491
3p
10
9
8
7
6
5
4
3
2
1
0
ppm

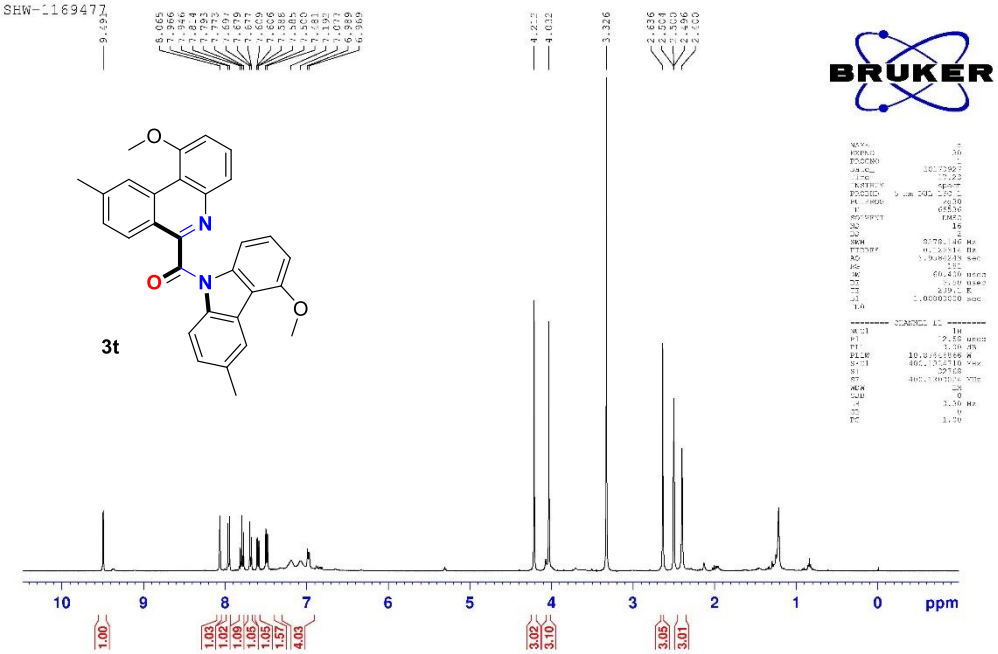

SHW-1169491
3p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

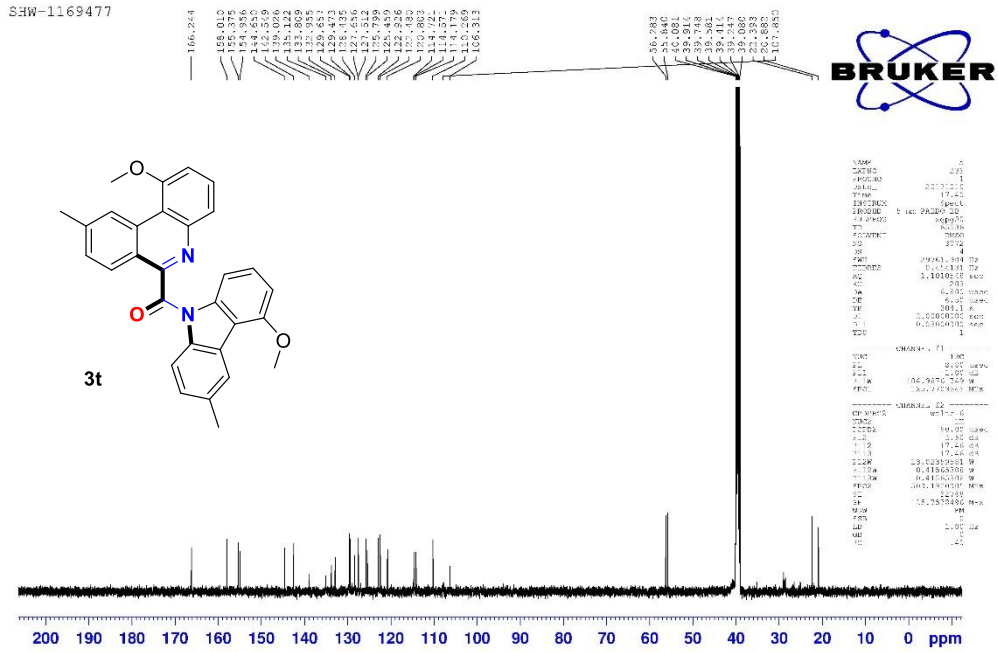

SHW-1169467
BRUKER
3r
3.363
2.501
2.011
1.724
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
2.00
1.01
2.03
1.01
1.03
1.03
1.01
3.20
1.06
3.08
3.06

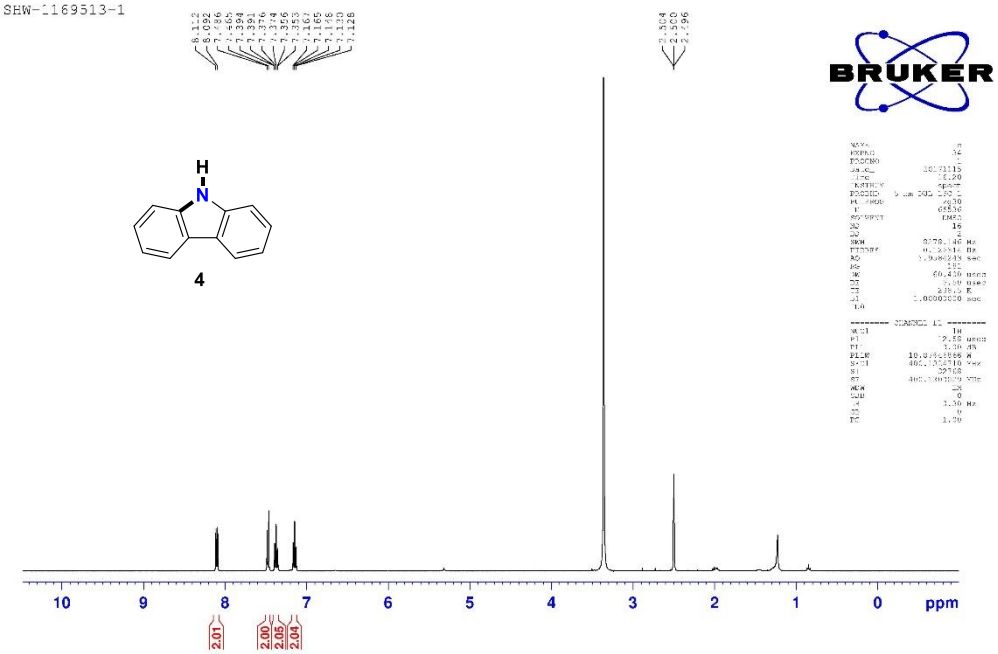

SHW-1169467
BRUKER
3r
167.388
20.342
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

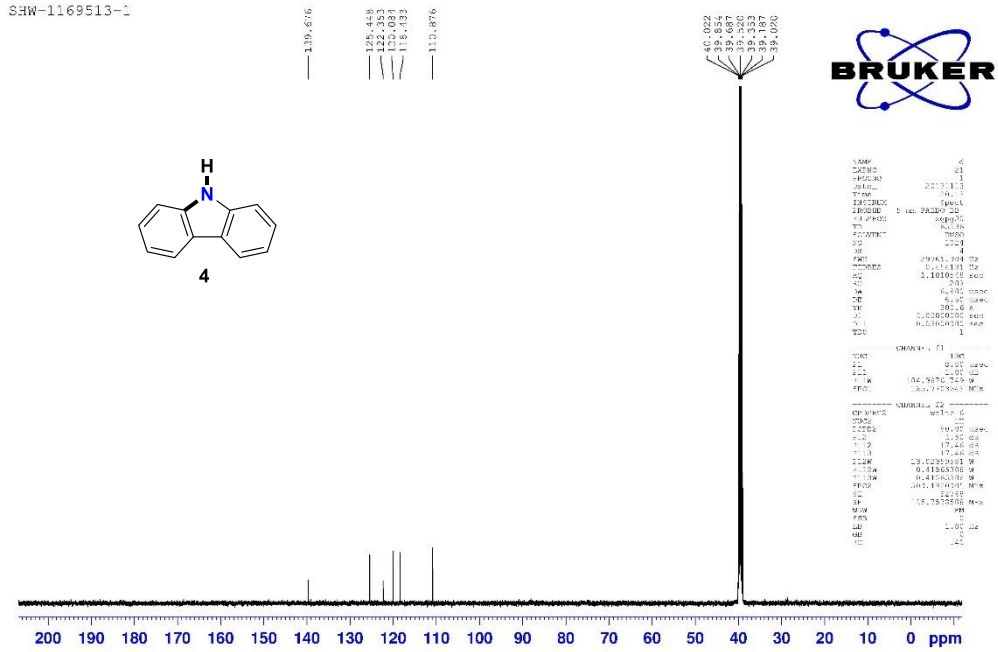

SHW-1169465
3s
ppm

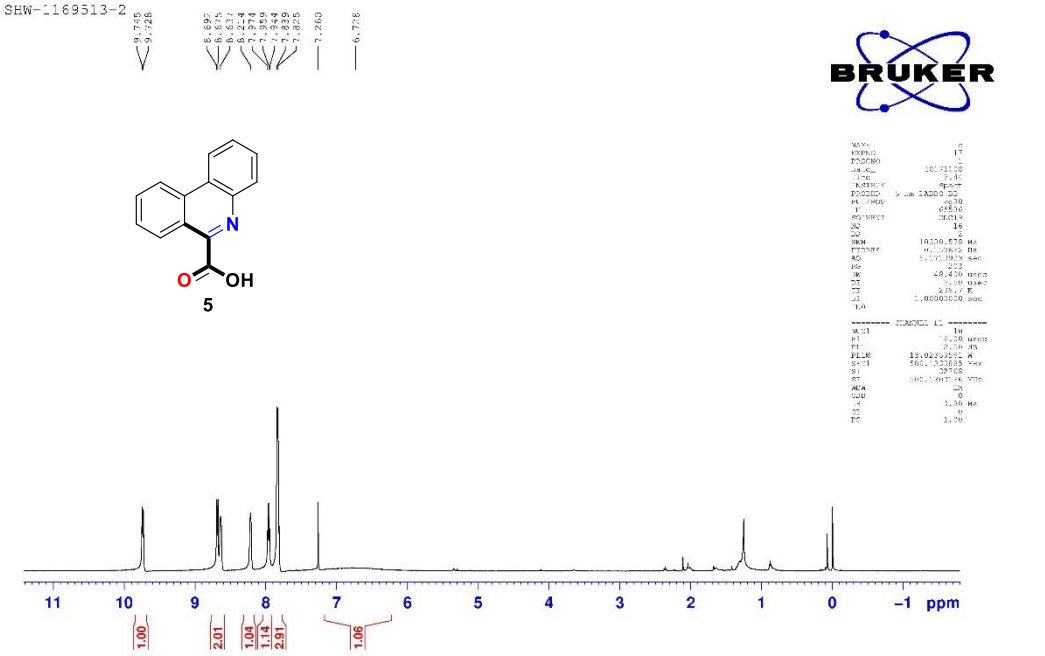

SHW-1169465
3s
ppm

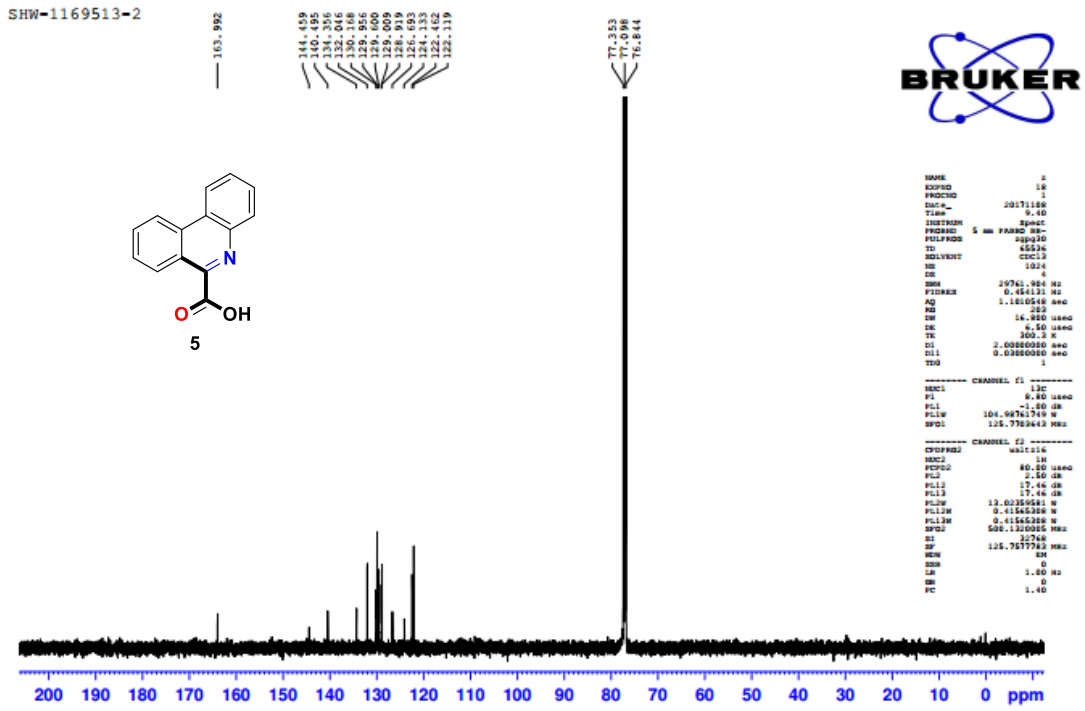

SHW-1169477
3t
ppm


SHW-1169477
3t
ppm


SHW-1169513-1
BRUKER
4
10 9 8 7 6 5 4 3 2 1 0 ppm
2.01
2.00
2.05
2.04


SHW-1169513-1
BRUKER
4
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


SHW-1169513-2
9.745
9.726
8.692
8.675
8.637
8.254
7.974
7.958
7.944
7.839
7.825
7.260
6.728
BRUKER
N
O
OH
5
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm
1.00
2.01
1.04
1.14
2.91
1.06


SHW-1169513-2
163.992
144.459
140.495
134.356
132.046
130.168
129.956
129.600
129.009
128.919
126.693
124.133
122.462
122.119
77.353
77.098
76.844
BRUKER
N
O
OH
5
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm